WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB EM Validation Report ⓘ

Oct 6, 2024 – 12:33 AM JST

PDB ID	:	5XXB
EMDB ID	:	EMD-6778
Title	:	Large subunit of Toxoplasma gondii ribosome
Authors	:	Li, Z.; Guo, Q.; Zheng, L.; Ji, Y.; Xie, Y.; Lai, D.; Lun, Z.; Suo, X.; Gao, N.
Deposited on	:	2017-07-03
Resolution	:	3.17 Å(reported)

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 3.17 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		1.5%
Sidechain outliers		4.8%
RNA backbone		0.46

Worse   *Better*

▉ Percentile relative to all structures
▯ Percentile relative to all EM structures
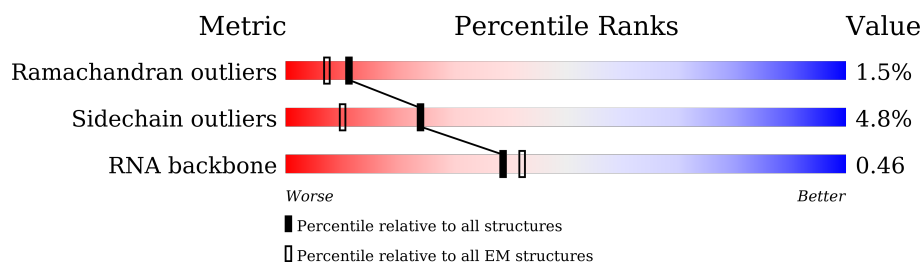
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	1	3477	67% 22% 12%
2	3	124	77% 18% 5%
3	4	158	7% 77% 22% •
4	A	260	91% • 5%
5	B	389	7% 89% 6% 5%
6	C	416	16% 91% • 5%
7	D	310	14% 81% • 16%
8	E	193	12% 62% • 36%
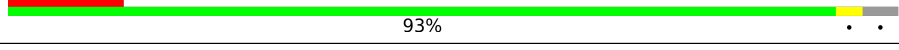
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Mol	Chain	Length	Quality of chain
9	F	258	14% / 93%
10	G	276	15% / 81% / 16%
11	H	190	12% / 94%
12	I	221	13% / 84% / 13%
13	J	175	39% / 91% / 5%
14	K	355	53% / 44%
15	L	134	13% / 90% / 7%
16	M	205	92% / 6%
17	N	269	5% / 71% / 26%
18	O	195	75% / 6% / 19%
19	P	187	5% / 94% / 5%
20	Q	187	18% / 93% / 6%
21	R	183	7% / 92% / 7%
22	S	157	9% / 92% / 6%
23	T	133	29% / 67% / 8% / 26%
24	U	139	8% / 90% / 7%
25	V	155	6% / 39% / 59%
26	W	167	7% / 71% / 5% / 24%
27	X	141	5% / 82% / 6% / 12%
28	Y	146	14% / 89% / 9%
29	Z	147	92% / 7%
30	a	54	13% / 85% / 6% / 9%
31	b	108	14% / 83% / 6% / 11%
32	c	120	6% / 82% / 7% / 11%
33	d	134	83% / 8% / 9%

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Mol	Chain	Length	Quality of chain
34	e	112	88% 6% 6%
35	f	134	6% 74% 6% 20%
36	g	123	11% 91% 7%
37	h	101	13% 93%
38	i	98	81% 8% 11%
39	j	84	21% 82% 14%
40	k	51	10% 84% 10%
41	l	129	38% 60%
42	n	105	8% 88% 5% 8%
43	o	96	5% 92% 6%
44	p	129	5% 92% 5%

2 Entry composition ⓘ

There are 44 unique types of molecules in this entry. The entry contains 121433 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 RNA chain called 25S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1	3077	65598	29312	11639	21570	3077	0	0

- Molecule 2 is a RNA chain called 5S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	3	118	2519	1123	452	826	118	0	0

- Molecule 3 is a RNA chain called 5.8S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	4	157	3339	1493	586	1103	157	0	0

- Molecule 4 is a protein called Ribosomal protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	246	1882	1170	379	324	9	0	0

- Molecule 5 is a protein called Ribosomal protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	B	369	2942	1867	561	496	18	0	0

- Molecule 6 is a protein called Ribosomal protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	C	394	3060	1897	621	528	14	0	0

- Molecule 7 is a protein called Ribosomal protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	261	Total	C	N	O	S	0	0
			2123	1336	406	375	6		

- Molecule 8 is a protein called Ribosomal protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	124	Total	C	N	O	S	0	0
			971	621	177	170	3		

- Molecule 9 is a protein called Ribosomal protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	250	Total	C	N	O	S	0	0
			2059	1324	389	338	8		

- Molecule 10 is a protein called Ribosomal protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	233	Total	C	N	O	S	0	0
			1877	1192	357	319	9		

- Molecule 11 is a protein called Ribosomal protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	187	Total	C	N	O	S	0	0
			1478	938	264	266	10		

- Molecule 12 is a protein called Ribosomal protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	193	Total	C	N	O	S	0	0
			1540	976	296	258	10		

- Molecule 13 is a protein called Ribosomal protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	166	Total	C	N	O	S	0	0
			1343	845	258	236	4		

- Molecule 14 is a protein called Ribosomal protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	199	Total 1593	C 1006	N 321	O 262	S 4	0	0

- Molecule 15 is a protein called Ribosomal protein eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	131	Total 1063	C 674	N 203	O 180	S 6	0	0

- Molecule 16 is a protein called Ribosomal protein eL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	202	Total 1683	C 1060	N 350	O 268	S 5	0	0

- Molecule 17 is a protein called Ribosomal protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	200	Total 1645	C 1034	N 330	O 272	S 9	0	0

- Molecule 18 is a protein called Ribosomal protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	158	Total 1286	C 805	N 249	O 222	S 10	0	0

- Molecule 19 is a protein called Ribosomal protein eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	186	Total 1477	C 918	N 306	O 246	S 7	0	0

- Molecule 20 is a protein called Ribosomal protein eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Q	176	Total 1473	C 918	N 309	O 236	S 10	0	0

- Molecule 21 is a protein called Ribosomal protein eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	R	182	Total	C	N	O	S	0	0
			1492	953	282	250	7		

- Molecule 22 is a protein called Ribosomal protein eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	S	154	Total	C	N	O	S	0	0
			1231	775	242	208	6		

- Molecule 23 is a protein called Ribosomal protein eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	T	99	Total	C	N	O	S	0	0
			827	531	147	145	4		

- Molecule 24 is a protein called Ribosomal protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	U	129	Total	C	N	O	S	0	0
			968	613	178	168	9		

- Molecule 25 is a protein called Ribosomal protein eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	V	63	Total	C	N	O	S	0	0
			533	344	104	82	3		

- Molecule 26 is a protein called Ribosomal protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	W	127	Total	C	N	O	S	0	0
			1038	655	194	186	3		

- Molecule 27 is a protein called Ribosomal protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	X	124	Total	C	N	O	S	0	0
			1011	629	207	172	3		

- Molecule 28 is a protein called Ribosomal protein eL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Y	144	Total 1163	C 751	N 214	O 191	S 7	0	0

- Molecule 29 is a protein called Ribosomal protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Z	145	Total 1136	C 724	N 221	O 186	S 5	0	0

- Molecule 30 is a protein called Ribosomal protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	a	49	Total 404	C 243	N 93	O 62	S 6	0	0

- Molecule 31 is a protein called Ribosomal protein eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	b	96	Total 725	C 450	N 134	O 134	S 7	0	0

- Molecule 32 is a protein called Ribosomal protein eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	c	107	Total 908	C 573	N 182	O 151	S 2	0	0

- Molecule 33 is a protein called Ribosomal protein eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	d	122	Total 1011	C 639	N 203	O 165	S 4	0	0

- Molecule 34 is a protein called Ribosomal protein eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	e	105	Total 854	C 546	N 167	O 140	S 1	0	0

- Molecule 35 is a protein called Ribosomal protein eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	f	107	863	535	191	132	5	0	0

- Molecule 36 is a protein called Ribosomal protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	g	121	981	615	199	165	2	0	0

- Molecule 37 is a protein called Ribosomal protein eL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	h	97	772	481	165	125	1	0	0

- Molecule 38 is a protein called Ribosomal protein eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	i	87	688	418	152	112	6	0	0

- Molecule 39 is a protein called Ribosomal protein eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	j	72	591	376	112	102	1	0	0

- Molecule 40 is a protein called Ribosomal protein eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	k	49	419	264	94	59	2	0	0

- Molecule 41 is a protein called Ribosomal protein eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	l	52	419	263	85	66	5	0	0

- Molecule 42 is a protein called Ribosomal protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	n	97	Total 790	C 503	N 157	O 125	S 5	0	0

• Molecule 43 is a protein called Ribosomal protein eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	o	90	Total 684	C 428	N 137	O 113	S 6	0	0

• Molecule 44 is a protein called Ribosomal protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	p	122	Total 974	C 607	N 197	O 161	S 9	0	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: 25S RNA
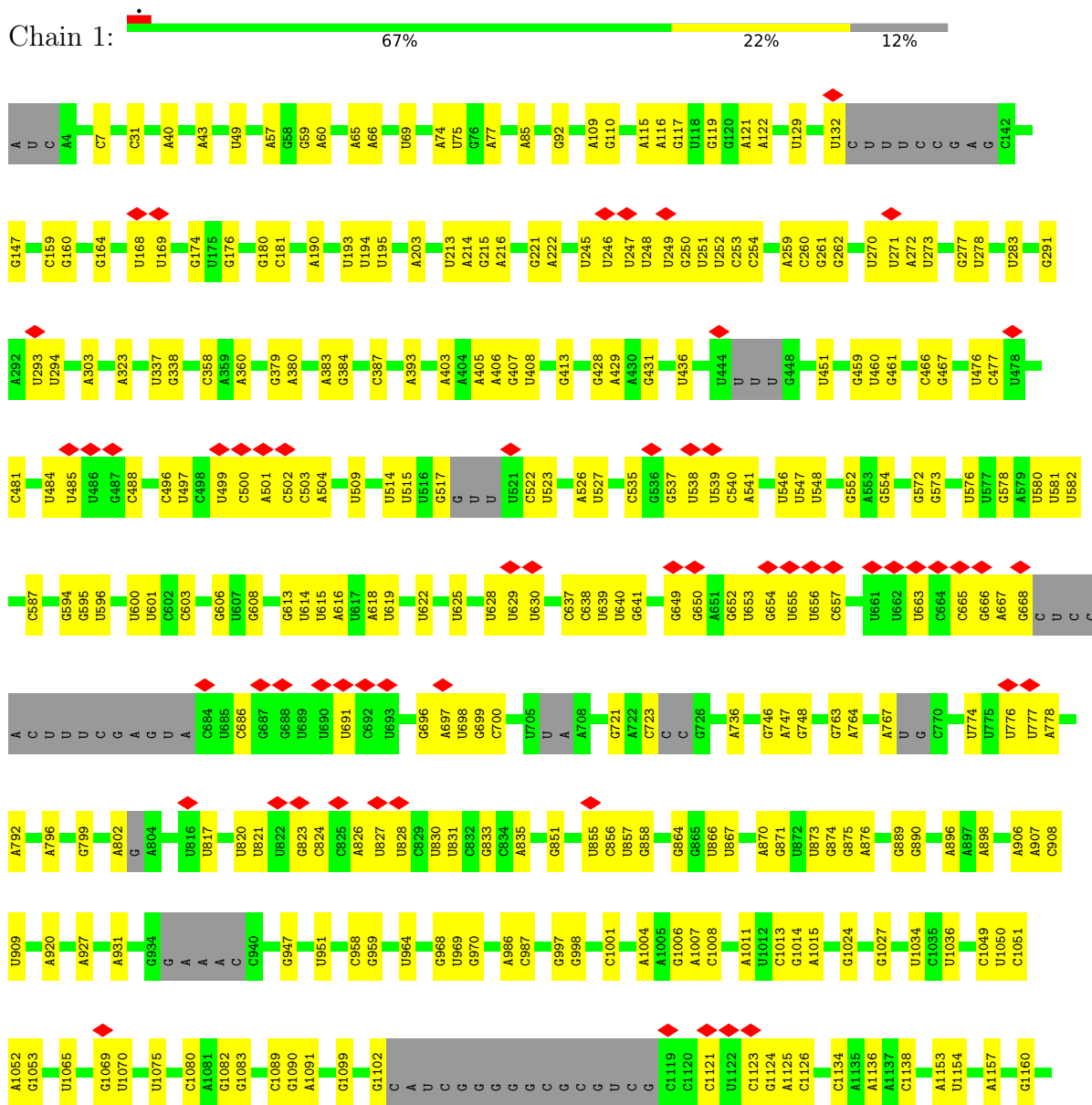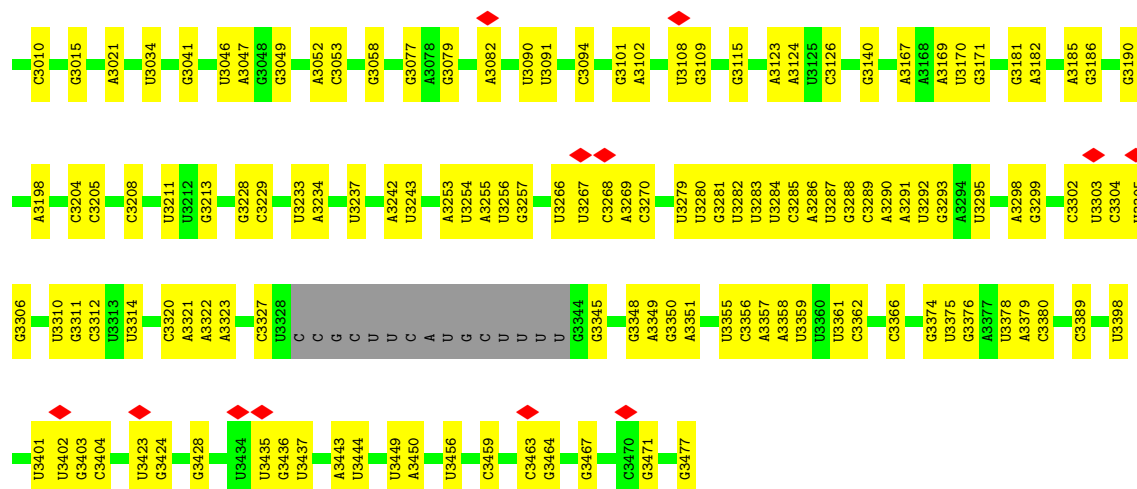
• Molecule 2: 5S RNA
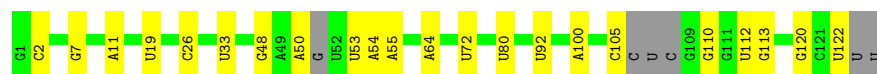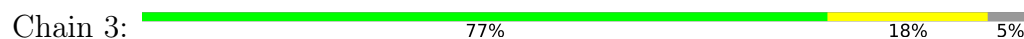
Chain 3:

77% 18% 5%

• Molecule 3: 5.8S RNA

Chain 4:

7% 77% 22%

• Molecule 4: Ribosomal protein uL2

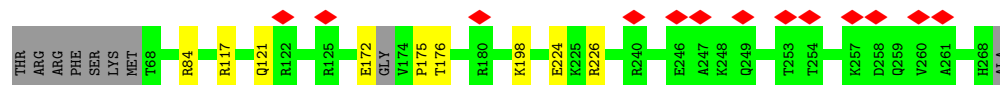Chain A:

91% 5%

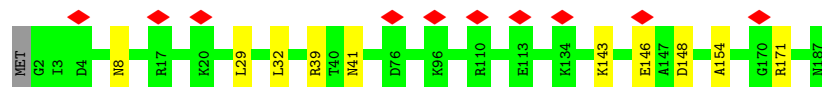
• Molecule 5: Ribosomal protein uL3

Chain B:

7% 89% 6% 5%

THR E276 A288 ASP P290 R291 E296 S297 D298 L299 H312 TYR G314 T315 V316 L321 L322 L323 K324 GLY CYS ILE VAL G329 T336 P343 R344 T345 T346 R347 A348 A349 L350 E351 S361 ALA LYS TRP G365 L382 K383 S384 ARG ALA ALA MET
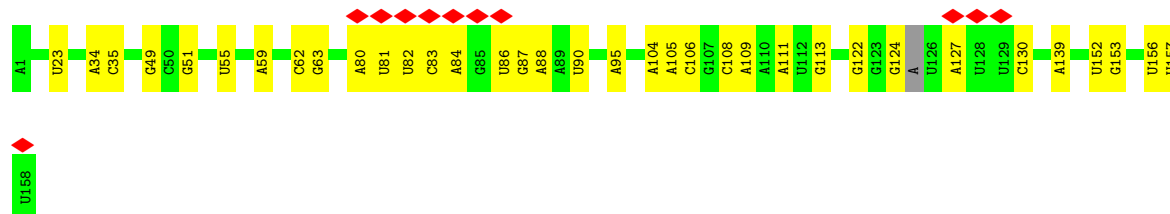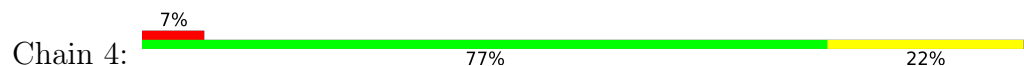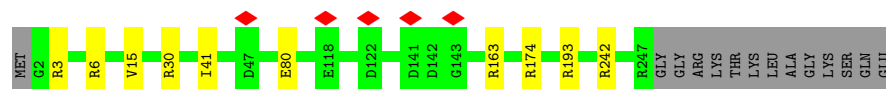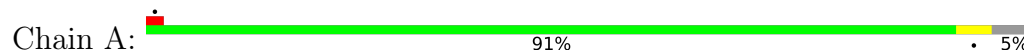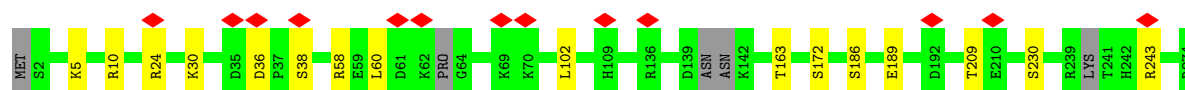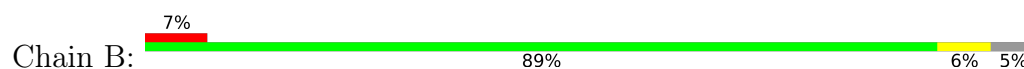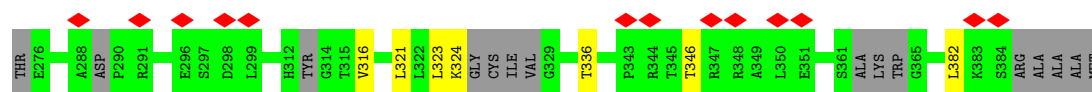
• Molecule 6: Ribosomal protein uL4

Chain C: 16%   91%   5%

MET A2 T3 A4 D15 G16 S19 P31 LEU R33 N57 V73 G82 GLY T84 H85 A90 ALA PHE G93 N94 M95 T107 W108 H122 L133 R140 GLY H142 D145 E172 L180 E181 R182 R191 D215 E229 D234 K259 T269

GLY T271 K277 A285 S288 N289 A290 D291 L292 S293 R294 E299 R303 A311 PRO GLN LYS LYS R316 G317 Q318 L323 K324 N325 H326 C330 R331 A336 R337 N338 L339 K340 I341 L342 A343 R344 T348 E349 G350 T351 K352 R359 K360 E366 K369 K370 H371

R372 Q373 R376 R377 A380 E381 A384 Q388 D388 K389 A392 E393 L394 E395 A396 A397 A398 R399 R400 K401 A402 E403 E404 A405 GLY ALA ILE ALA GLN ALA SER ALA GLU GLU GLU

• Molecule 7: Ribosomal protein uL18

Chain D: 14%   81%   16%

MET ALA PHE V4 K5 A6 L7 Y20 R21 Y44 L55 T68 I69 E70 K89 L92 Q112 E117 V122 E123 ALA T125 G126 E127 E133 N134 F135 G136 E137 D146 R151 N156 D167 Y182 SER LYS PRO GLU GLY GLU GLY GLU GLY S192 Y193

D194 P195 E196 D209 Y210 M211 E216 E217 D218 P219 E220 K221 Y222 S223 K233 I234 E235 A236 D237 D238 I239 E240 A241 M242 P254 D255 A256 V257 LYS LYS GLU ARG ALA ALA ASN VAL GLN ASN VAL ARG GLN GLY ASN VAL ILE LYS THR ALA LYS GLY GLN TYR VAL R283 K286

R295 Q298 K299 ILE ALA MET ILE ALA GLU GLN MET ALA GLU ALA

• Molecule 8: Ribosomal protein eL6

Chain E: 12%   62%   36%

MET ALA PRO THR ALA ALA ALA LEU ALA LYS LYS ARG LEU ARG THR ARG LYS PRO LYS ARG GLN LEU TYR LYS SER PRO ALA GLY ALA ALA LYS ARG M33 T41 L46 R54 L64 ALA P66 T73 GLY P75 T94 K97 V98 D99 ILE SER G102 V103 D104 V105 S106

S107 D110 G114 ALA SER LYS LYS GLU GLU GLY LYS PHE ALA GLU ARG LYS SER LEU ARG LYS LYS GLN ASP GLU GLY MET PHE VAL GLN GLN SER ASP SER LYS ALA LYS GLN ALA L147 F151 L154 Q155 D156 D159 K160 A161 L162 L163 A164 S167 K168 D169 K170 L171 L172 R179

G184 N185 M186 R187 K192 PHE

• Molecule 9: Ribosomal protein uL30

Chain F:

• Molecule 10: Ribosomal protein eL8

Chain G:

• Molecule 11: Ribosomal protein uL6

Chain H:

• Molecule 12: Ribosomal protein uL16
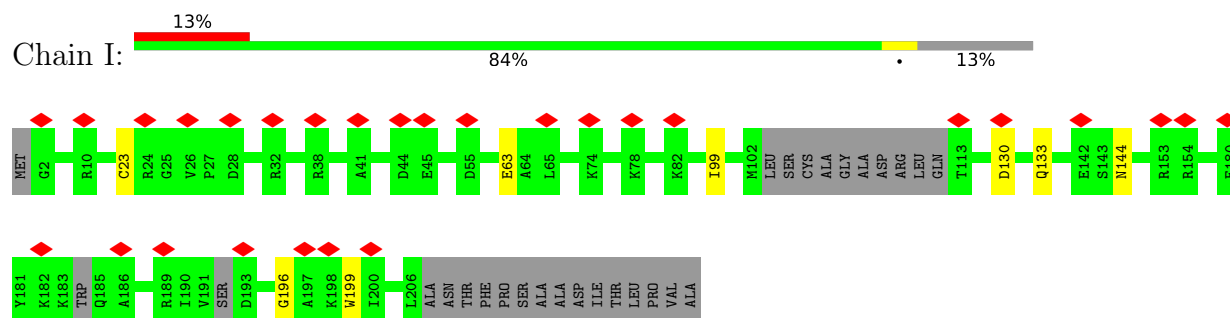
Chain I:

• Molecule 13: Ribosomal protein uL5
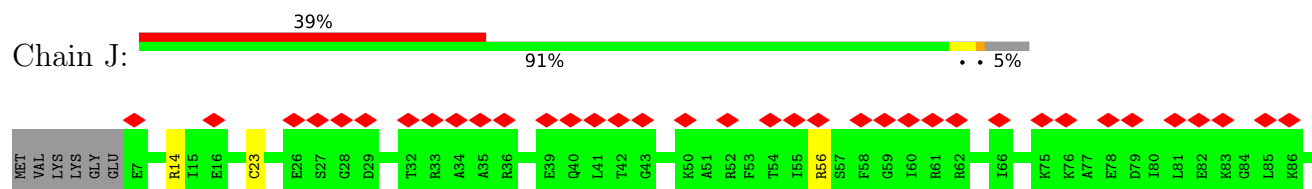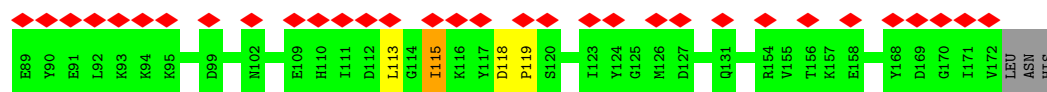
Chain J:

• Molecule 14: Ribosomal protein eL13

Chain K:

53%   44%
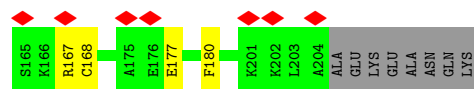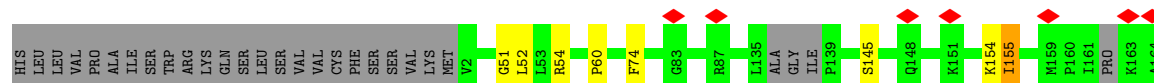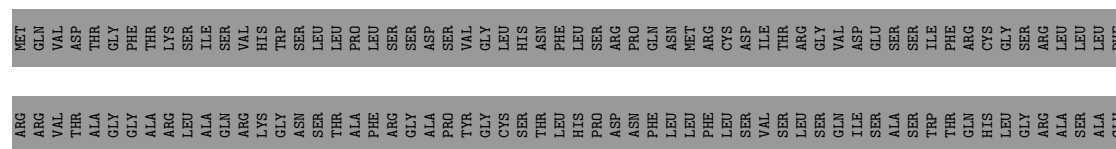
• Molecule 15: Ribosomal protein eL14

Chain L:

13%

90%   7%
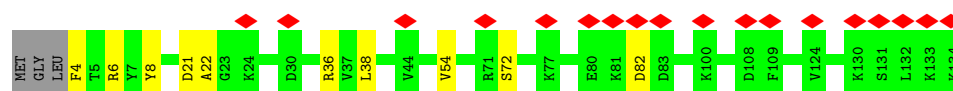
• Molecule 16: Ribosomal protein eL15

Chain M:

92%   6%

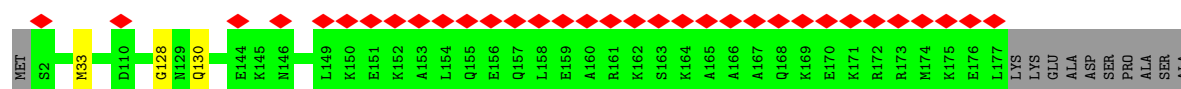• Molecule 17: Ribosomal protein uL13

Chain N:

5%

71%   26%
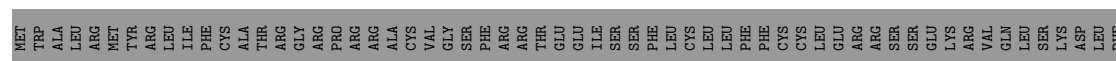
• Molecule 18: Ribosomal protein uL22

Chain O:

75%   6%   19%
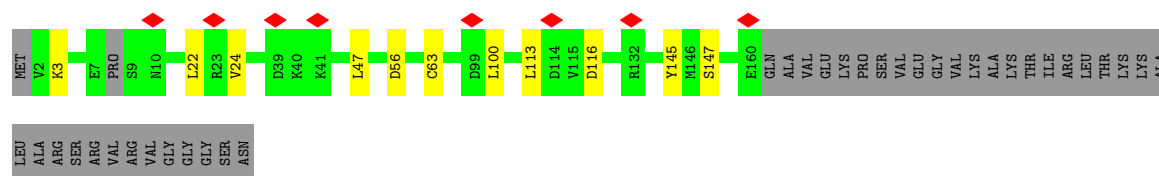
• Molecule 19: Ribosomal protein eL18

Chain P:

• Molecule 20: Ribosomal protein eL19

Chain Q:

• Molecule 21: Ribosomal protein eL20

Chain R:
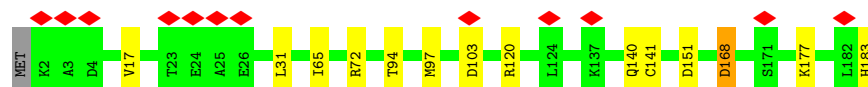
• Molecule 22: Ribosomal protein eL21

Chain S:

• Molecule 23: Ribosomal protein eL22

Chain T:
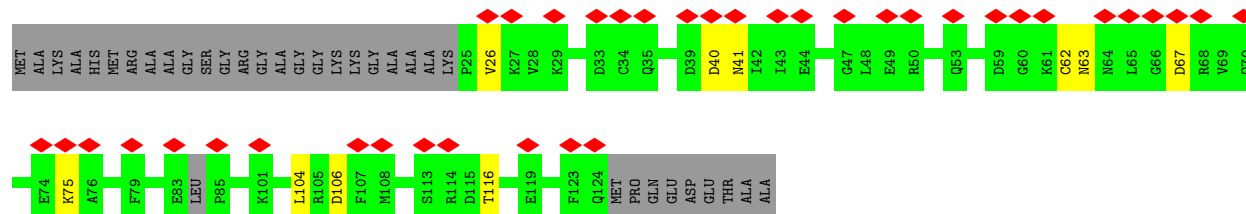
• Molecule 24: Ribosomal protein uL14

Chain U:

8%

90%

7%

• Molecule 25: Ribosomal protein eL24

Chain V:

6%

39%

59%

• Molecule 26: Ribosomal protein uL23

Chain W:

7%

71%

5%

24%

• Molecule 27: Ribosomal protein uL24

Chain X:

5%

82%

6%

12%

• Molecule 28: Ribosomal protein eL27

Chain Y:

14%

89%

9%

• Molecule 29: Ribosomal protein uL15

Chain Z:

92%

7%

• Molecule 30: Ribosomal protein eL29

Chain a:

13%

85%　　6%　9%

MET A2 K3 S4 K5 N6 N19 GLY I21 Q25 R26 K27 R28 K29 M30 R48 M51 LYS SER ASP

• Molecule 31: Ribosomal protein eL30

Chain b:

14%

83%　6%　11%

MET ALA LYS LYS ALA LYS LYS SER GLY SER E11 G12 R16 L17 Q18 K22 L28 K31 G40 L44 I47 C51 C68 G69 V70 H74 G75 D76 N77 N78 E79 D97 PRO G99 D100 S101 D102 R105 S106 V107 GLU
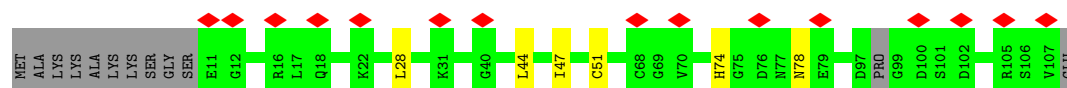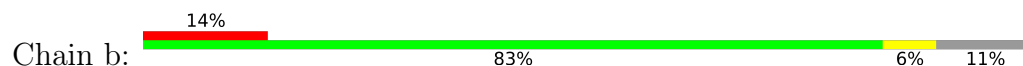
• Molecule 32: Ribosomal protein eL31

Chain c:

6%

82%　7%　11%

MET LYS GLY THR THR ARG LYS ALA GLN ASN LYS S12 D19 Y20 T21 E43 M52 I72 N88 ASP D90 E91 D92 S93 K94 L100 E110 N111 E119 GLU
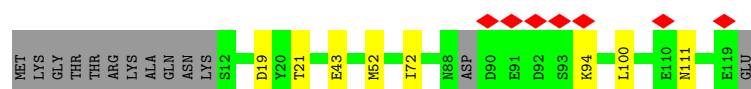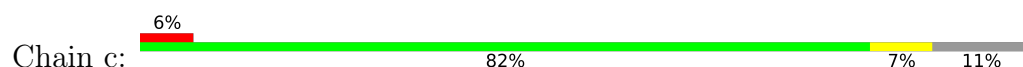
• Molecule 33: Ribosomal protein eL32

Chain d:

83%　8%　9%

MET ALA PRO VAL SER THR V7 K8 R9 S10 D25 K36 D41 N56 M68 L77 D83 N91 V121 R124 S125 A126 R127 L128 ASP THR ALA GLU ASP GLU
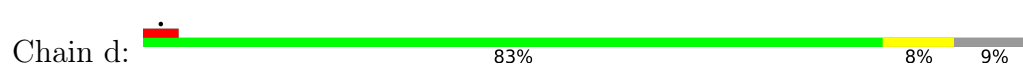
• Molecule 34: Ribosomal protein eL33

Chain e:

88%　6%　6%

MET LYS LYS SER GLY T6 V10 R11 Q28 L35 D45 R53 T62 GLU K64 N93 L107 N111 ILE
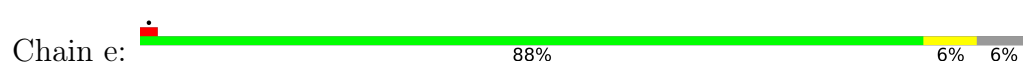
• Molecule 35: Ribosomal protein eL34

Chain f:

6%

74%　6%　20%

MET A2 P3 R4 L5 V31 Q38 R41 C47 H48 R49 I54 R68 E96 K102 Q103 V104 L105 Q106 V107 K108 GLU LYS GLN LYS LYS ASP GLU MET LYS ALA GLU SER LYS LYS SER LYS GLN LYS LYS SER SER LYS THR ALA LYS ALA
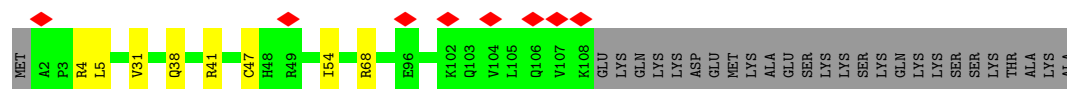
• Molecule 36: Ribosomal protein uL29

Chain g:

11%

91%　7%

MET VAL K3 E8 L21 K35 S39 A40 A41 S42 K43 L44 S45 L58 E67 G75 N81 D82 L83 R84 R94 L95 R101 L121 I122 A123
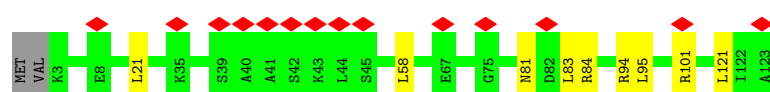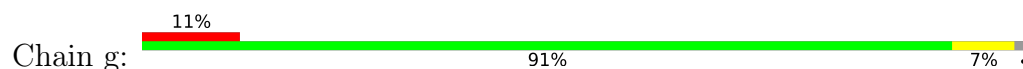
• Molecule 37: Ribosomal protein eL36

Chain h:
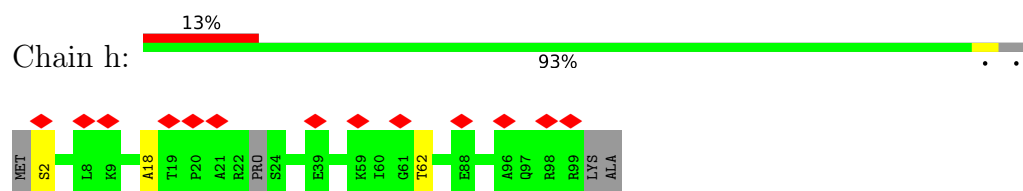
• Molecule 38: Ribosomal protein eL37

Chain i:
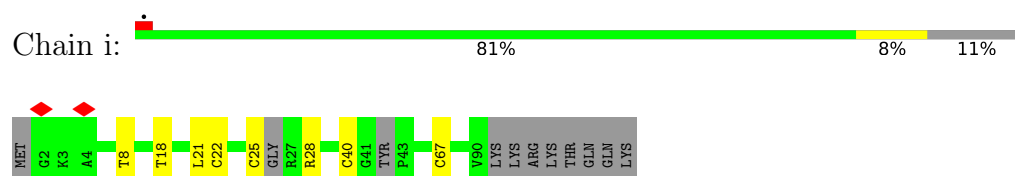
• Molecule 39: Ribosomal protein eL38

Chain j:
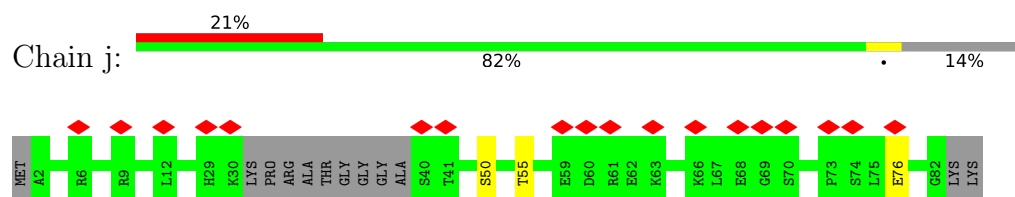
• Molecule 40: Ribosomal protein eL39

Chain k:
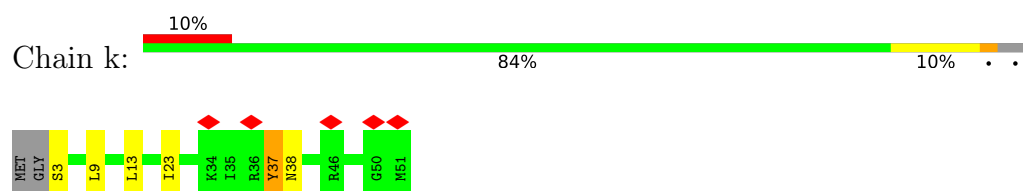
• Molecule 41: Ribosomal protein eL40

Chain l:
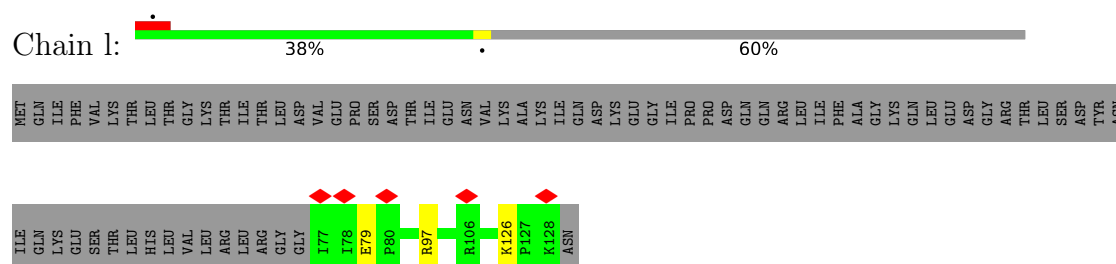
• Molecule 42: Ribosomal protein eL42

Chain n:
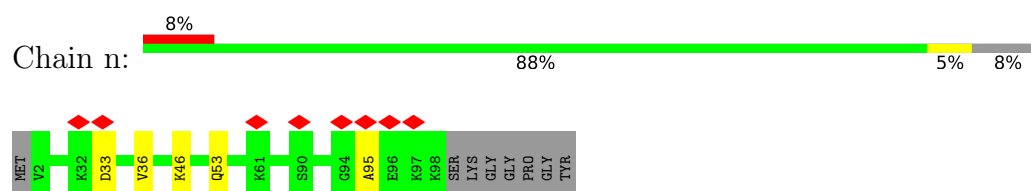
• Molecule 43: Ribosomal protein eL43

5%

Chain o:

92%   6%

MET A2 K13 R58 T73 K88 Q89 A90 G91 GLU ALA GLN ALA ALA
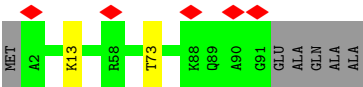
• Molecule 44: Ribosomal protein eL28

5%

Chain p:

92%   5%

MET V2 C16 R30 I44 K47 N53 G56 R84 M97 N112 K117 T121 GLY N123 S124 SER ASN LYS LYS GLU
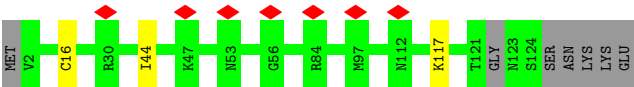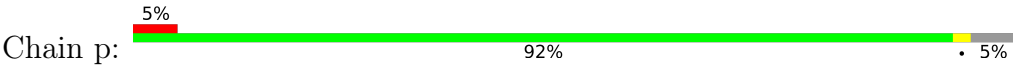
4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	108162	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.354	Depositor
Minimum map value	-0.211	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	1	0.22	0/73347	0.68	0/114257
2	3	0.20	0/2813	0.66	0/4379
3	4	0.23	0/3731	0.67	0/5808
4	A	0.33	0/1918	0.61	0/2572
5	B	0.37	0/3006	0.58	0/4023
6	C	0.35	0/3104	0.59	0/4164
7	D	0.35	0/2158	0.56	0/2891
8	E	0.35	0/981	0.54	0/1311
9	F	0.36	0/2102	0.55	0/2811
10	G	0.37	0/1905	0.57	0/2546
11	H	0.35	0/1500	0.53	0/2019
12	I	0.40	0/1570	0.62	0/2099
13	J	0.37	0/1366	0.54	0/1823
14	K	0.34	0/1621	0.60	0/2172
15	L	0.39	0/1077	0.63	0/1438
16	M	0.39	0/1715	0.65	0/2289
17	N	0.36	0/1671	0.59	0/2233
18	O	0.42	0/1308	0.66	0/1744
19	P	0.34	0/1498	0.62	0/1992
20	Q	0.34	0/1491	0.57	0/1970
21	R	0.37	0/1523	0.61	0/2043
22	S	0.40	0/1257	0.59	0/1685
23	T	0.39	0/840	0.59	0/1120
24	U	0.36	0/984	0.58	0/1326
25	V	0.37	0/547	0.59	0/728
26	W	0.36	0/1054	0.62	0/1420
27	X	0.38	0/1026	0.63	0/1367
28	Y	0.40	0/1182	0.59	0/1573
29	Z	0.48	0/1161	0.72	0/1549
30	a	0.30	0/408	0.59	0/531
31	b	0.39	0/732	0.56	0/980
32	c	0.38	0/925	0.65	0/1239
33	d	0.36	0/1029	0.71	0/1370
34	e	0.35	0/872	0.60	0/1170

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
35	f	0.37	0/881	0.68	0/1183
36	g	0.37	0/987	0.62	0/1306
37	h	0.37	0/779	0.66	0/1033
38	i	0.47	0/700	0.79	0/923
39	j	0.37	0/599	0.55	0/800
40	k	0.47	0/428	0.77	0/566
41	l	0.42	0/426	0.64	0/566
42	n	0.33	0/802	0.54	0/1057
43	o	0.36	0/693	0.60	0/923
44	p	0.34	0/984	0.60	0/1307
All	All	0.29	0/130701	0.66	0/192306

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	
4	A	244/260 (94%)	228 (93%)	15 (6%)	1 (0%)	30	62
5	B	351/389 (90%)	312 (89%)	33 (9%)	6 (2%)	7	33
6	C	380/416 (91%)	345 (91%)	30 (8%)	5 (1%)	10	39
7	D	253/310 (82%)	225 (89%)	24 (10%)	4 (2%)	8	35
8	E	114/193 (59%)	101 (89%)	12 (10%)	1 (1%)	14	47

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WORLDWIDE
wwPDB
PROTEIN DATA BANK

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	F	246/258 (95%)	226 (92%)	19 (8%)	1 (0%)	30	62
10	G	225/276 (82%)	209 (93%)	12 (5%)	4 (2%)	7	32
11	H	185/190 (97%)	169 (91%)	16 (9%)	0	100	100
12	I	185/221 (84%)	168 (91%)	15 (8%)	2 (1%)	12	42
13	J	164/175 (94%)	145 (88%)	16 (10%)	3 (2%)	7	32
14	K	193/355 (54%)	167 (86%)	20 (10%)	6 (3%)	3	20
15	L	129/134 (96%)	118 (92%)	8 (6%)	3 (2%)	5	27
16	M	196/205 (96%)	180 (92%)	15 (8%)	1 (0%)	25	58
17	N	196/269 (73%)	187 (95%)	6 (3%)	3 (2%)	8	36
18	O	154/195 (79%)	140 (91%)	13 (8%)	1 (1%)	22	55
19	P	184/187 (98%)	172 (94%)	10 (5%)	2 (1%)	12	42
20	Q	174/187 (93%)	165 (95%)	7 (4%)	2 (1%)	12	42
21	R	180/183 (98%)	159 (88%)	16 (9%)	5 (3%)	4	22
22	S	152/157 (97%)	141 (93%)	6 (4%)	5 (3%)	3	18
23	T	95/133 (71%)	85 (90%)	7 (7%)	3 (3%)	3	19
24	U	127/139 (91%)	117 (92%)	10 (8%)	0	100	100
25	V	61/155 (39%)	60 (98%)	1 (2%)	0	100	100
26	W	125/167 (75%)	107 (86%)	16 (13%)	2 (2%)	8	35
27	X	122/141 (86%)	111 (91%)	10 (8%)	1 (1%)	16	49
28	Y	140/146 (96%)	123 (88%)	11 (8%)	6 (4%)	2	14
29	Z	141/147 (96%)	126 (89%)	11 (8%)	4 (3%)	4	22
30	a	45/54 (83%)	42 (93%)	1 (2%)	2 (4%)	2	14
31	b	92/108 (85%)	83 (90%)	9 (10%)	0	100	100
32	c	103/120 (86%)	93 (90%)	7 (7%)	3 (3%)	3	21
33	d	120/134 (90%)	111 (92%)	6 (5%)	3 (2%)	4	25
34	e	101/112 (90%)	94 (93%)	6 (6%)	1 (1%)	13	45
35	f	105/134 (78%)	98 (93%)	6 (6%)	1 (1%)	13	45
36	g	119/123 (97%)	113 (95%)	4 (3%)	2 (2%)	7	33
37	h	93/101 (92%)	89 (96%)	2 (2%)	2 (2%)	5	27
38	i	81/98 (83%)	77 (95%)	3 (4%)	1 (1%)	11	41
39	j	68/84 (81%)	63 (93%)	4 (6%)	1 (2%)	8	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	k	47/51 (92%)	45 (96%)	1 (2%)	1 (2%)	5	29
41	l	50/129 (39%)	48 (96%)	1 (2%)	1 (2%)	6	29
42	n	95/105 (90%)	86 (90%)	7 (7%)	2 (2%)	5	29
43	o	88/96 (92%)	82 (93%)	5 (6%)	1 (1%)	12	42
44	p	118/129 (92%)	107 (91%)	10 (8%)	1 (1%)	16	49
All	All	6041/7166 (84%)	5517 (91%)	431 (7%)	93 (2%)	11	36

All (93) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	B	5	LYS
6	C	191	ARG
7	D	156	ASN
14	K	60	PRO
20	Q	130	GLN
21	R	151	ASP
22	S	12	ARG
23	T	26	VAL
28	Y	104	VAL
32	c	72	ILE
33	d	124	ARG
36	g	94	ARG
40	k	37	TYR
44	p	44	ILE
5	B	30	LYS
5	B	38	SER
12	I	144	ASN
13	J	115	ILE
14	K	74	PHE
14	K	154	LYS
14	K	155	ILE
15	L	22	ALA
16	M	197	GLN
17	N	176	THR
19	P	146	GLU
21	R	168	ASP
22	S	120	HIS
22	S	124	GLU
23	T	75	LYS
28	Y	8	GLY

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Mol	Chain	Res	Type
29	Z	77	LYS
29	Z	78	LEU
30	a	4	SER
32	c	111	ASN
38	i	28	ARG
43	o	13	LYS
6	C	85	HIS
7	D	20	TYR
7	D	21	ARG
7	D	44	TYR
13	J	119	PRO
15	L	8	TYR
17	N	198	LYS
20	Q	128	GLY
21	R	31	LEU
27	X	21	ALA
29	Z	47	LYS
29	Z	66	ASN
30	a	29	LYS
32	c	94	LYS
36	g	84	ARG
42	n	95	ALA
4	A	3	ARG
6	C	57	ASN
6	C	133	LEU
10	G	157	LYS
10	G	168	VAL
10	G	208	VAL
13	J	56	ARG
15	L	36	ARG
18	O	3	LYS
19	P	154	ALA
21	R	140	GLN
26	W	62	LYS
28	Y	35	ARG
28	Y	129	LYS
28	Y	134	SER
33	d	9	ARG
35	f	68	ARG
37	h	62	THR
41	l	79	GLU
5	B	24	ARG

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Mol	Chain	Res	Type
5	B	186	SER
5	B	316	VAL
6	C	323	LEU
14	K	145	SER
21	R	177	LYS
22	S	68	THR
23	T	41	ASN
26	W	141	ASP
28	Y	89	ASP
33	d	10	SER
39	j	76	GLU
34	e	10	VAL
37	h	18	ALA
22	S	81	GLY
10	G	132	GLY
14	K	51	GLY
17	N	175	PRO
42	n	36	VAL
9	F	237	GLU
12	I	196	GLY
8	E	184	GLY

5.3.2   Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	190/200 (95%)	181 (95%)	9 (5%)	22	52
5	B	315/330 (96%)	298 (95%)	17 (5%)	18	48
6	C	313/326 (96%)	302 (96%)	11 (4%)	31	60
7	D	218/253 (86%)	213 (98%)	5 (2%)	45	70
8	E	110/163 (68%)	106 (96%)	4 (4%)	30	59
9	F	216/223 (97%)	206 (95%)	10 (5%)	23	53
10	G	204/233 (88%)	198 (97%)	6 (3%)	37	65
11	H	167/169 (99%)	159 (95%)	8 (5%)	21	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	I	159/180 (88%)	153 (96%)	6 (4%)	28	58
13	J	141/151 (93%)	136 (96%)	5 (4%)	31	60
14	K	170/303 (56%)	163 (96%)	7 (4%)	26	56
15	L	116/118 (98%)	109 (94%)	7 (6%)	16	44
16	M	171/176 (97%)	159 (93%)	12 (7%)	12	39
17	N	178/240 (74%)	172 (97%)	6 (3%)	32	61
18	O	139/168 (83%)	129 (93%)	10 (7%)	12	38
19	P	154/155 (99%)	146 (95%)	8 (5%)	19	49
20	Q	154/162 (95%)	153 (99%)	1 (1%)	84	92
21	R	162/163 (99%)	152 (94%)	10 (6%)	15	44
22	S	134/137 (98%)	128 (96%)	6 (4%)	23	53
23	T	93/111 (84%)	86 (92%)	7 (8%)	11	37
24	U	100/105 (95%)	96 (96%)	4 (4%)	27	56
25	V	56/131 (43%)	54 (96%)	2 (4%)	30	59
26	W	116/139 (84%)	110 (95%)	6 (5%)	19	49
27	X	113/128 (88%)	106 (94%)	7 (6%)	15	44
28	Y	128/130 (98%)	119 (93%)	9 (7%)	12	39
29	Z	116/118 (98%)	110 (95%)	6 (5%)	19	49
30	a	44/48 (92%)	43 (98%)	1 (2%)	45	70
31	b	80/89 (90%)	74 (92%)	6 (8%)	11	37
32	c	99/110 (90%)	94 (95%)	5 (5%)	20	49
33	d	112/122 (92%)	104 (93%)	8 (7%)	12	38
34	e	91/97 (94%)	85 (93%)	6 (7%)	14	41
35	f	91/115 (79%)	84 (92%)	7 (8%)	10	36
36	g	103/105 (98%)	96 (93%)	7 (7%)	13	40
37	h	79/82 (96%)	78 (99%)	1 (1%)	65	82
38	i	69/79 (87%)	62 (90%)	7 (10%)	6	23
39	j	66/73 (90%)	64 (97%)	2 (3%)	36	64
40	k	44/45 (98%)	38 (86%)	6 (14%)	3	14
41	l	47/116 (40%)	45 (96%)	2 (4%)	25	54
42	n	88/93 (95%)	85 (97%)	3 (3%)	32	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	o	68/71 (96%)	67 (98%)	1 (2%)	60	79
44	p	108/114 (95%)	106 (98%)	2 (2%)	52	74
All	All	5322/6071 (88%)	5069 (95%)	253 (5%)	24	52

All (253) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	6	ARG
4	A	15	VAL
4	A	30	ARG
4	A	41	ILE
4	A	80	GLU
4	A	163	ARG
4	A	174	ARG
4	A	193	ARG
4	A	242	ARG
5	B	10	ARG
5	B	36	ASP
5	B	58	ARG
5	B	60	LEU
5	B	102	LEU
5	B	163	THR
5	B	172	SER
5	B	189	GLU
5	B	209	THR
5	B	230	SER
5	B	243	ARG
5	B	321	LEU
5	B	323	LEU
5	B	324	LYS
5	B	336	THR
5	B	346	THR
5	B	382	LEU
6	C	73	VAL
6	C	95	MET
6	C	107	THR
6	C	108	TRP
6	C	122	HIS
6	C	140	ARG
6	C	180	LEU
6	C	182	ARG

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Mol	Chain	Res	Type
6	C	191	ARG
6	C	277	LYS
6	C	372	ARG
7	D	68	THR
7	D	122	VAL
7	D	151	ARG
7	D	196	GLU
7	D	240	GLU
8	E	46	LEU
8	E	54	ARG
8	E	94	THR
8	E	179	ARG
9	F	21	ARG
9	F	110	LYS
9	F	144	ILE
9	F	153	THR
9	F	172	HIS
9	F	173	SER
9	F	222	ASN
9	F	232	ARG
9	F	246	ARG
9	F	255	GLN
10	G	70	LEU
10	G	161	LEU
10	G	189	CYS
10	G	192	LYS
10	G	214	VAL
10	G	218	ASP
11	H	23	ARG
11	H	40	HIS
11	H	57	GLU
11	H	65	ASP
11	H	138	ASN
11	H	141	ASP
11	H	170	ASP
11	H	176	ASP
12	I	23	CYS
12	I	63	GLU
12	I	99	ILE
12	I	130	ASP
12	I	133	GLN
12	I	199	TRP

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Mol	Chain	Res	Type
13	J	14	ARG
13	J	23	CYS
13	J	113	LEU
13	J	115	ILE
13	J	118	ASP
14	K	52	LEU
14	K	54	ARG
14	K	155	ILE
14	K	167	ARG
14	K	168	CYS
14	K	177	GLU
14	K	180	PHE
15	L	4	PHE
15	L	6	ARG
15	L	21	ASP
15	L	38	LEU
15	L	54	VAL
15	L	72	SER
15	L	82	ASP
16	M	10	LEU
16	M	39	CYS
16	M	66	VAL
16	M	75	VAL
16	M	104	GLU
16	M	118	ASN
16	M	146	ASP
16	M	160	ARG
16	M	161	GLU
16	M	175	LEU
16	M	185	LEU
16	M	189	ARG
17	N	84	ARG
17	N	117	ARG
17	N	121	GLN
17	N	172	GLU
17	N	224	GLU
17	N	226	ARG
18	O	22	LEU
18	O	24	VAL
18	O	47	LEU
18	O	56	ASP
18	O	63	CYS

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Mol	Chain	Res	Type
18	O	100	LEU
18	O	113	LEU
18	O	116	ASP
18	O	145	TYR
18	O	147	SER
19	P	8	ASN
19	P	29	LEU
19	P	32	LEU
19	P	39	ARG
19	P	41	ASN
19	P	143	LYS
19	P	148	ASP
19	P	171	ARG
20	Q	33	MET
21	R	17	VAL
21	R	65	ILE
21	R	72	ARG
21	R	94	THR
21	R	97	MET
21	R	103	ASP
21	R	120	ARG
21	R	141	CYS
21	R	168	ASP
21	R	183	HIS
22	S	13	GLN
22	S	67	VAL
22	S	68	THR
22	S	100	ARG
22	S	103	GLU
22	S	140	PHE
23	T	40	ASP
23	T	62	CYS
23	T	63	ASN
23	T	67	ASP
23	T	104	LEU
23	T	106	ASP
23	T	116	THR
24	U	47	CYS
24	U	73	LYS
24	U	77	MET
24	U	131	ILE
25	V	24	ARG

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Mol	Chain	Res	Type
25	V	56	LEU
26	W	68	TYR
26	W	78	LEU
26	W	111	ASP
26	W	137	LEU
26	W	139	ARG
26	W	149	ARG
27	X	6	GLN
27	X	23	SER
27	X	47	LEU
27	X	55	VAL
27	X	59	ARG
27	X	64	ASP
27	X	73	TYR
28	Y	65	MET
28	Y	72	LYS
28	Y	74	ILE
28	Y	80	MET
28	Y	89	ASP
28	Y	91	ASP
28	Y	98	GLU
28	Y	121	LYS
28	Y	123	THR
29	Z	11	ARG
29	Z	12	ARG
29	Z	73	VAL
29	Z	95	ASP
29	Z	116	LEU
29	Z	129	SER
30	a	6	ASN
31	b	28	LEU
31	b	44	LEU
31	b	47	ILE
31	b	51	CYS
31	b	74	HIS
31	b	78	ASN
32	c	19	ASP
32	c	21	THR
32	c	43	GLU
32	c	52	MET
32	c	100	LEU
33	d	7	VAL

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Mol	Chain	Res	Type
33	d	36	LYS
33	d	41	ASP
33	d	56	ASN
33	d	68	MET
33	d	77	LEU
33	d	91	ASN
33	d	121	VAL
34	e	11	ARG
34	e	28	GLN
34	e	35	LEU
34	e	53	ARG
34	e	93	ASN
34	e	107	LEU
35	f	4	ARG
35	f	5	LEU
35	f	31	VAL
35	f	38	GLN
35	f	41	ARG
35	f	47	CYS
35	f	54	ILE
36	g	21	LEU
36	g	58	LEU
36	g	81	ASN
36	g	83	LEU
36	g	95	LEU
36	g	101	ARG
36	g	121	LEU
37	h	2	SER
38	i	8	THR
38	i	18	THR
38	i	21	LEU
38	i	22	CYS
38	i	25	CYS
38	i	40	CYS
38	i	67	CYS
39	j	50	SER
39	j	55	THR
40	k	3	SER
40	k	9	LEU
40	k	13	LEU
40	k	23	ILE
40	k	37	TYR

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Mol	Chain	Res	Type
40	k	38	ASN
41	l	97	ARG
41	l	126	LYS
42	n	33	ASP
42	n	46	LYS
42	n	53	GLN
43	o	73	THR
44	p	16	CYS
44	p	117	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	209	HIS
5	B	55	HIS
5	B	152	ASN
5	B	260	GLN
5	B	268	GLN
6	C	50	GLN
6	C	94	ASN
9	F	130	ASN
9	F	214	ASN
9	F	251	ASN
10	G	93	HIS
12	I	185	GLN
13	J	40	GLN
13	J	131	GLN
13	J	137	ASN
14	K	18	GLN
14	K	32	GLN
16	M	124	GLN
17	N	162	GLN
18	O	20	GLN
18	O	143	ASN
18	O	151	HIS
19	P	8	ASN
19	P	41	ASN
20	Q	98	GLN
20	Q	129	ASN
21	R	21	GLN
21	R	81	ASN
21	R	147	GLN

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Mol	Chain	Res	Type
22	S	13	GLN
22	S	58	HIS
22	S	90	HIS
23	T	63	ASN
28	Y	78	HIS
29	Z	14	HIS
29	Z	25	HIS
29	Z	49	HIS
29	Z	60	HIS
30	a	6	ASN
30	a	17	HIS
32	c	64	ASN
33	d	91	ASN
33	d	116	GLN
34	e	28	GLN
35	f	34	ASN
36	g	99	GLN
40	k	38	ASN
40	k	43	HIS
42	n	47	GLN
42	n	53	GLN
44	p	55	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3053/3477 (87%)	732 (23%)	91 (2%)
2	3	115/124 (92%)	21 (18%)	1 (0%)
3	4	155/158 (98%)	35 (22%)	2 (1%)
All	All	3323/3759 (88%)	788 (23%)	94 (2%)

All (788) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	7	C
1	1	31	C
1	1	40	A
1	1	43	A
1	1	49	U
1	1	57	A
1	1	59	G

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Mol	Chain	Res	Type
1	1	60	A
1	1	65	A
1	1	66	A
1	1	69	U
1	1	74	A
1	1	75	U
1	1	77	A
1	1	85	A
1	1	92	G
1	1	109	A
1	1	110	G
1	1	115	A
1	1	116	A
1	1	117	G
1	1	119	G
1	1	121	A
1	1	122	A
1	1	129	U
1	1	132	U
1	1	147	G
1	1	159	C
1	1	160	G
1	1	164	G
1	1	168	U
1	1	169	U
1	1	174	G
1	1	176	G
1	1	180	G
1	1	181	C
1	1	190	A
1	1	193	U
1	1	194	U
1	1	195	U
1	1	203	A
1	1	213	U
1	1	214	A
1	1	215	G
1	1	216	A
1	1	221	G
1	1	222	A
1	1	245	U
1	1	246	U

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Mol	Chain	Res	Type
1	1	247	U
1	1	248	U
1	1	249	U
1	1	250	G
1	1	251	U
1	1	252	U
1	1	253	C
1	1	254	C
1	1	259	A
1	1	260	C
1	1	261	G
1	1	262	G
1	1	270	U
1	1	271	U
1	1	272	A
1	1	273	U
1	1	277	G
1	1	278	U
1	1	283	U
1	1	291	G
1	1	293	U
1	1	294	U
1	1	303	A
1	1	323	A
1	1	337	U
1	1	338	G
1	1	358	C
1	1	360	A
1	1	379	G
1	1	380	A
1	1	383	A
1	1	384	G
1	1	387	C
1	1	393	A
1	1	403	A
1	1	405	A
1	1	406	A
1	1	408	U
1	1	428	G
1	1	429	A
1	1	431	G
1	1	436	U

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Mol	Chain	Res	Type
1	1	451	U
1	1	459	G
1	1	461	G
1	1	466	C
1	1	467	G
1	1	476	U
1	1	477	C
1	1	481	C
1	1	484	U
1	1	485	U
1	1	488	C
1	1	496	C
1	1	497	U
1	1	499	U
1	1	500	C
1	1	501	A
1	1	502	C
1	1	503	C
1	1	504	A
1	1	509	U
1	1	514	U
1	1	515	U
1	1	517	G
1	1	522	C
1	1	523	U
1	1	526	A
1	1	527	U
1	1	535	C
1	1	537	G
1	1	538	U
1	1	539	U
1	1	540	C
1	1	541	A
1	1	546	U
1	1	547	U
1	1	548	U
1	1	552	G
1	1	554	G
1	1	572	G
1	1	573	G
1	1	576	U
1	1	580	U

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Mol	Chain	Res	Type
1	1	581	U
1	1	582	U
1	1	587	C
1	1	594	G
1	1	595	G
1	1	596	U
1	1	600	U
1	1	601	U
1	1	603	C
1	1	606	G
1	1	608	G
1	1	613	G
1	1	615	U
1	1	616	A
1	1	618	A
1	1	619	U
1	1	622	U
1	1	625	U
1	1	628	U
1	1	629	U
1	1	630	U
1	1	637	C
1	1	638	C
1	1	639	U
1	1	640	U
1	1	641	G
1	1	649	G
1	1	650	G
1	1	652	G
1	1	653	U
1	1	655	U
1	1	656	U
1	1	657	C
1	1	663	U
1	1	665	C
1	1	666	G
1	1	667	A
1	1	668	G
1	1	686	C
1	1	691	U
1	1	696	G
1	1	697	A

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Mol	Chain	Res	Type
1	1	698	U
1	1	699	G
1	1	700	C
1	1	721	G
1	1	723	C
1	1	736	A
1	1	746	G
1	1	747	A
1	1	763	G
1	1	764	A
1	1	767	A
1	1	774	U
1	1	776	U
1	1	777	U
1	1	778	A
1	1	792	A
1	1	796	A
1	1	799	G
1	1	802	A
1	1	817	U
1	1	820	U
1	1	821	U
1	1	824	C
1	1	826	A
1	1	827	U
1	1	828	U
1	1	830	U
1	1	831	U
1	1	833	G
1	1	835	A
1	1	851	G
1	1	855	U
1	1	856	C
1	1	857	U
1	1	858	G
1	1	864	G
1	1	866	U
1	1	867	U
1	1	870	A
1	1	871	G
1	1	873	U
1	1	874	G

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Mol	Chain	Res	Type
1	1	875	G
1	1	876	A
1	1	889	G
1	1	896	A
1	1	898	A
1	1	907	A
1	1	908	C
1	1	909	U
1	1	920	A
1	1	927	A
1	1	931	A
1	1	947	G
1	1	951	U
1	1	958	C
1	1	959	G
1	1	964	U
1	1	968	G
1	1	969	U
1	1	970	G
1	1	986	A
1	1	987	C
1	1	997	G
1	1	998	G
1	1	1001	C
1	1	1004	A
1	1	1006	G
1	1	1007	A
1	1	1008	C
1	1	1011	A
1	1	1013	C
1	1	1014	G
1	1	1015	A
1	1	1024	G
1	1	1027	G
1	1	1034	U
1	1	1036	U
1	1	1049	C
1	1	1050	U
1	1	1051	C
1	1	1052	A
1	1	1053	G
1	1	1065	U

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Mol	Chain	Res	Type
1	1	1069	G
1	1	1070	U
1	1	1075	U
1	1	1080	C
1	1	1082	G
1	1	1083	G
1	1	1089	C
1	1	1090	G
1	1	1091	A
1	1	1099	G
1	1	1102	G
1	1	1121	C
1	1	1123	C
1	1	1124	G
1	1	1125	A
1	1	1126	C
1	1	1134	C
1	1	1136	A
1	1	1138	C
1	1	1153	A
1	1	1154	U
1	1	1157	A
1	1	1160	G
1	1	1164	A
1	1	1165	C
1	1	1168	C
1	1	1170	U
1	1	1171	U
1	1	1183	A
1	1	1184	U
1	1	1185	U
1	1	1186	A
1	1	1191	G
1	1	1202	G
1	1	1204	G
1	1	1209	U
1	1	1218	G
1	1	1231	U
1	1	1240	C
1	1	1246	A
1	1	1249	C
1	1	1250	U

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Mol	Chain	Res	Type
1	1	1268	U
1	1	1269	G
1	1	1278	U
1	1	1279	C
1	1	1283	U
1	1	1284	A
1	1	1288	U
1	1	1289	A
1	1	1293	G
1	1	1296	G
1	1	1299	G
1	1	1304	A
1	1	1305	U
1	1	1382	G
1	1	1388	A
1	1	1392	U
1	1	1394	G
1	1	1396	U
1	1	1400	G
1	1	1403	G
1	1	1404	A
1	1	1409	G
1	1	1417	A
1	1	1427	A
1	1	1431	C
1	1	1432	U
1	1	1435	U
1	1	1436	A
1	1	1437	A
1	1	1438	U
1	1	1439	U
1	1	1440	A
1	1	1441	U
1	1	1442	C
1	1	1443	A
1	1	1449	C
1	1	1451	U
1	1	1452	U
1	1	1453	U
1	1	1454	U
1	1	1455	G
1	1	1456	U

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Mol	Chain	Res	Type
1	1	1489	G
1	1	1496	U
1	1	1498	G
1	1	1514	G
1	1	1516	A
1	1	1517	C
1	1	1531	G
1	1	1533	U
1	1	1534	C
1	1	1543	A
1	1	1547	G
1	1	1549	A
1	1	1552	U
1	1	1570	G
1	1	1572	A
1	1	1578	A
1	1	1579	A
1	1	1580	G
1	1	1599	G
1	1	1605	C
1	1	1620	U
1	1	1624	C
1	1	1628	C
1	1	1630	U
1	1	1633	G
1	1	1636	A
1	1	1637	C
1	1	1639	G
1	1	1644	A
1	1	1650	U
1	1	1651	A
1	1	1652	U
1	1	1653	A
1	1	1654	C
1	1	1672	C
1	1	1674	U
1	1	1675	U
1	1	1676	U
1	1	1678	G
1	1	1681	A
1	1	1683	A
1	1	1687	A

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Mol	Chain	Res	Type
1	1	1691	G
1	1	1714	C
1	1	1717	G
1	1	1718	G
1	1	1722	C
1	1	1723	U
1	1	1724	G
1	1	1726	A
1	1	1731	A
1	1	1733	C
1	1	1736	A
1	1	1737	A
1	1	1751	C
1	1	1777	G
1	1	1794	G
1	1	1818	C
1	1	1826	C
1	1	1829	G
1	1	1831	G
1	1	1841	G
1	1	1842	C
1	1	1843	U
1	1	1851	A
1	1	1852	G
1	1	1859	U
1	1	1861	G
1	1	1872	U
1	1	1877	G
1	1	1878	G
1	1	1882	G
1	1	1884	U
1	1	1899	A
1	1	1911	A
1	1	1916	U
1	1	1917	G
1	1	1918	U
1	1	1919	U
1	1	1920	A
1	1	1921	U
1	1	1922	U
1	1	1932	G
1	1	1942	A

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Mol	Chain	Res	Type
1	1	1944	A
1	1	1945	A
1	1	1949	C
1	1	1950	A
1	1	1953	A
1	1	1961	A
1	1	1962	A
1	1	1969	U
1	1	1974	U
1	1	1981	G
1	1	1983	U
1	1	1987	A
1	1	1989	A
1	1	1996	A
1	1	2009	G
1	1	2011	A
1	1	2013	A
1	1	2029	C
1	1	2033	A
1	1	2042	G
1	1	2055	G
1	1	2213	A
1	1	2215	C
1	1	2216	U
1	1	2217	C
1	1	2224	G
1	1	2225	G
1	1	2226	A
1	1	2227	G
1	1	2228	C
1	1	2232	C
1	1	2235	G
1	1	2236	G
1	1	2245	A
1	1	2258	A
1	1	2263	A
1	1	2264	G
1	1	2272	A
1	1	2274	G
1	1	2278	A
1	1	2283	U
1	1	2299	U

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Mol	Chain	Res	Type
1	1	2307	G
1	1	2314	G
1	1	2318	U
1	1	2338	U
1	1	2357	A
1	1	2359	G
1	1	2362	G
1	1	2365	A
1	1	2373	U
1	1	2385	G
1	1	2386	G
1	1	2387	U
1	1	2398	C
1	1	2401	G
1	1	2419	C
1	1	2420	G
1	1	2423	U
1	1	2426	A
1	1	2427	U
1	1	2428	G
1	1	2431	U
1	1	2448	G
1	1	2449	U
1	1	2476	A
1	1	2485	A
1	1	2486	A
1	1	2487	C
1	1	2488	G
1	1	2504	G
1	1	2506	G
1	1	2510	A
1	1	2514	A
1	1	2515	A
1	1	2516	G
1	1	2517	A
1	1	2518	C
1	1	2519	C
1	1	2524	U
1	1	2525	G
1	1	2535	C
1	1	2537	A
1	1	2548	G

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Mol	Chain	Res	Type
1	1	2550	G
1	1	2624	A
1	1	2627	U
1	1	2628	A
1	1	2636	A
1	1	2638	G
1	1	2645	C
1	1	2646	U
1	1	2647	C
1	1	2651	C
1	1	2652	U
1	1	2653	C
1	1	2655	G
1	1	2656	C
1	1	2657	A
1	1	2658	U
1	1	2659	G
1	1	2660	U
1	1	2661	G
1	1	2662	U
1	1	2663	U
1	1	2664	U
1	1	2665	U
1	1	2666	G
1	1	2667	G
1	1	2672	A
1	1	2673	A
1	1	2679	C
1	1	2695	A
1	1	2696	C
1	1	2702	A
1	1	2704	A
1	1	2705	C
1	1	2706	A
1	1	2717	G
1	1	2718	G
1	1	2725	G
1	1	2730	G
1	1	2731	G
1	1	2739	A
1	1	2749	C
1	1	2759	G

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Mol	Chain	Res	Type
1	1	2763	U
1	1	2766	U
1	1	2767	A
1	1	2768	A
1	1	2785	A
1	1	2788	G
1	1	2791	A
1	1	2800	U
1	1	2801	G
1	1	2802	A
1	1	2805	A
1	1	2807	A
1	1	2816	A
1	1	2820	U
1	1	2825	G
1	1	2827	U
1	1	2830	U
1	1	2836	U
1	1	2839	G
1	1	2840	U
1	1	2860	G
1	1	2863	U
1	1	2864	G
1	1	2866	C
1	1	2873	A
1	1	2883	U
1	1	2884	C
1	1	2888	G
1	1	2889	A
1	1	2907	G
1	1	2908	U
1	1	2911	G
1	1	2912	A
1	1	2913	A
1	1	2914	A
1	1	2915	A
1	1	2921	C
1	1	2925	G
1	1	2927	G
1	1	2928	A
1	1	2932	C
1	1	2949	A

Continued on next page...

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Mol	Chain	Res	Type
1	1	2953	U
1	1	2954	U
1	1	2955	C
1	1	2956	A
1	1	2960	C
1	1	2974	G
1	1	2978	C
1	1	2982	G
1	1	2983	A
1	1	2984	U
1	1	2987	C
1	1	2998	A
1	1	3010	C
1	1	3015	G
1	1	3021	A
1	1	3034	U
1	1	3041	G
1	1	3046	U
1	1	3047	A
1	1	3049	G
1	1	3052	A
1	1	3053	C
1	1	3058	G
1	1	3077	G
1	1	3079	G
1	1	3082	A
1	1	3091	U
1	1	3094	C
1	1	3101	G
1	1	3102	A
1	1	3108	U
1	1	3109	G
1	1	3115	G
1	1	3123	A
1	1	3124	A
1	1	3126	C
1	1	3140	G
1	1	3169	A
1	1	3170	U
1	1	3171	G
1	1	3181	G
1	1	3182	A

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Mol	Chain	Res	Type
1	1	3185	A
1	1	3186	G
1	1	3190	G
1	1	3198	A
1	1	3204	C
1	1	3205	C
1	1	3208	C
1	1	3211	U
1	1	3213	G
1	1	3228	G
1	1	3229	C
1	1	3234	A
1	1	3237	U
1	1	3242	A
1	1	3243	U
1	1	3253	A
1	1	3254	U
1	1	3255	A
1	1	3256	U
1	1	3257	G
1	1	3266	U
1	1	3267	U
1	1	3268	C
1	1	3269	A
1	1	3270	C
1	1	3279	U
1	1	3280	U
1	1	3282	U
1	1	3283	U
1	1	3284	U
1	1	3285	C
1	1	3286	A
1	1	3287	U
1	1	3288	G
1	1	3289	C
1	1	3290	A
1	1	3291	A
1	1	3292	U
1	1	3293	G
1	1	3295	U
1	1	3298	A
1	1	3299	G

Continued from previous page...

Mol	Chain	Res	Type
1	1	3302	C
1	1	3303	U
1	1	3304	C
1	1	3305	U
1	1	3306	G
1	1	3310	U
1	1	3311	G
1	1	3312	C
1	1	3314	U
1	1	3320	C
1	1	3321	A
1	1	3322	A
1	1	3323	A
1	1	3327	C
1	1	3345	G
1	1	3349	A
1	1	3350	G
1	1	3351	A
1	1	3355	U
1	1	3356	C
1	1	3357	A
1	1	3359	U
1	1	3361	U
1	1	3366	C
1	1	3374	G
1	1	3375	U
1	1	3376	G
1	1	3378	U
1	1	3379	A
1	1	3380	C
1	1	3389	C
1	1	3398	U
1	1	3401	U
1	1	3402	U
1	1	3403	G
1	1	3404	C
1	1	3423	U
1	1	3424	G
1	1	3428	G
1	1	3435	U
1	1	3436	G
1	1	3437	U

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Mol	Chain	Res	Type
1	1	3443	A
1	1	3444	U
1	1	3449	U
1	1	3450	A
1	1	3456	U
1	1	3459	C
1	1	3463	C
1	1	3464	G
1	1	3467	G
1	1	3471	G
1	1	3477	G
2	3	2	C
2	3	7	G
2	3	11	A
2	3	19	U
2	3	26	C
2	3	33	U
2	3	48	G
2	3	50	A
2	3	53	U
2	3	54	A
2	3	55	A
2	3	64	A
2	3	72	U
2	3	80	U
2	3	92	U
2	3	100	A
2	3	105	C
2	3	110	G
2	3	113	G
2	3	120	G
2	3	122	U
3	4	23	U
3	4	34	A
3	4	35	C
3	4	49	G
3	4	51	G
3	4	55	U
3	4	59	A
3	4	62	C
3	4	63	G
3	4	80	A

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Mol	Chain	Res	Type
3	4	81	U
3	4	82	U
3	4	83	C
3	4	84	A
3	4	86	U
3	4	87	G
3	4	88	A
3	4	90	U
3	4	95	A
3	4	104	A
3	4	105	A
3	4	106	C
3	4	108	C
3	4	109	A
3	4	111	A
3	4	113	G
3	4	122	G
3	4	124	G
3	4	127	A
3	4	130	C
3	4	139	A
3	4	152	U
3	4	153	G
3	4	156	U
3	4	157	U

All (94) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	116	A
1	1	180	G
1	1	193	U
1	1	259	A
1	1	405	A
1	1	407	G
1	1	413	G
1	1	460	U
1	1	537	G
1	1	547	U
1	1	578	G
1	1	580	U
1	1	581	U

Continued from previous page...

Mol	Chain	Res	Type
1	1	614	U
1	1	649	G
1	1	654	G
1	1	748	G
1	1	823	G
1	1	826	A
1	1	873	U
1	1	874	G
1	1	875	G
1	1	890	G
1	1	906	A
1	1	986	A
1	1	1006	G
1	1	1027	G
1	1	1049	C
1	1	1051	C
1	1	1082	G
1	1	1089	C
1	1	1153	A
1	1	1239	G
1	1	1241	U
1	1	1277	A
1	1	1283	U
1	1	1403	G
1	1	1436	A
1	1	1439	U
1	1	1440	A
1	1	1651	A
1	1	1675	U
1	1	1699	A
1	1	1723	U
1	1	1724	G
1	1	1737	A
1	1	1751	C
1	1	1825	G
1	1	1841	G
1	1	1897	U
1	1	1915	U
1	1	1937	U
1	1	1944	A
1	1	1961	A
1	1	1982	A

Continued from previous page...

Mol	Chain	Res	Type
1	1	2212	U
1	1	2215	C
1	1	2224	G
1	1	2226	A
1	1	2258	A
1	1	2427	U
1	1	2485	A
1	1	2487	C
1	1	2635	U
1	1	2651	C
1	1	2663	U
1	1	2664	U
1	1	2704	A
1	1	2738	C
1	1	2791	A
1	1	2800	U
1	1	2806	A
1	1	2839	G
1	1	2997	U
1	1	3090	U
1	1	3167	A
1	1	3204	C
1	1	3205	C
1	1	3233	U
1	1	3254	U
1	1	3255	A
1	1	3269	A
1	1	3281	G
1	1	3288	G
1	1	3290	A
1	1	3302	C
1	1	3348	G
1	1	3356	C
1	1	3358	A
1	1	3362	C
1	1	3456	U
2	3	112	U
3	4	83	C
3	4	87	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 oligosaccharides in this entry.

5.6   Ligand geometry ⓘ

There are no ligands in this entry.

5.7   Other polymers ⓘ

There are no such residues in this entry.

5.8   Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-6778. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections ⓘ

6.1.1 Primary map

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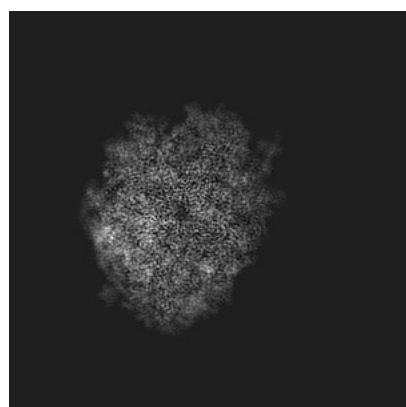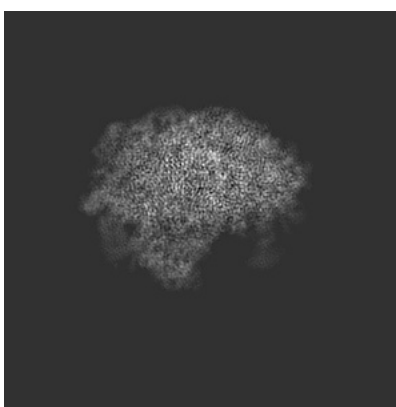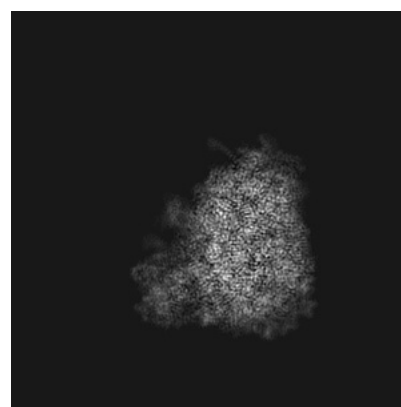
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
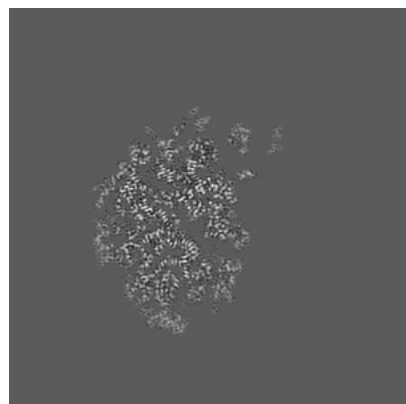
6.2.1 Primary map
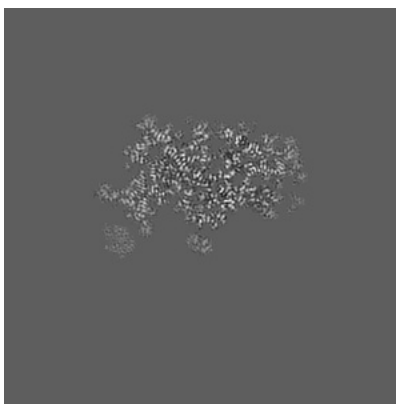
| X Index: 160 | Y Index: 160 | Z Index: 160 |

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

6.3 Largest variance slices ⓘ
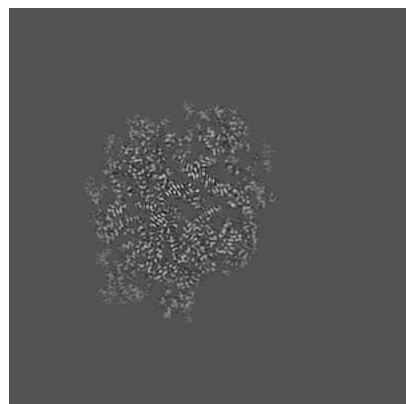
6.3.1 Primary map
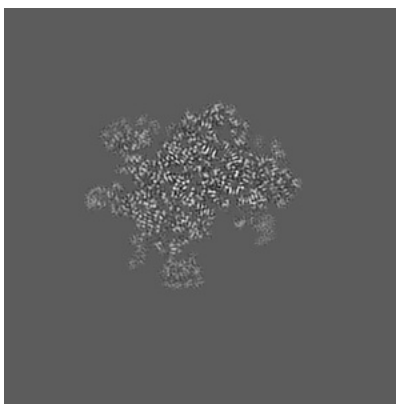
| X Index: 187 | Y Index: 111 | Z Index: 171 |
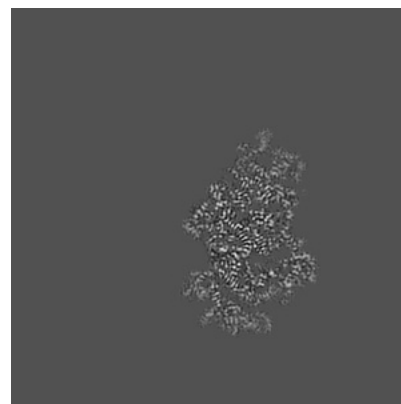
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map

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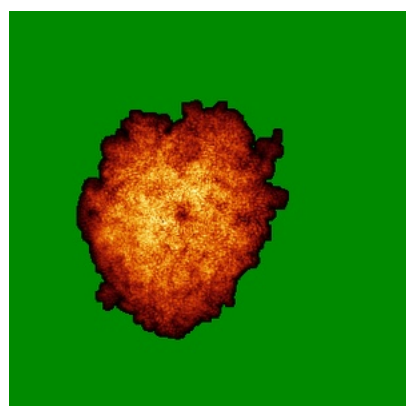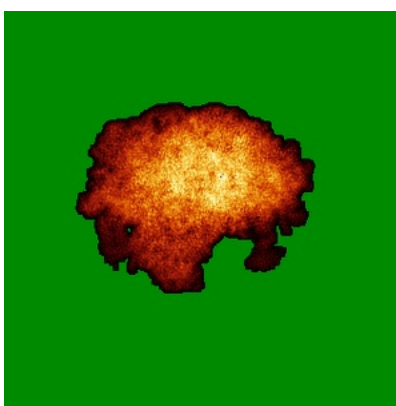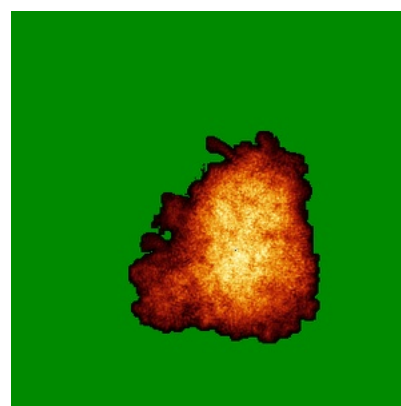
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views ⓘ
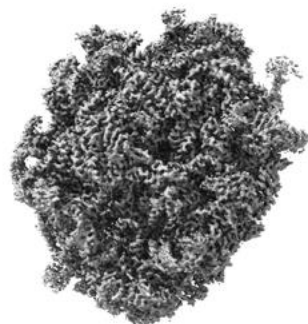
6.5.1 Primary map

X　　　　　　　　　　　　　Y　　　　　　　　　　　　　Z
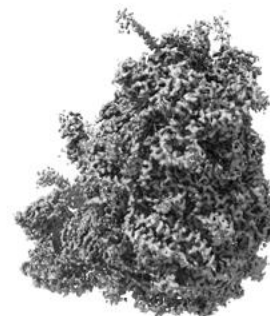
The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.6 Mask visualisation ⓘ

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_6778_msk_1.map ⓘ

X Y Z
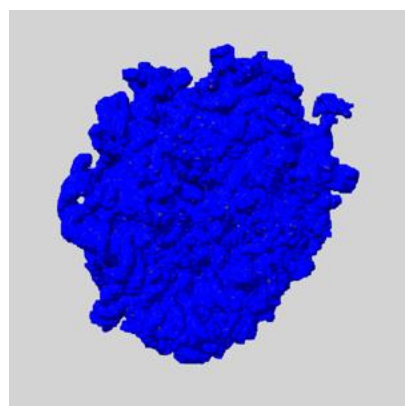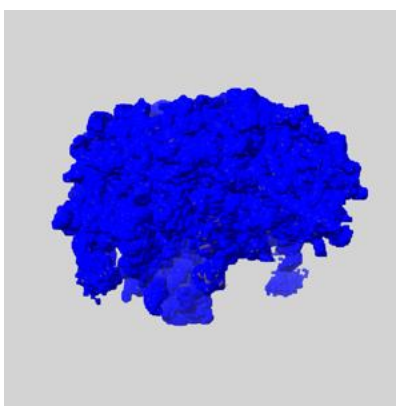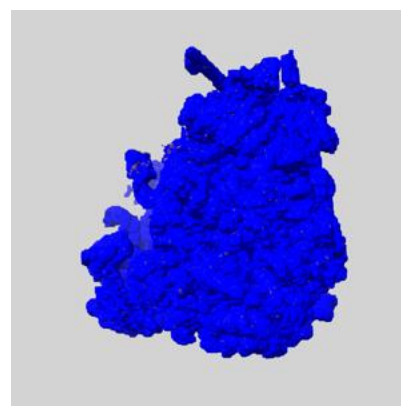
7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

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

7.2 Volume estimate ⓘ
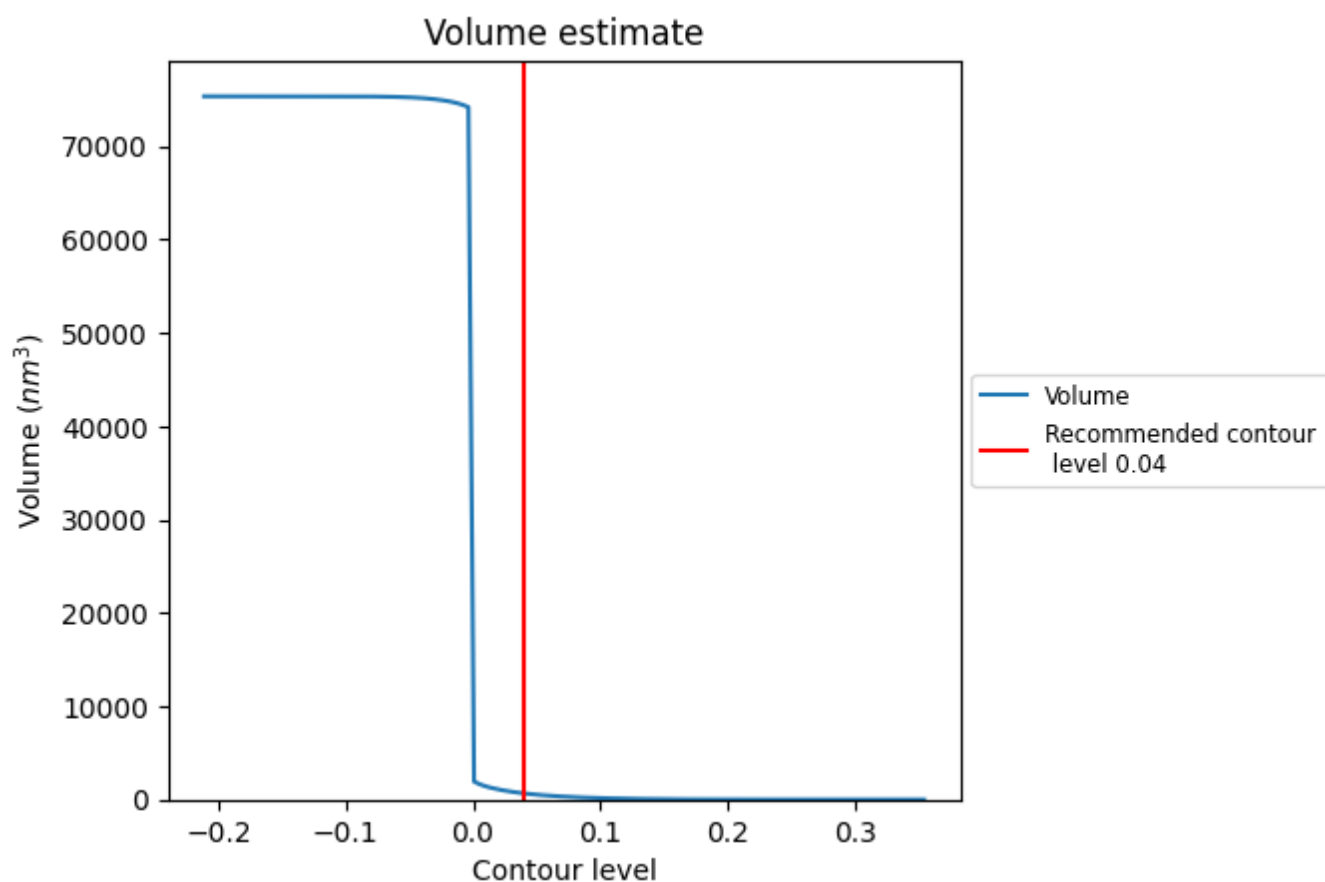
The volume at the recommended contour level is 664 nm^3; this corresponds to an approximate mass of 600 kDa.

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 ⓘ
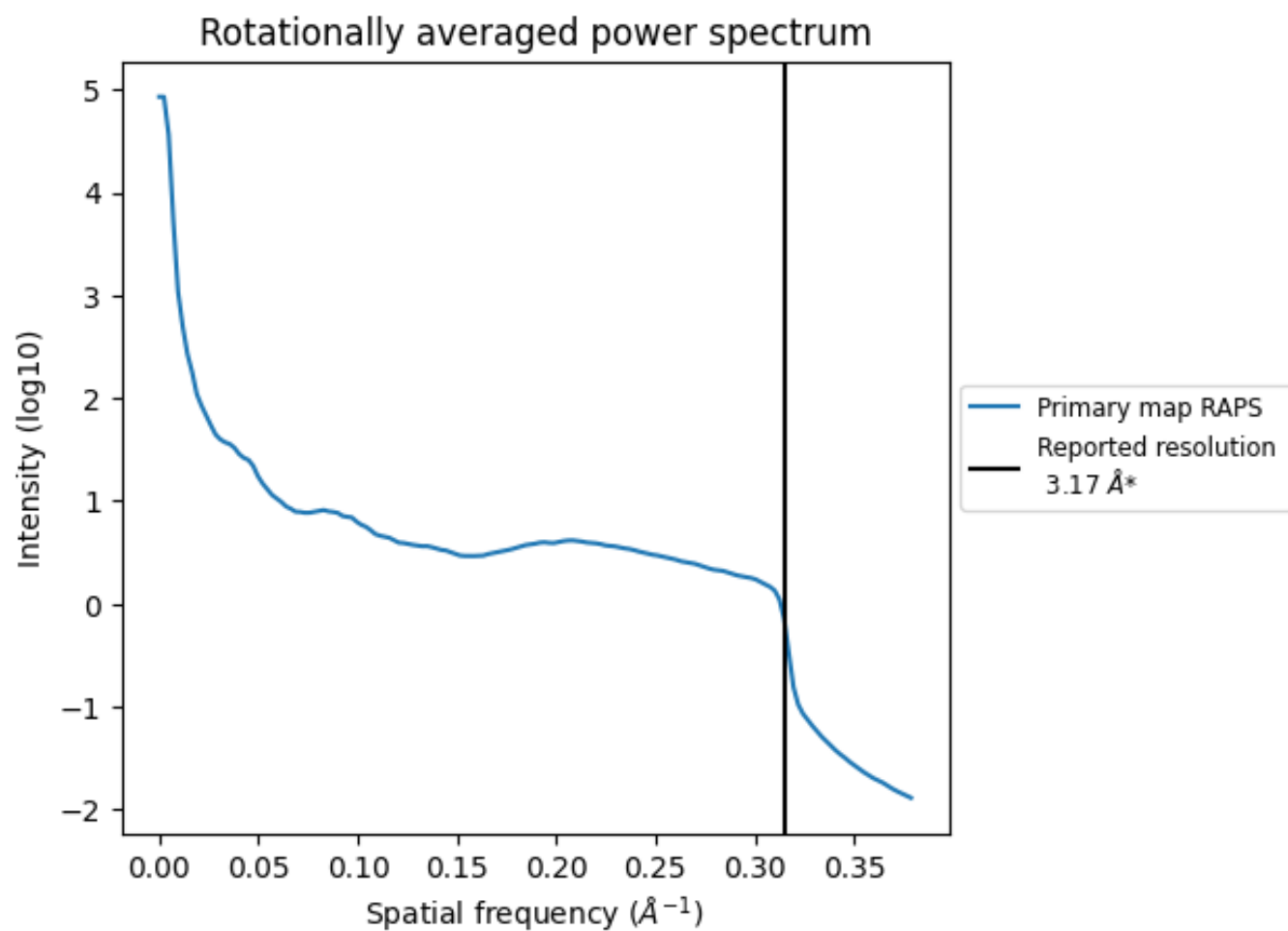
*Reported resolution corresponds to spatial frequency of 0.315 Å^{-1}

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 ⓘ
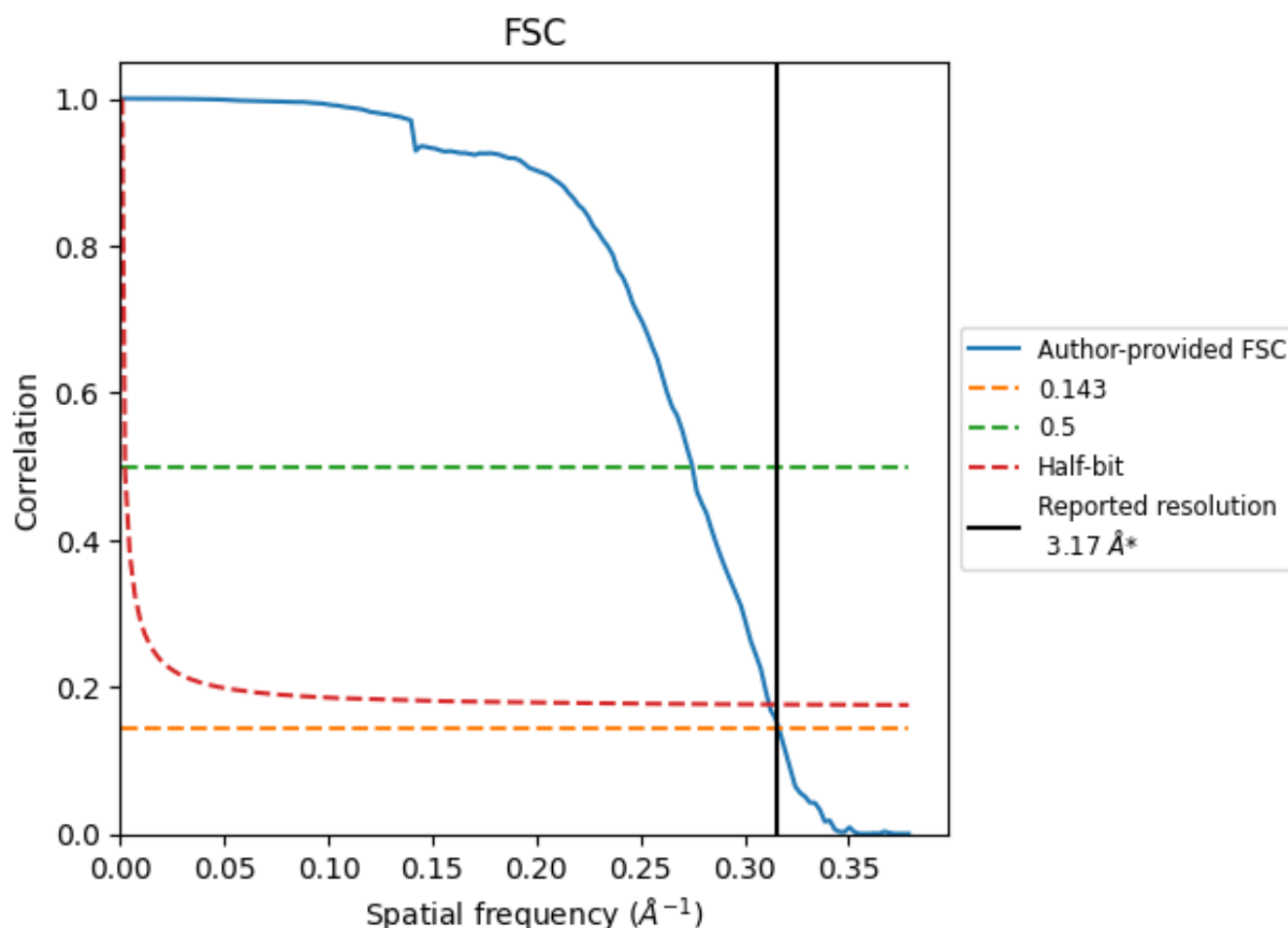
*Reported resolution corresponds to spatial frequency of 0.315 Å^{-1}

8.2 Resolution estimates ⓘ

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.17	-	-
Author-provided FSC curve	3.16	3.64	3.21
Unmasked-calculated*	-	-	-

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

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-6778 and PDB model 5XXB. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay ⓘ
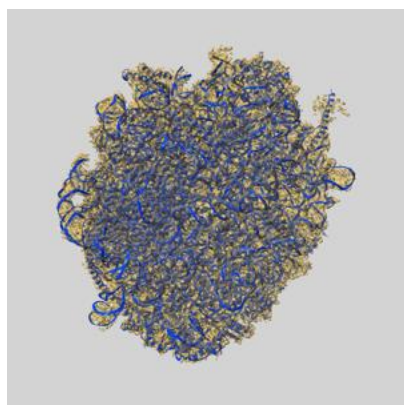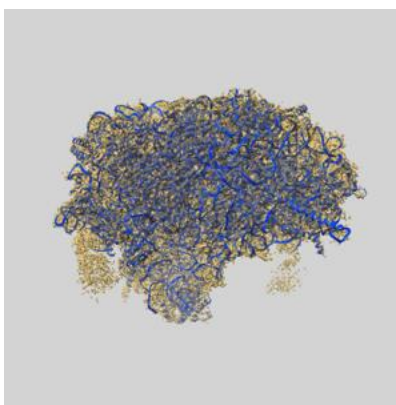
X   Y   Z
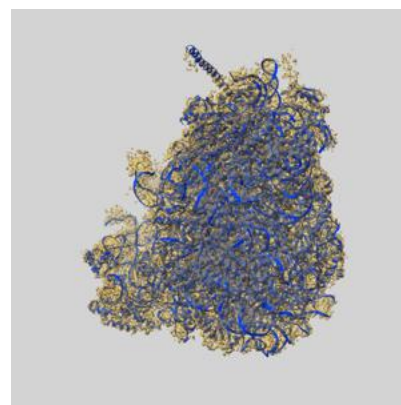
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2   Q-score mapped to coordinate model ⓘ

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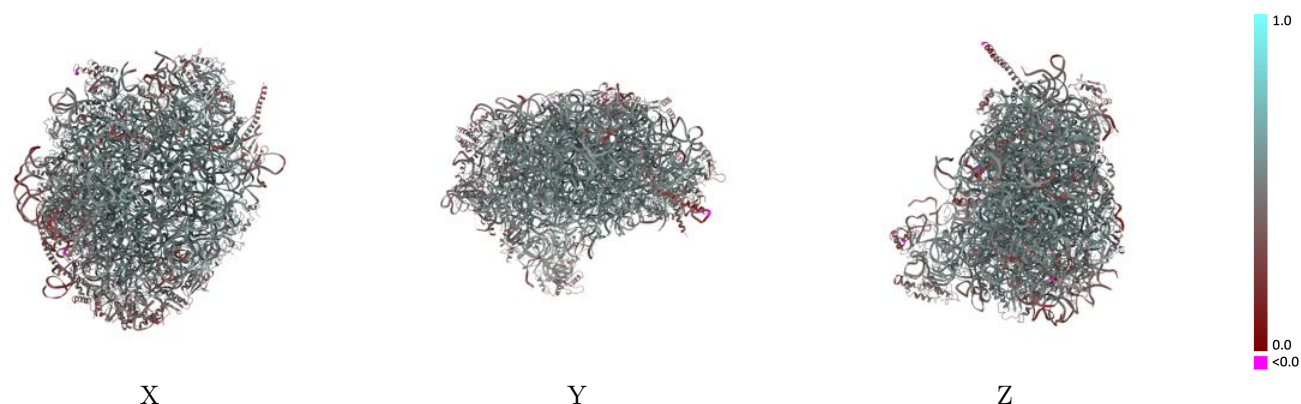
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3   Atom inclusion mapped to coordinate model ⓘ

X   Y   Z
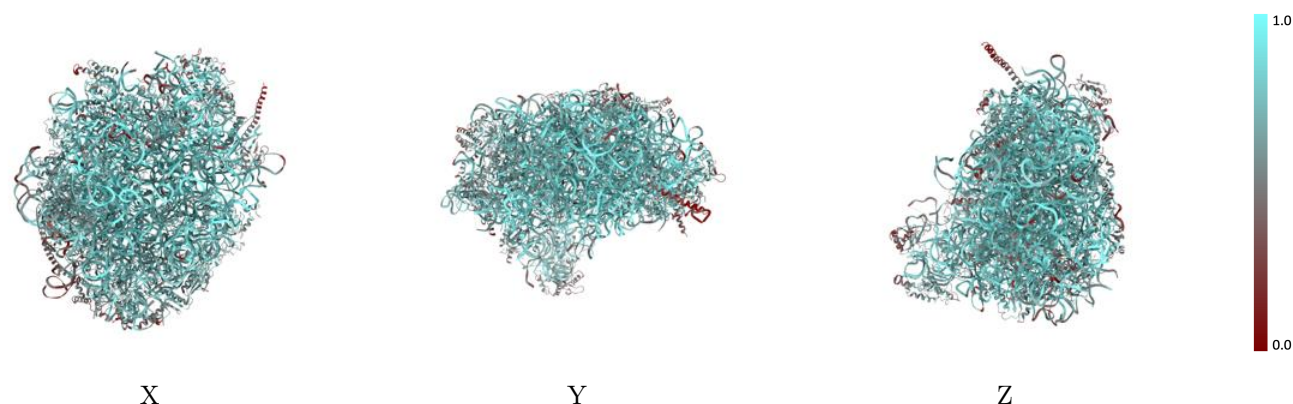
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

9.4 Atom inclusion ⓘ
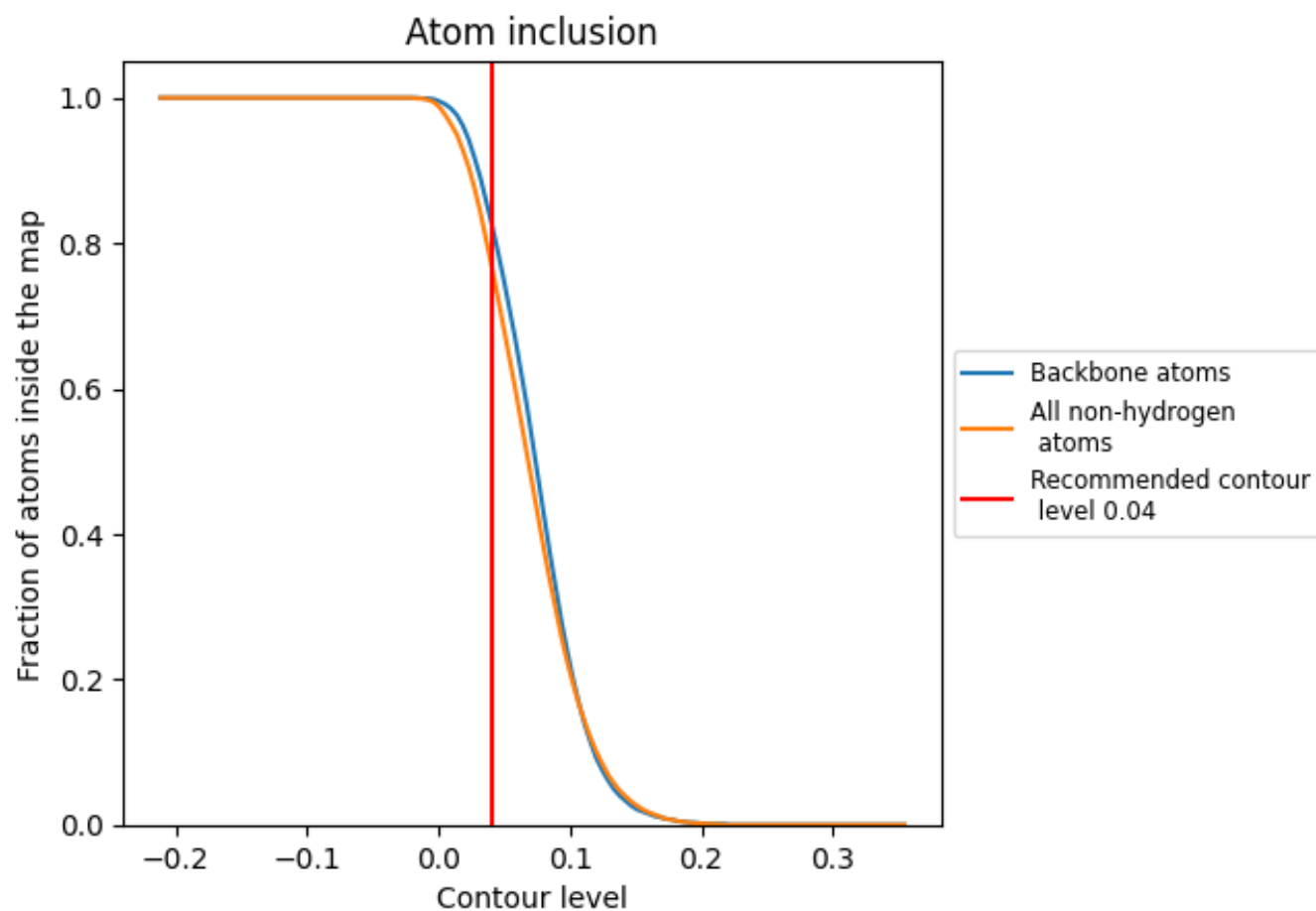
At the recommended contour level, 83% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7730	0.5070
1	0.8450	0.5240
3	0.8350	0.4940
4	0.8480	0.5300
A	0.7680	0.5420
B	0.7140	0.5060
C	0.6490	0.4720
D	0.5930	0.4270
E	0.5770	0.4330
F	0.6460	0.4740
G	0.6260	0.4550
H	0.6130	0.4500
I	0.6260	0.4630
J	0.4530	0.3490
K	0.7050	0.4850
L	0.6380	0.4410
M	0.7980	0.5520
N	0.6840	0.5000
O	0.7190	0.5180
P	0.7030	0.5080
Q	0.6200	0.4670
R	0.6760	0.4990
S	0.6710	0.4930
T	0.4880	0.4010
U	0.6650	0.5060
V	0.6580	0.4900
W	0.6940	0.4930
X	0.6930	0.4980
Y	0.6560	0.4730
Z	0.7840	0.5380
a	0.6990	0.5310
b	0.6050	0.4520
c	0.6990	0.4980
d	0.7250	0.5210
e	0.7640	0.5270

1.0

0.0
<0.0

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W O R L D W I D E
wwPDB
PROTEIN DATA BANK

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Chain	Atom inclusion	Q-score
f	0.7420	0.5120
g	0.6680	0.4930
h	0.6370	0.4530
i	0.8110	0.5500
j	0.5380	0.4240
k	0.7690	0.5400
l	0.6730	0.4910
n	0.6530	0.4910
o	0.7120	0.5210
p	0.6550	0.4710