W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB EM Validation Report ⓘ

Mar 20, 2024 – 08:29 am GMT

PDB ID	:	8CD1
EMDB ID	:	EMD-16566
Title	:	70S-PHIKZ014
Authors	:	Gerovac, M.; Vogel, J.
Deposited on	:	2023-01-29
Resolution	:	3.00 Å(reported)

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

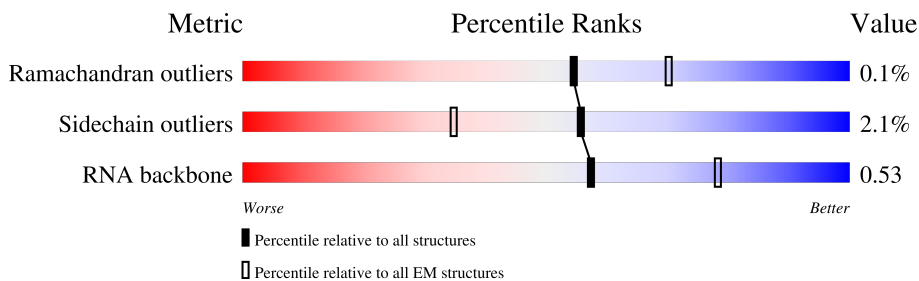|		
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1   Overall quality at a glance ⓘ

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

The reported resolution of this entry is 3.00 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	Percentile Ranks	Value
Ramachandran outliers		0.1%
Sidechain outliers		2.1%
RNA backbone		0.53

Worse   Better

▮ Percentile relative to all structures

▯ Percentile relative to all EM structures

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	2	60	87% • 12%
2	4	44	98% •
3	5	64	8% 97% • •
4	6	38	97% •
5	A	2888	74% 25% •
6	B	120	76% 24%
7	C	273	99% • •
8	D	211	97% • •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	Dt	76	87% / 62% 33% 5%
10	E	200	99%
11	F	179	95%
12	G	177	97%
13	H	148	45% / 53% 47%
14	J	142	96%
15	K	122	98%
16	L	144	99%
17	Le	71	13% / 92%
18	M	137	99%
19	N	129	91% 9%
20	O	116	99%
21	P	116	97%
22	Q	118	98%
23	R	103	98%
24	S	110	99%
25	T	99	89% 7%
26	U	104	8% / 94% 5%
27	V	204	89% 8%
28	W	85	87% 11%
29	X	78	97%
30	Y	63	81% 13% 6%
31	Z	58	98%
32	a	1526	80% 20%
33	b	246	14% / 94% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	c	228	90% 10%
35	d	206	98%
36	e	166	92% 6%
37	f	139	75% 24%
38	g	156	6% 97%
39	h	130	99%
40	i	130	93% 5%
41	j	103	32% 89% 7%
42	k	129	89% 11%
43	l	123	96%
44	m	118	87% 6% 7%
45	n	101	97%
46	o	89	97%
47	p	83	94% 6%
48	q	88	83% 14%
49	r	76	12% 88% 7%
50	s	91	87% 12%
51	t	91	93% 7%
52	u	71	35% 85% 13%
53	v	370	12% 69% 27%

2 Entry composition ⓘ

There are 54 unique types of molecules in this entry. The entry contains 144789 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 L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	53	Total 423	C 254	N 90	O 78	S 1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	4	44	Total 376	C 228	N 91	O 55	S 2	1	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	5	63	Total 506	C 314	N 108	O 81	S 3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	6	38	Total 303	C 184	N 69	O 46	S 4	0	0

- Molecule 5 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	2883	Total 61859	C 27600	N 11347	O 20030	P 2882	0	0

- Molecule 6 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	120	Total 2555	C 1141	N 455	O 839	P 120	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	271	Total	C	N	O	S	0	0
			2048	1258	422	362	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	207	Total	C	N	O	S	0	0
			1549	960	297	287	5		

- Molecule 9 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Dt	76	Total	C	N	O	P	0	0
			1623	723	290	534	76		

- Molecule 10 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	E	199	Total	C	N	O	S	0	0
			1509	948	281	278	2		

- Molecule 11 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	174	Total	C	N	O	S	0	0
			1288	811	228	246	3		

- Molecule 12 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	173	Total	C	N	O	S	0	0
			1294	815	238	239	2		

- Molecule 13 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	H	78	Total	C	N	O	0	0
			577	363	104	110		

- Molecule 14 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	141	Total	C	N	O	S	0	0
			1122	713	205	201	3		

- Molecule 15 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	120	Total	C	N	O	S	0	0
			922	576	178	162	6		

- Molecule 16 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	143	Total	C	N	O	S	0	0
			1055	648	213	192	2		

- Molecule 17 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Le	68	Total	C	N	O	S	0	0
			531	334	95	96	6		

- Molecule 18 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	M	135	Total	C	N	O	S	0	0
			1069	679	209	178	3		

- Molecule 19 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	N	118	Total	C	N	O	S	0	0
			945	590	190	160	5		

- Molecule 20 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	O	115	Total	C	N	O	S	0	0
			881	544	174	161	2		

- Molecule 21 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	P	113	Total	C	N	O	S	0	0
			891	563	168	159	1		

- Molecule 22 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	Q	117	Total	C	N	O	0	0
			936	592	196	148		

- Molecule 23 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	R	102	Total	C	N	O	S	0	0
			801	509	154	136	2		

- Molecule 24 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	S	109	Total	C	N	O	S	0	0
			825	510	160	152	3		

- Molecule 25 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	T	92	Total	C	N	O	0	0
			701	449	124	128		

- Molecule 26 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	U	103	Total	C	N	O	S	0	0
			800	503	152	143	2		

- Molecule 27 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	V	188	Total	C	N	O	S	0	0
			1396	887	254	253	2		

- Molecule 28 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	W	76	Total 575	C 364	N 111	O 100	0	0

- Molecule 29 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	X	77	Total 626	C 389	N 134	O 101	S 2	0	0

- Molecule 30 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Y	59	Total 473	C 291	N 94	O 87	S 1	0	0

- Molecule 31 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Z	57	Total 445	C 277	N 87	O 79	S 2	0	0

- Molecule 32 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	1526	Total 32744	C 14606	N 6011	O 10602	P 1525	0	0

- Molecule 33 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	234	Total 1821	C 1145	N 329	O 337	S 10	0	0

- Molecule 34 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	c	205	Total 1627	C 1028	N 307	O 287	S 5	0	0

- Molecule 35 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	d	205	Total 1603	C 991	N 311	O 296	S 5	0	0

- Molecule 36 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	e	156	Total 1145	C 720	N 209	O 210	S 6	0	0

- Molecule 37 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	f	105	Total 853	C 531	N 158	O 159	S 5	0	0

- Molecule 38 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	g	154	Total 1190	C 747	N 227	O 211	S 5	0	0

- Molecule 39 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	h	129	Total 982	C 618	N 173	O 185	S 6	0	0

- Molecule 40 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	i	127	Total 1010	C 625	N 203	O 181	S 1	0	0

- Molecule 41 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	j	96	Total 765	C 479	N 143	O 142	S 1	0	0

- Molecule 42 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	k	115	Total 838	C 517	N 163	O 156	S 2	0	0

- Molecule 43 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	l	121	Total 949	C 582	N 196	O 167	S 4	0	0

- Molecule 44 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	m	110	Total 859	C 524	N 174	O 157	S 4	0	0

- Molecule 45 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	n	98	Total 777	C 479	N 163	O 132	S 3	0	0

- Molecule 46 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	o	86	Total 686	C 425	N 134	O 126	S 1	0	0

- Molecule 47 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	p	78	Total 610	C 381	N 121	O 108	0	0

- Molecule 48 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	q	76	Total 619	C 387	N 120	O 110	S 2	0	0

- Molecule 49 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	r	71	Total 566	C 361	N 107	O 97	S 1	0	0

- Molecule 50 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	s	80	Total 635	C 405	N 121	O 106	S 3	0	0

- Molecule 51 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	t	85	Total 654	C 404	N 135	O 113	S 2	0	0

- Molecule 52 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	u	62	Total 519	C 320	N 112	O 86	S 1	0	0

- Molecule 53 is a protein called PHIKZ014.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	v	271	Total 2262	C 1436	N 410	O 409	S 7	0	0

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
54	A	150	Total 150	Mg 150	0
54	C	1	Total 1	Mg 1	0
54	D	1	Total 1	Mg 1	0
54	P	1	Total 1	Mg 1	0
54	U	1	Total 1	Mg 1	0
54	a	17	Total 17	Mg 17	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.
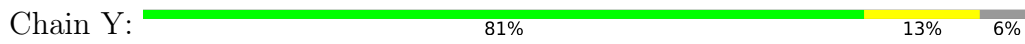
- Molecule 1: 50S ribosomal protein L32
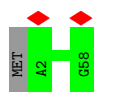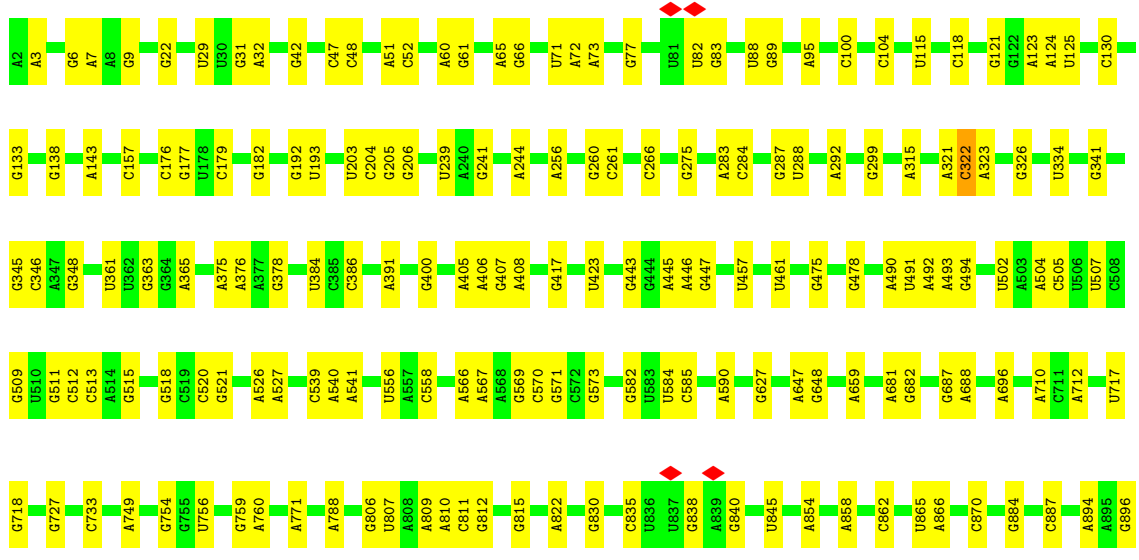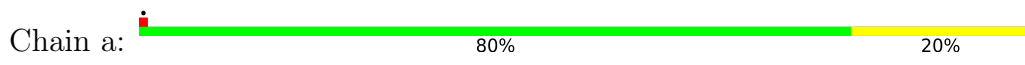
Chain 2:
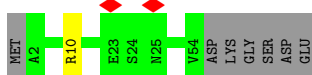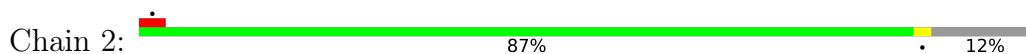
- Molecule 2: 50S ribosomal protein L34

Chain 4:

- Molecule 3: 50S ribosomal protein L35

Chain 5:
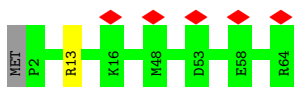
- Molecule 4: 50S ribosomal protein L36

Chain 6:

- Molecule 5: 23S rRNA

Chain A:

- Molecule 6: 5S rRNA

Chain B:
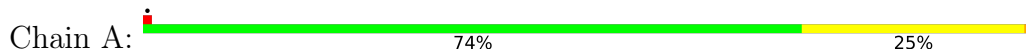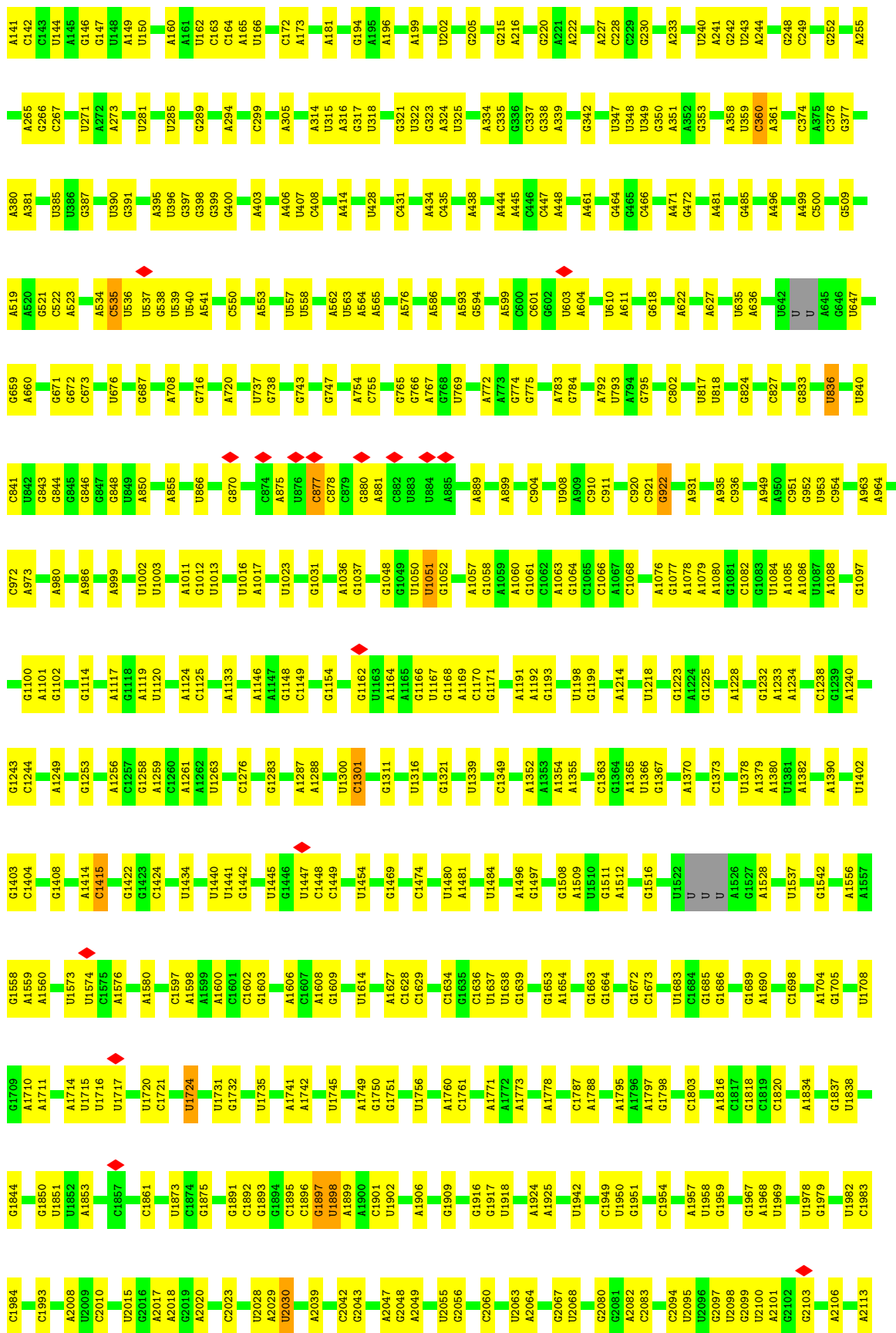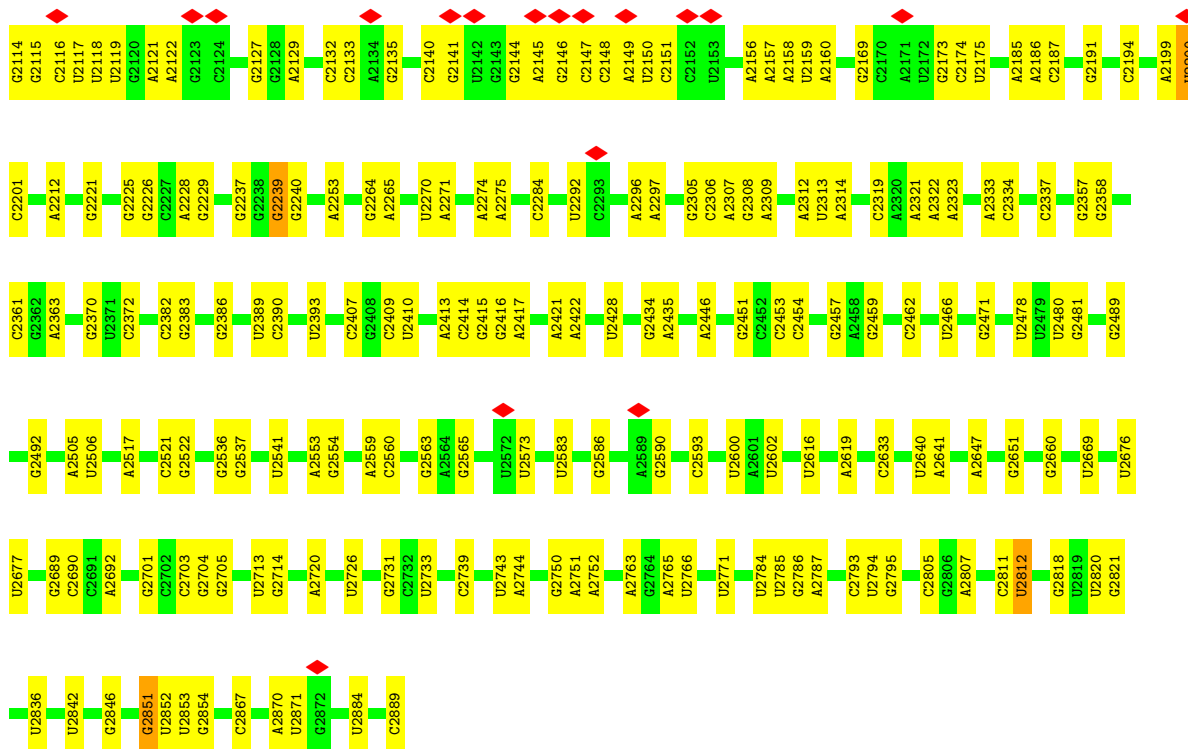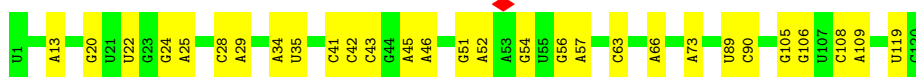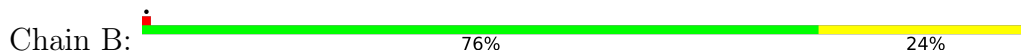
- Molecule 7: 50S ribosomal protein L2

Chain C:

- Molecule 8: 50S ribosomal protein L3

Chain D:

- Molecule 9: tRNA

Chain Dt:

G1 C2 C3 C4 G5 G6 A7 U8 A9 G10 C11 U12 C13 A14 G15 U16 C17 G18 G19 U20 A21 G22 A23 G24 C25 A26 G27 C28 G29 G30 A31 U32 U33 A36 A37 A38 U39 C40 C41 C42 C43 G44 U45 G46 U47 C48 C49 U50 U51 G52 G53 U54 U55 C56 G57 A58 U59 U60 C61

C62 G63 A64 G65 U66 C67 C68 G69 G70 G71 C72 A73 C74 C75 A76
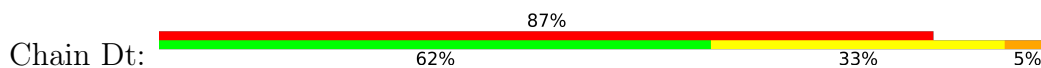
• Molecule 10: 50S ribosomal protein L4

Chain E: 99%

MET Q2 A8 R60 D138 G200
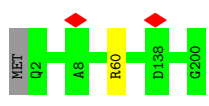
• Molecule 11: 50S ribosomal protein L5

Chain F: 95%

MET ALA R3 I7 T32 A43 E81 R102 R110 E140 I141 D142 Y143 D144 K145 L149 T162 P176 PHE ARG ASN
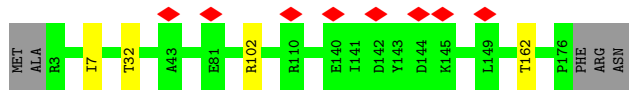
• Molecule 12: 50S ribosomal protein L6

Chain G: 97%

MET S2 A13 L33 D46 G82 E167 A174 LYS LYS LYS
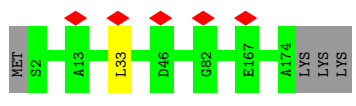
• Molecule 13: 50S ribosomal protein L9

Chain H: 45% / 53% / 47%

MET E2 V3 I4 L5 L6 E7 K8 V9 A10 N11 L12 G13 N14 L15 G16 D17 K18 V19 N20 L31 P32 Q33 G34 K35 A36 T37 V38 A39 T40 A41 E42 N43 V44 A45 A46 F47 E48 A49 R50 R51 A52 E53 L54 E55 K56 A57 A58 A59 E60 K61 K62 A63 A64 A65 E66 A67 R68 A69

A70 Q71 L72 S73 E74 L75 V76 V77 T78 L79 GLY ALA HIS ALA GLY ASP GLU GLY LYS LEU PHE GLY SER ILE GLY THR ARG ASP ILE ALA GLU ALA VAL SER ALA ALA GLY TYR PRO LEU GLU LYS ALA GLU VAL ARG LEU PRO ASN GLY ALA LEU ARG ASN THR GLY GLU PHE ASP VAL

ALA VAL HIS LEU HIS THR ASP VAL GLU THR THR LEU LYS LEU LEU ILE ILE VAL ALA GLU

• Molecule 14: 50S ribosomal protein L13

Chain J: 96%

MET K2 T45 T50 R116 K141 I142
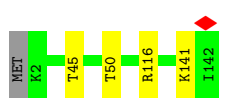
• Molecule 15: 50S ribosomal protein L14

Chain K:

98%
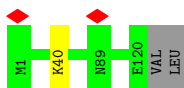
• Molecule 16: 50S ribosomal protein L15

Chain L:

99%

• Molecule 17: 50S ribosomal protein L31

Chain Le:

13%

92%
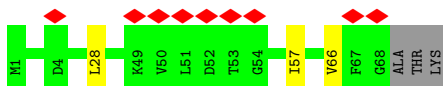
• Molecule 18: 50S ribosomal protein L16

Chain M:

99%
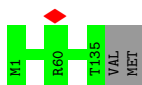
• Molecule 19: 50S ribosomal protein L17

Chain N:

91%

9%
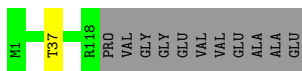
• Molecule 20: 50S ribosomal protein L18

Chain O:

99%
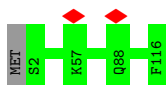
• Molecule 21: 50S ribosomal protein L19

Chain P:

97%
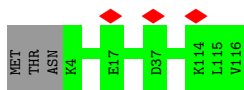
• Molecule 22: 50S ribosomal protein L20

Chain Q:
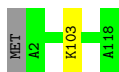
• Molecule 23: 50S ribosomal protein L21

Chain R:
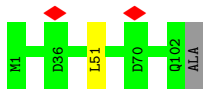
• Molecule 24: Large ribosomal subunit protein uL22

Chain S:
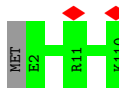
• Molecule 25: 50S ribosomal protein L23

Chain T:

• Molecule 26: 50S ribosomal protein L24

Chain U:
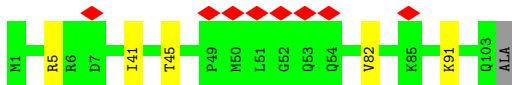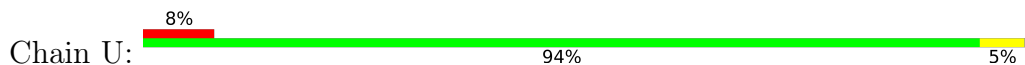
• Molecule 27: 50S ribosomal protein L25

Chain V:
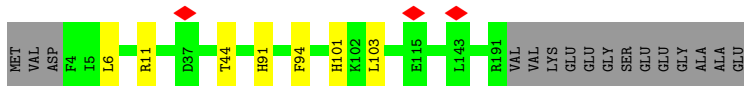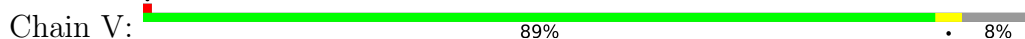
• Molecule 28: 50S ribosomal protein L27

Chain W:

87%   11%

MET ALA HIS LYS LYS ALA GLY GLY SER T10 Q40 R41 A85
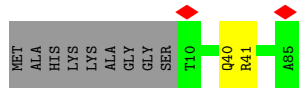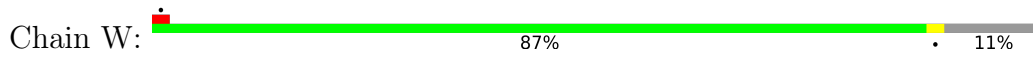
• Molecule 29: 50S ribosomal protein L28

Chain X:

97%

MET S2 R27 F78
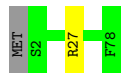
• Molecule 30: 50S ribosomal protein L29

Chain Y:

81%   13%   6%

MET K1 S9 V10 E15 Q16 L17 L18 G19 L20 T33 Q59 ALA GLY LYS

• Molecule 31: 50S ribosomal protein L30

Chain Z:

98%

MET A2 G58

• Molecule 32: 16S rRNA

Chain a:

80%   20%

A2 A3 G6 A7 A8 G9 G22 U29 U30 G31 A32 G42 C47 C48 A51 C52 A60 G61 A65 G66 U71 A72 A73 G77 U81 U82 G83 U88 G89 A95 C100 C104 U115 C118 G121 G122 A123 A124 U125 C130

G133 G138 A143 C157 C176 G177 U178 C179 G182 G192 U193 U203 C204 G205 G206 U239 A240 G241 A244 A256 G260 C261 C266 G275 A283 C284 G287 U288 A292 C299 A315 A321 C322 A323 G326 U334 G341

G345 C346 A347 G348 U361 U362 G363 G364 A365 A375 A376 A377 G378 U384 C385 C386 A391 G400 A405 A406 G407 A408 G417 U423 G443 G444 A445 A446 G447 U457 U461 G475 G478 A490 U491 A492 A493 G494 U502 A503 A504 C505 U506 U507 C508

G509 U510 G511 C512 C513 A514 G515 G518 C519 G520 G521 A526 A527 C539 A540 A541 U556 A557 C558 A566 A567 A568 G569 C570 G571 C572 G573 G582 U583 U584 C585 A590 G627 A647 G648 A659 A681 G682 G687 A688 A696 A710 C711 A712 U717

G718 G727 C733 A749 G754 G755 U756 G759 A760 A771 A788 G806 U807 A808 A809 A810 C811 C812 G815 A822 G830 C835 U836 U837 G838 A839 G840 U845 A854 A858 C862 U865 A866 C870 G884 C887 A894 A895 G896

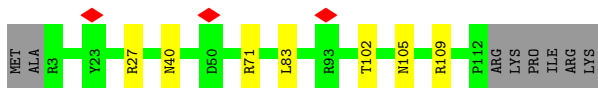• Molecule 33: 30S ribosomal protein S2

Chain b:
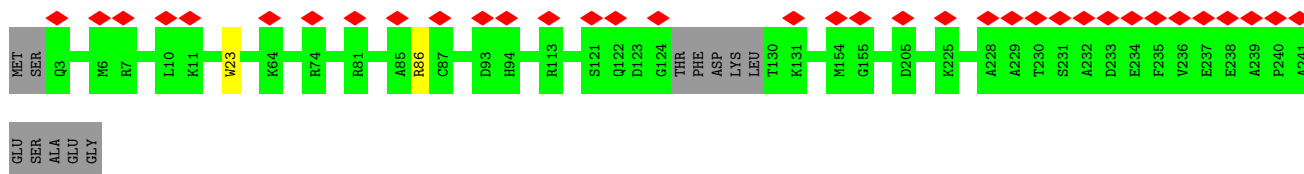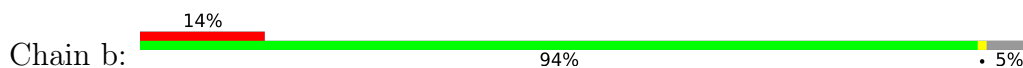
• Molecule 34: 30S ribosomal protein S3

Chain c:
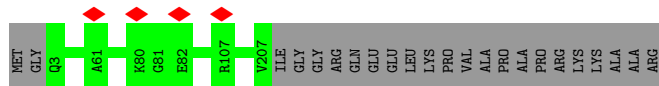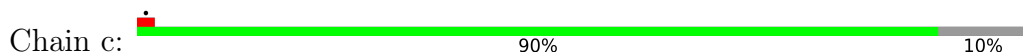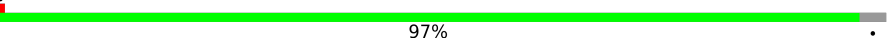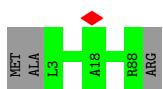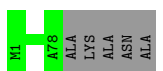

• Molecule 35: 30S ribosomal protein S4

Chain d:
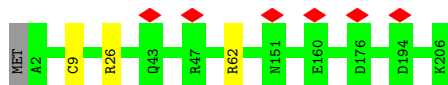
• Molecule 36: 30S ribosomal protein S5

Chain e:
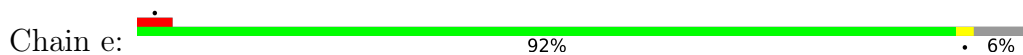
• Molecule 37: 30S ribosomal protein S6

Chain f:

MET R2 L9 E31 L103 K104 A105 E106 GLU SER ARG ASN GLU ARG ARG GLU ARG ARG GLU ARG ARG PRO ASN ASP ASN ALA GLU GLY ALA ASP GLY ASP ASP ASN SER SER ASP ASP ASN ALA ASP GLU
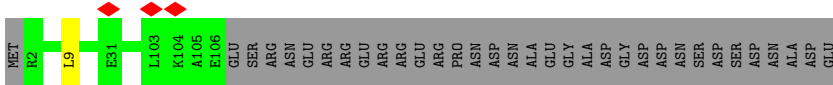
• Molecule 38: 30S ribosomal protein S7

Chain g:
6%
97%

MET PRO R3 R4 R5 V12 L13 K55 V80 G81 G82 A83 E129 R143 E146 A147 N148 F156
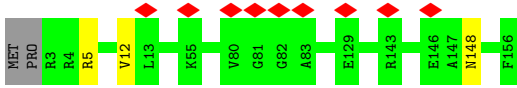
• Molecule 39: 30S ribosomal protein S8

Chain h:
99%

MET S2 E54 F130
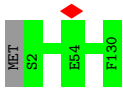
• Molecule 40: 30S ribosomal protein S9

Chain i:
93% 5%

MET SER ALA T4 Q5 R12 K27 I28 R41 M46 V47 G117 R130
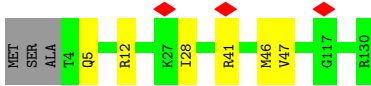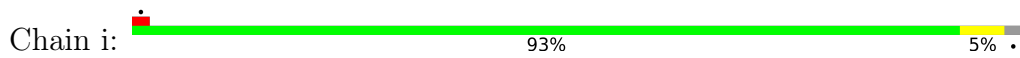
• Molecule 41: 30S ribosomal protein S10

Chain j:
32%
89% 7%

MET GLN ASN GLN GLN ILE ARG I8 R16 L17 I18 D19 I25 K30 R31 T32 G33 A34 Q35 V36 R37 R45 R48 K59 D60 A61 R62 D63 Q64 Y65 E66 I67 V77 Q78 P79 T80 D81 K82 T83 V84 D85 A86 K89 L90 D91 L92 G95 V96 G103
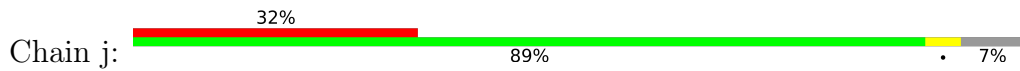
• Molecule 42: 30S ribosomal protein S11

Chain k:
89% 11%

MET ALA LYS PRO ALA ARG PRO LYS LYS VAL LYS K14 D18 R37 R128 VAL
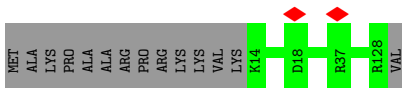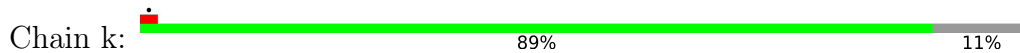
• Molecule 43: 30S ribosomal protein S12

Chain l:
96%

MET A2 R14 M15 V16 D17 R114 P122 LYS
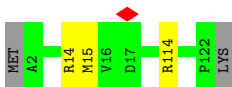
• Molecule 44: 30S ribosomal protein S13

Chain m:

87% 6% 7%

MET ALA R3 Y23 R27 N40 D50 R71 L83 R93 T102 N105 R109 P112 ARG LYS PRO ILE ARG LYS

• Molecule 45: 30S ribosomal protein S14

Chain n:

97%

MET ALA K3 S100 TRP

• Molecule 46: 30S ribosomal protein S15

Chain o:

97%

MET ALA L3 A18 R88 ARG

• Molecule 47: 30S ribosomal protein S16

Chain p:

94% 6%

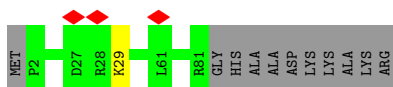M1 A78 ALA LYS ALA ASN ALA

• Molecule 48: 30S ribosomal protein S17

Chain q:

83% 14%

MET ALA GLU ALA GLN LYS THR VAL R9 N54 R65 R68 R84 ALA VAL GLU VAL

• Molecule 49: 30S ribosomal protein S18

Chain r:

12%

88% 7%

MET ALA ARG F4 F5 R6 R7 R8 K9 F10 C11 R12 F13 G17 V18 H74 GLY ARG
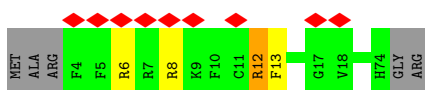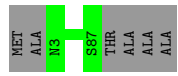
• Molecule 50: 30S ribosomal protein S19

Chain s:

87% 12%
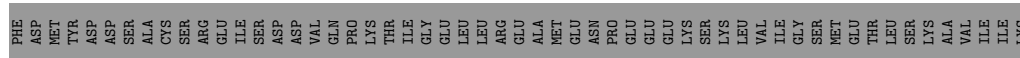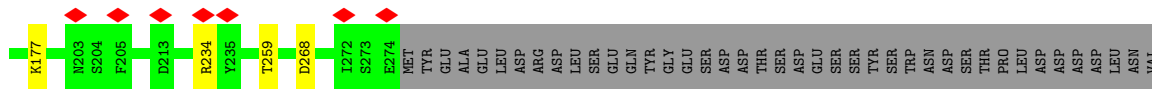
MET P2 D27 R28 K29 L61 R81 GLY HIS ALA ALA ASP LYS LYS ALA LYS ARG

• Molecule 51: 30S ribosomal protein S20

Chain t:

93% 7%

MET ALA N3 S87 THR ALA ALA ALA

• Molecule 52: 30S ribosomal protein S21

35%

Chain u:

85% 13%

MET PRO ALA VAL K4 E7 ASN E10 P11 V14 A15 L16 R17 R18 R21 E24 K25 A26 G27 V28 L29 A30 R33 S34 R35 R45 K46 R47 K48 R62 E63 Q64 R65 R66 R67 GLU ARG TYR

• Molecule 53: PHIKZ014

12%

Chain v:

69% 27%

MET LYS GLN Y4 S49 L50 R51 Y52 L53 N56 E57 T71 D88 M89 P90 C91 D92 L93 T94 E95 S96 R97 E114 E122 E123 S124 T125 E126 Y127 D128 R129 N130 H131 K138 R143 E146 G147 T157 W158 E161 F162 D163 Y164 N165 R166 A167 V168 D169 P170

K17 N203 S204 F205 D213 R234 Y235 T259 D268 I272 S273 E274 MET TYR GLU ALA GLU LEU ASP ARG ASP LEU SER GLU GLN TYR GLY GLU SER ASP ASP THR SER ASP GLU SER SER TYR SER TRP ASN ASP SER THR PRO LEU ASP ASP ASP ASP LEU ASN VAL

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

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	169672	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 $(e^-/\text{Å}^2)$	88.28	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	26.120	Depositor
Minimum map value	-7.773	Depositor
Average map value	-0.008	Depositor
Map value standard deviation	0.894	Depositor
Recommended contour level	3.46	Depositor
Map size (Å)	544.512, 544.512, 544.512	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0635, 1.0635, 1.0635	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	2	0.24	0/429	0.62	0/572
2	4	0.25	0/379	0.77	0/496
3	5	0.24	0/511	0.66	0/668
4	6	0.26	0/304	0.70	0/399
5	A	0.25	4/69275 (0.0%)	0.84	62/108063 (0.1%)
6	B	0.24	0/2855	0.85	3/4447 (0.1%)
7	C	0.26	0/2084	0.64	0/2800
8	D	0.26	0/1572	0.61	0/2118
9	Dt	0.36	1/1813 (0.1%)	0.99	12/2823 (0.4%)
10	E	0.25	0/1529	0.56	0/2060
11	F	0.27	0/1304	0.58	0/1766
12	G	0.26	0/1311	0.58	0/1767
13	H	0.26	0/580	0.52	0/781
14	J	0.26	0/1148	0.56	0/1549
15	K	0.26	0/931	0.65	0/1247
16	L	0.26	0/1067	0.63	0/1422
17	Le	0.28	0/542	0.57	0/728
18	M	0.26	0/1089	0.62	0/1456
19	N	0.25	0/960	0.63	0/1282
20	O	0.25	0/888	0.63	0/1183
21	P	0.25	0/900	0.61	0/1203
22	Q	0.25	0/946	0.64	0/1257
23	R	0.26	0/814	0.60	0/1091
24	S	0.25	0/829	0.59	0/1104
25	T	0.26	0/710	0.52	0/953
26	U	0.27	0/808	0.58	0/1079
27	V	0.25	0/1419	0.56	0/1925
28	W	0.27	0/583	0.64	0/774
29	X	0.24	0/637	0.68	0/849
30	Y	0.34	0/474	0.60	0/632
31	Z	0.24	0/449	0.61	0/602
32	a	0.23	0/36667	0.81	12/57202 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	b	0.25	0/1849	0.55	0/2486
34	c	0.24	0/1656	0.60	0/2232
35	d	0.25	0/1622	0.60	0/2171
36	e	0.27	0/1159	0.62	1/1559 (0.1%)
37	f	0.25	0/867	0.57	0/1167
38	g	0.25	0/1207	0.59	0/1616
39	h	0.25	0/993	0.55	0/1332
40	i	0.26	0/1022	0.68	0/1365
41	j	0.26	0/775	0.60	0/1046
42	k	0.25	0/854	0.59	0/1159
43	l	0.27	0/963	0.68	0/1292
44	m	0.24	0/867	0.63	0/1165
45	n	0.25	0/787	0.64	0/1048
46	o	0.24	0/693	0.54	0/926
47	p	0.27	0/621	0.64	0/837
48	q	0.25	0/627	0.64	0/844
49	r	0.27	0/575	2.14	2/771 (0.3%)
50	s	0.23	0/649	0.58	0/874
51	t	0.25	0/661	0.54	0/881
52	u	0.25	0/524	0.66	0/689
53	v	0.26	0/2323	0.60	0/3138
All	All	0.25	5/157101 (0.0%)	0.79	92/234896 (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
5	A	1	0
8	D	0	1
23	R	0	1
49	r	0	1
All	All	1	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	Dt	1	G	OP3-P	-10.53	1.48	1.61
5	A	1897	G	C8-N7	-9.41	1.25	1.30
5	A	1897	G	N7-C5	-6.26	1.35	1.39
5	A	1897	G	C6-N1	-5.93	1.35	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1909	G	N1-C2	-5.50	1.33	1.37

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	r	12	ARG	O-C-N	-56.80	31.82	122.70
5	A	1897	G	N7-C8-N9	12.70	119.45	113.10
5	A	1897	G	C8-N9-C4	-10.79	102.08	106.40
5	A	1909	G	N1-C2-N2	-10.28	106.94	116.20
5	A	1896	C	C5-C6-N1	9.41	125.71	121.00
5	A	1897	G	C4-N9-C1'	9.13	138.37	126.50
5	A	877	C	C6-N1-C2	-9.06	116.67	120.30
5	A	2239	G	O4'-C1'-N9	8.76	115.21	108.20
5	A	1897	G	C6-C5-N7	-8.60	125.24	130.40
5	A	1909	G	N3-C2-N2	8.19	125.63	119.90
5	A	1909	G	C5-C6-N1	-7.75	107.63	111.50
5	A	1895	C	N3-C4-C5	7.68	124.97	121.90
5	A	1300	U	C2-N1-C1'	7.41	126.59	117.70
5	A	818	U	C2-N1-C1'	7.37	126.54	117.70
5	A	535	C	C6-N1-C2	-7.31	117.38	120.30
5	A	1897	G	N3-C4-N9	7.28	130.37	126.00
5	A	1897	G	N3-C4-C5	-7.15	125.02	128.60
5	A	2851	G	N3-C4-N9	7.08	130.25	126.00
5	A	1895	C	C2-N1-C1'	-7.07	111.03	118.80
9	Dt	8	U	C2-N1-C1'	7.05	126.16	117.70
5	A	1897	G	N1-C2-N2	-6.99	109.91	116.20
5	A	877	C	N1-C2-O2	6.99	123.09	118.90
5	A	1909	G	C8-N9-C4	-6.84	103.67	106.40
5	A	877	C	N3-C2-O2	-6.83	117.12	121.90
5	A	2812	U	N3-C2-O2	-6.69	117.52	122.20
49	r	12	ARG	C-N-CA	-6.69	104.98	121.70
5	A	1896	C	C2-N1-C1'	6.68	126.15	118.80
36	e	47	VAL	CG1-CB-CG2	6.68	121.58	110.90
5	A	1761	C	C6-N1-C2	-6.57	117.67	120.30
5	A	1909	G	C2-N3-C4	-6.57	108.62	111.90
5	A	1896	C	C6-N1-C2	-6.54	117.68	120.30
5	A	2100	U	C2-N1-C1'	6.54	125.54	117.70
5	A	1724	U	N3-C2-O2	-6.52	117.63	122.20
32	a	104	C	N1-C2-O2	6.42	122.75	118.90
9	Dt	32	U	C6-N1-C2	-6.30	117.22	121.00
5	A	1897	G	C4-C5-C6	6.28	122.56	118.80
5	A	2851	G	C4-N9-C1'	6.23	134.60	126.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	Dt	36	A	OP1-P-O3'	6.19	118.83	105.20
9	Dt	38	A	OP1-P-O3'	6.19	118.81	105.20
32	a	130	C	C6-N1-C2	-6.16	117.83	120.30
9	Dt	46	G	OP1-P-OP2	6.16	128.84	119.60
9	Dt	31	A	OP1-P-O3'	6.16	118.74	105.20
5	A	2851	G	C8-N9-C1'	-6.06	119.12	127.00
5	A	2812	U	N1-C2-O2	5.92	126.95	122.80
5	A	1897	G	C8-N9-C1'	-5.88	119.35	127.00
5	A	1909	G	N1-C2-N3	5.87	127.42	123.90
32	a	963	A	O4'-C1'-N9	5.87	112.89	108.20
32	a	104	C	C6-N1-C2	-5.83	117.97	120.30
32	a	104	C	N3-C2-O2	-5.74	117.88	121.90
9	Dt	32	U	N3-C2-O2	-5.73	118.19	122.20
32	a	1341	G	P-O3'-C3'	5.68	126.51	119.70
5	A	1896	C	N1-C2-O2	5.67	122.30	118.90
6	B	108	C	C6-N1-C2	-5.66	118.03	120.30
32	a	104	C	C2-N1-C1'	5.65	125.01	118.80
32	a	987	G	C4-N9-C1'	5.63	133.82	126.50
5	A	1724	U	C6-N1-C2	-5.60	117.64	121.00
5	A	1896	C	N3-C4-N4	5.58	121.91	118.00
5	A	1897	G	N1-C2-N3	5.58	127.25	123.90
6	B	119	U	N3-C2-O2	-5.56	118.31	122.20
9	Dt	16	U	OP1-P-OP2	5.55	127.93	119.60
5	A	836	U	N3-C2-O2	-5.50	118.35	122.20
5	A	535	C	C6-N1-C1'	5.45	127.34	120.80
5	A	1166	G	C4-N9-C1'	5.44	133.57	126.50
5	A	1724	U	N1-C2-O2	5.41	126.59	122.80
9	Dt	54	U	OP1-P-O3'	5.41	117.10	105.20
5	A	922	G	C4-N9-C1'	5.39	133.51	126.50
5	A	2023	C	C6-N1-C2	-5.38	118.15	120.30
5	A	1415	C	C6-N1-C2	-5.36	118.16	120.30
5	A	2812	U	C6-N1-C2	-5.36	117.79	121.00
5	A	1909	G	N1-C6-O6	5.33	123.10	119.90
5	A	1895	C	C4-C5-C6	-5.29	114.76	117.40
9	Dt	8	U	OP1-P-OP2	5.28	127.52	119.60
5	A	1897	G	C5-N7-C8	-5.27	101.66	104.30
5	A	1051	U	P-O3'-C3'	5.25	126.00	119.70
32	a	203	U	C2-N1-C1'	5.19	123.92	117.70
5	A	910	C	C6-N1-C2	-5.17	118.23	120.30
6	B	119	U	N1-C2-O2	5.10	126.37	122.80
32	a	322	C	P-O3'-C3'	5.09	125.81	119.70
5	A	360	C	P-O3'-C3'	5.09	125.81	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2583	U	N3-C2-O2	-5.09	118.64	122.20
5	A	2030	U	C2-N1-C1'	5.08	123.80	117.70
9	Dt	32	U	C5-C6-N1	5.08	125.24	122.70
9	Dt	7	A	OP1-P-O3'	-5.08	94.03	105.20
5	A	836	U	N1-C2-O2	5.08	126.35	122.80
5	A	1724	U	C5-C6-N1	5.07	125.24	122.70
5	A	1898	U	O5'-P-OP1	-5.07	101.13	105.70
5	A	1896	C	C2-N3-C4	5.06	122.43	119.90
5	A	1301	C	C6-N1-C2	-5.05	118.28	120.30
32	a	987	G	C8-N9-C1'	-5.03	120.46	127.00
5	A	1818	G	N3-C4-N9	5.02	129.01	126.00
32	a	976	U	P-O3'-C3'	5.01	125.72	119.70
5	A	2200	U	P-O3'-C3'	5.01	125.71	119.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	1897	G	C1'

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	D	151	THR	Peptide
23	R	51	LEU	Peptide
49	r	12	ARG	Mainchain

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2	51/60 (85%)	49 (96%)	2 (4%)	0	100	100
2	4	43/44 (98%)	42 (98%)	1 (2%)	0	100	100
3	5	61/64 (95%)	54 (88%)	7 (12%)	0	100	100
4	6	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
7	C	269/273 (98%)	255 (95%)	14 (5%)	0	100	100
8	D	205/211 (97%)	184 (90%)	21 (10%)	0	100	100
10	E	197/200 (98%)	190 (96%)	7 (4%)	0	100	100
11	F	172/179 (96%)	155 (90%)	17 (10%)	0	100	100
12	G	171/177 (97%)	164 (96%)	7 (4%)	0	100	100
13	H	76/148 (51%)	76 (100%)	0	0	100	100
14	J	139/142 (98%)	134 (96%)	5 (4%)	0	100	100
15	K	118/122 (97%)	111 (94%)	7 (6%)	0	100	100
16	L	141/144 (98%)	130 (92%)	11 (8%)	0	100	100
17	Le	66/71 (93%)	59 (89%)	6 (9%)	1 (2%)	10	42
18	M	133/137 (97%)	132 (99%)	1 (1%)	0	100	100
19	N	116/129 (90%)	105 (90%)	11 (10%)	0	100	100
20	O	113/116 (97%)	108 (96%)	5 (4%)	0	100	100
21	P	111/116 (96%)	104 (94%)	7 (6%)	0	100	100
22	Q	115/118 (98%)	109 (95%)	6 (5%)	0	100	100
23	R	100/103 (97%)	93 (93%)	7 (7%)	0	100	100
24	S	107/110 (97%)	107 (100%)	0	0	100	100
25	T	90/99 (91%)	84 (93%)	5 (6%)	1 (1%)	14	50
26	U	101/104 (97%)	94 (93%)	7 (7%)	0	100	100
27	V	186/204 (91%)	173 (93%)	13 (7%)	0	100	100
28	W	74/85 (87%)	57 (77%)	17 (23%)	0	100	100
29	X	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
30	Y	57/63 (90%)	54 (95%)	2 (4%)	1 (2%)	8	37
31	Z	55/58 (95%)	54 (98%)	1 (2%)	0	100	100
33	b	230/246 (94%)	214 (93%)	16 (7%)	0	100	100
34	c	203/228 (89%)	188 (93%)	15 (7%)	0	100	100
35	d	203/206 (98%)	190 (94%)	13 (6%)	0	100	100
36	e	154/166 (93%)	141 (92%)	13 (8%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	f	103/139 (74%)	98 (95%)	5 (5%)	0	100	100
38	g	152/156 (97%)	147 (97%)	5 (3%)	0	100	100
39	h	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
40	i	125/130 (96%)	110 (88%)	14 (11%)	1 (1%)	19	57
41	j	94/103 (91%)	88 (94%)	6 (6%)	0	100	100
42	k	113/129 (88%)	110 (97%)	3 (3%)	0	100	100
43	l	119/123 (97%)	111 (93%)	8 (7%)	0	100	100
44	m	108/118 (92%)	103 (95%)	5 (5%)	0	100	100
45	n	96/101 (95%)	91 (95%)	5 (5%)	0	100	100
46	o	84/89 (94%)	83 (99%)	1 (1%)	0	100	100
47	p	76/83 (92%)	73 (96%)	3 (4%)	0	100	100
48	q	74/88 (84%)	72 (97%)	2 (3%)	0	100	100
49	r	67/76 (88%)	65 (97%)	1 (2%)	1 (2%)	10	42
50	s	78/91 (86%)	71 (91%)	7 (9%)	0	100	100
51	t	83/91 (91%)	83 (100%)	0	0	100	100
52	u	58/71 (82%)	56 (97%)	1 (2%)	1 (2%)	9	39
53	v	269/370 (73%)	264 (98%)	5 (2%)	0	100	100
All	All	5794/6327 (92%)	5463 (94%)	325 (6%)	6 (0%)	54	85

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
25	T	71	ARG
30	Y	10	VAL
40	i	28	ILE
49	r	13	PHE
17	Le	66	VAL
52	u	28	VAL

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2	46/52 (88%)	45 (98%)	1 (2%)	52	81
2	4	38/37 (103%)	37 (97%)	1 (3%)	46	78
3	5	54/55 (98%)	53 (98%)	1 (2%)	57	84
4	6	33/34 (97%)	32 (97%)	1 (3%)	41	75
7	C	206/213 (97%)	204 (99%)	2 (1%)	76	91
8	D	157/162 (97%)	155 (99%)	2 (1%)	69	89
10	E	155/158 (98%)	154 (99%)	1 (1%)	86	95
11	F	124/153 (81%)	120 (97%)	4 (3%)	39	74
12	G	133/141 (94%)	132 (99%)	1 (1%)	81	93
13	H	55/107 (51%)	55 (100%)	0	100	100
14	J	118/119 (99%)	114 (97%)	4 (3%)	37	72
15	K	100/102 (98%)	99 (99%)	1 (1%)	76	91
16	L	104/106 (98%)	103 (99%)	1 (1%)	76	91
17	Le	59/61 (97%)	57 (97%)	2 (3%)	37	72
18	M	108/110 (98%)	108 (100%)	0	100	100
19	N	97/104 (93%)	96 (99%)	1 (1%)	76	91
20	O	86/87 (99%)	86 (100%)	0	100	100
21	P	94/98 (96%)	94 (100%)	0	100	100
22	Q	87/88 (99%)	86 (99%)	1 (1%)	73	90
23	R	82/86 (95%)	82 (100%)	0	100	100
24	S	86/87 (99%)	86 (100%)	0	100	100
25	T	73/82 (89%)	70 (96%)	3 (4%)	30	67
26	U	88/88 (100%)	83 (94%)	5 (6%)	20	56
27	V	143/164 (87%)	136 (95%)	7 (5%)	25	61
28	W	56/61 (92%)	54 (96%)	2 (4%)	35	70
29	X	65/67 (97%)	64 (98%)	1 (2%)	65	87
30	Y	52/55 (94%)	45 (86%)	7 (14%)	4	17
31	Z	48/49 (98%)	48 (100%)	0	100	100
33	b	191/202 (95%)	189 (99%)	2 (1%)	76	91
34	c	165/187 (88%)	165 (100%)	0	100	100
35	d	166/174 (95%)	163 (98%)	3 (2%)	59	85

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	e	114/124 (92%)	112 (98%)	2 (2%)	59	85
37	f	88/119 (74%)	87 (99%)	1 (1%)	73	90
38	g	116/122 (95%)	113 (97%)	3 (3%)	46	78
39	h	108/109 (99%)	108 (100%)	0	100	100
40	i	104/106 (98%)	99 (95%)	5 (5%)	25	62
41	j	85/92 (92%)	81 (95%)	4 (5%)	26	63
42	k	84/98 (86%)	84 (100%)	0	100	100
43	l	105/107 (98%)	102 (97%)	3 (3%)	42	76
44	m	92/99 (93%)	85 (92%)	7 (8%)	13	43
45	n	78/82 (95%)	78 (100%)	0	100	100
46	o	73/75 (97%)	73 (100%)	0	100	100
47	p	61/65 (94%)	61 (100%)	0	100	100
48	q	70/79 (89%)	67 (96%)	3 (4%)	29	66
49	r	56/64 (88%)	54 (96%)	2 (4%)	35	70
50	s	69/78 (88%)	68 (99%)	1 (1%)	67	88
51	t	67/70 (96%)	67 (100%)	0	100	100
52	u	51/60 (85%)	50 (98%)	1 (2%)	55	83
53	v	242/335 (72%)	227 (94%)	15 (6%)	18	52
All	All	4732/5173 (92%)	4631 (98%)	101 (2%)	56	82

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2	10	ARG
2	4	42	LEU
3	5	13	ARG
4	6	37	GLN
7	C	79	GLU
7	C	258	THR
8	D	13	THR
8	D	34	ARG
10	E	60	ARG
11	F	7	ILE
11	F	32	THR
11	F	102	ARG
11	F	162	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	G	33	LEU
14	J	45	THR
14	J	50	THR
14	J	116	ARG
14	J	141	LYS
15	K	40	LYS
16	L	7	ARG
17	Le	28	LEU
17	Le	57	ILE
19	N	37	THR
22	Q	103	LYS
25	T	5	ARG
25	T	8	LYS
25	T	40	LEU
26	U	5	ARG
26	U	41	ILE
26	U	45	THR
26	U	82	VAL
26	U	91	LYS
27	V	6	LEU
27	V	11	ARG
27	V	44	THR
27	V	91	HIS
27	V	94	PHE
27	V	101	HIS
27	V	103	LEU
28	W	40	GLN
28	W	41	ARG
29	X	27	ARG
30	Y	9	SER
30	Y	15	GLU
30	Y	16	GLN
30	Y	17	LEU
30	Y	18	LEU
30	Y	20	LEU
30	Y	33	THR
33	b	23	TRP
33	b	86	ARG
35	d	9	CYS
35	d	26	ARG
35	d	62	ARG
36	e	27	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	e	158	ARG
37	f	9	LEU
38	g	5	ARG
38	g	12	VAL
38	g	148	ASN
40	i	5	GLN
40	i	12	ARG
40	i	41	ARG
40	i	46	MET
40	i	47	VAL
41	j	16	ARG
41	j	59	LYS
41	j	67	ILE
41	j	82	LYS
43	l	14	ARG
43	l	15	MET
43	l	114	ARG
44	m	27	ARG
44	m	40	ASN
44	m	71	ARG
44	m	83	LEU
44	m	102	THR
44	m	105	ASN
44	m	109	ARG
48	q	54	ASN
48	q	65	ARG
48	q	68	ARG
49	r	6	ARG
49	r	8	ARG
50	s	29	LYS
52	u	45	ARG
53	v	50	LEU
53	v	53	LEU
53	v	71	THR
53	v	89	MET
53	v	94	THR
53	v	97	ARG
53	v	138	LYS
53	v	143	ARG
53	v	158	TRP
53	v	164	TYR
53	v	166	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	v	177	LYS
53	v	234	ARG
53	v	259	THR
53	v	268	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
2	4	26	ASN
7	C	261	ASN
8	D	150	GLN
12	G	60	GLN
14	J	58	ASN
15	K	88	ASN
16	L	54	GLN
22	Q	37	GLN
22	Q	101	ASN
23	R	66	HIS
26	U	44	HIS
28	W	29	GLN
30	Y	12	GLN
30	Y	16	GLN
31	Z	43	ASN
33	b	3	GLN
33	b	24	ASN
36	e	147	ASN
38	g	153	HIS
40	i	75	GLN
46	o	61	ASN
53	v	102	ASN
53	v	116	ASN

5.3.3　RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
32	a	1525/1526 (99%)	301 (19%)	0
5	A	2880/2888 (99%)	707 (24%)	49 (1%)
6	B	119/120 (99%)	26 (21%)	2 (1%)
9	Dt	75/76 (98%)	23 (30%)	0
All	All	4599/4610 (99%)	1057 (22%)	51 (1%)

All (1057) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	A	10	A
5	A	33	U
5	A	34	U
5	A	35	G
5	A	44	A
5	A	45	G
5	A	46	G
5	A	51	G
5	A	54	A
5	A	59	U
5	A	61	G
5	A	63	A
5	A	74	A
5	A	75	G
5	A	79	C
5	A	82	G
5	A	85	G
5	A	91	A
5	A	92	A
5	A	97	A
5	A	100	U
5	A	102	G
5	A	104	U
5	A	114	U
5	A	115	C
5	A	118	A
5	A	120	U
5	A	125	G
5	A	131	A
5	A	137	G
5	A	138	A
5	A	139	U
5	A	141	A
5	A	142	C
5	A	144	U
5	A	146	G
5	A	147	G
5	A	149	A
5	A	150	U
5	A	160	A
5	A	162	U
5	A	163	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	A	164	C
5	A	165	A
5	A	166	U
5	A	172	C
5	A	173	A
5	A	181	A
5	A	194	G
5	A	196	A
5	A	199	A
5	A	202	U
5	A	205	G
5	A	215	G
5	A	216	A
5	A	220	G
5	A	222	A
5	A	227	A
5	A	228	C
5	A	230	G
5	A	233	A
5	A	240	U
5	A	241	A
5	A	242	G
5	A	243	U
5	A	244	A
5	A	248	G
5	A	249	C
5	A	252	G
5	A	255	A
5	A	265	A
5	A	266	G
5	A	267	C
5	A	271	U
5	A	273	A
5	A	281	U
5	A	285	U
5	A	289	G
5	A	294	A
5	A	299	C
5	A	305	A
5	A	315	U
5	A	316	A
5	A	317	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	A	318	U
5	A	321	G
5	A	322	U
5	A	323	G
5	A	324	A
5	A	325	U
5	A	335	C
5	A	337	C
5	A	338	G
5	A	339	A
5	A	342	G
5	A	347	U
5	A	348	U
5	A	349	U
5	A	350	G
5	A	351	A
5	A	353	G
5	A	358	A
5	A	359	U
5	A	360	C
5	A	361	A
5	A	374	C
5	A	376	C
5	A	377	G
5	A	380	A
5	A	381	A
5	A	385	U
5	A	387	G
5	A	390	U
5	A	391	G
5	A	395	A
5	A	396	U
5	A	397	G
5	A	398	G
5	A	399	G
5	A	400	G
5	A	403	A
5	A	406	A
5	A	407	U
5	A	408	C
5	A	414	A
5	A	428	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	A	431	C
5	A	435	C
5	A	438	A
5	A	445	A
5	A	447	C
5	A	448	A
5	A	461	A
5	A	464	G
5	A	466	C
5	A	471	A
5	A	472	G
5	A	481	A
5	A	485	G
5	A	496	A
5	A	499	A
5	A	500	C
5	A	509	G
5	A	519	A
5	A	521	G
5	A	522	C
5	A	523	A
5	A	534	A
5	A	535	C
5	A	536	U
5	A	537	U
5	A	538	G
5	A	539	U
5	A	540	U
5	A	541	A
5	A	550	C
5	A	553	A
5	A	557	U
5	A	558	U
5	A	562	A
5	A	563	U
5	A	564	A
5	A	565	A
5	A	576	A
5	A	586	A
5	A	593	A
5	A	594	G
5	A	599	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	A	601	C
5	A	603	U
5	A	604	A
5	A	610	U
5	A	611	A
5	A	618	G
5	A	622	A
5	A	627	A
5	A	635	U
5	A	636	A
5	A	647	U
5	A	659	G
5	A	660	A
5	A	671	G
5	A	672	G
5	A	673	C
5	A	676	U
5	A	687	G
5	A	708	A
5	A	716	G
5	A	720	A
5	A	737	U
5	A	738	G
5	A	743	G
5	A	747	G
5	A	754	A
5	A	755	C
5	A	765	G
5	A	766	G
5	A	767	A
5	A	769	U
5	A	772	A
5	A	774	G
5	A	775	G
5	A	783	A
5	A	784	G
5	A	793	U
5	A	795	G
5	A	802	C
5	A	817	U
5	A	824	G
5	A	827	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	A	833	G
5	A	836	U
5	A	841	C
5	A	843	G
5	A	844	G
5	A	846	G
5	A	848	G
5	A	850	A
5	A	855	A
5	A	866	U
5	A	870	G
5	A	875	A
5	A	877	C
5	A	878	C
5	A	880	G
5	A	881	A
5	A	889	A
5	A	899	A
5	A	904	C
5	A	908	U
5	A	911	C
5	A	921	C
5	A	922	G
5	A	931	A
5	A	935	A
5	A	936	C
5	A	949	A
5	A	951	C
5	A	952	G
5	A	954	C
5	A	963	A
5	A	964	A
5	A	972	C
5	A	973	A
5	A	980	A
5	A	986	A
5	A	999	A
5	A	1002	U
5	A	1003	U
5	A	1011	A
5	A	1012	G
5	A	1013	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	A	1016	U
5	A	1017	A
5	A	1023	U
5	A	1031	G
5	A	1036	A
5	A	1037	G
5	A	1048	G
5	A	1050	U
5	A	1051	U
5	A	1052	G
5	A	1057	A
5	A	1058	G
5	A	1060	A
5	A	1061	G
5	A	1063	A
5	A	1064	G
5	A	1066	C
5	A	1068	C
5	A	1076	A
5	A	1077	G
5	A	1078	A
5	A	1079	A
5	A	1080	A
5	A	1082	C
5	A	1084	U
5	A	1085	A
5	A	1086	A
5	A	1088	A
5	A	1097	G
5	A	1100	G
5	A	1101	A
5	A	1102	G
5	A	1114	G
5	A	1117	A
5	A	1119	A
5	A	1120	U
5	A	1124	A
5	A	1125	C
5	A	1133	A
5	A	1146	A
5	A	1148	G
5	A	1149	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	A	1154	G
5	A	1162	G
5	A	1164	A
5	A	1167	U
5	A	1168	G
5	A	1170	C
5	A	1171	G
5	A	1191	A
5	A	1192	A
5	A	1193	G
5	A	1198	U
5	A	1199	G
5	A	1214	A
5	A	1218	U
5	A	1223	G
5	A	1225	G
5	A	1228	A
5	A	1232	G
5	A	1233	A
5	A	1234	A
5	A	1238	C
5	A	1240	A
5	A	1243	G
5	A	1244	C
5	A	1249	A
5	A	1253	G
5	A	1256	A
5	A	1258	G
5	A	1259	A
5	A	1261	A
5	A	1263	U
5	A	1276	C
5	A	1283	G
5	A	1287	A
5	A	1288	A
5	A	1301	C
5	A	1311	G
5	A	1316	U
5	A	1321	G
5	A	1339	U
5	A	1349	C
5	A	1352	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	A	1354	A
5	A	1355	A
5	A	1363	C
5	A	1365	A
5	A	1366	U
5	A	1367	G
5	A	1370	A
5	A	1373	C
5	A	1379	A
5	A	1380	A
5	A	1382	A
5	A	1390	A
5	A	1402	U
5	A	1403	G
5	A	1404	C
5	A	1408	G
5	A	1414	A
5	A	1415	C
5	A	1422	G
5	A	1424	C
5	A	1434	U
5	A	1440	U
5	A	1441	U
5	A	1442	G
5	A	1445	U
5	A	1447	U
5	A	1448	C
5	A	1449	C
5	A	1454	U
5	A	1469	G
5	A	1474	C
5	A	1480	U
5	A	1481	A
5	A	1484	U
5	A	1496	A
5	A	1497	G
5	A	1508	G
5	A	1509	A
5	A	1511	G
5	A	1512	A
5	A	1516	G
5	A	1528	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	A	1537	U
5	A	1542	G
5	A	1556	A
5	A	1558	G
5	A	1559	A
5	A	1560	A
5	A	1573	U
5	A	1574	U
5	A	1576	A
5	A	1580	A
5	A	1597	C
5	A	1598	A
5	A	1600	A
5	A	1602	C
5	A	1603	G
5	A	1606	A
5	A	1608	A
5	A	1609	G
5	A	1614	U
5	A	1628	C
5	A	1629	C
5	A	1634	C
5	A	1636	C
5	A	1637	U
5	A	1638	U
5	A	1639	G
5	A	1654	A
5	A	1663	G
5	A	1664	G
5	A	1673	C
5	A	1683	U
5	A	1685	G
5	A	1686	G
5	A	1689	G
5	A	1690	A
5	A	1698	C
5	A	1704	A
5	A	1705	G
5	A	1708	U
5	A	1711	A
5	A	1714	A
5	A	1716	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	A	1717	U
5	A	1720	U
5	A	1721	C
5	A	1724	U
5	A	1731	U
5	A	1732	G
5	A	1735	U
5	A	1741	A
5	A	1742	A
5	A	1745	U
5	A	1749	A
5	A	1750	G
5	A	1751	G
5	A	1756	U
5	A	1760	A
5	A	1771	A
5	A	1773	A
5	A	1778	A
5	A	1787	C
5	A	1788	A
5	A	1795	A
5	A	1797	A
5	A	1798	G
5	A	1803	C
5	A	1816	A
5	A	1820	C
5	A	1834	A
5	A	1837	G
5	A	1838	U
5	A	1844	G
5	A	1850	G
5	A	1851	U
5	A	1853	A
5	A	1861	C
5	A	1873	U
5	A	1875	G
5	A	1892	C
5	A	1893	G
5	A	1897	G
5	A	1898	U
5	A	1899	A
5	A	1901	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	A	1902	U
5	A	1906	A
5	A	1916	G
5	A	1917	G
5	A	1918	U
5	A	1924	A
5	A	1925	A
5	A	1942	U
5	A	1949	C
5	A	1950	U
5	A	1951	G
5	A	1954	C
5	A	1957	A
5	A	1958	U
5	A	1959	G
5	A	1967	G
5	A	1968	A
5	A	1969	U
5	A	1978	U
5	A	1979	G
5	A	1982	U
5	A	1983	C
5	A	1984	C
5	A	1993	C
5	A	2008	A
5	A	2010	C
5	A	2015	U
5	A	2017	A
5	A	2018	A
5	A	2020	A
5	A	2028	U
5	A	2030	U
5	A	2039	A
5	A	2042	C
5	A	2043	G
5	A	2047	A
5	A	2048	G
5	A	2049	A
5	A	2055	U
5	A	2056	G
5	A	2060	C
5	A	2063	U

Continued from previous page...

Mol	Chain	Res	Type
5	A	2064	A
5	A	2067	G
5	A	2068	U
5	A	2080	G
5	A	2082	A
5	A	2083	C
5	A	2094	C
5	A	2095	U
5	A	2097	G
5	A	2098	U
5	A	2099	G
5	A	2101	A
5	A	2103	G
5	A	2106	A
5	A	2113	A
5	A	2114	G
5	A	2115	G
5	A	2116	C
5	A	2117	U
5	A	2118	U
5	A	2119	U
5	A	2121	A
5	A	2122	A
5	A	2127	G
5	A	2129	A
5	A	2132	C
5	A	2133	C
5	A	2135	G
5	A	2140	C
5	A	2141	G
5	A	2144	G
5	A	2145	A
5	A	2146	G
5	A	2147	C
5	A	2148	C
5	A	2149	A
5	A	2150	U
5	A	2151	C
5	A	2156	A
5	A	2157	A
5	A	2158	A
5	A	2159	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	A	2160	A
5	A	2169	G
5	A	2173	G
5	A	2174	C
5	A	2175	U
5	A	2185	A
5	A	2186	A
5	A	2187	C
5	A	2191	G
5	A	2194	C
5	A	2199	A
5	A	2201	C
5	A	2212	A
5	A	2221	G
5	A	2225	G
5	A	2226	G
5	A	2229	G
5	A	2237	G
5	A	2239	G
5	A	2240	G
5	A	2253	A
5	A	2264	G
5	A	2265	A
5	A	2270	U
5	A	2271	A
5	A	2274	A
5	A	2275	A
5	A	2284	C
5	A	2292	U
5	A	2296	A
5	A	2297	A
5	A	2305	G
5	A	2306	C
5	A	2307	A
5	A	2308	G
5	A	2309	A
5	A	2312	A
5	A	2313	U
5	A	2314	A
5	A	2319	C
5	A	2321	A
5	A	2322	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	A	2323	A
5	A	2333	A
5	A	2334	C
5	A	2337	C
5	A	2357	G
5	A	2358	G
5	A	2361	C
5	A	2363	A
5	A	2370	G
5	A	2372	C
5	A	2382	C
5	A	2383	G
5	A	2386	G
5	A	2389	U
5	A	2390	C
5	A	2393	U
5	A	2407	C
5	A	2409	C
5	A	2410	U
5	A	2413	A
5	A	2414	C
5	A	2415	G
5	A	2416	G
5	A	2417	A
5	A	2421	A
5	A	2422	A
5	A	2428	U
5	A	2434	G
5	A	2435	A
5	A	2446	A
5	A	2451	G
5	A	2453	C
5	A	2454	C
5	A	2457	G
5	A	2459	G
5	A	2462	C
5	A	2466	U
5	A	2471	G
5	A	2478	U
5	A	2480	U
5	A	2481	G
5	A	2489	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	A	2492	G
5	A	2505	A
5	A	2506	U
5	A	2517	A
5	A	2521	C
5	A	2522	G
5	A	2537	G
5	A	2541	U
5	A	2553	A
5	A	2554	G
5	A	2559	A
5	A	2560	C
5	A	2563	G
5	A	2565	G
5	A	2573	U
5	A	2586	G
5	A	2590	G
5	A	2593	C
5	A	2600	U
5	A	2602	U
5	A	2616	U
5	A	2619	A
5	A	2633	C
5	A	2640	U
5	A	2641	A
5	A	2647	A
5	A	2651	G
5	A	2660	G
5	A	2669	U
5	A	2676	U
5	A	2677	U
5	A	2689	G
5	A	2690	C
5	A	2692	A
5	A	2701	G
5	A	2703	C
5	A	2704	G
5	A	2705	G
5	A	2713	U
5	A	2714	G
5	A	2720	A
5	A	2726	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	A	2731	G
5	A	2733	U
5	A	2739	C
5	A	2743	U
5	A	2744	A
5	A	2751	A
5	A	2752	A
5	A	2763	A
5	A	2765	A
5	A	2766	U
5	A	2771	U
5	A	2784	U
5	A	2785	U
5	A	2786	G
5	A	2787	A
5	A	2794	U
5	A	2795	G
5	A	2805	C
5	A	2807	A
5	A	2811	C
5	A	2812	U
5	A	2818	G
5	A	2820	U
5	A	2821	G
5	A	2836	U
5	A	2842	U
5	A	2846	G
5	A	2851	G
5	A	2852	U
5	A	2854	G
5	A	2867	C
5	A	2870	A
5	A	2871	U
5	A	2884	U
5	A	2889	C
6	B	13	A
6	B	20	G
6	B	22	U
6	B	24	G
6	B	25	A
6	B	28	C
6	B	29	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	B	35	U
6	B	41	C
6	B	42	C
6	B	43	C
6	B	45	A
6	B	46	A
6	B	51	G
6	B	52	A
6	B	54	G
6	B	56	G
6	B	57	A
6	B	63	C
6	B	66	A
6	B	73	A
6	B	89	U
6	B	90	C
6	B	105	G
6	B	106	G
6	B	109	A
9	Dt	4	C
9	Dt	8	U
9	Dt	11	C
9	Dt	15	G
9	Dt	16	U
9	Dt	17	C
9	Dt	19	G
9	Dt	20	U
9	Dt	21	A
9	Dt	22	G
9	Dt	32	U
9	Dt	39	U
9	Dt	44	G
9	Dt	46	G
9	Dt	47	U
9	Dt	49	C
9	Dt	52	G
9	Dt	55	U
9	Dt	58	A
9	Dt	72	C
9	Dt	74	C
9	Dt	75	C
9	Dt	76	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	a	3	A
32	a	6	G
32	a	7	A
32	a	9	G
32	a	22	G
32	a	29	U
32	a	31	G
32	a	32	A
32	a	42	G
32	a	47	C
32	a	48	C
32	a	51	A
32	a	52	C
32	a	60	A
32	a	61	G
32	a	65	A
32	a	66	G
32	a	71	U
32	a	72	A
32	a	73	A
32	a	77	G
32	a	82	U
32	a	83	G
32	a	88	U
32	a	89	G
32	a	95	A
32	a	100	C
32	a	115	U
32	a	118	C
32	a	121	G
32	a	123	A
32	a	124	A
32	a	125	U
32	a	133	G
32	a	138	G
32	a	143	A
32	a	157	C
32	a	176	C
32	a	177	G
32	a	179	C
32	a	182	G
32	a	192	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	a	193	U
32	a	204	C
32	a	205	G
32	a	206	G
32	a	239	U
32	a	241	G
32	a	244	A
32	a	256	A
32	a	260	G
32	a	261	C
32	a	266	C
32	a	275	G
32	a	283	A
32	a	284	C
32	a	287	G
32	a	288	U
32	a	292	A
32	a	299	G
32	a	315	A
32	a	321	A
32	a	322	C
32	a	323	A
32	a	326	G
32	a	334	U
32	a	341	G
32	a	345	G
32	a	346	C
32	a	348	G
32	a	361	U
32	a	363	G
32	a	365	A
32	a	375	A
32	a	376	A
32	a	378	G
32	a	384	U
32	a	386	C
32	a	391	A
32	a	400	G
32	a	405	A
32	a	406	A
32	a	407	G
32	a	408	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	a	417	G
32	a	423	U
32	a	443	G
32	a	445	A
32	a	446	A
32	a	447	G
32	a	457	U
32	a	461	U
32	a	475	G
32	a	478	G
32	a	490	A
32	a	491	U
32	a	492	A
32	a	493	A
32	a	494	G
32	a	502	U
32	a	504	A
32	a	505	C
32	a	507	U
32	a	509	G
32	a	511	G
32	a	512	C
32	a	513	C
32	a	515	G
32	a	518	G
32	a	520	C
32	a	521	G
32	a	526	A
32	a	527	A
32	a	539	C
32	a	540	A
32	a	541	A
32	a	556	U
32	a	558	C
32	a	566	A
32	a	567	A
32	a	569	G
32	a	570	C
32	a	571	G
32	a	573	G
32	a	582	G
32	a	584	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	a	585	C
32	a	590	A
32	a	627	G
32	a	647	A
32	a	648	G
32	a	659	A
32	a	681	A
32	a	682	G
32	a	687	G
32	a	688	A
32	a	696	A
32	a	710	A
32	a	712	A
32	a	717	U
32	a	718	G
32	a	727	G
32	a	733	C
32	a	749	A
32	a	754	G
32	a	756	U
32	a	759	G
32	a	760	A
32	a	771	A
32	a	788	A
32	a	806	G
32	a	807	U
32	a	809	A
32	a	810	A
32	a	811	C
32	a	812	G
32	a	815	G
32	a	822	A
32	a	830	G
32	a	835	C
32	a	838	G
32	a	840	G
32	a	845	U
32	a	854	A
32	a	858	A
32	a	862	C
32	a	865	U
32	a	866	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	a	870	C
32	a	884	G
32	a	887	C
32	a	894	A
32	a	896	G
32	a	908	A
32	a	920	G
32	a	921	G
32	a	928	C
32	a	929	A
32	a	932	A
32	a	936	G
32	a	939	G
32	a	954	U
32	a	955	U
32	a	956	C
32	a	960	G
32	a	963	A
32	a	964	C
32	a	966	C
32	a	967	G
32	a	968	A
32	a	969	A
32	a	970	G
32	a	971	A
32	a	975	U
32	a	977	A
32	a	988	A
32	a	990	A
32	a	998	A
32	a	1004	C
32	a	1015	U
32	a	1017	G
32	a	1023	U
32	a	1025	C
32	a	1026	G
32	a	1027	G
32	a	1039	C
32	a	1044	G
32	a	1049	A
32	a	1059	U
32	a	1073	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	a	1075	G
32	a	1078	G
32	a	1079	U
32	a	1080	U
32	a	1086	A
32	a	1088	G
32	a	1089	U
32	a	1090	C
32	a	1095	A
32	a	1118	G
32	a	1119	U
32	a	1124	A
32	a	1127	A
32	a	1130	U
32	a	1133	G
32	a	1134	G
32	a	1149	A
32	a	1152	C
32	a	1153	U
32	a	1160	G
32	a	1162	C
32	a	1163	A
32	a	1164	A
32	a	1165	A
32	a	1175	G
32	a	1178	G
32	a	1184	G
32	a	1190	A
32	a	1191	A
32	a	1196	U
32	a	1207	A
32	a	1214	G
32	a	1219	A
32	a	1221	A
32	a	1222	C
32	a	1229	U
32	a	1230	A
32	a	1232	A
32	a	1234	U
32	a	1235	G
32	a	1248	G
32	a	1250	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	a	1251	U
32	a	1252	G
32	a	1254	C
32	a	1264	G
32	a	1266	U
32	a	1272	U
32	a	1273	A
32	a	1281	A
32	a	1293	A
32	a	1294	G
32	a	1297	C
32	a	1299	G
32	a	1314	C
32	a	1332	G
32	a	1334	A
32	a	1342	U
32	a	1347	G
32	a	1358	U
32	a	1362	A
32	a	1381	G
32	a	1388	A
32	a	1391	C
32	a	1397	C
32	a	1413	G
32	a	1414	U
32	a	1418	U
32	a	1419	U
32	a	1423	C
32	a	1424	C
32	a	1428	A
32	a	1440	A
32	a	1446	A
32	a	1448	G
32	a	1469	G
32	a	1470	A
32	a	1486	A
32	a	1487	A
32	a	1491	G
32	a	1497	A
32	a	1498	G
32	a	1499	G
32	a	1500	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	a	1501	A
32	a	1502	G
32	a	1511	G
32	a	1514	C
32	a	1523	G
32	a	1525	A
32	a	1526	U

All (51) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	A	81	G
5	A	87	C
5	A	114	U
5	A	227	A
5	A	243	U
5	A	266	G
5	A	314	A
5	A	334	A
5	A	348	U
5	A	360	C
5	A	434	A
5	A	444	A
5	A	538	G
5	A	540	U
5	A	774	G
5	A	783	A
5	A	792	A
5	A	840	U
5	A	920	C
5	A	953	U
5	A	963	A
5	A	1003	U
5	A	1016	U
5	A	1051	U
5	A	1169	A
5	A	1232	G
5	A	1233	A
5	A	1378	U
5	A	1448	C
5	A	1627	A
5	A	1653	G

Continued from previous page...

Mol	Chain	Res	Type
5	A	1672	G
5	A	1710	A
5	A	1715	U
5	A	1741	A
5	A	1891	G
5	A	1897	G
5	A	1917	G
5	A	2029	A
5	A	2149	A
5	A	2200	U
5	A	2228	A
5	A	2274	A
5	A	2536	G
5	A	2703	C
5	A	2750	G
5	A	2784	U
5	A	2793	C
5	A	2853	U
6	B	34	A
6	B	51	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 ⓘ

Of 171 ligands modelled in this entry, 171 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7   Other polymers ⓘ

There are no such residues in this entry.

5.8   Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
49	r	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	r	11:CYS	C	12:ARG	N	3.53

6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-16566. 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
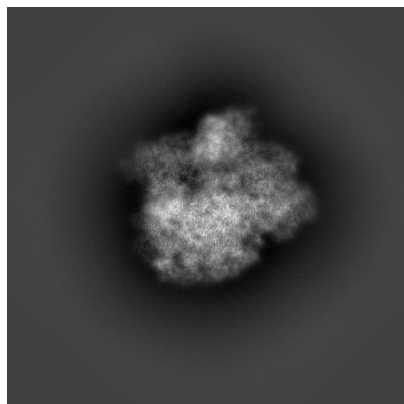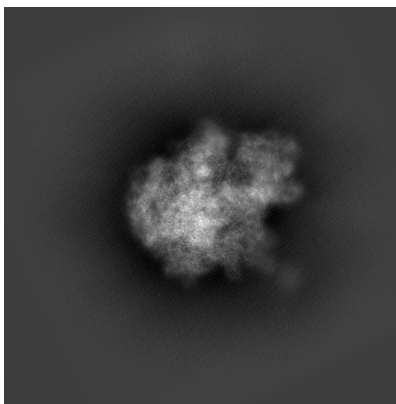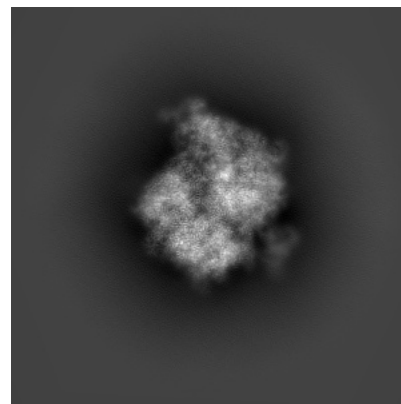
| X | Y | Z |

6.1.2 Raw map

| X | Y | Z |
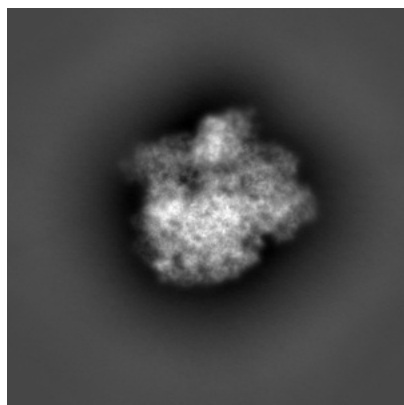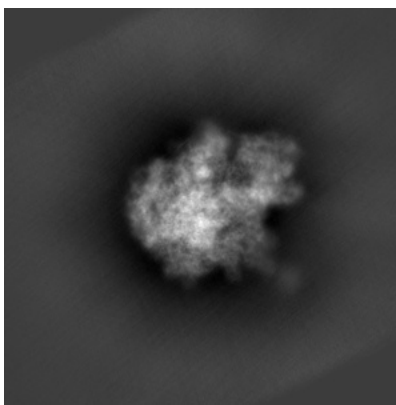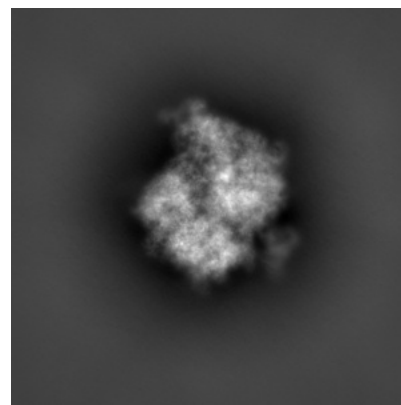
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
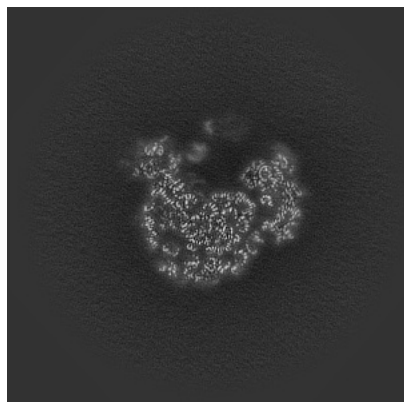
6.2.1 Primary map
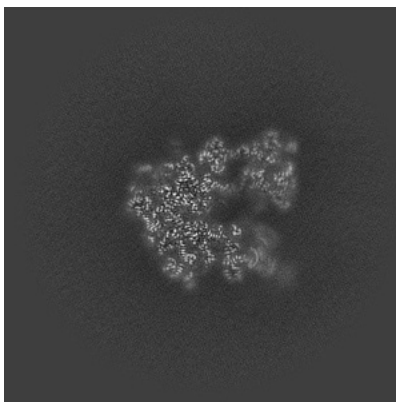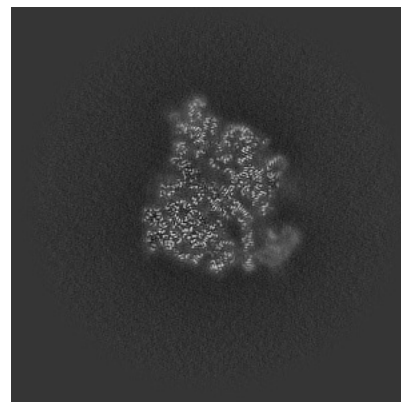
| X Index: 256 | Y Index: 256 | Z Index: 256 |

6.2.2 Raw map
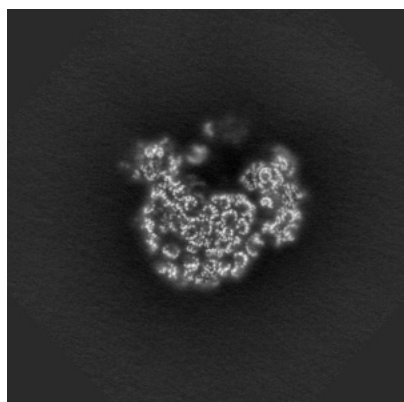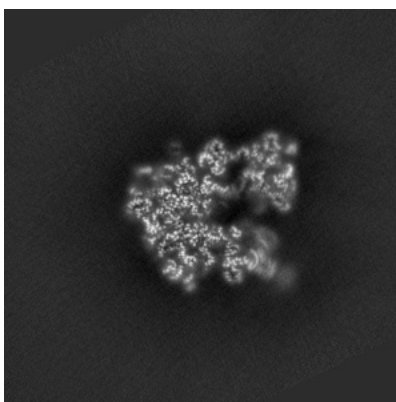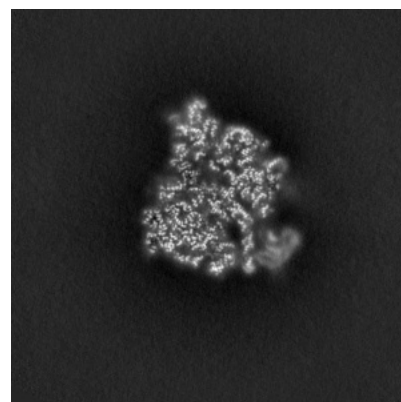
| X Index: 256 | Y Index: 256 | Z Index: 256 |

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

6.3　Largest variance slices ⓘ

6.3.1　Primary map
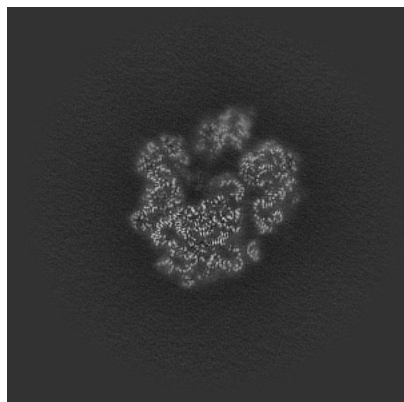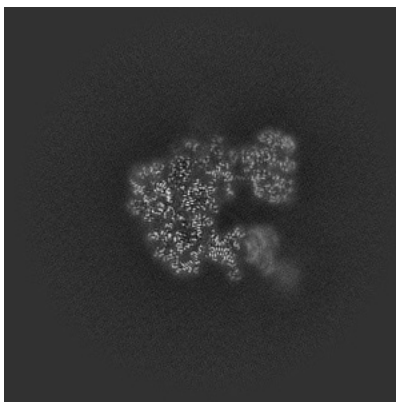
| X Index: 268 | Y Index: 267 | Z Index: 250 |
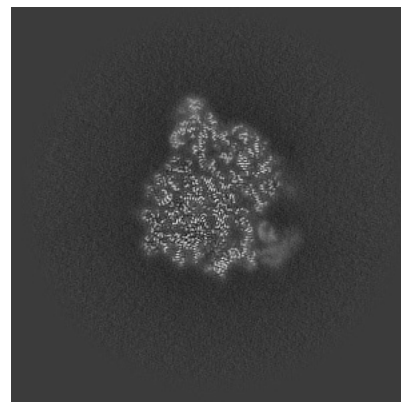
6.3.2　Raw map
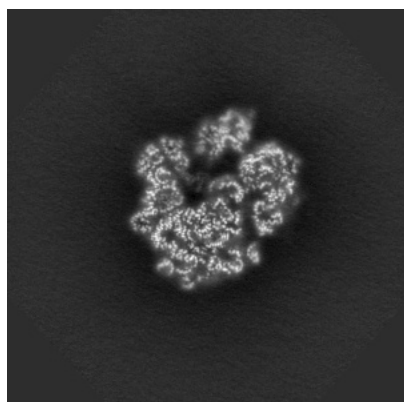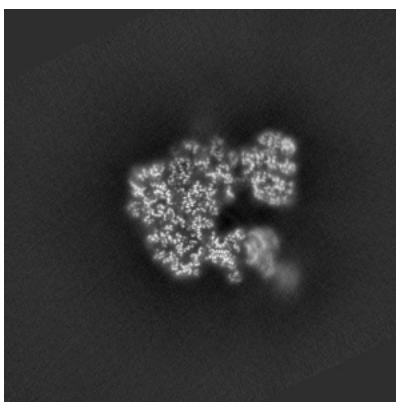
| X Index: 269 | Y Index: 267 | Z Index: 250 |
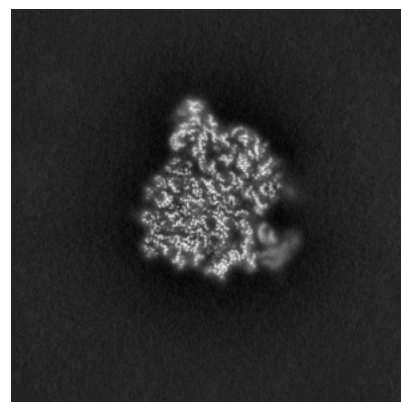
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1　Primary map
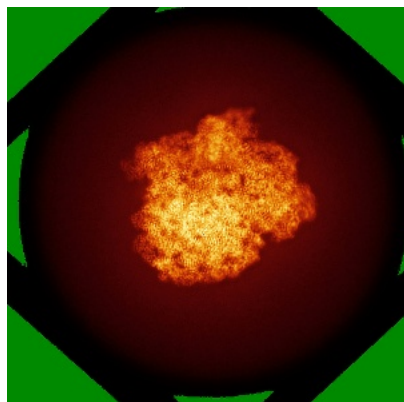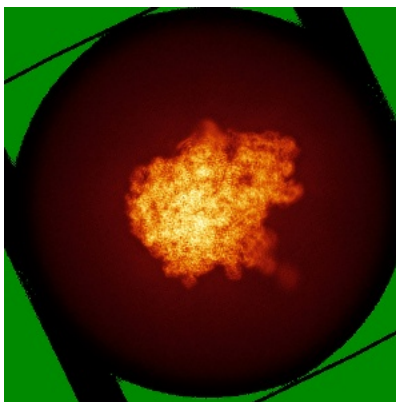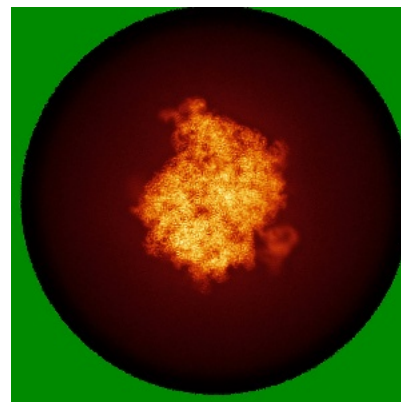
X　　　　　　　　　　Y　　　　　　　　　　Z

6.4.2　Raw map

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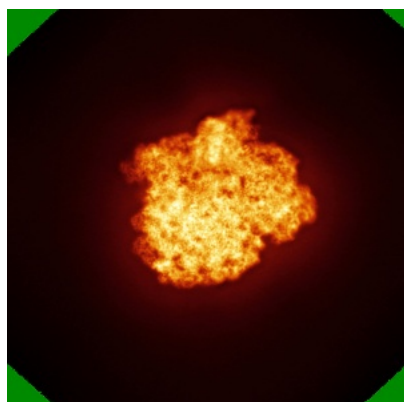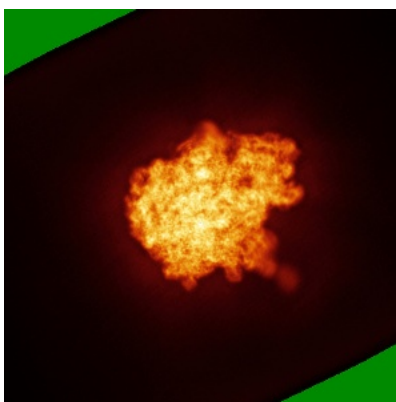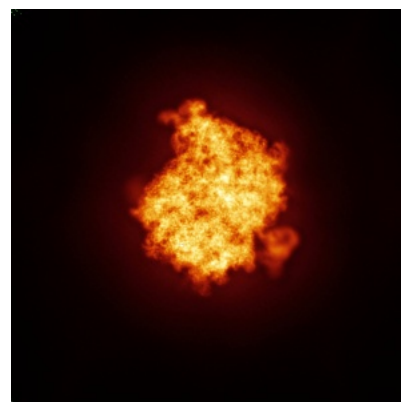
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X   Y   Z
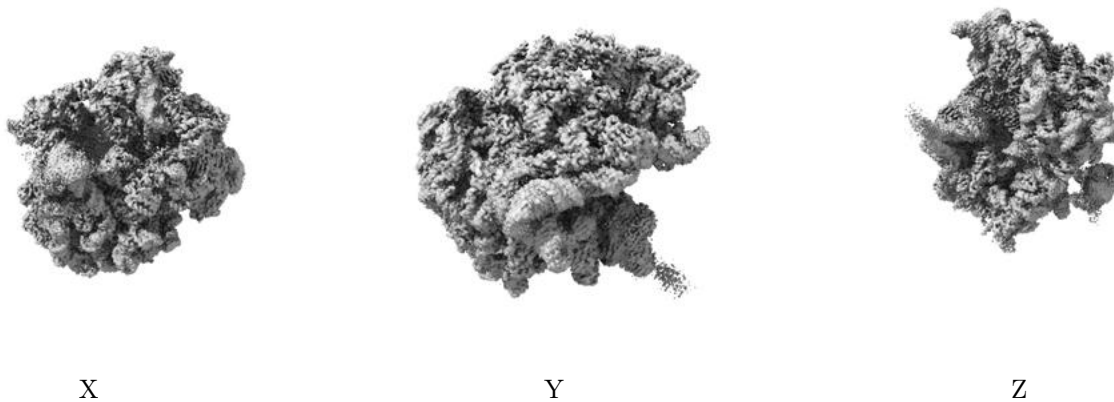
The images above show the 3D surface view of the map at the recommended contour level 3.46. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

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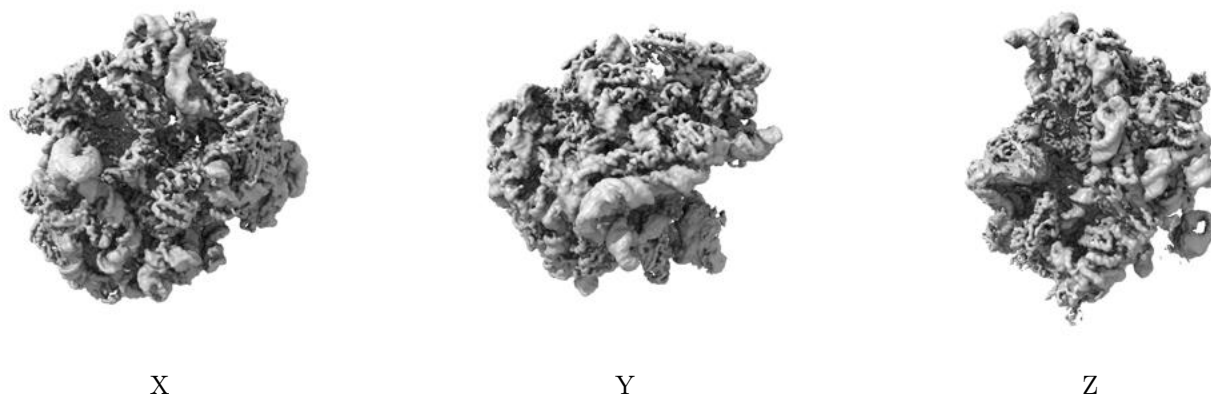
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation (i)

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

7 Map analysis ⓘ

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

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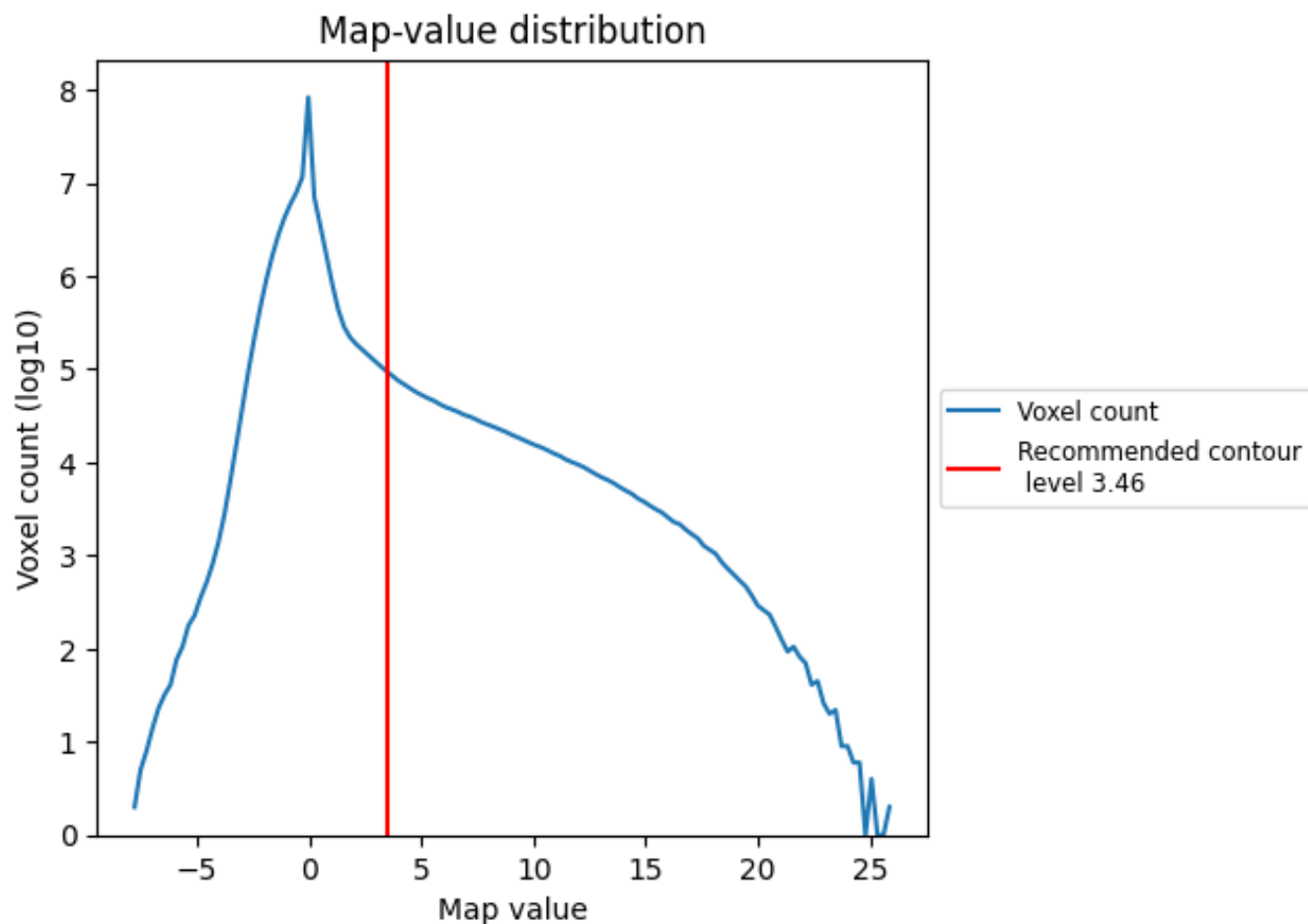
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate ⓘ
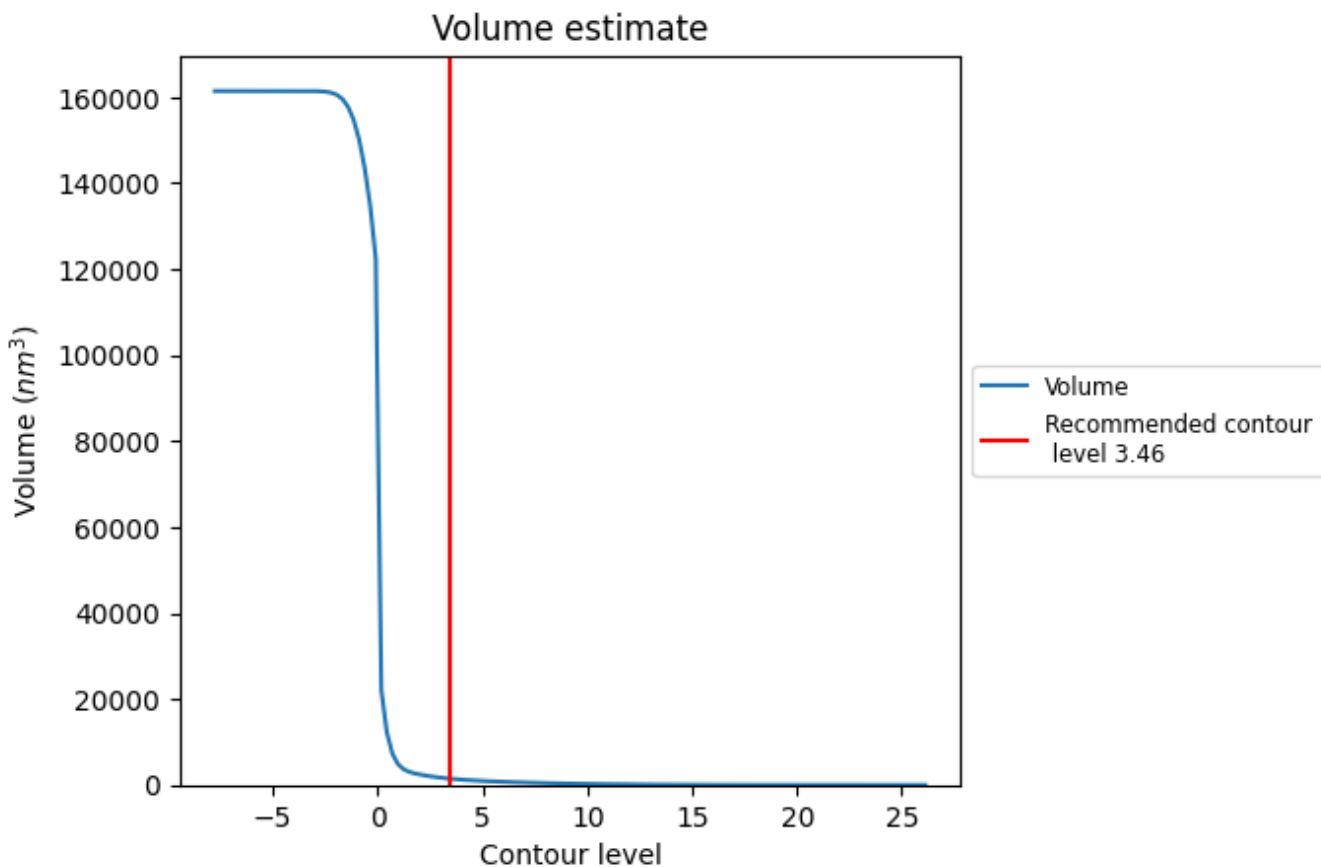
The volume at the recommended contour level is 1459 nm^3; this corresponds to an approximate mass of 1318 kDa.

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 ⓘ
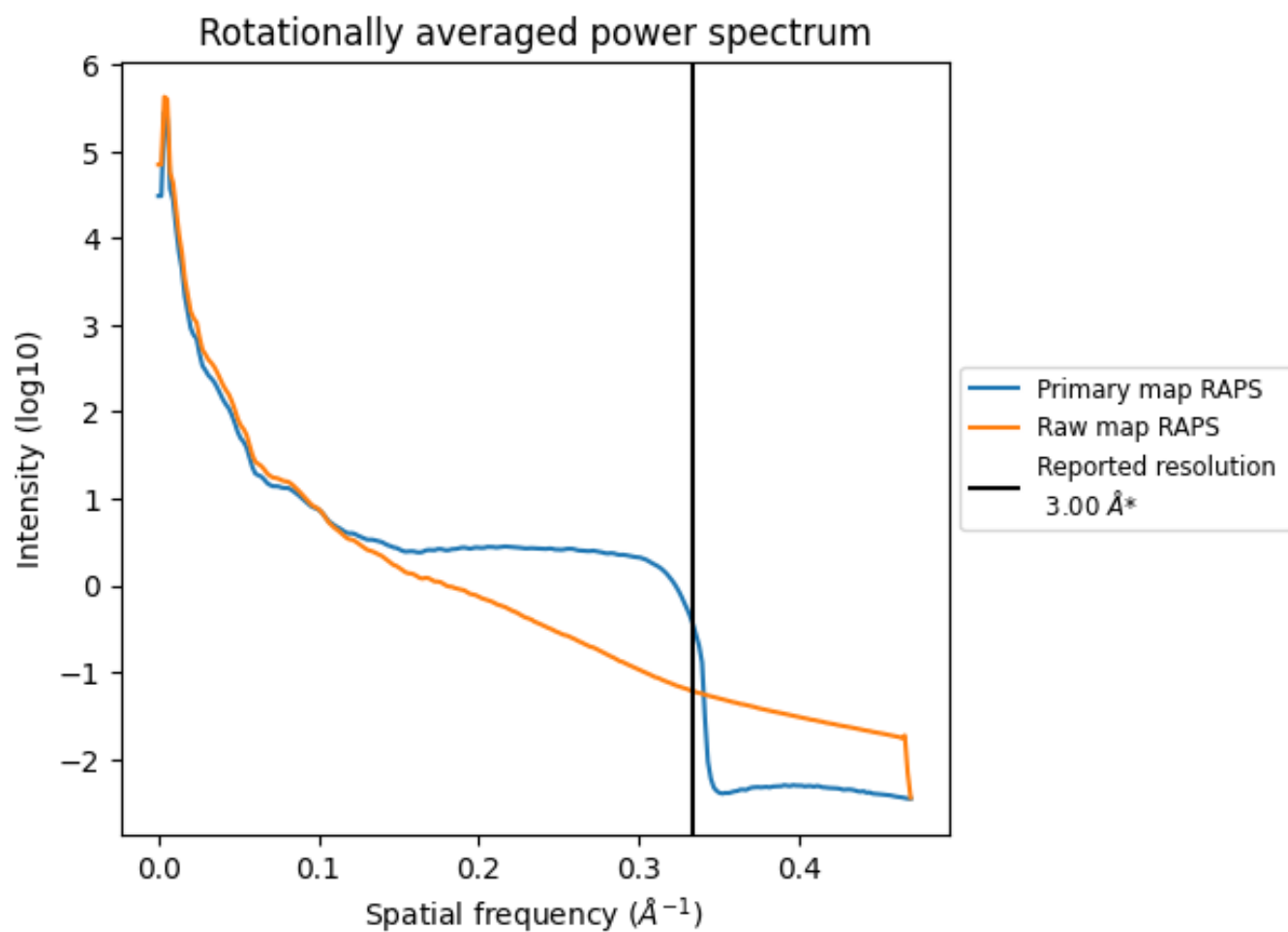
*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

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 ⓘ
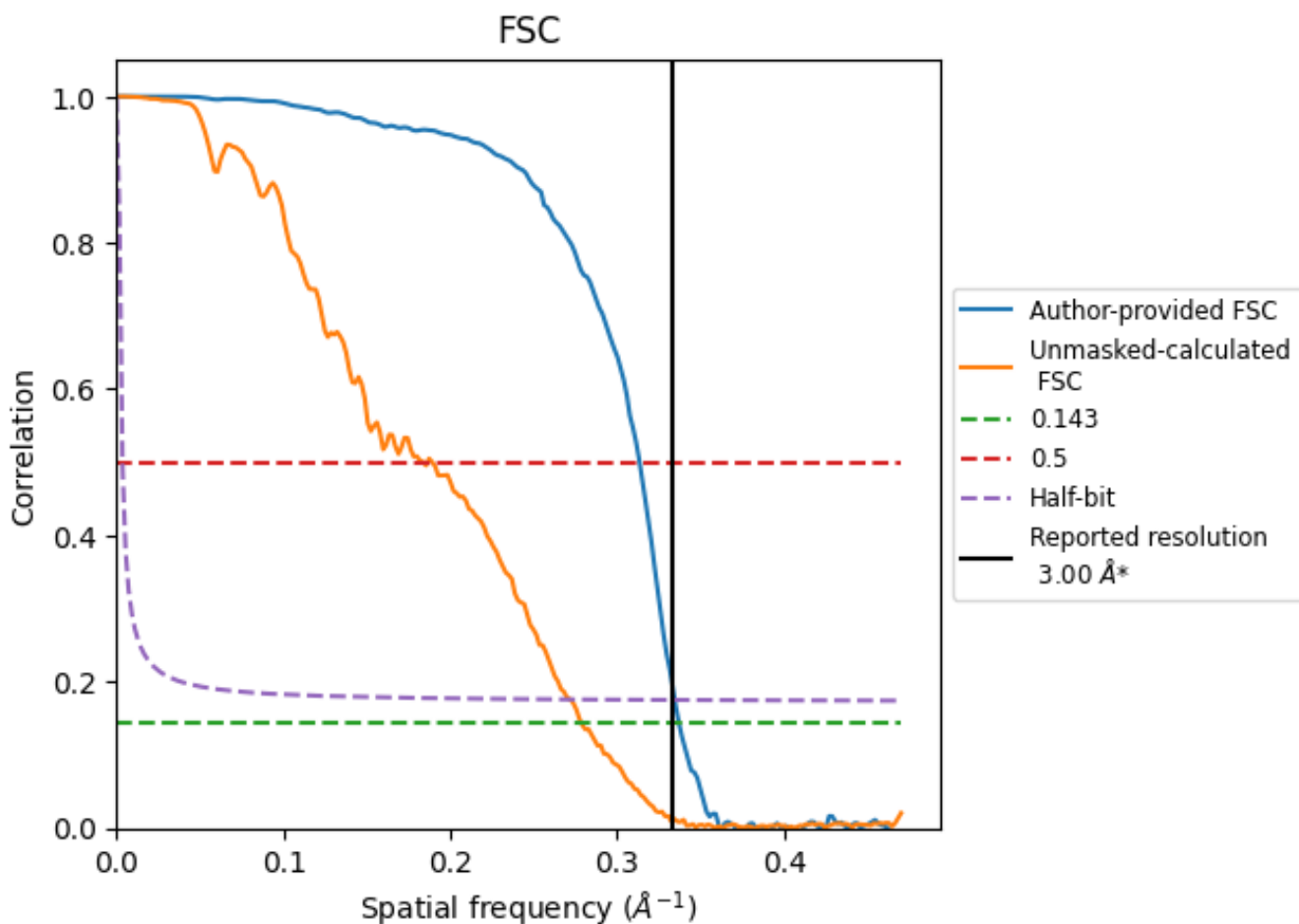
*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8.2 Resolution estimates ⓘ

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.97	3.19	2.99
Unmasked-calculated*	3.59	5.44	3.68

*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 3.59 differs from the reported value 3.0 by more than 10 %

9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-16566 and PDB model 8CD1. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay (i)

| X | Y | Z |
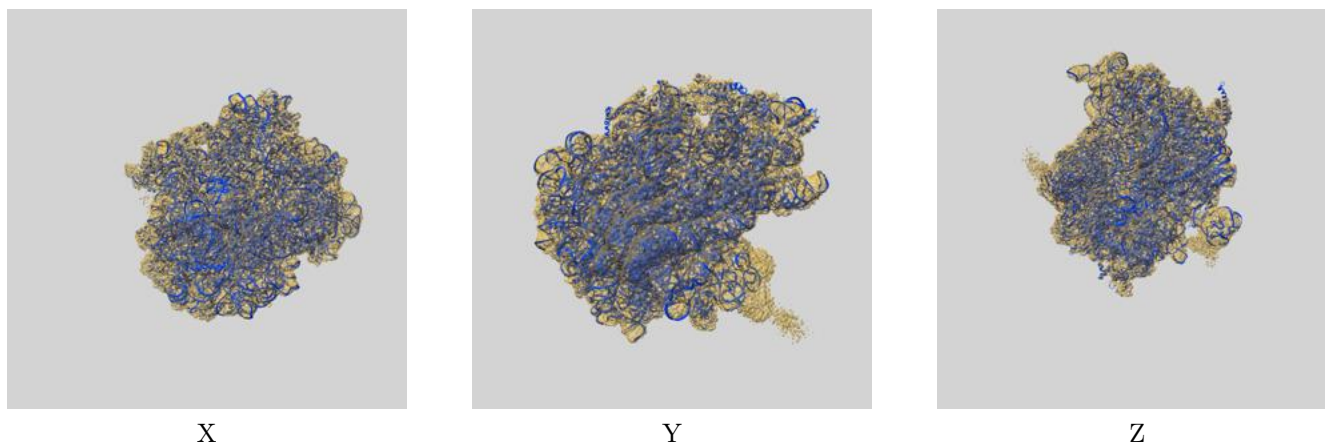
The images above show the 3D surface view of the map at the recommended contour level 3.46 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2　Q-score mapped to coordinate model ⓘ
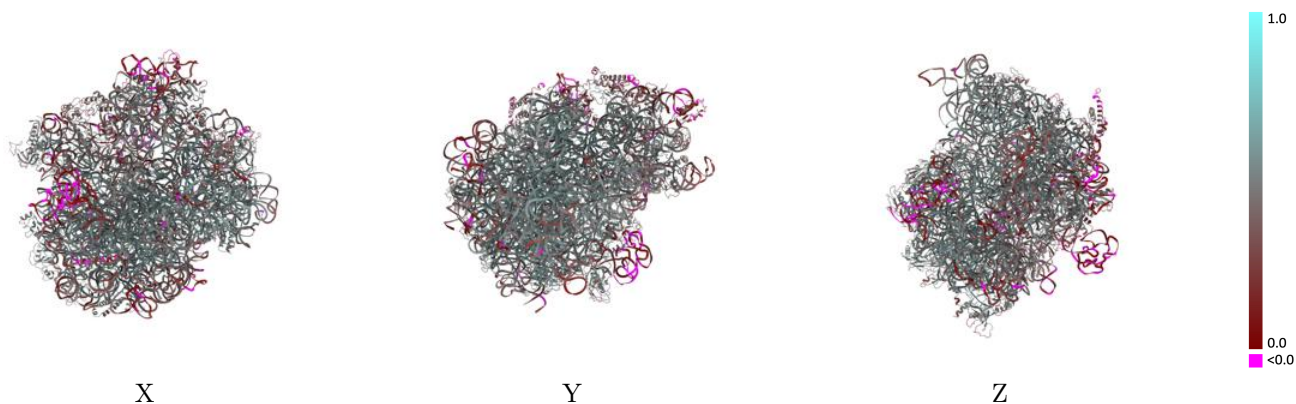
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 ⓘ
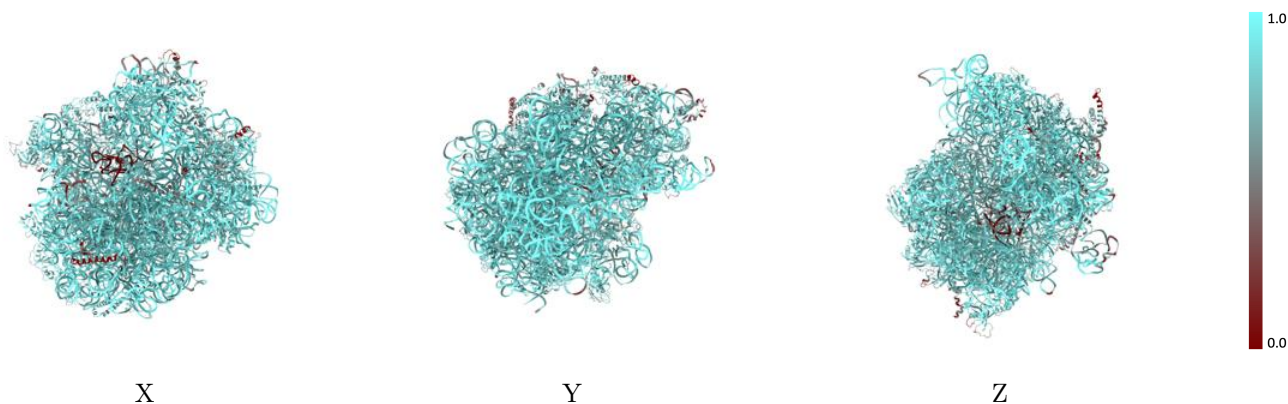
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.46).

9.4   Atom inclusion ⓘ
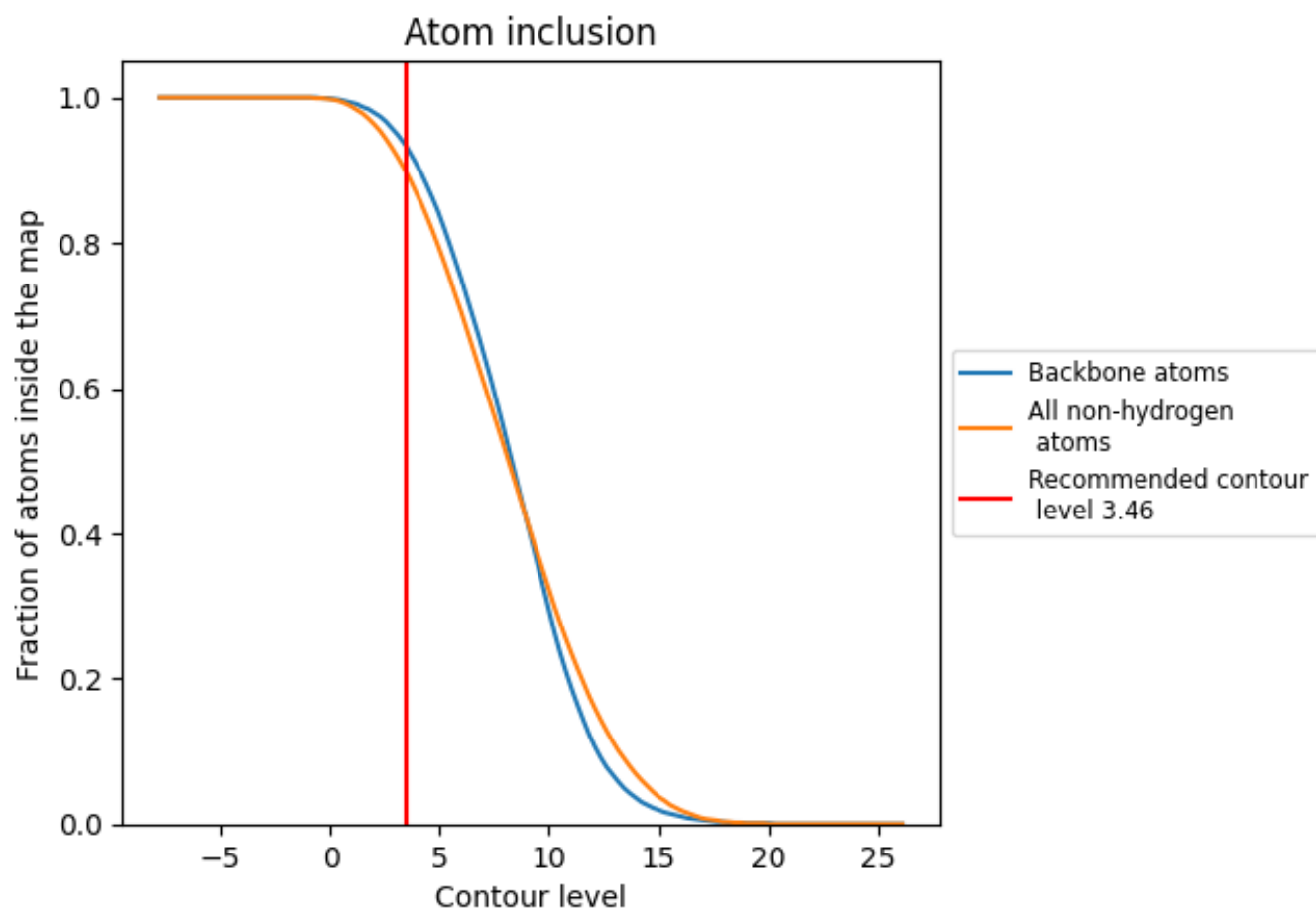
At the recommended contour level, 93% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (3.46) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8980	0.4610
2	0.8800	0.5090
4	0.9330	0.5560
5	0.6800	0.4950
6	0.8960	0.5200
A	0.9400	0.4550
B	0.9300	0.4200
C	0.9020	0.5320
D	0.8950	0.5120
Dt	0.1470	0.3840
E	0.8990	0.5220
F	0.7810	0.3700
G	0.8210	0.4400
H	0.1530	0.2090
J	0.9060	0.5310
K	0.8330	0.4870
L	0.8800	0.4960
Le	0.7180	0.3440
M	0.8750	0.5400
N	0.9200	0.5360
O	0.8660	0.4610
P	0.8550	0.4940
Q	0.9290	0.5520
R	0.8940	0.5230
S	0.8790	0.5210
T	0.9020	0.5250
U	0.8180	0.4650
V	0.8200	0.4580
W	0.8750	0.5090
X	0.9000	0.5260
Y	0.8850	0.4640
Z	0.9140	0.5280
a	0.9630	0.4840
b	0.6390	0.3340
c	0.8060	0.4230

1.0

0.0
<0.0

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
d	0.8360	0.4510
e	0.8150	0.4450
f	0.7900	0.4050
g	0.7650	0.3770
h	0.8740	0.4970
i	0.8530	0.4170
j	0.5110	0.1420
k	0.8480	0.4720
l	0.8320	0.4750
m	0.7860	0.3550
n	0.8650	0.4270
o	0.8730	0.4910
p	0.9250	0.5130
q	0.8600	0.4860
r	0.8000	0.4290
s	0.8260	0.3850
t	0.8990	0.5050
u	0.4290	0.3630
v	0.6920	0.4530