Full wwPDB EM Validation Report ⓘ

Dec 10, 2022 – 09:29 am GMT

PDB ID	:	5APO
EMDB ID	:	EMD-3151
Title	:	Structure of the yeast 60S ribosomal subunit in complex with Arx1, Alb1 and C-terminally tagged Rei1
Authors	:	Greber, B.J.; Gerhardy, S.; Leitner, A.; Leibundgut, M.; Salem, M.; Boehringer, D.; Leulliot, N.; Aebersold, R.; Panse, V.G.; Ban, N.
Deposited on	:	2015-09-17
Resolution	:	3.41 Å(reported)

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

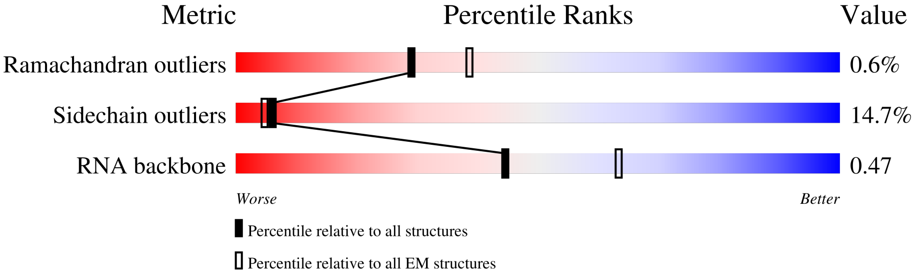
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance

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

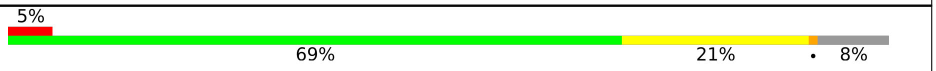
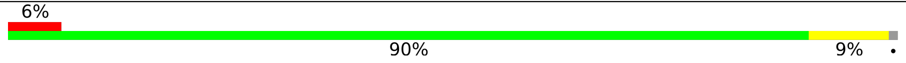
The reported resolution of this entry is 3.41 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	5	3396	
2	7	121	
3	8	158	
4	A	254	
5	B	387	
6	C	362	
7	D	297	
8	E	176	

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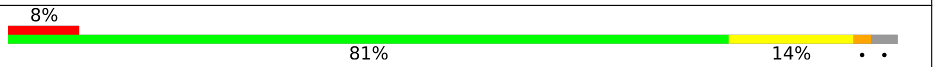
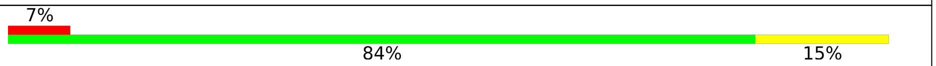
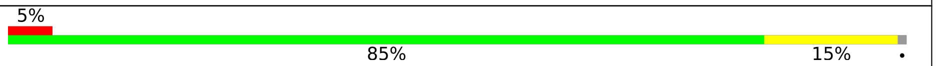
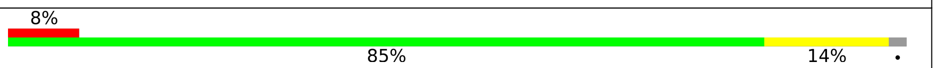
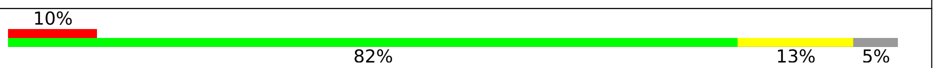
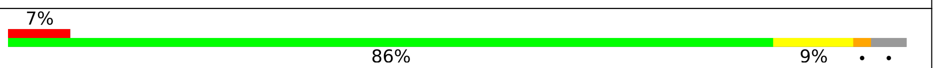
Mol	Chain	Length	Quality of chain
9	F	244	 • 83% 8% 9%
10	G	256	 • 79% 11% 10%
11	H	191	 • 87% 13%
12	I	221	 • 85% 12% •
13	J	174	 8% 81% 14% • •
14	L	199	 • 82% 16% •
15	M	138	 • 90% 9% •
16	N	204	 7% 84% 15%
17	O	199	 83% 16% •
18	P	184	 5% 85% 15% •
19	Q	186	 • 87% 13% •
20	R	189	 • 70% 13% 17%
21	S	172	 • 85% 14% •
22	T	160	 • 84% 16% •
23	U	121	 • 77% 7% 16%
24	V	137	 • 91% 8% •
25	W	155	 • 38% • 59%
26	X	142	 • 72% 13% 15%
27	Y	127	 88% 10% ••
28	Z	136	 • 81% 17% ••
29	a	149	 • 91% 9% •
30	b	59	 8% 85% 14% •
31	c	105	 10% 82% 13% 5%
32	d	113	 7% 86% 9% • •
33	e	130	 • 87% 12% •

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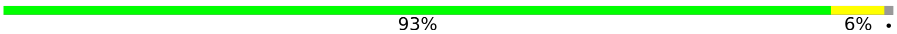
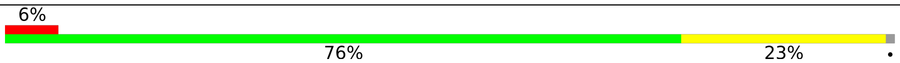
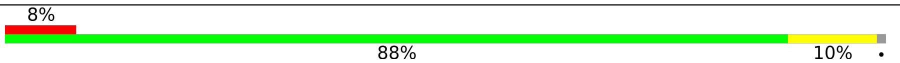
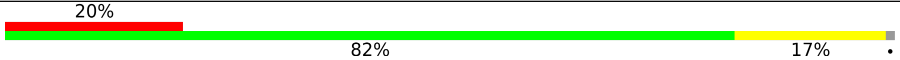
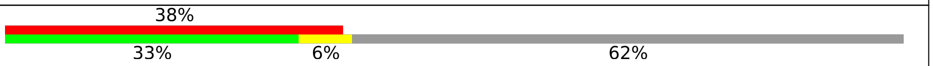
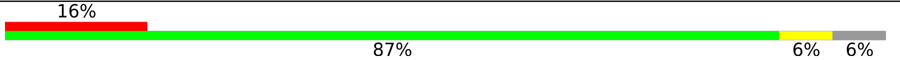
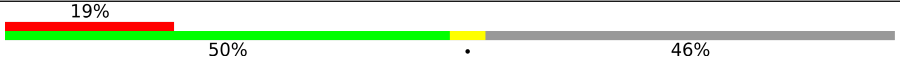
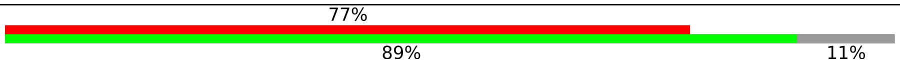
Mol	Chain	Length	Quality of chain
34	f	107	
35	g	121	
36	h	120	
37	i	100	
38	j	88	
39	k	78	
40	l	51	
41	m	128	
42	o	106	
43	p	92	
44	q	312	
45	x	616	
46	y	401	
47	z	95	

2 Entry composition (i)

There are 49 unique types of molecules in this entry. The entry contains 129386 atoms, of which 3 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 ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	5	3112	66537	29736	11996	21694	3111	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	7	121	2579	1152	461	845	121	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	8	158	3353	1500	586	1109	158	0	0

- Molecule 4 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	212	1630	1021	325	283	1	0	0

- Molecule 5 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	B	386	3075	1950	584	533	8	0	0

- Molecule 6 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	C	361	2748	1729	522	494	3	0	0

- Molecule 7 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	D	294	2359	1489	412	456	2	0	0

- Molecule 8 is a protein called 60S RIBOSOMAL PROTEIN EL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	E	175	1356	878	242	235	1	0	0

- Molecule 9 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	F	223	1791	1155	325	310	1	0	0

- Molecule 10 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	G	231	1763	1130	316	314	3	0	0

- Molecule 11 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	H	191	1518	963	274	277	4	0	0

- Molecule 12 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	I	213	1722	1094	325	297	6	0	0

- Molecule 13 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	J	169	1353	847	253	249	4	0	0

- Molecule 14 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	L	194	Total 1548	C 965	N 316	O 267	0	0

- Molecule 15 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	137	Total 1059	C 678	N 200	O 179	S 2	0	0

- Molecule 16 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	203	Total 1720	C 1077	N 361	O 281	S 1	0	0

- Molecule 17 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	197	Total 1555	C 1003	N 289	O 262	S 1	0	0

- Molecule 18 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	P	183	Total 1442	C 896	N 287	O 259	0	0

- Molecule 19 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Q	185	Total 1441	C 908	N 290	O 241	S 2	0	0

- Molecule 20 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	R	156	Total 1258	C 781	N 265	O 212	0	0

- Molecule 21 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	171	Total 1437	C 925	N 266	O 243	S 3	0	0

- Molecule 22 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T	159	Total 1276	C 805	N 246	O 221	S 4	0	0

- Molecule 23 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	U	102	Total 808	C 524	N 132	O 152	0	0

- Molecule 24 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	V	136	Total 1003	C 628	N 189	O 179	S 7	0	0

- Molecule 25 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	W	63	Total 521	C 336	N 102	O 82	S 1	0	0

- Molecule 26 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	X	120	Total 959	C 617	N 168	O 172	S 2	0	0

- Molecule 27 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	Y	126	Total 993	C 625	N 192	O 176	0	0

- Molecule 28 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	Z	135	Total 1092	C 710	N 202	O 180	0	0

- Molecule 29 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	a	148	Total 1173	C 749	N 231	O 190	S 3	0	0

- Molecule 30 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	b	58	Total 462	C 289	N 100	O 73	0	0

- Molecule 31 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	c	100	Total 767	C 492	N 128	O 146	S 1	0	0

- Molecule 32 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	109	Total 883	C 559	N 167	O 156	S 1	0	0

- Molecule 33 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	e	129	Total 1034	C 655	N 207	O 171	S 1	0	0

- Molecule 34 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	106	Total 850	C 540	N 165	O 144	S 1	0	0

- Molecule 35 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	g	112	Total	C	N	O	S	0	0
			880	545	179	152	4		

- Molecule 36 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	h	119	Total	C	N	O	S	0	0
			965	612	185	167	1		

- Molecule 37 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	i	99	Total	C	N	O	S	0	0
			770	481	156	131	2		

- Molecule 38 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	j	87	Total	C	N	O	S	0	0
			681	414	148	114	5		

- Molecule 39 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	k	77	Total	C	N	O	0	0
			608	388	114	106		

- Molecule 40 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	l	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 41 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	m	52	Total	C	N	O	S	0	0
			417	259	86	67	5		

- Molecule 42 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	o	105	847	534	170	138	5	0	0

- Molecule 43 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	p	91	694	429	138	121	6	0	0

- Molecule 44 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	q	120	962	618	169	172	3	0	0

- Molecule 45 is a protein called Probable metalloprotease ARX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	x	579	4477	2823	772	867	15	0	0

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
x	-22	MET	-	initiating methionine	UNP Q03862
x	-21	GLY	-	expression tag	UNP Q03862
x	-20	SER	-	expression tag	UNP Q03862
x	-19	SER	-	expression tag	UNP Q03862
x	-18	HIS	-	expression tag	UNP Q03862
x	-17	HIS	-	expression tag	UNP Q03862
x	-16	HIS	-	expression tag	UNP Q03862
x	-15	HIS	-	expression tag	UNP Q03862
x	-14	HIS	-	expression tag	UNP Q03862
x	-13	HIS	-	expression tag	UNP Q03862
x	-12	SER	-	expression tag	UNP Q03862
x	-11	SER	-	expression tag	UNP Q03862
x	-10	GLY	-	expression tag	UNP Q03862
x	-9	LEU	-	expression tag	UNP Q03862
x	-8	VAL	-	expression tag	UNP Q03862
x	-7	PRO	-	expression tag	UNP Q03862
x	-6	ARG	-	expression tag	UNP Q03862
x	-5	GLY	-	expression tag	UNP Q03862
x	-4	SER	-	expression tag	UNP Q03862

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Chain	Residue	Modelled	Actual	Comment	Reference
x	-3	HIS	-	expression tag	UNP Q03862
x	-2	MET	-	expression tag	UNP Q03862
x	-1	LEU	-	expression tag	UNP Q03862
x	0	GLU	-	expression tag	UNP Q03862

- Molecule 46 is a protein called CYTOPLASMIC 60S SUBUNIT BIOGENESIS FACTOR REI1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
46	y	217	1788	1131	3	324	322	8	0	0

- Molecule 47 is a protein called ALB1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
47	z	85	510	340	85	85	0	0

- Molecule 48 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
48	5	259	259	259	0
48	7	6	6	6	0
48	8	7	7	7	0
48	B	2	2	2	0
48	C	1	1	1	0
48	N	1	1	1	0
48	P	1	1	1	0
48	R	1	1	1	0
48	V	1	1	1	0
48	y	1	1	1	0

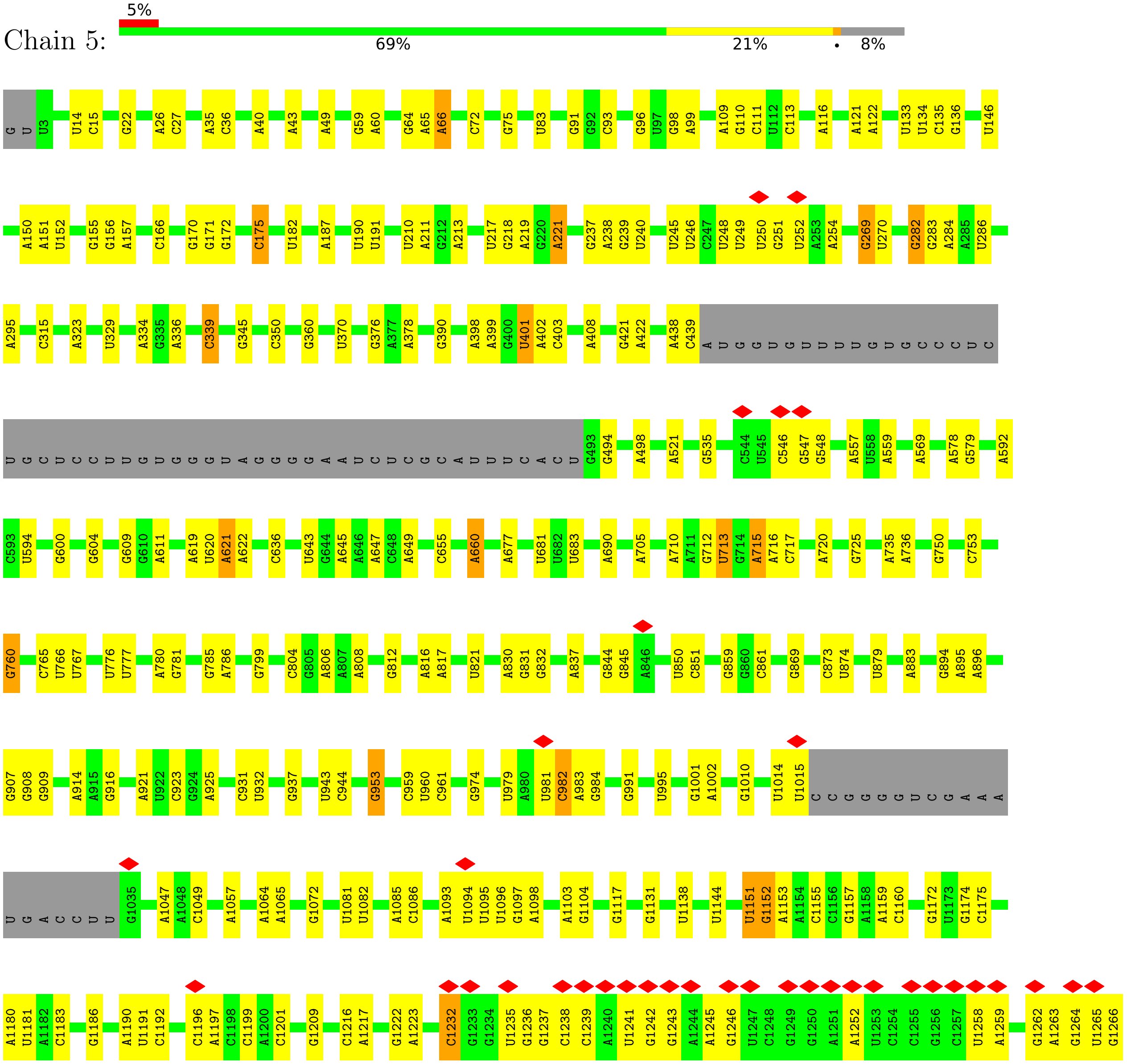
- Molecule 49 is ZINC ION (three-letter code: ZN) (formula: Zn).

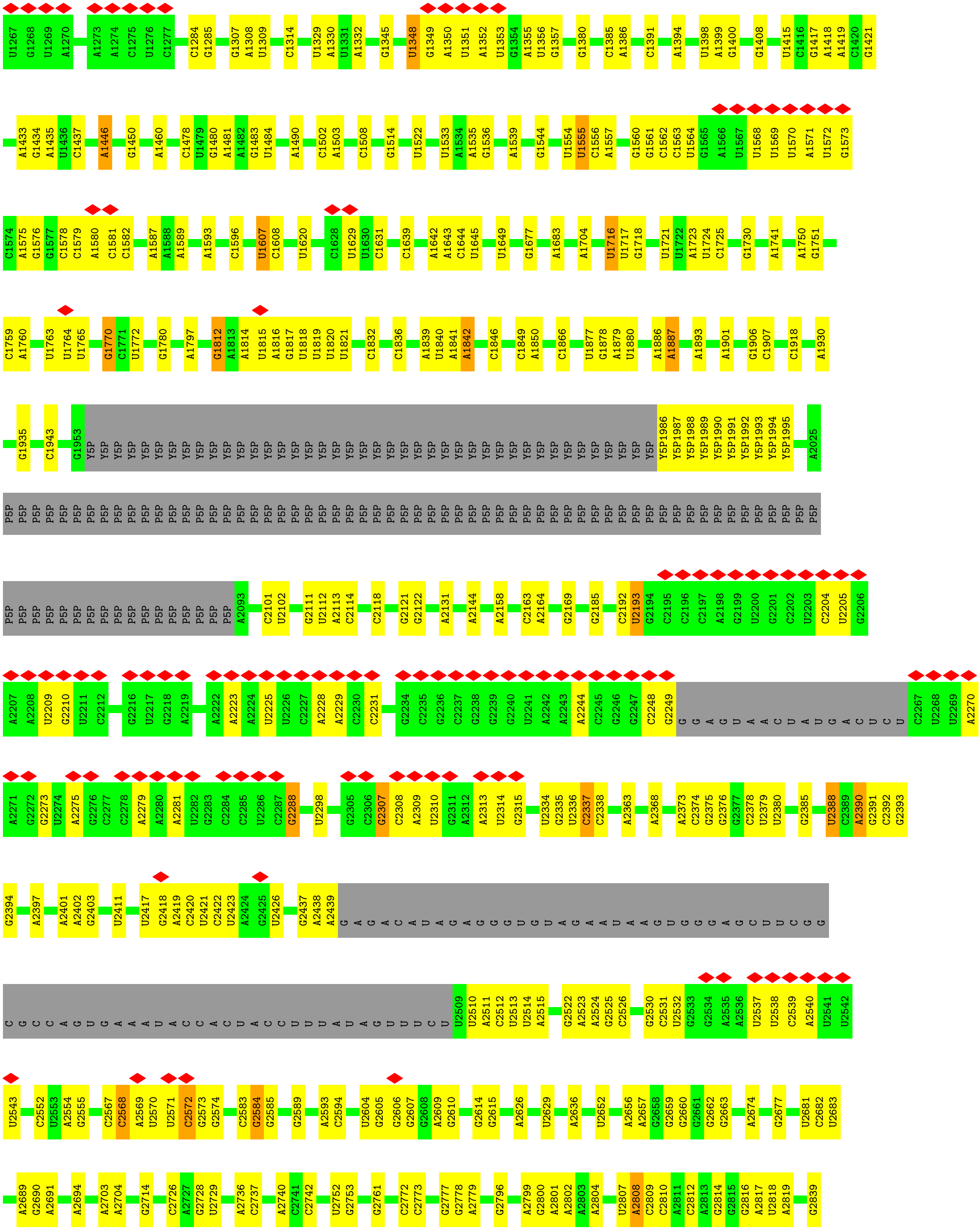
Mol	Chain	Residues	Atoms	AltConf
49	j	1	Total Zn 1 1	0
49	m	1	Total Zn 1 1	0
49	o	1	Total Zn 1 1	0
49	p	1	Total Zn 1 1	0
49	y	2	Total Zn 2 2	0

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 ribosomal RNA




U1267
G1268
U1269
A1270
A1273
A1274
C1275
U1276
C1277
C1284
G1285
G1307
A1308
U1309
C1314
U1329
A1330
U1331
A1332
G1345
U1348
G1349
A1350
U1351
A1352
U1353
G1354
A1355
U1356
G1357
G1380
C1385
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A1643
C1644
U1645
U1649
G1677
A1683
A1704
U1716
U1717
G1718
U1721
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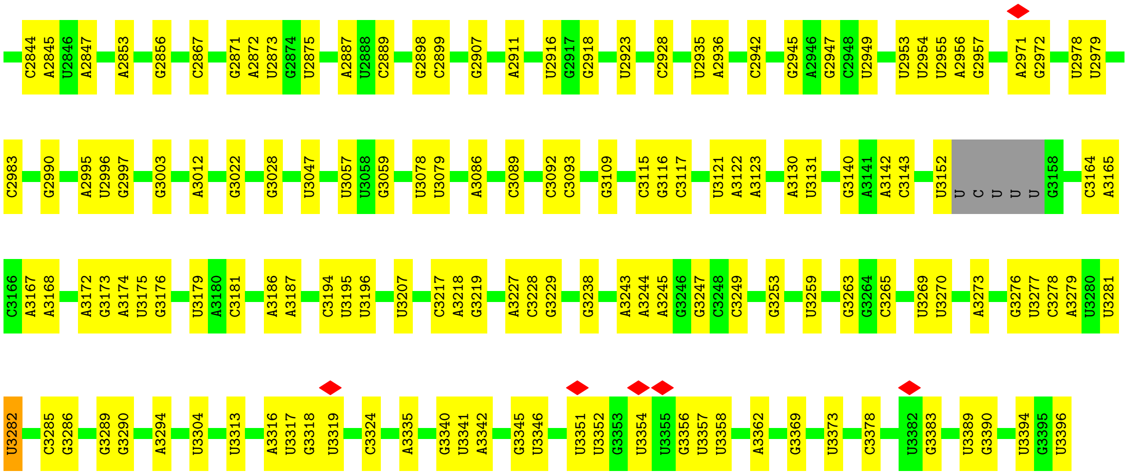
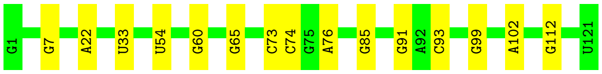


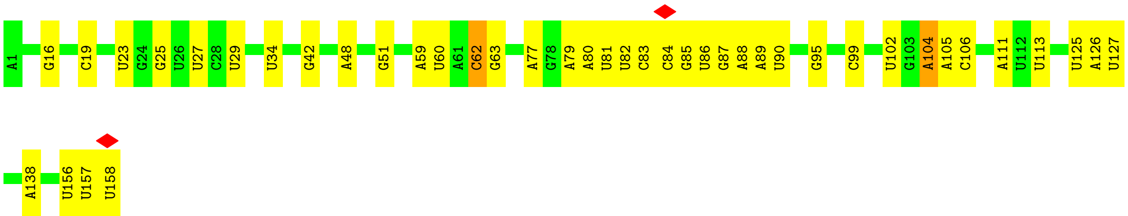
- Molecule 2: 5S ribosomal RNA

Chain 7:



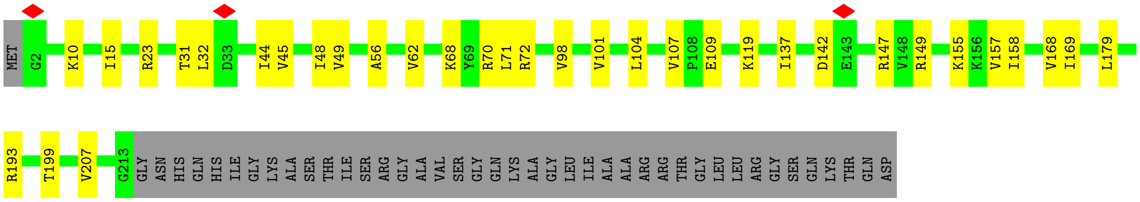
- Molecule 3: 5.8S ribosomal RNA

Chain 8:



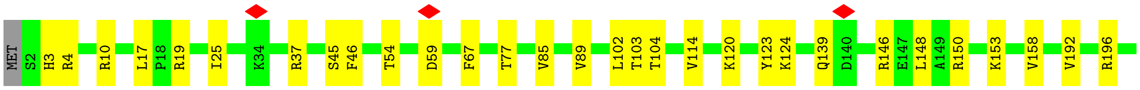
- Molecule 4: 60S ribosomal protein L2-A

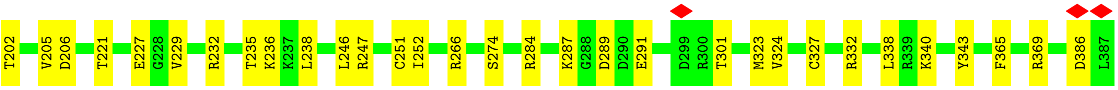
Chain A:



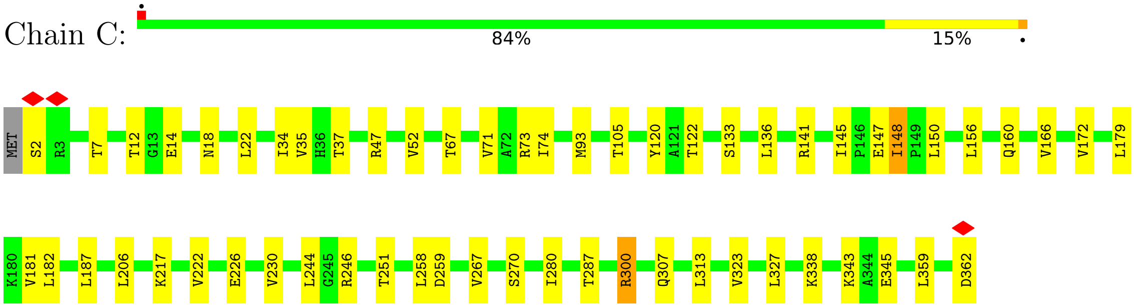
- Molecule 5: 60S ribosomal protein L3

Chain B:

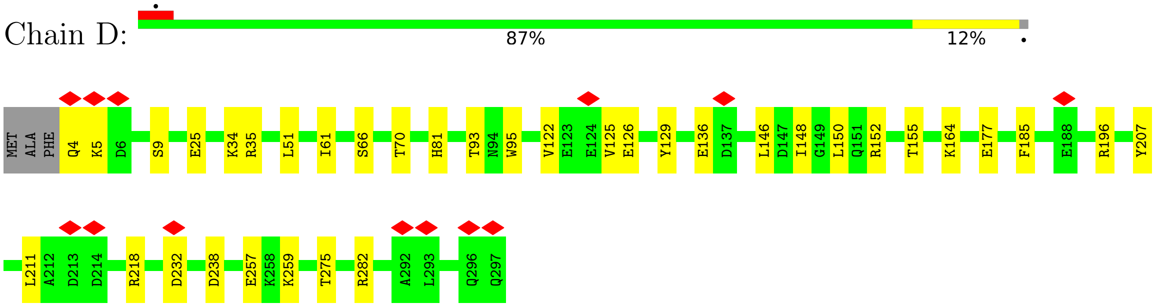




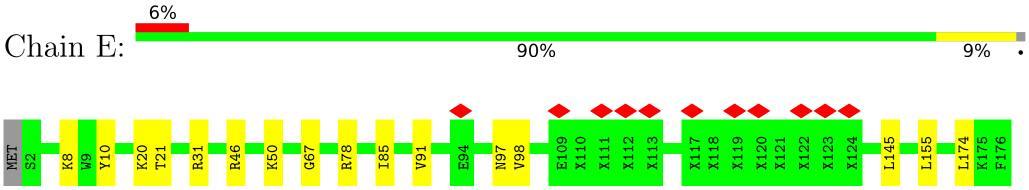
- Molecule 6: 60S ribosomal protein L4-A



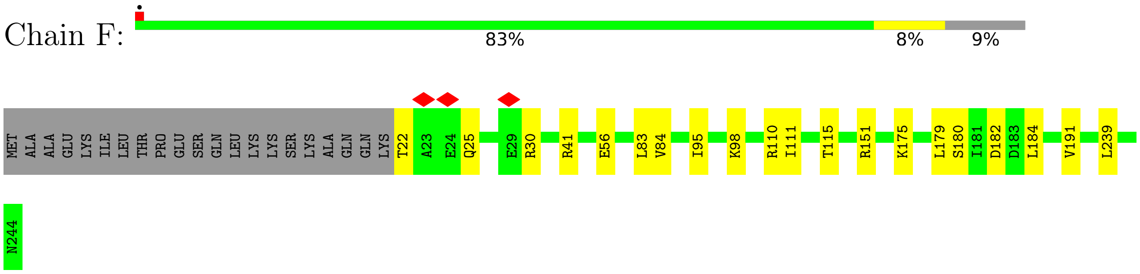
- Molecule 7: 60S ribosomal protein L5



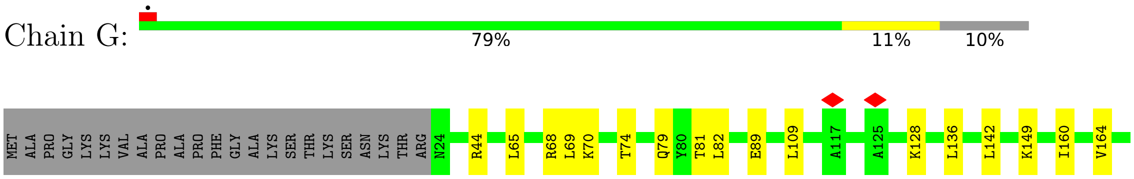
- Molecule 8: 60S RIBOSOMAL PROTEIN EL6

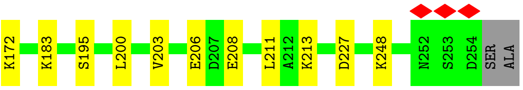


- Molecule 9: 60S ribosomal protein L7-A

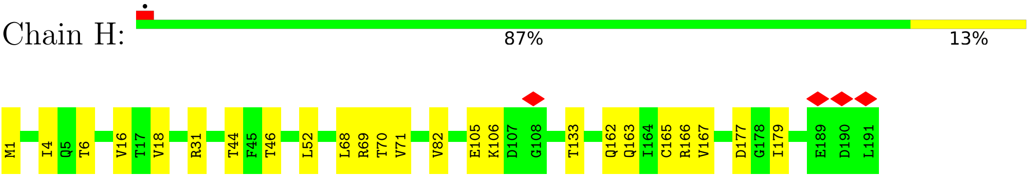


- Molecule 10: 60S ribosomal protein L8-A

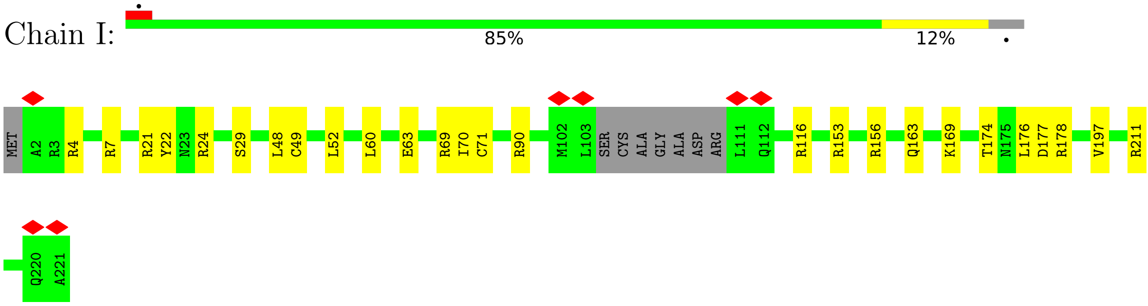




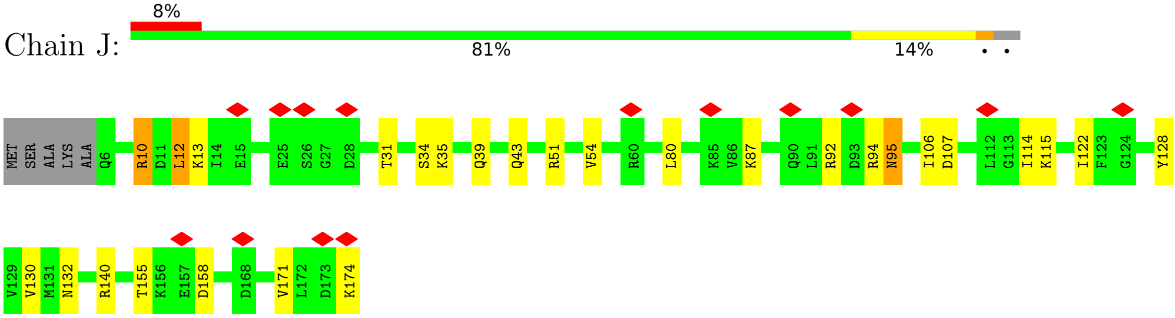
• Molecule 11: 60S ribosomal protein L9-A



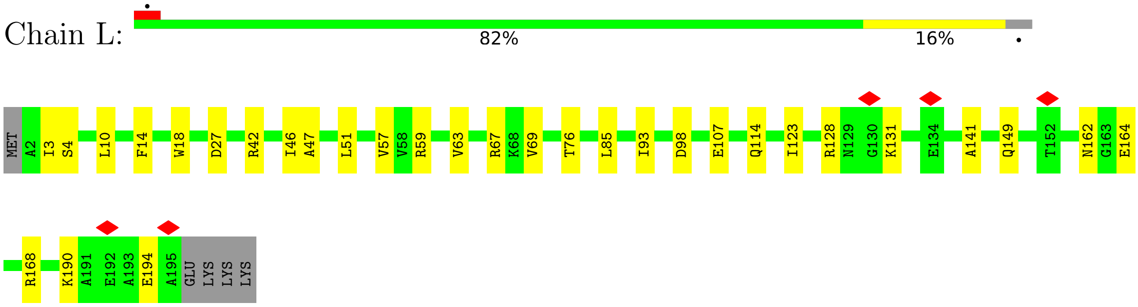
• Molecule 12: 60S ribosomal protein L10



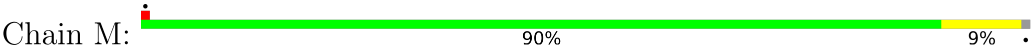
• Molecule 13: 60S ribosomal protein L11-A

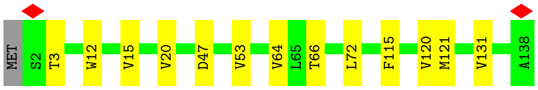


• Molecule 14: 60S ribosomal protein L13-A



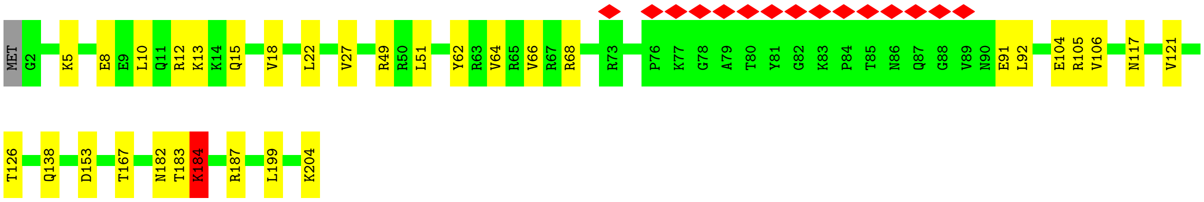
• Molecule 15: 60S ribosomal protein L14-A





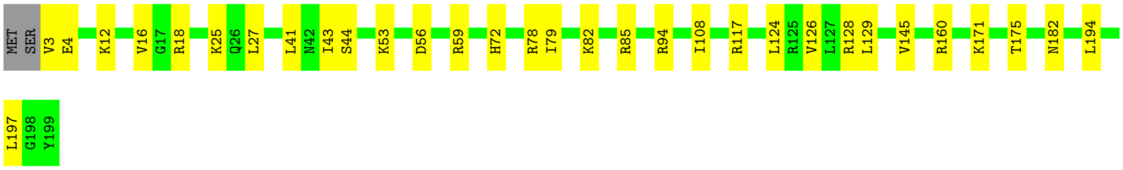
- Molecule 16: 60S ribosomal protein L15-A

Chain N:



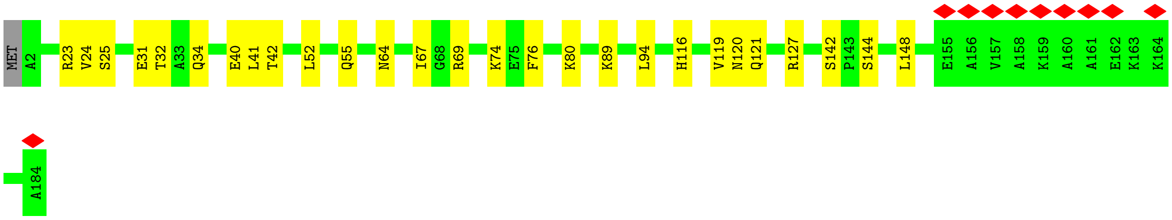
- Molecule 17: 60S ribosomal protein L16-A

Chain O:



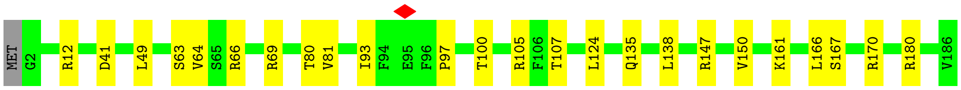
- Molecule 18: 60S ribosomal protein L17-A

Chain P:



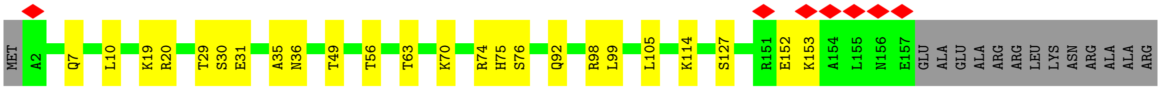
- Molecule 19: 60S ribosomal protein L18-A

Chain Q:



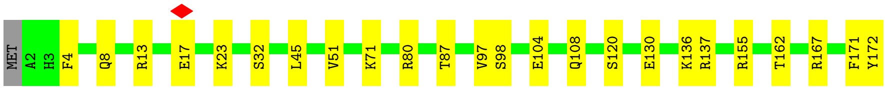
- Molecule 20: 60S ribosomal protein L19-A

Chain R:



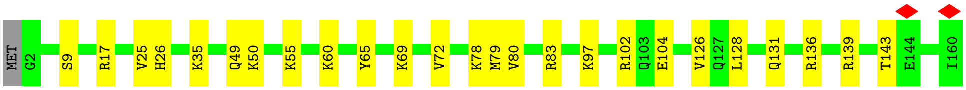
- Molecule 21: 60S ribosomal protein L20-A

Chain S:



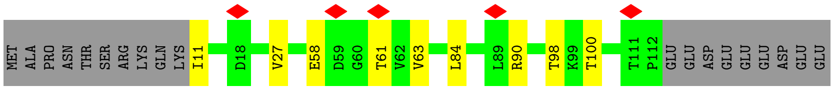
- Molecule 22: 60S ribosomal protein L21-A

Chain T:



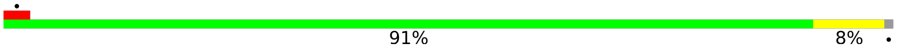
- Molecule 23: 60S ribosomal protein L22-A

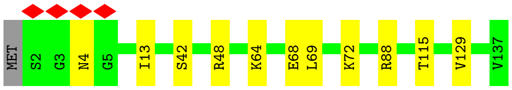
Chain U:



- Molecule 24: 60S ribosomal protein L23-A

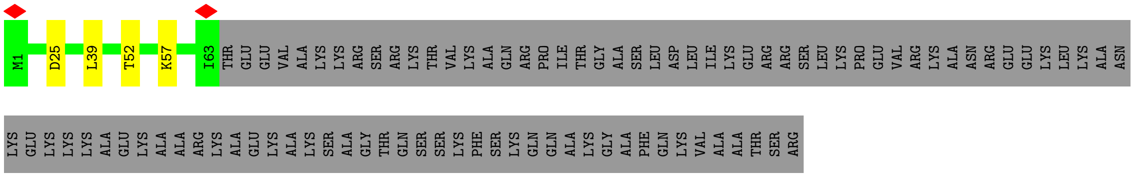
Chain V:





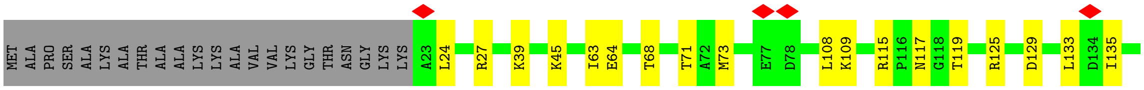
- Molecule 25: 60S ribosomal protein L24-A

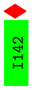
Chain W:



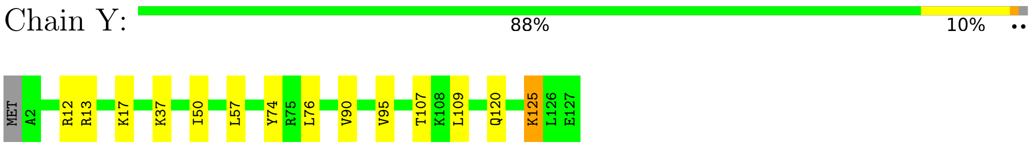
- Molecule 26: 60S ribosomal protein L25

Chain X:

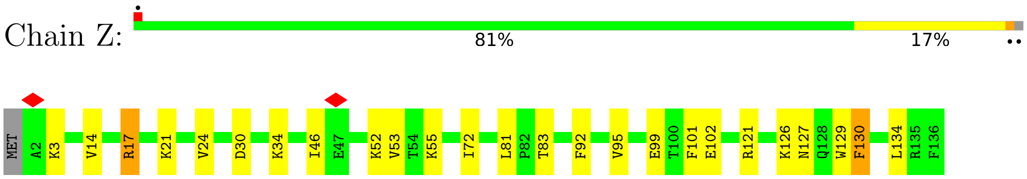




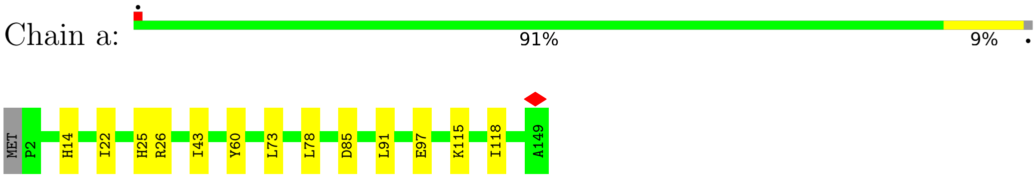
- Molecule 27: 60S ribosomal protein L26-A



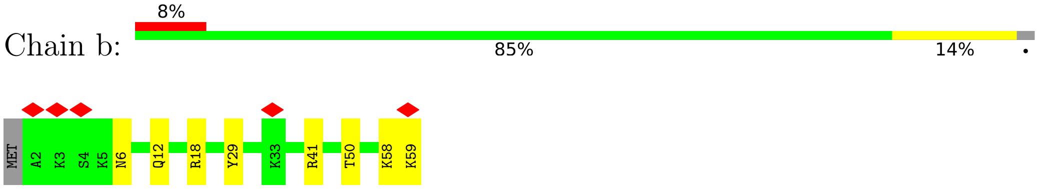
- Molecule 28: 60S ribosomal protein L27-A



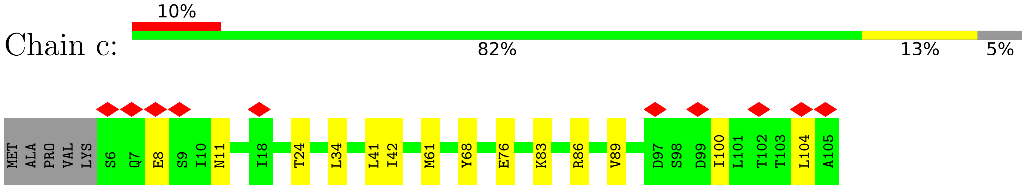
- Molecule 29: 60S ribosomal protein L28



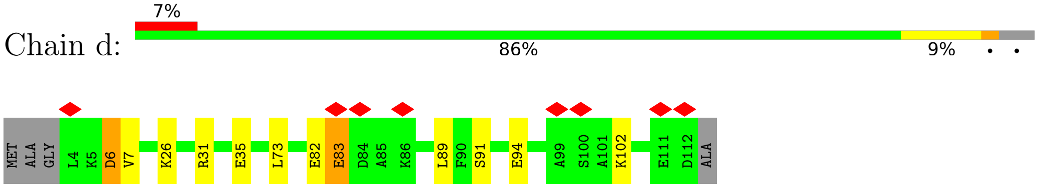
- Molecule 30: 60S ribosomal protein L29



- Molecule 31: 60S ribosomal protein L30

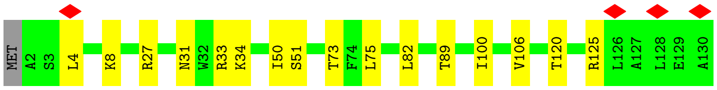


- Molecule 32: 60S ribosomal protein L31-A



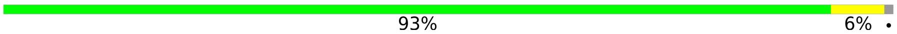
- Molecule 33: 60S ribosomal protein L32

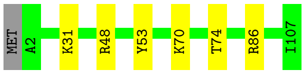
Chain e:



- Molecule 34: 60S ribosomal protein L33-A

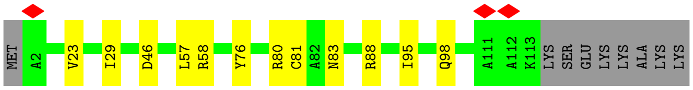
Chain f:





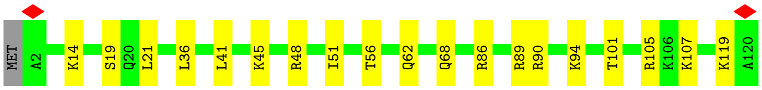
- Molecule 35: 60S ribosomal protein L34-A

Chain g:



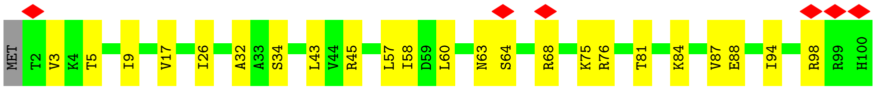
- Molecule 36: 60S ribosomal protein L35-A

Chain h:



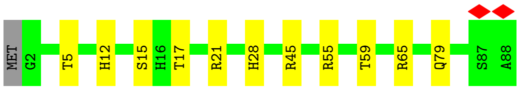
- Molecule 37: 60S ribosomal protein L36-A

Chain i:



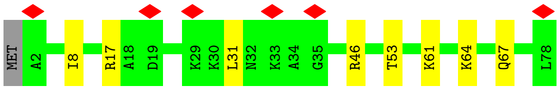
- Molecule 38: 60S ribosomal protein L37-A

Chain j:

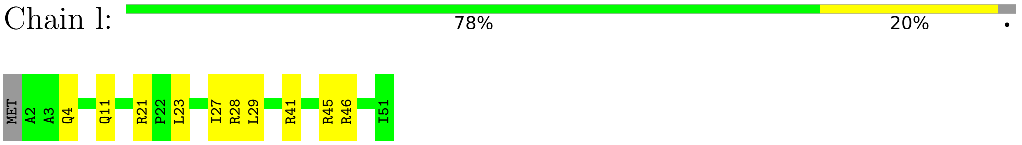


- Molecule 39: 60S ribosomal protein L38

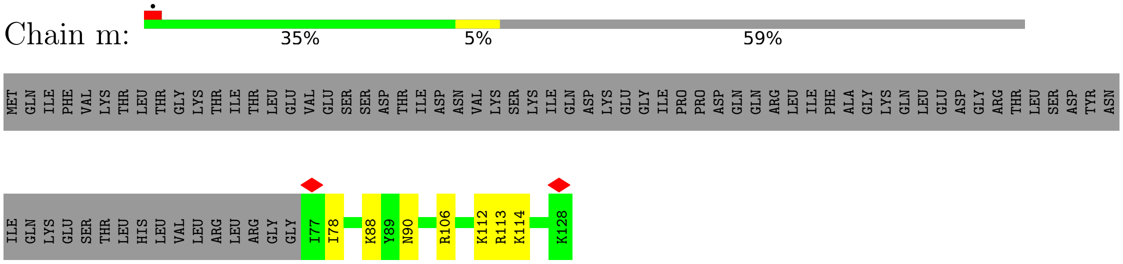
Chain k:



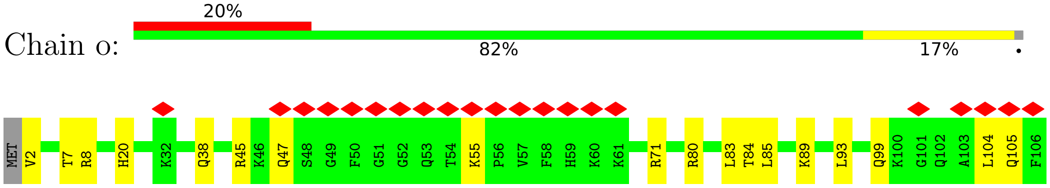
- Molecule 40: 60S ribosomal protein L39



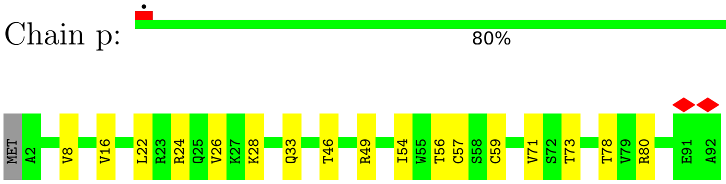
- Molecule 41: Ubiquitin-60S ribosomal protein L40



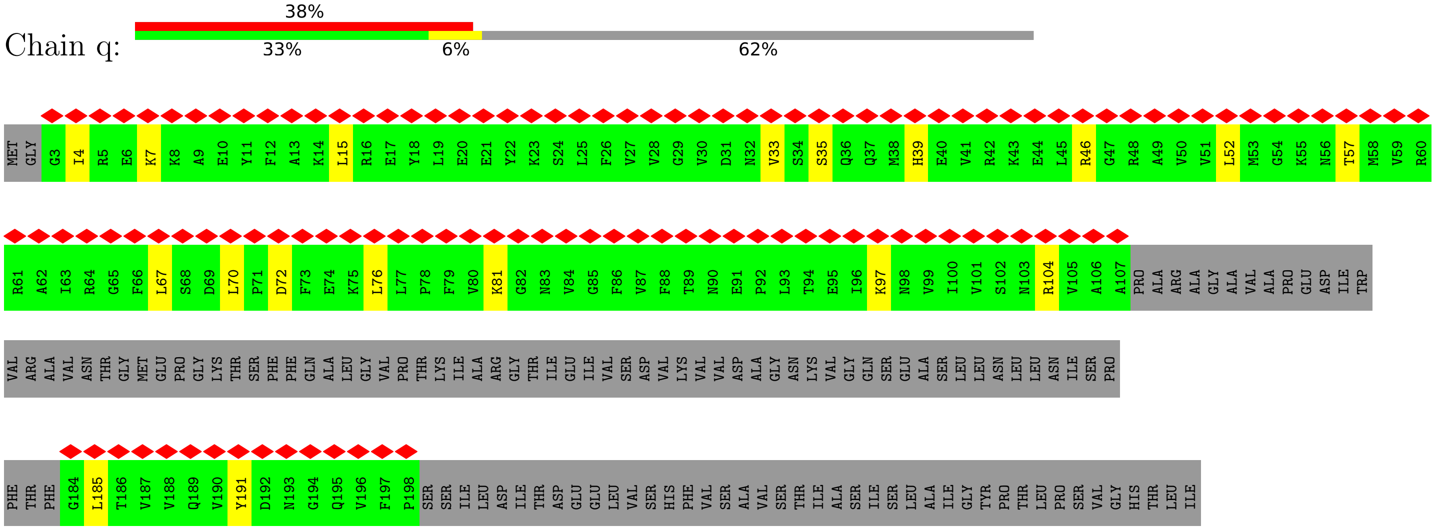
- Molecule 42: 60S ribosomal protein L42-A

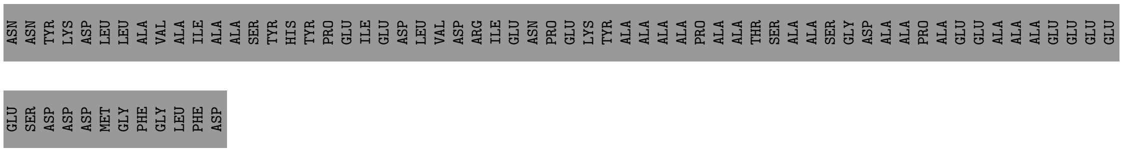


- Molecule 43: 60S ribosomal protein L43-A

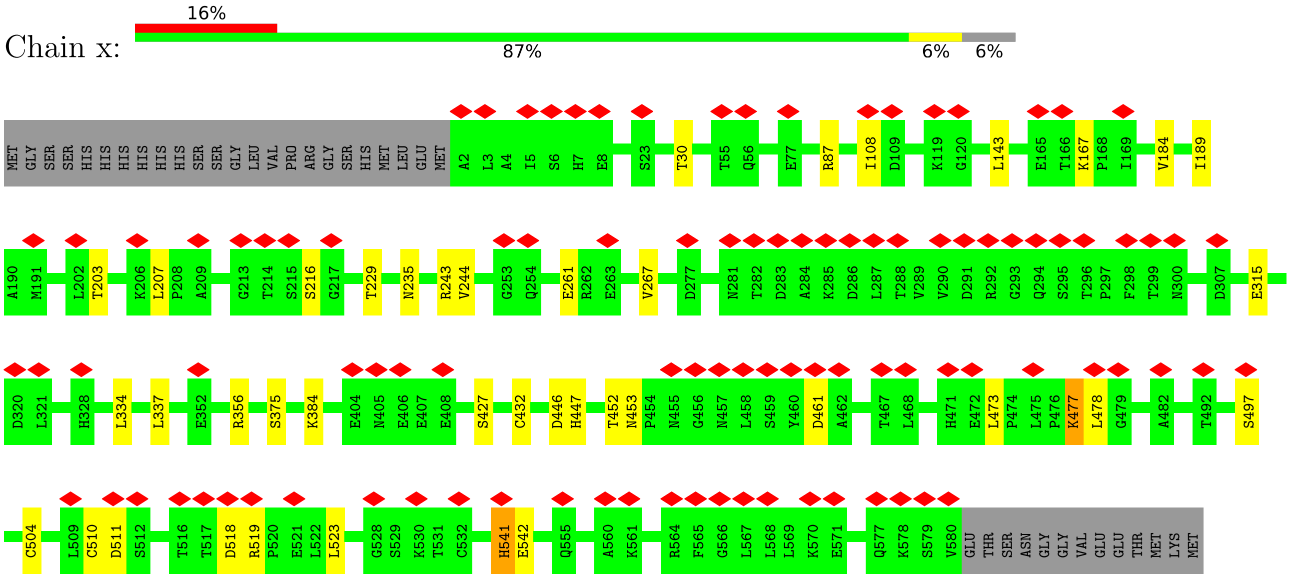


- Molecule 44: 60S acidic ribosomal protein P0

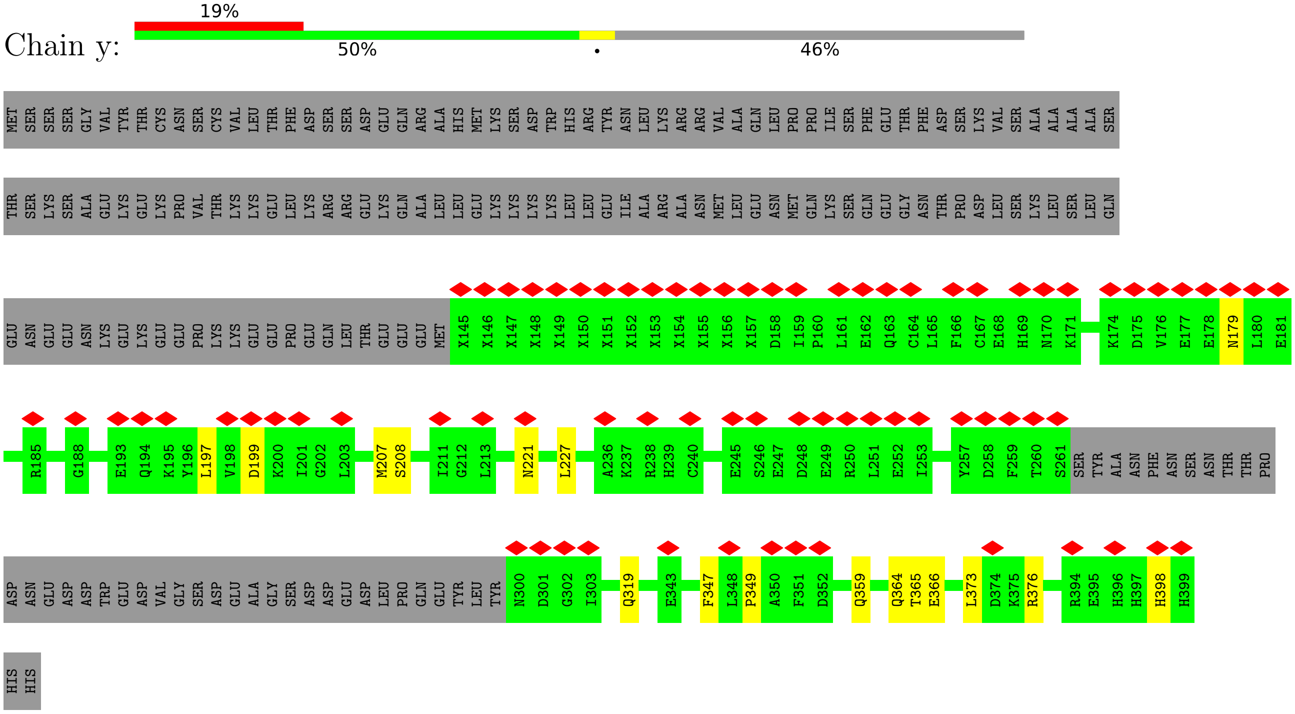




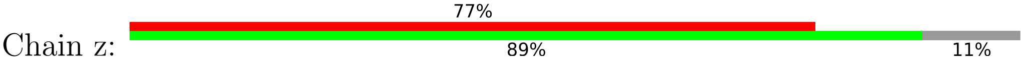
- Molecule 45: Probable metalloprotease ARX1

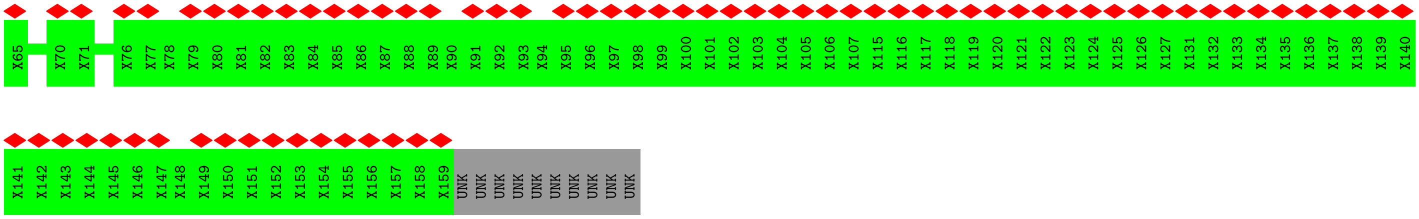


- Molecule 46: CYTOPLASMIC 60S SUBUNIT BIOGENESIS FACTOR REI1



- Molecule 47: ALB1

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4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	134701	Depositor
Resolution determination method	Not provided	
CTF correction method	PER DETECTOR FRAME	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	20	Depositor
Minimum defocus (nm)	800.00	Depositor
Maximum defocus (nm)	3000.00	Depositor
Magnification	100720	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	1.020	Depositor
Minimum map value	-0.642	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.055	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	300.24, 300.24, 300.24	wwPDB
Map dimensions	216, 216, 216	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, Y5P, MG, P5P

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	5	0.66	12/74039 (0.0%)	1.09	121/115426 (0.1%)
2	7	0.41	0/2883	0.90	1/4491 (0.0%)
3	8	0.69	0/3746	1.12	8/5832 (0.1%)
4	A	0.41	0/1662	0.60	0/2236
5	B	0.46	0/3146	0.59	0/4228
6	C	0.47	0/2800	0.67	1/3790 (0.0%)
7	D	0.34	0/2408	0.50	0/3248
8	E	0.39	0/1269	0.58	0/1705
9	F	0.46	0/1828	0.58	0/2461
10	G	0.38	0/1795	0.58	0/2429
11	H	0.40	0/1539	0.54	0/2073
12	I	0.36	0/1758	0.57	0/2358
13	J	0.34	0/1374	0.55	0/1842
14	L	0.46	0/1573	0.61	0/2113
15	M	0.38	0/1074	0.55	0/1446
16	N	0.52	0/1757	0.65	0/2354
17	O	0.48	0/1585	0.63	1/2128 (0.0%)
18	P	0.50	0/1465	0.60	0/1968
19	Q	0.42	0/1465	0.61	0/1965
20	R	0.39	0/1275	0.52	0/1702
21	S	0.45	0/1473	0.59	0/1980
22	T	0.42	0/1300	0.56	0/1743
23	U	0.36	0/825	0.56	0/1120
24	V	0.43	0/1018	0.60	0/1369
25	W	0.40	0/533	0.53	0/707
26	X	0.42	0/974	0.62	0/1314
27	Y	0.43	0/1004	0.62	0/1341
28	Z	0.38	0/1118	0.62	0/1497
29	a	0.47	0/1204	0.64	0/1612
30	b	0.39	0/473	0.53	0/629
31	c	0.35	0/775	0.52	0/1040
32	d	0.46	0/897	0.62	0/1205

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	e	0.52	0/1055	0.63	0/1413
34	f	0.52	0/868	0.67	0/1168
35	g	0.43	0/890	0.63	0/1189
36	h	0.42	0/974	0.58	0/1297
37	i	0.35	0/777	0.55	0/1033
38	j	0.51	0/696	0.65	0/923
39	k	0.34	0/614	0.53	0/822
40	l	0.46	0/443	0.57	0/588
41	m	0.40	0/423	0.55	0/562
42	o	0.41	0/860	0.56	0/1136
43	p	0.46	0/701	0.62	0/934
44	q	0.58	0/977	0.61	0/1313
45	x	0.37	0/4557	0.57	0/6189
46	y	0.39	0/1746	0.54	0/2346
All	All	0.57	12/137616 (0.0%)	0.93	132/202265 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	C	0	3
8	E	0	1
14	L	0	1
16	N	0	1
27	Y	0	1
28	Z	0	1
32	d	0	3
37	i	0	1
45	x	0	3
46	y	0	1
All	All	0	16

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	1152	G	N9-C4	-7.14	1.32	1.38
1	5	2368	A	N9-C4	-6.55	1.33	1.37
1	5	336	A	N9-C4	-6.44	1.33	1.37
1	5	2392	C	N1-C6	-6.25	1.33	1.37
1	5	1446	A	N9-C4	-6.19	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	1886	A	N9-C4	-5.73	1.34	1.37
1	5	660	A	N9-C4	-5.60	1.34	1.37
1	5	1723	A	N9-C4	-5.55	1.34	1.37
1	5	1197	A	N9-C4	-5.41	1.34	1.37
1	5	1842	A	N9-C4	-5.32	1.34	1.37
1	5	2368	A	N3-C4	-5.19	1.31	1.34
1	5	408	A	C6-N1	-5.03	1.32	1.35

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	1152	G	N3-C4-C5	10.03	133.61	128.60
1	5	408	A	N1-C6-N6	-8.94	113.24	118.60
1	5	1232	C	O4'-C1'-N1	8.59	115.07	108.20
1	5	2193	U	N1-C2-N3	8.32	119.89	114.90
3	8	62	C	C6-N1-C2	8.32	123.63	120.30
1	5	2307	G	C4-N9-C1'	-8.29	115.72	126.50
1	5	1152	G	N3-C4-N9	-8.06	121.16	126.00
3	8	27	U	C5-C6-N1	-7.88	118.76	122.70
1	5	64	G	N3-C4-N9	7.87	130.72	126.00
1	5	2307	G	C8-N9-C1'	7.73	137.05	127.00
1	5	1555	U	N3-C2-O2	-7.54	116.92	122.20
1	5	1812	G	N3-C4-N9	-7.10	121.74	126.00
1	5	1836	C	C6-N1-C2	-6.94	117.52	120.30
1	5	1607	U	P-O3'-C3'	6.82	127.89	119.70
1	5	1522	U	C5-C6-N1	-6.72	119.34	122.70
1	5	1631	C	C2-N1-C1'	-6.71	111.42	118.80
1	5	2808	A	O4'-C1'-N9	6.71	113.56	108.20
1	5	339	C	N1-C2-O2	-6.59	114.94	118.90
1	5	982	C	C6-N1-C2	-6.59	117.67	120.30
1	5	643	U	C5-C6-N1	-6.54	119.43	122.70
1	5	982	C	N3-C2-O2	-6.54	117.33	121.90
1	5	621	A	C8-N9-C4	-6.53	103.19	105.80
1	5	894	G	C8-N9-C4	6.50	109.00	106.40
1	5	894	G	N3-C4-C5	6.48	131.84	128.60
1	5	753	C	C6-N1-C2	-6.28	117.79	120.30
1	5	767	U	O4'-C1'-N1	6.28	113.22	108.20
1	5	1332	A	C8-N9-C4	-6.28	103.29	105.80
1	5	821	U	N1-C2-O2	-6.22	118.44	122.80
1	5	953	G	N1-C6-O6	-6.20	116.18	119.90
1	5	821	U	C2-N1-C1'	-6.15	110.32	117.70
1	5	35	A	N1-C2-N3	6.10	132.35	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	1172	G	N3-C4-C5	-6.07	125.57	128.60
1	5	1631	C	C6-N1-C1'	6.06	128.08	120.80
1	5	931	C	N1-C2-O2	-6.04	115.27	118.90
1	5	408	A	N9-C4-C5	6.04	108.22	105.80
1	5	1151	U	C4-C5-C6	6.03	123.32	119.70
1	5	1555	U	P-O3'-C3'	6.02	126.92	119.70
1	5	99	A	N1-C2-N3	6.00	132.30	129.30
2	7	85	G	C8-N9-C4	5.93	108.77	106.40
1	5	645	A	C2-N3-C4	5.92	113.56	110.60
1	5	1175	C	C5-C6-N1	-5.91	118.05	121.00
1	5	2949	U	C5-C6-N1	-5.91	119.75	122.70
1	5	2307	G	N3-C4-N9	-5.90	122.46	126.00
1	5	360	G	N3-C4-C5	-5.89	125.66	128.60
1	5	645	A	N3-C4-C5	-5.88	122.68	126.80
1	5	64	G	N3-C4-C5	-5.87	125.66	128.60
1	5	3335	A	C8-N9-C4	-5.83	103.47	105.80
1	5	2379	U	C5-C6-N1	-5.79	119.80	122.70
1	5	72	C	C5-C6-N1	-5.78	118.11	121.00
1	5	1174	G	C4-N9-C1'	5.71	133.93	126.50
1	5	2193	U	C2-N3-C4	-5.71	123.57	127.00
1	5	2659	G	C8-N9-C4	5.71	108.69	106.40
1	5	3373	U	C5-C6-N1	-5.71	119.84	122.70
3	8	99	C	C6-N1-C2	5.67	122.57	120.30
1	5	66	A	C8-N9-C4	5.65	108.06	105.80
1	5	943	U	C5-C6-N1	-5.64	119.88	122.70
1	5	1723	A	C2-N3-C4	-5.56	107.82	110.60
1	5	2380	U	C5-C6-N1	-5.55	119.92	122.70
1	5	1151	U	N1-C2-N3	5.55	118.23	114.90
1	5	3089	C	C6-N1-C2	5.54	122.52	120.30
1	5	282	G	N3-C4-C5	-5.54	125.83	128.60
1	5	1555	U	N1-C2-O2	5.53	126.67	122.80
1	5	1348	U	N1-C1'-C2'	-5.51	105.93	112.00
1	5	1172	G	C4-N9-C1'	5.50	133.65	126.50
1	5	645	A	C6-N1-C2	-5.47	115.32	118.60
1	5	339	C	N1-C2-N3	5.43	123.00	119.20
1	5	1199	C	C6-N1-C2	5.43	122.47	120.30
1	5	1832	C	C6-N1-C2	5.41	122.46	120.30
1	5	816	A	C4-C5-C6	5.39	119.69	117.00
1	5	760	G	O4'-C1'-N9	5.38	112.51	108.20
1	5	931	C	C5-C6-N1	-5.38	118.31	121.00
1	5	1836	C	N3-C2-O2	-5.37	118.14	121.90
1	5	2231	C	C6-N1-C2	-5.34	118.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	3047	U	C5-C6-N1	-5.34	120.03	122.70
1	5	2584	G	C4-N9-C1’	5.34	133.44	126.50
1	5	1812	G	N3-C4-C5	5.34	131.27	128.60
1	5	2288	G	C4-N9-C1’	5.34	133.44	126.50
1	5	1348	U	C3’-C2’-C1’	-5.33	97.24	101.50
1	5	655	C	N1-C2-O2	-5.33	115.70	118.90
1	5	713	U	N3-C2-O2	-5.31	118.48	122.20
1	5	2307	G	C6-C5-N7	5.31	133.59	130.40
1	5	1174	G	N3-C4-C5	-5.31	125.95	128.60
1	5	1478	C	C6-N1-C2	5.31	122.42	120.30
1	5	175	C	C2-N1-C1’	5.29	124.61	118.80
1	5	93	C	C6-N1-C2	5.27	122.41	120.30
1	5	1152	G	C4-N9-C1’	-5.24	119.68	126.50
3	8	16	G	N9-C4-C5	-5.24	103.31	105.40
1	5	1418	A	C8-N9-C4	5.23	107.89	105.80
3	8	19	C	N3-C4-C5	5.22	123.99	121.90
1	5	72	C	C6-N1-C2	5.21	122.39	120.30
1	5	2390	A	C2-N3-C4	-5.21	108.00	110.60
1	5	621	A	N7-C8-N9	5.20	116.40	113.80
17	O	27	LEU	CA-CB-CG	-5.20	103.34	115.30
1	5	3140	G	C4-N9-C1’	5.19	133.24	126.50
1	5	2659	G	N9-C4-C5	-5.18	103.33	105.40
1	5	2388	U	C2-N3-C4	-5.18	123.89	127.00
1	5	715	A	P-O3’-C3’	5.17	125.91	119.70
1	5	64	G	C8-N9-C1’	-5.17	120.28	127.00
1	5	2307	G	N3-C4-C5	5.17	131.19	128.60
1	5	1716	U	P-O3’-C3’	5.16	125.90	119.70
1	5	401	U	C5-C6-N1	-5.16	120.12	122.70
6	C	244	LEU	CA-CB-CG	-5.16	103.44	115.30
1	5	2572	C	N1-C2-O2	5.16	121.99	118.90
1	5	1172	G	N3-C4-N9	5.15	129.09	126.00
1	5	831	G	C8-N9-C4	-5.15	104.34	106.40
1	5	2376	G	C4-C5-N7	5.14	112.86	110.80
1	5	1770	G	C4-N9-C1’	5.14	133.19	126.50
1	5	645	A	C5-C6-N1	5.14	120.27	117.70
1	5	804	C	C4-C5-C6	5.14	119.97	117.40
1	5	3282	U	C2-N1-C1’	5.14	123.86	117.70
1	5	821	U	C5-C6-N1	-5.13	120.13	122.70
1	5	1535	A	N1-C6-N6	-5.13	115.52	118.60
1	5	35	A	C6-N1-C2	-5.13	115.52	118.60
1	5	1152	G	C2-N3-C4	-5.12	109.34	111.90
1	5	27	C	C6-N1-C2	5.11	122.34	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	2568	C	O4'-C1'-N1	5.10	112.28	108.20
1	5	36	C	C2-N3-C4	-5.10	117.35	119.90
1	5	2660	G	N9-C4-C5	-5.10	103.36	105.40
1	5	269	G	C8-N9-C4	5.09	108.44	106.40
1	5	345	G	C4-C5-C6	5.08	121.85	118.80
1	5	360	G	N3-C4-N9	5.08	129.05	126.00
1	5	1887	A	C8-N9-C4	5.08	107.83	105.80
1	5	1417	G	C8-N9-C4	5.07	108.43	106.40
3	8	104	A	C8-N9-C4	5.07	107.83	105.80
1	5	221	A	N1-C6-N6	-5.07	115.56	118.60
1	5	2337	C	N1-C2-O2	-5.06	115.86	118.90
1	5	3022	G	O4'-C1'-N9	5.05	112.24	108.20
3	8	29	U	C5-C6-N1	-5.04	120.18	122.70
1	5	3093	C	C6-N1-C2	5.02	122.31	120.30
3	8	104	A	C6-N1-C2	-5.02	115.59	118.60
1	5	859	G	C8-N9-C4	-5.01	104.40	106.40
1	5	2193	U	C6-N1-C1'	5.00	128.20	121.20

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	C	145	ILE	Peptide
6	C	148	ILE	Peptide
6	C	300	ARG	Peptide
8	E	67	GLY	Peptide
14	L	141	ALA	Peptide
16	N	184	LYS	Peptide
27	Y	125	LYS	Peptide
28	Z	101	PHE	Peptide
32	d	6	ASP	Peptide
32	d	82	GLU	Peptide
32	d	89	LEU	Peptide
37	i	32	ALA	Peptide
45	x	473	LEU	Peptide
45	x	477	LYS	Peptide
45	x	541	HIS	Peptide
46	y	349	PRO	Peptide

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	210/254 (83%)	195 (93%)	14 (7%)	1 (0%)	29	65
5	B	384/387 (99%)	367 (96%)	17 (4%)	0	100	100
6	C	359/362 (99%)	329 (92%)	28 (8%)	2 (1%)	25	61
7	D	292/297 (98%)	282 (97%)	8 (3%)	2 (1%)	22	58
8	E	155/176 (88%)	143 (92%)	9 (6%)	3 (2%)	8	37
9	F	221/244 (91%)	210 (95%)	10 (4%)	1 (0%)	29	65
10	G	229/256 (90%)	200 (87%)	28 (12%)	1 (0%)	34	69
11	H	189/191 (99%)	178 (94%)	10 (5%)	1 (0%)	29	65
12	I	209/221 (95%)	193 (92%)	16 (8%)	0	100	100
13	J	167/174 (96%)	143 (86%)	18 (11%)	6 (4%)	3	25
14	L	192/199 (96%)	170 (88%)	20 (10%)	2 (1%)	15	51
15	M	135/138 (98%)	133 (98%)	2 (2%)	0	100	100
16	N	201/204 (98%)	187 (93%)	13 (6%)	1 (0%)	29	65
17	O	195/199 (98%)	193 (99%)	2 (1%)	0	100	100
18	P	181/184 (98%)	176 (97%)	5 (3%)	0	100	100
19	Q	183/186 (98%)	174 (95%)	8 (4%)	1 (0%)	29	65
20	R	154/189 (82%)	148 (96%)	5 (3%)	1 (1%)	25	61
21	S	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
22	T	157/160 (98%)	151 (96%)	4 (2%)	2 (1%)	12	45
23	U	100/121 (83%)	95 (95%)	5 (5%)	0	100	100
24	V	134/137 (98%)	130 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	W	61/155 (39%)	57 (93%)	3 (5%)	1 (2%)	9	41
26	X	118/142 (83%)	109 (92%)	9 (8%)	0	100	100
27	Y	124/127 (98%)	118 (95%)	5 (4%)	1 (1%)	19	56
28	Z	133/136 (98%)	112 (84%)	18 (14%)	3 (2%)	6	34
29	a	146/149 (98%)	132 (90%)	13 (9%)	1 (1%)	22	58
30	b	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
31	c	98/105 (93%)	92 (94%)	6 (6%)	0	100	100
32	d	107/113 (95%)	97 (91%)	8 (8%)	2 (2%)	8	37
33	e	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
34	f	104/107 (97%)	100 (96%)	4 (4%)	0	100	100
35	g	110/121 (91%)	104 (94%)	5 (4%)	1 (1%)	17	53
36	h	117/120 (98%)	109 (93%)	8 (7%)	0	100	100
37	i	97/100 (97%)	86 (89%)	8 (8%)	3 (3%)	4	28
38	j	85/88 (97%)	77 (91%)	8 (9%)	0	100	100
39	k	75/78 (96%)	70 (93%)	4 (5%)	1 (1%)	12	45
40	l	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
41	m	50/128 (39%)	46 (92%)	3 (6%)	1 (2%)	7	36
42	o	103/106 (97%)	94 (91%)	9 (9%)	0	100	100
43	p	89/92 (97%)	82 (92%)	7 (8%)	0	100	100
44	q	116/312 (37%)	111 (96%)	4 (3%)	1 (1%)	17	53
45	x	577/616 (94%)	544 (94%)	32 (6%)	1 (0%)	47	80
46	y	201/401 (50%)	191 (95%)	10 (5%)	0	100	100
All	All	6958/7887 (88%)	6511 (94%)	407 (6%)	40 (1%)	29	61

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	E	98	VAL
13	J	10	ARG
13	J	95	ASN
16	N	184	LYS
25	W	25	ASP
14	L	18	TRP
28	Z	17	ARG

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Mol	Chain	Res	Type
28	Z	130	PHE
13	J	115	LYS
27	Y	125	LYS
28	Z	129	TRP
29	a	78	LEU
35	g	83	ASN
37	i	34	SER
37	i	63	ASN
39	k	17	ARG
6	C	71	VAL
9	F	191	VAL
20	R	35	ALA
32	d	83	GLU
37	i	64	SER
13	J	12	LEU
14	L	47	ALA
22	T	69	LYS
22	T	136	ARG
32	d	7	VAL
8	E	97	ASN
13	J	94	ARG
10	G	203	VAL
6	C	148	ILE
7	D	125	VAL
19	Q	97	PRO
45	x	519	ARG
4	A	56	ALA
8	E	10	TYR
11	H	167	VAL
13	J	114	ILE
41	m	78	ILE
44	q	33	VAL
7	D	122	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	
4	A	166/196 (85%)	133 (80%)	33 (20%)	1	5
5	B	321/323 (99%)	260 (81%)	61 (19%)	1	6
6	C	288/289 (100%)	234 (81%)	54 (19%)	1	6
7	D	243/245 (99%)	209 (86%)	34 (14%)	3	17
8	E	135/136 (99%)	123 (91%)	12 (9%)	9	37
9	F	187/205 (91%)	168 (90%)	19 (10%)	7	30
10	G	177/208 (85%)	150 (85%)	27 (15%)	2	15
11	H	171/171 (100%)	148 (86%)	23 (14%)	4	19
12	I	179/187 (96%)	153 (86%)	26 (14%)	3	16
13	J	147/150 (98%)	122 (83%)	25 (17%)	2	10
14	L	154/159 (97%)	126 (82%)	28 (18%)	1	7
15	M	108/109 (99%)	95 (88%)	13 (12%)	5	23
16	N	175/176 (99%)	143 (82%)	32 (18%)	1	7
17	O	160/162 (99%)	129 (81%)	31 (19%)	1	6
18	P	145/146 (99%)	118 (81%)	27 (19%)	1	7
19	Q	150/151 (99%)	127 (85%)	23 (15%)	2	15
20	R	129/154 (84%)	106 (82%)	23 (18%)	2	8
21	S	155/156 (99%)	131 (84%)	24 (16%)	2	14
22	T	136/137 (99%)	113 (83%)	23 (17%)	2	10
23	U	89/107 (83%)	80 (90%)	9 (10%)	7	31
24	V	104/105 (99%)	93 (89%)	11 (11%)	6	29
25	W	55/129 (43%)	52 (94%)	3 (6%)	21	54
26	X	104/118 (88%)	86 (83%)	18 (17%)	2	9
27	Y	109/110 (99%)	96 (88%)	13 (12%)	5	23
28	Z	115/116 (99%)	92 (80%)	23 (20%)	1	5
29	a	118/119 (99%)	106 (90%)	12 (10%)	7	30
30	b	46/47 (98%)	38 (83%)	8 (17%)	2	9
31	c	84/88 (96%)	70 (83%)	14 (17%)	2	10
32	d	94/97 (97%)	85 (90%)	9 (10%)	8	33
33	e	110/111 (99%)	94 (86%)	16 (14%)	3	16
34	f	90/91 (99%)	84 (93%)	6 (7%)	16	49
35	g	95/103 (92%)	84 (88%)	11 (12%)	5	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	h	103/105 (98%)	84 (82%)	19 (18%)	1	7
37	i	80/82 (98%)	61 (76%)	19 (24%)	0	3
38	j	70/71 (99%)	59 (84%)	11 (16%)	2	14
39	k	67/69 (97%)	60 (90%)	7 (10%)	7	30
40	l	45/46 (98%)	35 (78%)	10 (22%)	1	3
41	m	47/116 (40%)	41 (87%)	6 (13%)	4	20
42	o	90/91 (99%)	72 (80%)	18 (20%)	1	5
43	p	71/72 (99%)	54 (76%)	17 (24%)	0	3
44	q	105/254 (41%)	88 (84%)	17 (16%)	2	12
45	x	508/540 (94%)	469 (92%)	39 (8%)	13	42
46	y	187/355 (53%)	171 (91%)	16 (9%)	10	38
All	All	5912/6602 (90%)	5042 (85%)	870 (15%)	6	16

All (870) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	10	LYS
4	A	15	ILE
4	A	23	ARG
4	A	31	THR
4	A	32	LEU
4	A	44	ILE
4	A	45	VAL
4	A	48	ILE
4	A	49	VAL
4	A	62	VAL
4	A	68	LYS
4	A	70	ARG
4	A	71	LEU
4	A	72	ARG
4	A	98	VAL
4	A	101	VAL
4	A	104	LEU
4	A	107	VAL
4	A	109	GLU
4	A	119	LYS
4	A	137	ILE
4	A	142	ASP

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Mol	Chain	Res	Type
4	A	147	ARG
4	A	149	ARG
4	A	155	LYS
4	A	157	VAL
4	A	158	ILE
4	A	168	VAL
4	A	169	ILE
4	A	179	LEU
4	A	193	ARG
4	A	199	THR
4	A	207	VAL
5	B	3	HIS
5	B	4	ARG
5	B	10	ARG
5	B	17	LEU
5	B	19	ARG
5	B	25	ILE
5	B	37	ARG
5	B	45	SER
5	B	46	PHE
5	B	54	THR
5	B	59	ASP
5	B	67	PHE
5	B	77	THR
5	B	85	VAL
5	B	89	VAL
5	B	102	LEU
5	B	103	THR
5	B	104	THR
5	B	114	VAL
5	B	120	LYS
5	B	123	TYR
5	B	124	LYS
5	B	139	GLN
5	B	146	ARG
5	B	148	LEU
5	B	150	ARG
5	B	153	LYS
5	B	158	VAL
5	B	192	VAL
5	B	196	ARG
5	B	202	THR

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Mol	Chain	Res	Type
5	B	205	VAL
5	B	206	ASP
5	B	221	THR
5	B	227	GLU
5	B	229	VAL
5	B	232	ARG
5	B	235	THR
5	B	236	LYS
5	B	238	LEU
5	B	246	LEU
5	B	247	ARG
5	B	251	CYS
5	B	252	ILE
5	B	266	ARG
5	B	274	SER
5	B	284	ARG
5	B	287	LYS
5	B	289	ASP
5	B	291	GLU
5	B	301	THR
5	B	323	MET
5	B	324	VAL
5	B	327	CYS
5	B	332	ARG
5	B	338	LEU
5	B	340	LYS
5	B	343	TYR
5	B	365	PHE
5	B	369	ARG
5	B	386	ASP
6	C	2	SER
6	C	7	THR
6	C	12	THR
6	C	14	GLU
6	C	18	ASN
6	C	22	LEU
6	C	34	ILE
6	C	35	VAL
6	C	37	THR
6	C	47	ARG
6	C	52	VAL
6	C	67	THR

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Mol	Chain	Res	Type
6	C	73	ARG
6	C	74	ILE
6	C	93	MET
6	C	105	THR
6	C	120	TYR
6	C	122	THR
6	C	133	SER
6	C	136	LEU
6	C	141	ARG
6	C	147	GLU
6	C	150	LEU
6	C	156	LEU
6	C	160	GLN
6	C	166	VAL
6	C	172	VAL
6	C	179	LEU
6	C	181	VAL
6	C	182	LEU
6	C	187	LEU
6	C	206	LEU
6	C	217	LYS
6	C	222	VAL
6	C	226	GLU
6	C	230	VAL
6	C	246	ARG
6	C	251	THR
6	C	258	LEU
6	C	259	ASP
6	C	267	VAL
6	C	270	SER
6	C	280	ILE
6	C	287	THR
6	C	300	ARG
6	C	307	GLN
6	C	313	LEU
6	C	323	VAL
6	C	327	LEU
6	C	338	LYS
6	C	343	LYS
6	C	345	GLU
6	C	359	LEU
6	C	362	ASP

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Mol	Chain	Res	Type
7	D	4	GLN
7	D	5	LYS
7	D	9	SER
7	D	25	GLU
7	D	34	LYS
7	D	35	ARG
7	D	51	LEU
7	D	61	ILE
7	D	66	SER
7	D	70	THR
7	D	81	HIS
7	D	93	THR
7	D	95	TRP
7	D	126	GLU
7	D	129	TYR
7	D	136	GLU
7	D	146	LEU
7	D	148	ILE
7	D	150	LEU
7	D	152	ARG
7	D	155	THR
7	D	164	LYS
7	D	177	GLU
7	D	185	PHE
7	D	196	ARG
7	D	207	TYR
7	D	211	LEU
7	D	218	ARG
7	D	232	ASP
7	D	238	ASP
7	D	257	GLU
7	D	259	LYS
7	D	275	THR
7	D	282	ARG
8	E	8	LYS
8	E	20	LYS
8	E	21	THR
8	E	31	ARG
8	E	46	ARG
8	E	50	LYS
8	E	78	ARG
8	E	85	ILE

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Mol	Chain	Res	Type
8	E	91	VAL
8	E	145	LEU
8	E	155	LEU
8	E	174	LEU
9	F	22	THR
9	F	25	GLN
9	F	30	ARG
9	F	41	ARG
9	F	56	GLU
9	F	83	LEU
9	F	84	VAL
9	F	95	ILE
9	F	98	LYS
9	F	110	ARG
9	F	111	ILE
9	F	115	THR
9	F	151	ARG
9	F	175	LYS
9	F	179	LEU
9	F	180	SER
9	F	182	ASP
9	F	184	LEU
9	F	239	LEU
10	G	44	ARG
10	G	65	LEU
10	G	68	ARG
10	G	69	LEU
10	G	70	LYS
10	G	74	THR
10	G	79	GLN
10	G	81	THR
10	G	82	LEU
10	G	89	GLU
10	G	109	LEU
10	G	128	LYS
10	G	136	LEU
10	G	142	LEU
10	G	149	LYS
10	G	160	ILE
10	G	164	VAL
10	G	172	LYS
10	G	183	LYS

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Mol	Chain	Res	Type
10	G	195	SER
10	G	200	LEU
10	G	206	GLU
10	G	208	GLU
10	G	211	LEU
10	G	213	LYS
10	G	227	ASP
10	G	248	LYS
11	H	1	MET
11	H	4	ILE
11	H	6	THR
11	H	16	VAL
11	H	18	VAL
11	H	31	ARG
11	H	44	THR
11	H	46	THR
11	H	52	LEU
11	H	68	LEU
11	H	69	ARG
11	H	70	THR
11	H	71	VAL
11	H	82	VAL
11	H	105	GLU
11	H	106	LYS
11	H	133	THR
11	H	162	GLN
11	H	163	GLN
11	H	165	CYS
11	H	166	ARG
11	H	177	ASP
11	H	179	ILE
12	I	4	ARG
12	I	7	ARG
12	I	21	ARG
12	I	22	TYR
12	I	24	ARG
12	I	29	SER
12	I	48	LEU
12	I	49	CYS
12	I	52	LEU
12	I	60	LEU
12	I	63	GLU

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Mol	Chain	Res	Type
12	I	69	ARG
12	I	70	ILE
12	I	71	CYS
12	I	90	ARG
12	I	116	ARG
12	I	153	ARG
12	I	156	ARG
12	I	163	GLN
12	I	169	LYS
12	I	174	THR
12	I	176	LEU
12	I	177	ASP
12	I	178	ARG
12	I	197	VAL
12	I	211	ARG
13	J	10	ARG
13	J	12	LEU
13	J	13	LYS
13	J	31	THR
13	J	34	SER
13	J	35	LYS
13	J	39	GLN
13	J	43	GLN
13	J	51	ARG
13	J	54	VAL
13	J	80	LEU
13	J	87	LYS
13	J	92	ARG
13	J	95	ASN
13	J	106	ILE
13	J	107	ASP
13	J	122	ILE
13	J	128	TYR
13	J	130	VAL
13	J	132	ASN
13	J	140	ARG
13	J	155	THR
13	J	158	ASP
13	J	171	VAL
13	J	174	LYS
14	L	3	ILE
14	L	4	SER

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Mol	Chain	Res	Type
14	L	10	LEU
14	L	14	PHE
14	L	27	ASP
14	L	42	ARG
14	L	46	ILE
14	L	51	LEU
14	L	57	VAL
14	L	59	ARG
14	L	63	VAL
14	L	67	ARG
14	L	69	VAL
14	L	76	THR
14	L	85	LEU
14	L	93	ILE
14	L	98	ASP
14	L	107	GLU
14	L	114	GLN
14	L	123	ILE
14	L	128	ARG
14	L	131	LYS
14	L	149	GLN
14	L	162	ASN
14	L	164	GLU
14	L	168	ARG
14	L	190	LYS
14	L	194	GLU
15	M	3	THR
15	M	12	TRP
15	M	15	VAL
15	M	20	VAL
15	M	47	ASP
15	M	53	VAL
15	M	64	VAL
15	M	66	THR
15	M	72	LEU
15	M	115	PHE
15	M	120	VAL
15	M	121	MET
15	M	131	VAL
16	N	5	LYS
16	N	8	GLU
16	N	10	LEU

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Mol	Chain	Res	Type
16	N	12	ARG
16	N	13	LYS
16	N	15	GLN
16	N	18	VAL
16	N	22	LEU
16	N	27	VAL
16	N	49	ARG
16	N	51	LEU
16	N	62	TYR
16	N	64	VAL
16	N	66	VAL
16	N	68	ARG
16	N	91	GLU
16	N	92	LEU
16	N	104	GLU
16	N	105	ARG
16	N	106	VAL
16	N	117	ASN
16	N	121	VAL
16	N	126	THR
16	N	138	GLN
16	N	153	ASP
16	N	167	THR
16	N	182	ASN
16	N	183	THR
16	N	184	LYS
16	N	187	ARG
16	N	199	LEU
16	N	204	LYS
17	O	3	VAL
17	O	4	GLU
17	O	12	LYS
17	O	16	VAL
17	O	18	ARG
17	O	25	LYS
17	O	41	LEU
17	O	43	ILE
17	O	44	SER
17	O	53	LYS
17	O	56	ASP
17	O	59	ARG
17	O	72	HIS

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Mol	Chain	Res	Type
17	O	78	ARG
17	O	79	ILE
17	O	82	LYS
17	O	85	ARG
17	O	94	ARG
17	O	108	ILE
17	O	117	ARG
17	O	124	LEU
17	O	126	VAL
17	O	128	ARG
17	O	129	LEU
17	O	145	VAL
17	O	160	ARG
17	O	171	LYS
17	O	175	THR
17	O	182	ASN
17	O	194	LEU
17	O	197	LEU
18	P	23	ARG
18	P	24	VAL
18	P	25	SER
18	P	31	GLU
18	P	32	THR
18	P	34	GLN
18	P	40	GLU
18	P	41	LEU
18	P	42	THR
18	P	52	LEU
18	P	55	GLN
18	P	64	ASN
18	P	67	ILE
18	P	69	ARG
18	P	74	LYS
18	P	76	PHE
18	P	80	LYS
18	P	89	LYS
18	P	94	LEU
18	P	116	HIS
18	P	119	VAL
18	P	120	ASN
18	P	121	GLN
18	P	127	ARG

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Mol	Chain	Res	Type
18	P	142	SER
18	P	144	SER
18	P	148	LEU
19	Q	12	ARG
19	Q	41	ASP
19	Q	49	LEU
19	Q	63	SER
19	Q	64	VAL
19	Q	66	ARG
19	Q	69	ARG
19	Q	80	THR
19	Q	81	VAL
19	Q	93	ILE
19	Q	100	THR
19	Q	105	ARG
19	Q	107	THR
19	Q	124	LEU
19	Q	135	GLN
19	Q	138	LEU
19	Q	147	ARG
19	Q	150	VAL
19	Q	161	LYS
19	Q	166	LEU
19	Q	167	SER
19	Q	170	ARG
19	Q	180	ARG
20	R	7	GLN
20	R	10	LEU
20	R	19	LYS
20	R	20	ARG
20	R	29	THR
20	R	30	SER
20	R	31	GLU
20	R	36	ASN
20	R	49	THR
20	R	56	THR
20	R	63	THR
20	R	70	LYS
20	R	74	ARG
20	R	75	HIS
20	R	76	SER
20	R	92	GLN

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Mol	Chain	Res	Type
20	R	98	ARG
20	R	99	LEU
20	R	105	LEU
20	R	114	LYS
20	R	127	SER
20	R	152	GLU
20	R	153	LYS
21	S	4	PHE
21	S	8	GLN
21	S	13	ARG
21	S	17	GLU
21	S	23	LYS
21	S	32	SER
21	S	45	LEU
21	S	51	VAL
21	S	71	LYS
21	S	80	ARG
21	S	87	THR
21	S	97	VAL
21	S	98	SER
21	S	104	GLU
21	S	108	GLN
21	S	120	SER
21	S	130	GLU
21	S	136	LYS
21	S	137	ARG
21	S	155	ARG
21	S	162	THR
21	S	167	ARG
21	S	171	PHE
21	S	172	TYR
22	T	9	SER
22	T	17	ARG
22	T	25	VAL
22	T	26	HIS
22	T	35	LYS
22	T	49	GLN
22	T	50	LYS
22	T	55	LYS
22	T	60	LYS
22	T	65	TYR
22	T	72	VAL

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Mol	Chain	Res	Type
22	T	78	LYS
22	T	79	MET
22	T	80	VAL
22	T	83	ARG
22	T	97	LYS
22	T	102	ARG
22	T	104	GLU
22	T	126	VAL
22	T	128	LEU
22	T	131	GLN
22	T	139	ARG
22	T	143	THR
23	U	11	ILE
23	U	27	VAL
23	U	58	GLU
23	U	61	THR
23	U	63	VAL
23	U	84	LEU
23	U	90	ARG
23	U	98	THR
23	U	100	THR
24	V	4	ASN
24	V	13	ILE
24	V	42	SER
24	V	48	ARG
24	V	64	LYS
24	V	68	GLU
24	V	69	LEU
24	V	72	LYS
24	V	88	ARG
24	V	115	THR
24	V	129	VAL
25	W	39	LEU
25	W	52	THR
25	W	57	LYS
26	X	24	LEU
26	X	27	ARG
26	X	39	LYS
26	X	45	LYS
26	X	63	ILE
26	X	64	GLU
26	X	68	THR

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Mol	Chain	Res	Type
26	X	71	THR
26	X	73	MET
26	X	108	LEU
26	X	109	LYS
26	X	115	ARG
26	X	117	ASN
26	X	119	THR
26	X	125	ARG
26	X	129	ASP
26	X	133	LEU
26	X	135	ILE
27	Y	12	ARG
27	Y	13	ARG
27	Y	17	LYS
27	Y	37	LYS
27	Y	50	ILE
27	Y	57	LEU
27	Y	74	TYR
27	Y	76	LEU
27	Y	90	VAL
27	Y	95	VAL
27	Y	107	THR
27	Y	109	LEU
27	Y	120	GLN
28	Z	3	LYS
28	Z	14	VAL
28	Z	17	ARG
28	Z	21	LYS
28	Z	24	VAL
28	Z	30	ASP
28	Z	34	LYS
28	Z	46	ILE
28	Z	52	LYS
28	Z	53	VAL
28	Z	55	LYS
28	Z	72	ILE
28	Z	81	LEU
28	Z	83	THR
28	Z	92	PHE
28	Z	95	VAL
28	Z	99	GLU
28	Z	102	GLU

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Mol	Chain	Res	Type
28	Z	121	ARG
28	Z	126	LYS
28	Z	127	ASN
28	Z	130	PHE
28	Z	134	LEU
29	a	14	HIS
29	a	22	ILE
29	a	25	HIS
29	a	26	ARG
29	a	43	ILE
29	a	60	TYR
29	a	73	LEU
29	a	85	ASP
29	a	91	LEU
29	a	97	GLU
29	a	115	LYS
29	a	118	ILE
30	b	6	ASN
30	b	12	GLN
30	b	18	ARG
30	b	29	TYR
30	b	41	ARG
30	b	50	THR
30	b	58	LYS
30	b	59	LYS
31	c	8	GLU
31	c	11	ASN
31	c	24	THR
31	c	34	LEU
31	c	41	LEU
31	c	42	ILE
31	c	61	MET
31	c	68	TYR
31	c	76	GLU
31	c	83	LYS
31	c	86	ARG
31	c	89	VAL
31	c	100	ILE
31	c	104	LEU
32	d	6	ASP
32	d	26	LYS
32	d	31	ARG

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Mol	Chain	Res	Type
32	d	35	GLU
32	d	73	LEU
32	d	83	GLU
32	d	91	SER
32	d	94	GLU
32	d	102	LYS
33	e	4	LEU
33	e	8	LYS
33	e	27	ARG
33	e	31	ASN
33	e	33	ARG
33	e	34	LYS
33	e	50	ILE
33	e	51	SER
33	e	73	THR
33	e	75	LEU
33	e	82	LEU
33	e	89	THR
33	e	100	ILE
33	e	106	VAL
33	e	120	THR
33	e	125	ARG
34	f	31	LYS
34	f	48	ARG
34	f	53	TYR
34	f	70	LYS
34	f	74	THR
34	f	86	ARG
35	g	23	VAL
35	g	29	ILE
35	g	46	ASP
35	g	57	LEU
35	g	58	ARG
35	g	76	TYR
35	g	80	ARG
35	g	81	CYS
35	g	88	ARG
35	g	95	ILE
35	g	98	GLN
36	h	14	LYS
36	h	19	SER
36	h	21	LEU

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Mol	Chain	Res	Type
36	h	36	LEU
36	h	41	LEU
36	h	45	LYS
36	h	48	ARG
36	h	51	ILE
36	h	56	THR
36	h	62	GLN
36	h	68	GLN
36	h	86	ARG
36	h	89	ARG
36	h	90	ARG
36	h	94	LYS
36	h	101	THR
36	h	105	ARG
36	h	107	LYS
36	h	119	LYS
37	i	3	VAL
37	i	5	THR
37	i	9	ILE
37	i	17	VAL
37	i	26	ILE
37	i	43	LEU
37	i	45	ARG
37	i	57	LEU
37	i	58	ILE
37	i	60	LEU
37	i	68	ARG
37	i	75	LYS
37	i	76	ARG
37	i	81	THR
37	i	84	LYS
37	i	87	VAL
37	i	88	GLU
37	i	94	ILE
37	i	98	ARG
38	j	5	THR
38	j	12	HIS
38	j	15	SER
38	j	17	THR
38	j	21	ARG
38	j	28	HIS
38	j	45	ARG

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Mol	Chain	Res	Type
38	j	55	ARG
38	j	59	THR
38	j	65	ARG
38	j	79	GLN
39	k	8	ILE
39	k	31	LEU
39	k	46	ARG
39	k	53	THR
39	k	61	LYS
39	k	64	LYS
39	k	67	GLN
40	l	4	GLN
40	l	11	GLN
40	l	21	ARG
40	l	23	LEU
40	l	27	ILE
40	l	28	ARG
40	l	29	LEU
40	l	41	ARG
40	l	45	ARG
40	l	46	ARG
41	m	88	LYS
41	m	90	ASN
41	m	106	ARG
41	m	112	LYS
41	m	113	ARG
41	m	114	LYS
42	o	2	VAL
42	o	7	THR
42	o	8	ARG
42	o	20	HIS
42	o	38	GLN
42	o	45	ARG
42	o	47	GLN
42	o	55	LYS
42	o	71	ARG
42	o	80	ARG
42	o	83	LEU
42	o	84	THR
42	o	85	LEU
42	o	89	LYS
42	o	93	LEU

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Mol	Chain	Res	Type
42	o	99	GLN
42	o	104	LEU
42	o	105	GLN
43	p	8	VAL
43	p	16	VAL
43	p	22	LEU
43	p	24	ARG
43	p	26	VAL
43	p	28	LYS
43	p	33	GLN
43	p	46	THR
43	p	49	ARG
43	p	54	ILE
43	p	56	THR
43	p	57	CYS
43	p	59	CYS
43	p	71	VAL
43	p	73	THR
43	p	78	THR
43	p	80	ARG
44	q	4	ILE
44	q	7	LYS
44	q	15	LEU
44	q	35	SER
44	q	39	HIS
44	q	46	ARG
44	q	52	LEU
44	q	57	THR
44	q	67	LEU
44	q	70	LEU
44	q	72	ASP
44	q	76	LEU
44	q	81	LYS
44	q	97	LYS
44	q	104	ARG
44	q	185	LEU
44	q	191	TYR
45	x	30	THR
45	x	87	ARG
45	x	108	ILE
45	x	143	LEU
45	x	167	LYS

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Mol	Chain	Res	Type
45	x	184	VAL
45	x	189	ILE
45	x	203	THR
45	x	207	LEU
45	x	216	SER
45	x	229	THR
45	x	235	ASN
45	x	243	ARG
45	x	244	VAL
45	x	261	GLU
45	x	267	VAL
45	x	315	GLU
45	x	334	LEU
45	x	337	LEU
45	x	356	ARG
45	x	375	SER
45	x	384	LYS
45	x	427	SER
45	x	432	CYS
45	x	446	ASP
45	x	447	HIS
45	x	452	THR
45	x	453	ASN
45	x	461	ASP
45	x	477	LYS
45	x	478	LEU
45	x	497	SER
45	x	504	CYS
45	x	510	CYS
45	x	511	ASP
45	x	518	ASP
45	x	523	LEU
45	x	541	HIS
45	x	542	GLU
46	y	179	ASN
46	y	197	LEU
46	y	199	ASP
46	y	207	MET
46	y	208	SER
46	y	221	ASN
46	y	227	LEU
46	y	319	GLN

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Mol	Chain	Res	Type
46	y	347	PHE
46	y	359	GLN
46	y	364	GLN
46	y	365	THR
46	y	366	GLU
46	y	373	LEU
46	y	376	ARG
46	y	398	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (107) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	47	GLN
4	A	97	ASN
4	A	132	ASN
4	A	139	HIS
4	A	194	ASN
4	A	209	HIS
5	B	11	HIS
5	B	121	ASN
5	B	211	GLN
5	B	243	HIS
5	B	273	HIS
6	C	5	GLN
6	C	114	ASN
6	C	221	ASN
6	C	260	GLN
6	C	291	ASN
6	C	311	HIS
7	D	40	HIS
7	D	57	ASN
7	D	63	GLN
8	E	172	HIS
9	F	25	GLN
9	F	37	ASN
9	F	159	GLN
9	F	194	HIS
10	G	41	GLN
10	G	221	ASN
10	G	240	ASN
10	G	243	GLN
11	H	8	GLN

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Mol	Chain	Res	Type
11	H	50	ASN
11	H	100	ASN
11	H	169	ASN
11	H	183	HIS
12	I	12	GLN
12	I	59	GLN
13	J	132	ASN
14	L	13	HIS
14	L	19	GLN
14	L	114	GLN
14	L	120	GLN
14	L	149	GLN
16	N	15	GLN
16	N	90	ASN
17	O	26	GLN
17	O	29	ASN
17	O	31	GLN
17	O	50	ASN
17	O	122	GLN
18	P	55	GLN
18	P	96	GLN
18	P	125	GLN
19	Q	73	GLN
19	Q	135	GLN
20	R	58	HIS
21	S	8	GLN
21	S	138	GLN
22	T	16	GLN
22	T	49	GLN
22	T	77	ASN
22	T	95	HIS
22	T	98	HIS
23	U	109	GLN
25	W	42	GLN
25	W	58	HIS
26	X	65	GLN
27	Y	120	GLN
28	Z	36	HIS
28	Z	57	HIS
28	Z	106	GLN
29	a	44	ASN
30	b	6	ASN

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Mol	Chain	Res	Type
31	c	75	ASN
33	e	52	GLN
34	f	5	HIS
34	f	13	HIS
34	f	77	ASN
35	g	3	GLN
35	g	18	ASN
36	h	20	GLN
36	h	68	GLN
36	h	99	GLN
36	h	104	GLN
36	h	108	GLN
40	l	25	GLN
40	l	38	ASN
42	o	22	GLN
43	p	34	HIS
44	q	37	GLN
45	x	18	ASN
45	x	51	HIS
45	x	118	ASN
45	x	146	HIS
45	x	188	HIS
45	x	235	ASN
45	x	281	ASN
45	x	294	GLN
45	x	366	GLN
45	x	377	GLN
45	x	405	ASN
45	x	429	ASN
45	x	447	HIS
45	x	471	HIS
46	y	172	HIS
46	y	182	HIS
46	y	239	HIS
46	y	319	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	5	3084/3396 (90%)	669 (21%)	73 (2%)
2	7	120/121 (99%)	14 (11%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	8	157/158 (99%)	36 (22%)	5 (3%)
All	All	3361/3675 (91%)	719 (21%)	78 (2%)

All (719) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	5	14	U
1	5	15	C
1	5	22	G
1	5	26	A
1	5	40	A
1	5	43	A
1	5	49	A
1	5	59	G
1	5	60	A
1	5	65	A
1	5	66	A
1	5	75	G
1	5	83	U
1	5	91	G
1	5	96	G
1	5	98	G
1	5	109	A
1	5	110	G
1	5	111	C
1	5	113	C
1	5	116	A
1	5	121	A
1	5	122	A
1	5	133	U
1	5	134	U
1	5	135	C
1	5	136	G
1	5	146	U
1	5	150	A
1	5	152	U
1	5	155	G
1	5	156	G
1	5	157	A
1	5	166	C
1	5	170	G
1	5	171	G

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Mol	Chain	Res	Type
1	5	172	G
1	5	175	C
1	5	182	U
1	5	187	A
1	5	190	U
1	5	191	U
1	5	210	U
1	5	211	A
1	5	213	A
1	5	218	G
1	5	219	A
1	5	221	A
1	5	237	G
1	5	239	G
1	5	240	U
1	5	245	U
1	5	246	U
1	5	248	U
1	5	249	U
1	5	250	U
1	5	251	G
1	5	252	U
1	5	254	A
1	5	269	G
1	5	270	U
1	5	282	G
1	5	283	G
1	5	284	A
1	5	286	U
1	5	295	A
1	5	315	C
1	5	323	A
1	5	329	U
1	5	334	A
1	5	339	C
1	5	350	C
1	5	370	U
1	5	376	G
1	5	378	A
1	5	390	G
1	5	398	A
1	5	399	A

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Mol	Chain	Res	Type
1	5	401	U
1	5	402	A
1	5	403	C
1	5	421	G
1	5	422	A
1	5	438	A
1	5	439	C
1	5	494	G
1	5	498	A
1	5	521	A
1	5	535	G
1	5	546	C
1	5	547	G
1	5	548	G
1	5	557	A
1	5	559	A
1	5	569	A
1	5	578	A
1	5	579	G
1	5	592	A
1	5	594	U
1	5	600	G
1	5	604	G
1	5	609	G
1	5	611	A
1	5	619	A
1	5	620	U
1	5	621	A
1	5	622	A
1	5	636	C
1	5	647	A
1	5	649	A
1	5	660	A
1	5	677	A
1	5	681	U
1	5	683	U
1	5	690	A
1	5	705	A
1	5	710	A
1	5	712	G
1	5	713	U
1	5	715	A

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Mol	Chain	Res	Type
1	5	716	A
1	5	717	C
1	5	720	A
1	5	725	G
1	5	735	A
1	5	736	A
1	5	750	G
1	5	760	G
1	5	766	U
1	5	776	U
1	5	777	U
1	5	780	A
1	5	781	G
1	5	785	G
1	5	786	A
1	5	799	G
1	5	806	A
1	5	808	A
1	5	812	G
1	5	817	A
1	5	830	A
1	5	832	G
1	5	837	A
1	5	844	G
1	5	845	G
1	5	851	C
1	5	861	C
1	5	869	G
1	5	873	C
1	5	874	U
1	5	879	U
1	5	883	A
1	5	895	A
1	5	896	A
1	5	907	G
1	5	908	G
1	5	909	G
1	5	914	A
1	5	916	G
1	5	921	A
1	5	923	C
1	5	925	A

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Mol	Chain	Res	Type
1	5	932	U
1	5	937	G
1	5	944	C
1	5	953	G
1	5	959	C
1	5	960	U
1	5	961	C
1	5	974	G
1	5	979	U
1	5	982	C
1	5	983	A
1	5	984	G
1	5	991	G
1	5	995	U
1	5	1001	G
1	5	1002	A
1	5	1010	G
1	5	1014	U
1	5	1015	U
1	5	1047	A
1	5	1049	C
1	5	1057	A
1	5	1064	A
1	5	1065	A
1	5	1072	G
1	5	1081	U
1	5	1082	U
1	5	1085	A
1	5	1086	C
1	5	1093	A
1	5	1094	U
1	5	1095	U
1	5	1096	U
1	5	1097	G
1	5	1098	A
1	5	1103	A
1	5	1104	G
1	5	1117	G
1	5	1131	G
1	5	1138	U
1	5	1144	U
1	5	1151	U

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Mol	Chain	Res	Type
1	5	1152	G
1	5	1153	A
1	5	1155	C
1	5	1157	G
1	5	1159	A
1	5	1160	C
1	5	1180	A
1	5	1181	U
1	5	1183	C
1	5	1186	G
1	5	1190	A
1	5	1191	U
1	5	1192	C
1	5	1196	C
1	5	1201	C
1	5	1209	G
1	5	1216	C
1	5	1217	A
1	5	1222	G
1	5	1223	A
1	5	1232	C
1	5	1235	U
1	5	1236	G
1	5	1237	G
1	5	1239	C
1	5	1241	U
1	5	1242	G
1	5	1243	G
1	5	1245	A
1	5	1246	G
1	5	1252	A
1	5	1258	U
1	5	1259	A
1	5	1262	G
1	5	1263	A
1	5	1264	G
1	5	1265	U
1	5	1266	G
1	5	1285	G
1	5	1307	G
1	5	1308	A
1	5	1309	U

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Mol	Chain	Res	Type
1	5	1314	C
1	5	1329	U
1	5	1330	A
1	5	1345	G
1	5	1348	U
1	5	1349	G
1	5	1350	A
1	5	1351	U
1	5	1352	A
1	5	1353	U
1	5	1356	U
1	5	1357	G
1	5	1380	G
1	5	1385	C
1	5	1386	A
1	5	1391	C
1	5	1394	A
1	5	1398	U
1	5	1399	A
1	5	1400	G
1	5	1408	G
1	5	1415	U
1	5	1419	A
1	5	1421	G
1	5	1433	A
1	5	1434	G
1	5	1435	A
1	5	1437	C
1	5	1446	A
1	5	1450	G
1	5	1460	A
1	5	1480	G
1	5	1481	A
1	5	1483	G
1	5	1484	U
1	5	1490	A
1	5	1502	C
1	5	1503	A
1	5	1508	C
1	5	1514	G
1	5	1533	U
1	5	1536	G

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Mol	Chain	Res	Type
1	5	1539	A
1	5	1544	G
1	5	1554	U
1	5	1555	U
1	5	1556	C
1	5	1557	A
1	5	1560	G
1	5	1561	G
1	5	1562	C
1	5	1563	C
1	5	1564	U
1	5	1568	U
1	5	1569	U
1	5	1570	U
1	5	1571	A
1	5	1572	U
1	5	1573	G
1	5	1575	A
1	5	1576	G
1	5	1578	C
1	5	1579	C
1	5	1581	C
1	5	1582	C
1	5	1587	A
1	5	1589	A
1	5	1593	A
1	5	1596	C
1	5	1607	U
1	5	1608	C
1	5	1620	U
1	5	1629	U
1	5	1639	C
1	5	1642	A
1	5	1643	A
1	5	1644	C
1	5	1645	U
1	5	1649	U
1	5	1677	G
1	5	1683	A
1	5	1704	A
1	5	1716	U
1	5	1717	U

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Mol	Chain	Res	Type
1	5	1718	G
1	5	1721	U
1	5	1724	U
1	5	1725	C
1	5	1730	G
1	5	1741	A
1	5	1750	A
1	5	1751	G
1	5	1759	C
1	5	1760	A
1	5	1763	U
1	5	1764	U
1	5	1765	U
1	5	1770	G
1	5	1772	U
1	5	1780	G
1	5	1797	A
1	5	1812	G
1	5	1814	A
1	5	1815	U
1	5	1816	A
1	5	1817	G
1	5	1818	U
1	5	1820	U
1	5	1821	U
1	5	1839	A
1	5	1840	U
1	5	1841	A
1	5	1842	A
1	5	1846	C
1	5	1849	C
1	5	1850	A
1	5	1866	C
1	5	1877	U
1	5	1878	G
1	5	1879	A
1	5	1880	U
1	5	1887	A
1	5	1893	A
1	5	1901	A
1	5	1906	G
1	5	1907	C

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Mol	Chain	Res	Type
1	5	1918	C
1	5	1930	A
1	5	1935	G
1	5	1943	C
1	5	2101	C
1	5	2102	U
1	5	2111	G
1	5	2112	U
1	5	2113	A
1	5	2114	C
1	5	2118	C
1	5	2121	G
1	5	2122	G
1	5	2131	A
1	5	2144	A
1	5	2158	A
1	5	2163	C
1	5	2164	A
1	5	2169	G
1	5	2185	G
1	5	2192	C
1	5	2193	U
1	5	2205	U
1	5	2210	G
1	5	2223	A
1	5	2225	U
1	5	2228	A
1	5	2229	A
1	5	2244	A
1	5	2249	G
1	5	2270	A
1	5	2273	G
1	5	2275	A
1	5	2279	A
1	5	2281	A
1	5	2288	G
1	5	2298	U
1	5	2307	G
1	5	2308	C
1	5	2309	A
1	5	2310	U
1	5	2313	A

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Mol	Chain	Res	Type
1	5	2314	U
1	5	2315	G
1	5	2334	U
1	5	2335	G
1	5	2336	U
1	5	2337	C
1	5	2338	C
1	5	2363	A
1	5	2373	A
1	5	2374	C
1	5	2375	G
1	5	2378	C
1	5	2385	G
1	5	2388	U
1	5	2390	A
1	5	2391	G
1	5	2393	G
1	5	2394	G
1	5	2397	A
1	5	2401	A
1	5	2402	A
1	5	2403	G
1	5	2411	U
1	5	2417	U
1	5	2418	G
1	5	2419	A
1	5	2420	C
1	5	2421	U
1	5	2422	C
1	5	2423	U
1	5	2426	U
1	5	2437	G
1	5	2438	A
1	5	2439	A
1	5	2510	U
1	5	2511	A
1	5	2512	C
1	5	2514	U
1	5	2515	A
1	5	2522	G
1	5	2523	A
1	5	2524	A

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Mol	Chain	Res	Type
1	5	2525	G
1	5	2526	C
1	5	2530	G
1	5	2531	C
1	5	2532	U
1	5	2537	U
1	5	2538	U
1	5	2539	C
1	5	2540	A
1	5	2543	U
1	5	2552	C
1	5	2554	A
1	5	2555	G
1	5	2567	C
1	5	2568	C
1	5	2569	A
1	5	2570	U
1	5	2571	U
1	5	2572	C
1	5	2573	G
1	5	2574	G
1	5	2584	G
1	5	2585	G
1	5	2589	G
1	5	2593	A
1	5	2594	C
1	5	2604	U
1	5	2605	G
1	5	2606	G
1	5	2607	G
1	5	2609	A
1	5	2610	G
1	5	2614	G
1	5	2615	G
1	5	2626	A
1	5	2629	U
1	5	2636	A
1	5	2652	U
1	5	2656	A
1	5	2657	A
1	5	2662	G
1	5	2663	G

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Mol	Chain	Res	Type
1	5	2674	A
1	5	2677	G
1	5	2681	U
1	5	2683	U
1	5	2689	A
1	5	2690	G
1	5	2691	A
1	5	2694	A
1	5	2703	A
1	5	2704	A
1	5	2714	G
1	5	2726	C
1	5	2728	G
1	5	2729	U
1	5	2736	A
1	5	2737	C
1	5	2740	A
1	5	2742	C
1	5	2752	U
1	5	2753	G
1	5	2761	G
1	5	2772	C
1	5	2773	C
1	5	2777	G
1	5	2778	G
1	5	2779	A
1	5	2796	G
1	5	2799	A
1	5	2800	G
1	5	2801	A
1	5	2802	A
1	5	2804	A
1	5	2807	U
1	5	2808	A
1	5	2809	C
1	5	2810	C
1	5	2812	C
1	5	2814	G
1	5	2816	G
1	5	2817	A
1	5	2818	U
1	5	2819	A

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Mol	Chain	Res	Type
1	5	2839	G
1	5	2844	C
1	5	2845	A
1	5	2847	A
1	5	2853	A
1	5	2856	G
1	5	2867	C
1	5	2871	G
1	5	2872	A
1	5	2873	U
1	5	2875	U
1	5	2887	A
1	5	2889	C
1	5	2898	G
1	5	2899	C
1	5	2907	G
1	5	2911	A
1	5	2916	U
1	5	2918	G
1	5	2923	U
1	5	2928	C
1	5	2935	U
1	5	2936	A
1	5	2942	C
1	5	2945	G
1	5	2947	G
1	5	2953	U
1	5	2954	U
1	5	2955	U
1	5	2956	A
1	5	2957	G
1	5	2971	A
1	5	2972	G
1	5	2978	U
1	5	2979	U
1	5	2983	C
1	5	2990	G
1	5	2996	U
1	5	2997	G
1	5	3003	G
1	5	3012	A
1	5	3028	G

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Mol	Chain	Res	Type
1	5	3057	U
1	5	3059	G
1	5	3078	U
1	5	3079	U
1	5	3086	A
1	5	3092	C
1	5	3109	G
1	5	3116	G
1	5	3117	C
1	5	3122	A
1	5	3123	A
1	5	3130	A
1	5	3131	U
1	5	3142	A
1	5	3143	C
1	5	3152	U
1	5	3164	C
1	5	3165	A
1	5	3168	A
1	5	3172	A
1	5	3173	G
1	5	3174	A
1	5	3175	U
1	5	3176	G
1	5	3179	U
1	5	3181	C
1	5	3186	A
1	5	3187	A
1	5	3194	C
1	5	3195	U
1	5	3196	U
1	5	3207	U
1	5	3217	C
1	5	3218	A
1	5	3219	G
1	5	3227	A
1	5	3228	C
1	5	3229	G
1	5	3238	G
1	5	3243	A
1	5	3244	A
1	5	3245	A

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Mol	Chain	Res	Type
1	5	3247	G
1	5	3249	C
1	5	3253	G
1	5	3259	U
1	5	3263	G
1	5	3265	C
1	5	3269	U
1	5	3270	U
1	5	3273	A
1	5	3276	G
1	5	3277	U
1	5	3278	C
1	5	3279	A
1	5	3281	U
1	5	3282	U
1	5	3285	C
1	5	3286	G
1	5	3289	G
1	5	3290	G
1	5	3294	A
1	5	3304	U
1	5	3313	U
1	5	3316	A
1	5	3317	U
1	5	3318	G
1	5	3319	U
1	5	3324	C
1	5	3341	U
1	5	3342	A
1	5	3345	G
1	5	3346	U
1	5	3351	U
1	5	3352	U
1	5	3354	U
1	5	3356	G
1	5	3357	U
1	5	3358	U
1	5	3362	A
1	5	3369	G
1	5	3378	C
1	5	3383	G
1	5	3389	U

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Mol	Chain	Res	Type
1	5	3390	G
1	5	3394	U
1	5	3396	U
2	7	7	G
2	7	22	A
2	7	33	U
2	7	54	U
2	7	60	G
2	7	65	G
2	7	73	C
2	7	74	C
2	7	76	A
2	7	91	G
2	7	93	C
2	7	99	G
2	7	102	A
2	7	112	G
3	8	23	U
3	8	25	G
3	8	34	U
3	8	42	G
3	8	48	A
3	8	51	G
3	8	59	A
3	8	60	U
3	8	62	C
3	8	63	G
3	8	77	A
3	8	80	A
3	8	81	U
3	8	82	U
3	8	83	C
3	8	84	C
3	8	85	G
3	8	86	U
3	8	87	G
3	8	88	A
3	8	89	A
3	8	90	U
3	8	95	G
3	8	102	U
3	8	104	A

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Mol	Chain	Res	Type
3	8	105	A
3	8	106	C
3	8	111	A
3	8	113	U
3	8	125	U
3	8	126	A
3	8	127	U
3	8	138	A
3	8	156	U
3	8	157	U
3	8	158	U

All (78) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	5	151	A
1	5	190	U
1	5	210	U
1	5	217	U
1	5	238	A
1	5	282	G
1	5	438	A
1	5	546	C
1	5	620	U
1	5	621	A
1	5	715	A
1	5	735	A
1	5	765	C
1	5	850	U
1	5	873	C
1	5	981	U
1	5	982	C
1	5	1064	A
1	5	1081	U
1	5	1094	U
1	5	1222	G
1	5	1238	C
1	5	1241	U
1	5	1284	C
1	5	1307	G
1	5	1329	U
1	5	1352	A

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Mol	Chain	Res	Type
1	5	1355	A
1	5	1555	U
1	5	1568	U
1	5	1571	A
1	5	1580	A
1	5	1607	U
1	5	1716	U
1	5	1724	U
1	5	1816	A
1	5	1819	U
1	5	2101	C
1	5	2112	U
1	5	2204	C
1	5	2209	U
1	5	2248	C
1	5	2307	G
1	5	2418	G
1	5	2422	C
1	5	2438	A
1	5	2513	U
1	5	2539	C
1	5	2583	C
1	5	2593	A
1	5	2604	U
1	5	2662	G
1	5	2682	C
1	5	2772	C
1	5	2807	U
1	5	2817	A
1	5	2871	G
1	5	2872	A
1	5	2954	U
1	5	2971	A
1	5	2995	A
1	5	3078	U
1	5	3115	C
1	5	3121	U
1	5	3167	A
1	5	3195	U
1	5	3218	A
1	5	3228	C
1	5	3269	U

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Mol	Chain	Res	Type
1	5	3289	G
1	5	3340	G
1	5	3341	U
1	5	3357	U
3	8	79	A
3	8	80	A
3	8	88	A
3	8	126	A
3	8	156	U

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

20 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	P5P	5	2019	1	16,23,24	0.79	0	14,33,36	0.80	0
1	Y5P	5	1992	1	14,19,20	2.22	1 (7%)	18,26,29	1.04	1 (5%)
1	P5P	5	2017	1	16,23,24	0.78	0	14,33,36	0.77	0
1	Y5P	5	1989	1	14,19,20	2.31	1 (7%)	18,26,29	0.98	1 (5%)
1	Y5P	5	1988	1	14,19,20	2.28	1 (7%)	18,26,29	1.03	1 (5%)
1	Y5P	5	1986	1	14,19,20	2.27	1 (7%)	18,26,29	1.02	1 (5%)
1	P5P	5	2025	1	16,23,24	0.77	0	14,33,36	0.75	0
1	Y5P	5	1995	1	14,19,20	2.31	1 (7%)	18,26,29	0.97	1 (5%)
1	P5P	5	2020	1	16,23,24	0.77	0	14,33,36	0.78	0
1	P5P	5	2024	1	16,23,24	0.77	0	14,33,36	0.77	0
1	P5P	5	2023	1	16,23,24	0.81	0	14,33,36	0.83	0
1	Y5P	5	1994	1	14,19,20	2.30	1 (7%)	18,26,29	1.06	1 (5%)
1	Y5P	5	1991	1	14,19,20	2.35	1 (7%)	18,26,29	1.01	1 (5%)
1	Y5P	5	1990	1	14,19,20	2.28	1 (7%)	18,26,29	1.06	1 (5%)
1	P5P	5	2022	1	16,23,24	0.78	0	14,33,36	0.79	0
1	P5P	5	2018	1	16,23,24	0.79	0	14,33,36	0.77	0
1	Y5P	5	1987	1	14,19,20	2.32	1 (7%)	18,26,29	1.03	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
1	Y5P	5	1993	1	14,19,20	2.34	1 (7%)	18,26,29	1.01	1 (5%)
1	P5P	5	2021	1	16,23,24	0.78	0	14,33,36	0.75	0
1	P5P	5	2016	1	16,23,24	0.77	0	14,33,36	0.76	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	P5P	5	2019	1	-	0/3/25/26	0/3/3/3
1	Y5P	5	1992	1	-	1/7/33/34	0/2/2/2
1	P5P	5	2017	1	-	0/3/25/26	0/3/3/3
1	Y5P	5	1989	1	-	1/7/33/34	0/2/2/2
1	Y5P	5	1988	1	-	1/7/33/34	0/2/2/2
1	Y5P	5	1986	1	-	1/7/33/34	0/2/2/2
1	P5P	5	2025	1	-	0/3/25/26	0/3/3/3
1	Y5P	5	1995	1	-	1/7/33/34	0/2/2/2
1	P5P	5	2020	1	-	0/3/25/26	0/3/3/3
1	P5P	5	2024	1	-	0/3/25/26	0/3/3/3
1	P5P	5	2023	1	-	0/3/25/26	0/3/3/3
1	Y5P	5	1994	1	-	1/7/33/34	0/2/2/2
1	Y5P	5	1991	1	-	1/7/33/34	0/2/2/2
1	Y5P	5	1990	1	-	1/7/33/34	0/2/2/2
1	P5P	5	2022	1	-	0/3/25/26	0/3/3/3
1	P5P	5	2018	1	-	0/3/25/26	0/3/3/3
1	Y5P	5	1987	1	-	1/7/33/34	0/2/2/2
1	Y5P	5	1993	1	-	1/7/33/34	0/2/2/2
1	P5P	5	2021	1	-	0/3/25/26	0/3/3/3
1	P5P	5	2016	1	-	0/3/25/26	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	1991	Y5P	C4-N3	-8.62	1.38	1.46
1	5	1993	Y5P	C4-N3	-8.54	1.38	1.46
1	5	1987	Y5P	C4-N3	-8.51	1.38	1.46
1	5	1995	Y5P	C4-N3	-8.46	1.38	1.46
1	5	1989	Y5P	C4-N3	-8.45	1.38	1.46
1	5	1994	Y5P	C4-N3	-8.43	1.38	1.46
1	5	1988	Y5P	C4-N3	-8.34	1.38	1.46
1	5	1990	Y5P	C4-N3	-8.34	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	1986	Y5P	C4-N3	-8.31	1.38	1.46
1	5	1992	Y5P	C4-N3	-8.14	1.38	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	1986	Y5P	N1-C2-N3	-3.75	114.34	125.33
1	5	1994	Y5P	N1-C2-N3	-3.74	114.37	125.33
1	5	1992	Y5P	N1-C2-N3	-3.69	114.50	125.33
1	5	1990	Y5P	N1-C2-N3	-3.68	114.53	125.33
1	5	1988	Y5P	N1-C2-N3	-3.66	114.61	125.33
1	5	1993	Y5P	N1-C2-N3	-3.55	114.93	125.33
1	5	1989	Y5P	N1-C2-N3	-3.53	114.99	125.33
1	5	1987	Y5P	N1-C2-N3	-3.51	115.03	125.33
1	5	1995	Y5P	N1-C2-N3	-3.50	115.08	125.33
1	5	1991	Y5P	N1-C2-N3	-3.40	115.36	125.33

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	5	1987	Y5P	O4'-C1'-N1-C2
1	5	1989	Y5P	O4'-C1'-N1-C2
1	5	1990	Y5P	O4'-C1'-N1-C2
1	5	1991	Y5P	O4'-C1'-N1-C2
1	5	1993	Y5P	O4'-C1'-N1-C2
1	5	1995	Y5P	O4'-C1'-N1-C2
1	5	1986	Y5P	O4'-C1'-N1-C2
1	5	1988	Y5P	O4'-C1'-N1-C2
1	5	1992	Y5P	O4'-C1'-N1-C2
1	5	1994	Y5P	O4'-C1'-N1-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 286 ligands modelled in this entry, 286 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
47	z	2
1	5	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	z	107:UNK	C	115:UNK	N	20.22
1	5	1995:Y5P	O3'	2016:P5P	P	17.42
1	z	127:UNK	C	131:UNK	N	9.67

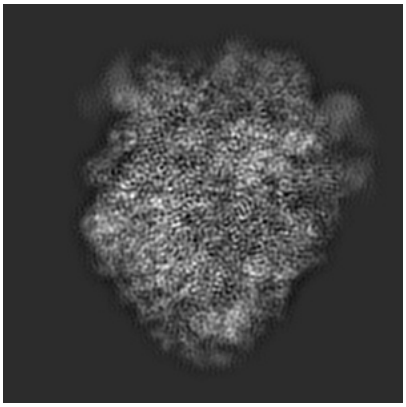
6 Map visualisation

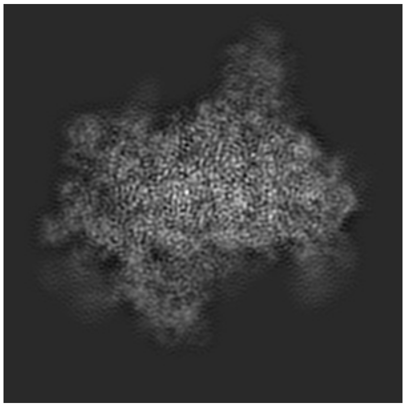
This section contains visualisations of the EMDB entry EMD-3151. These allow visual inspection of the internal detail of the map and identification of artifacts.

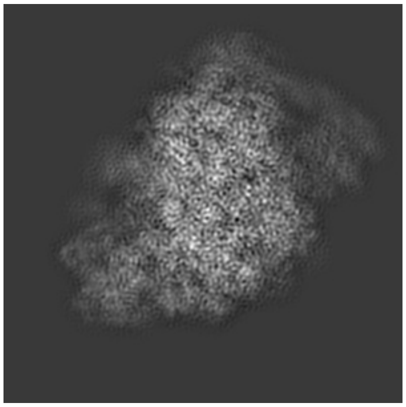
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

6.1.1 Primary map


X

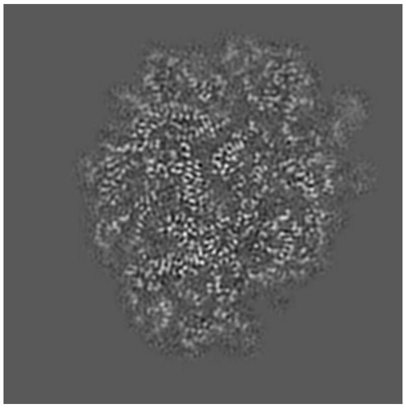

Y

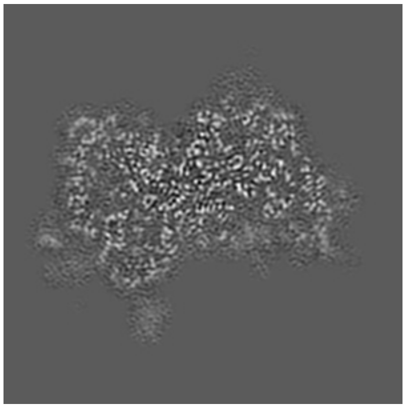

Z

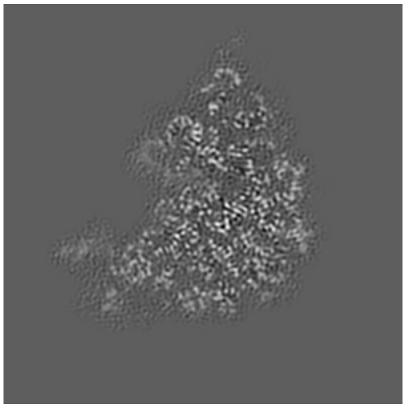
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map


X Index: 108

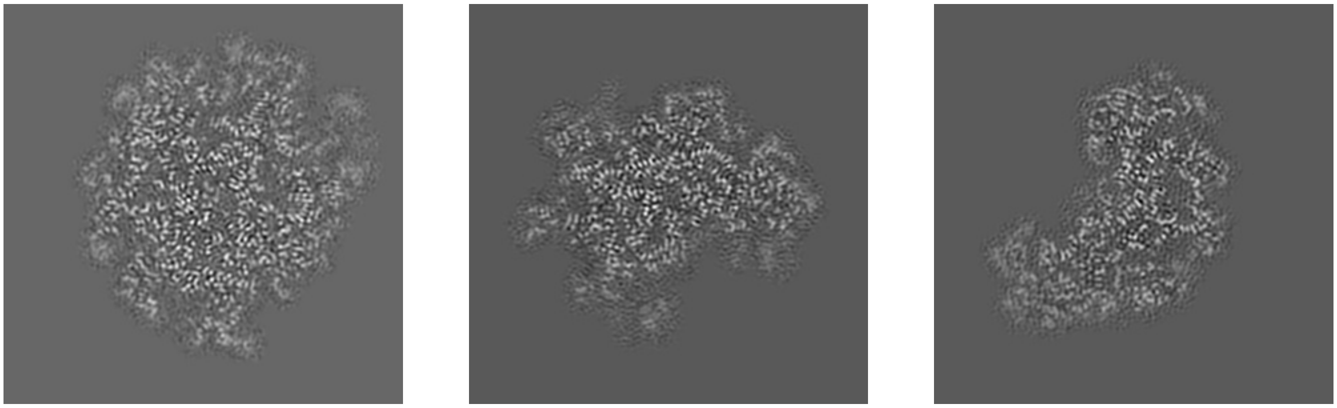

Y Index: 108


Z Index: 108

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

6.3 Largest variance slices ⓘ

6.3.1 Primary map

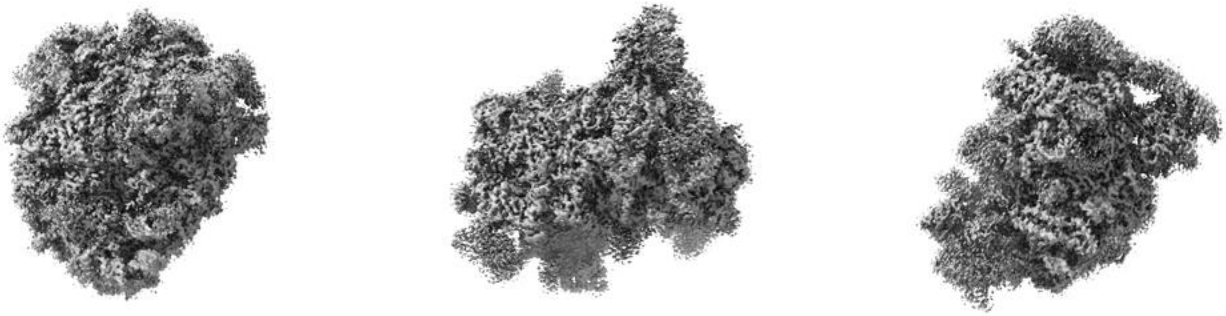


X Index: 116 Y Index: 91 Z Index: 94

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

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

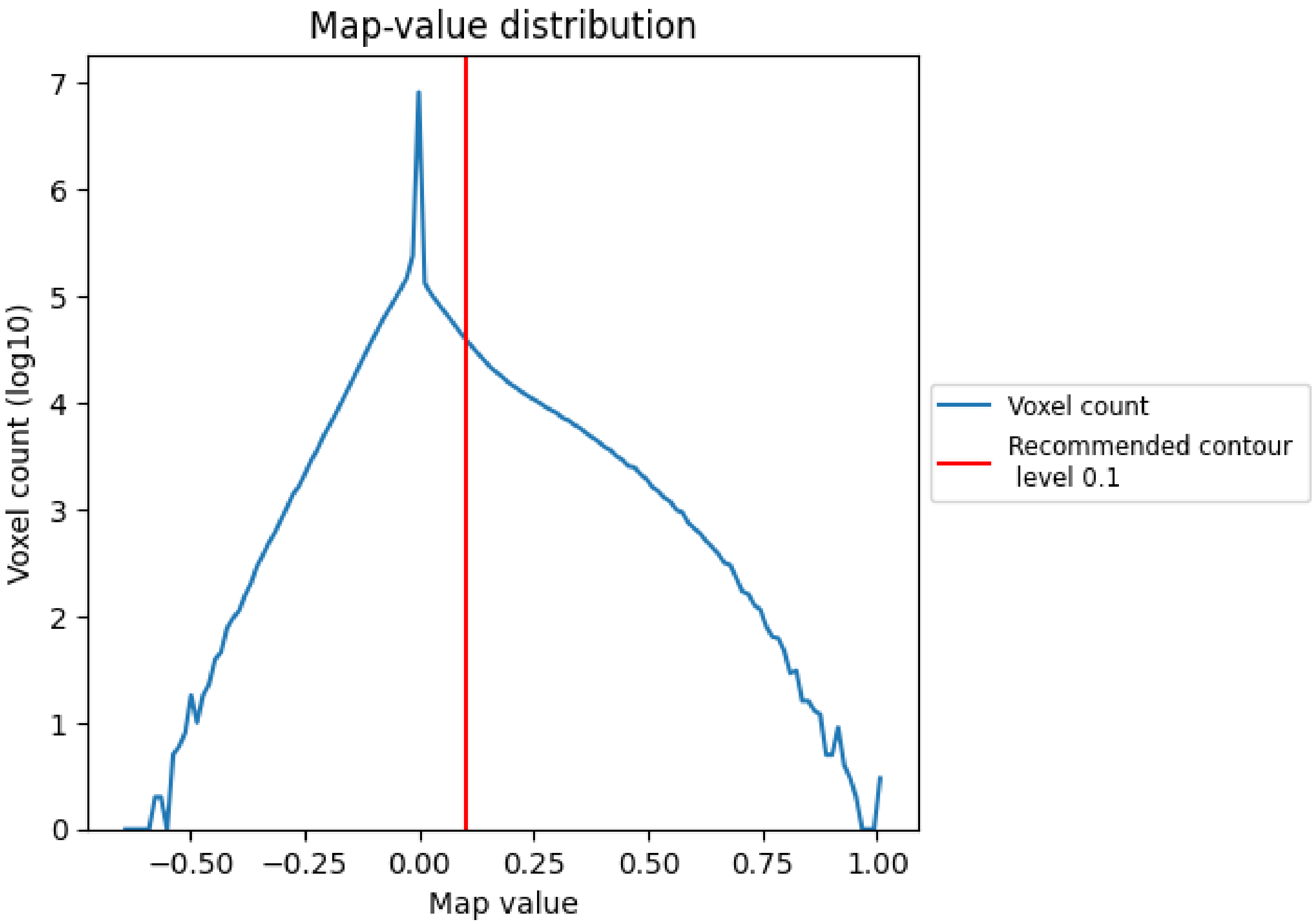
6.5 Mask visualisation ⓘ

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

7 Map analysis ⓘ

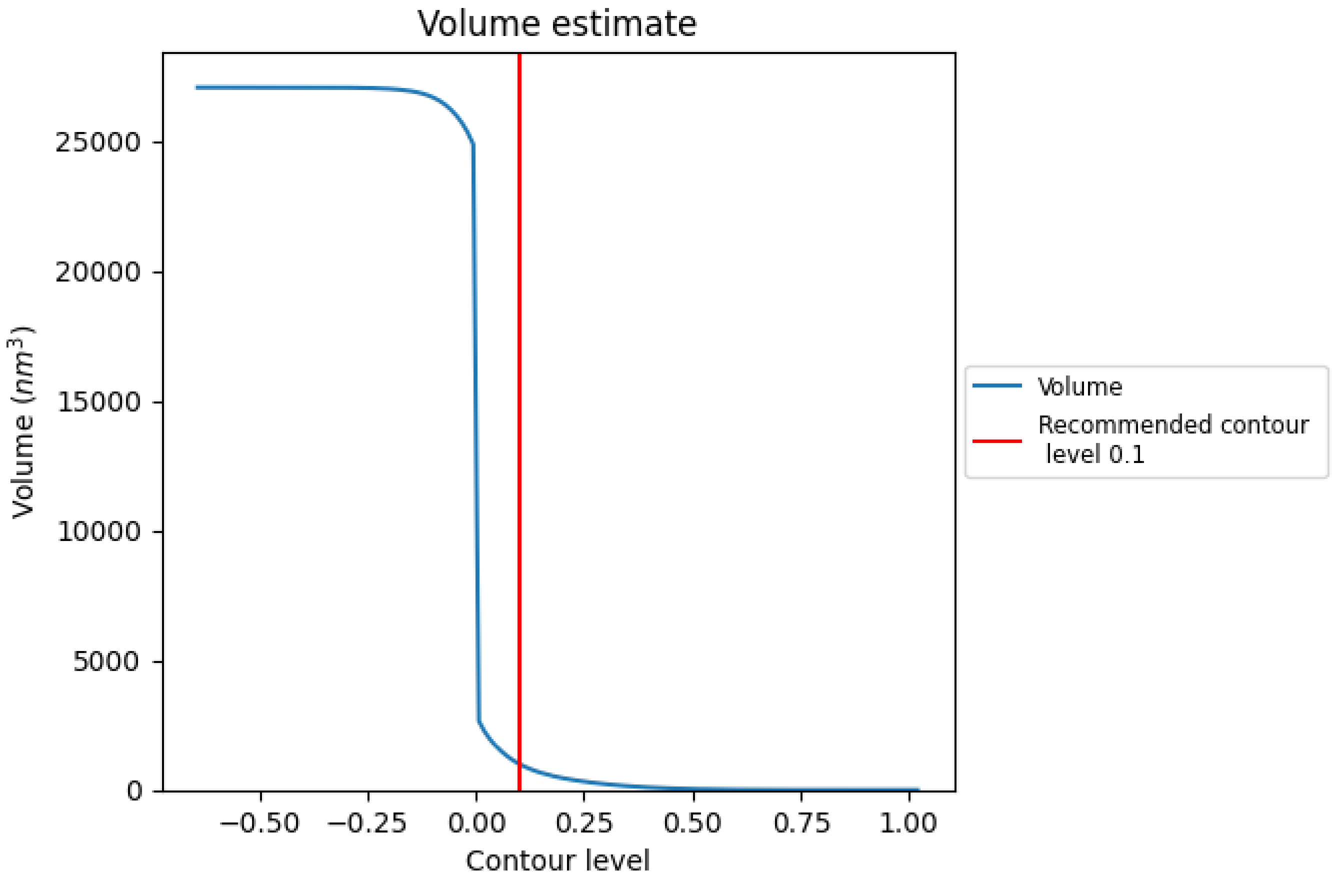
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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

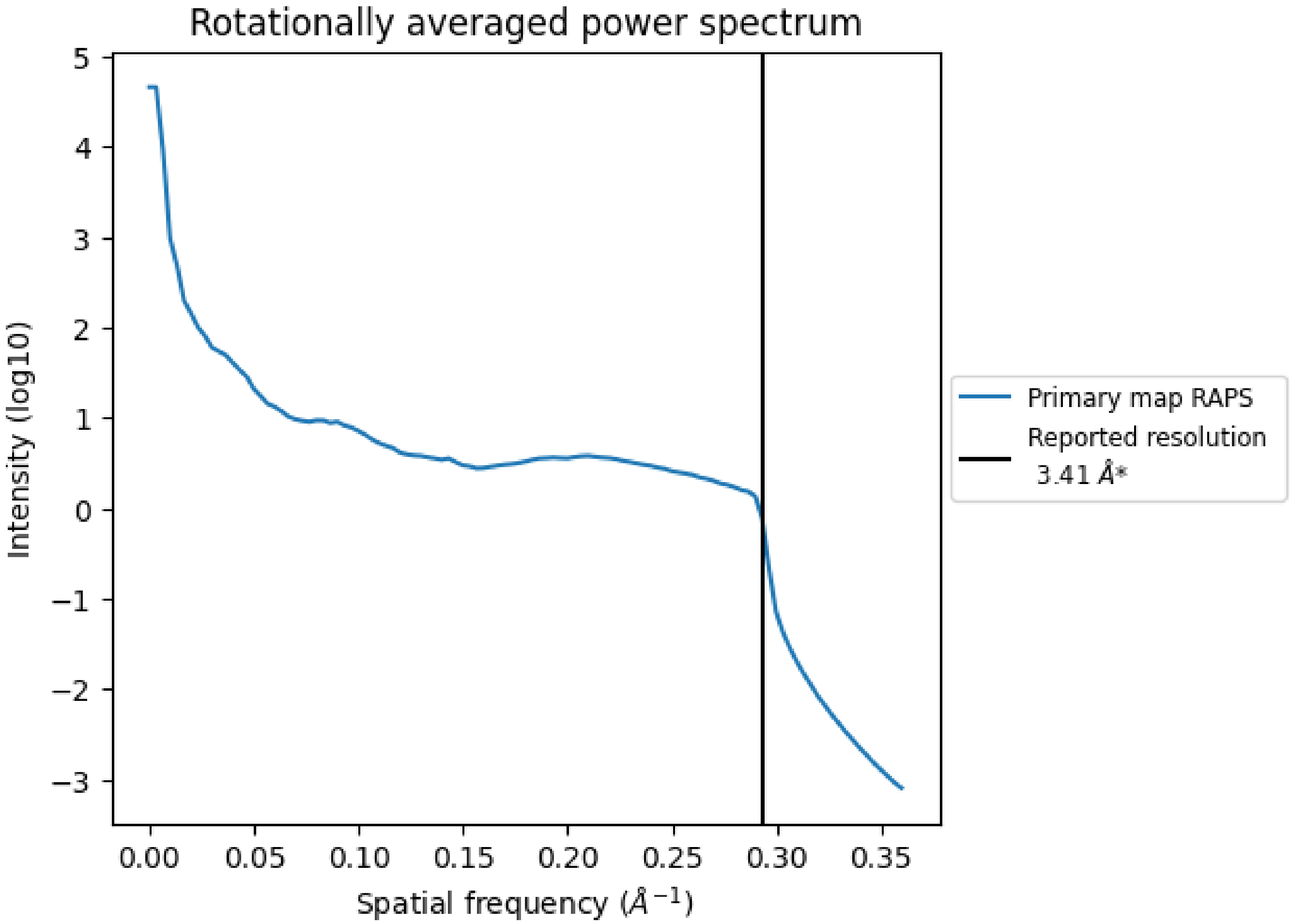
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 1001 nm^3; this corresponds to an approximate mass of 904 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 0.293 $Å^{-1}$

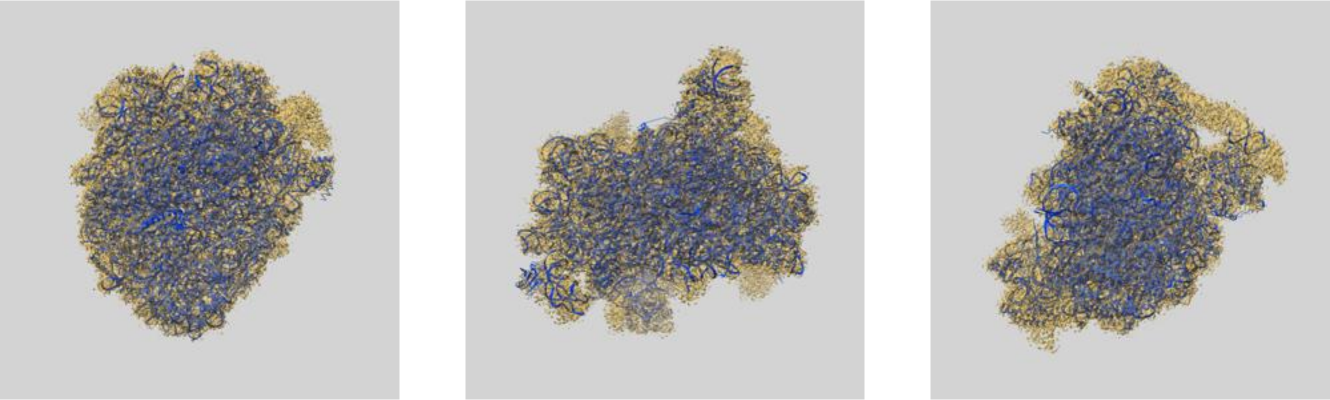
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-3151 and PDB model 5APO. Per-residue inclusion information can be found in section 3 on page 14.

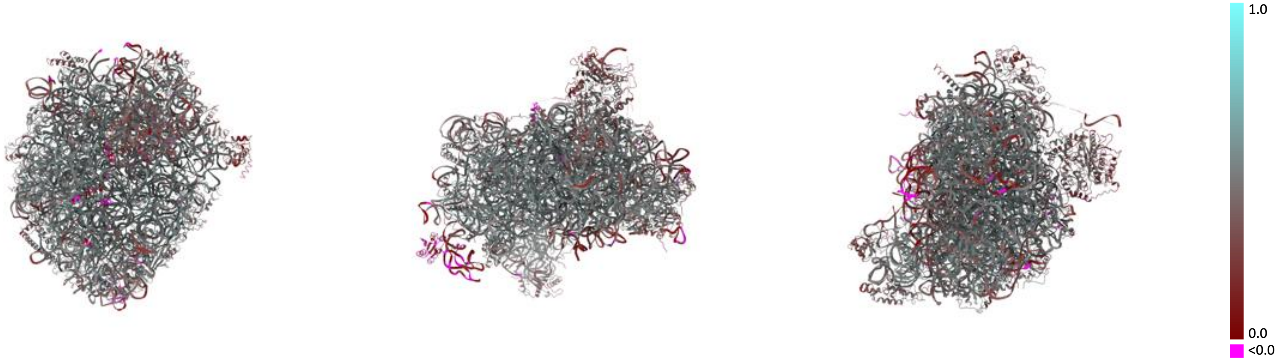
9.1 Map-model overlay ⓘ



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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.

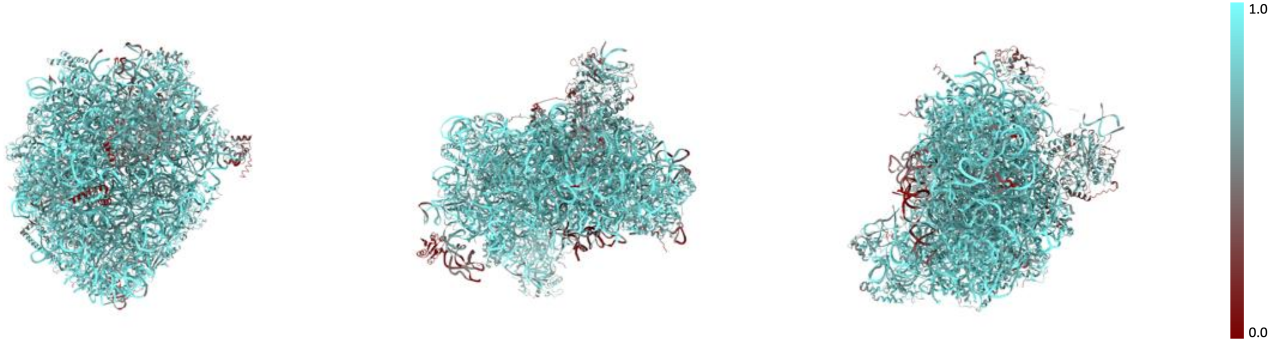
9.2 Q-score mapped to coordinate model ⓘ



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.

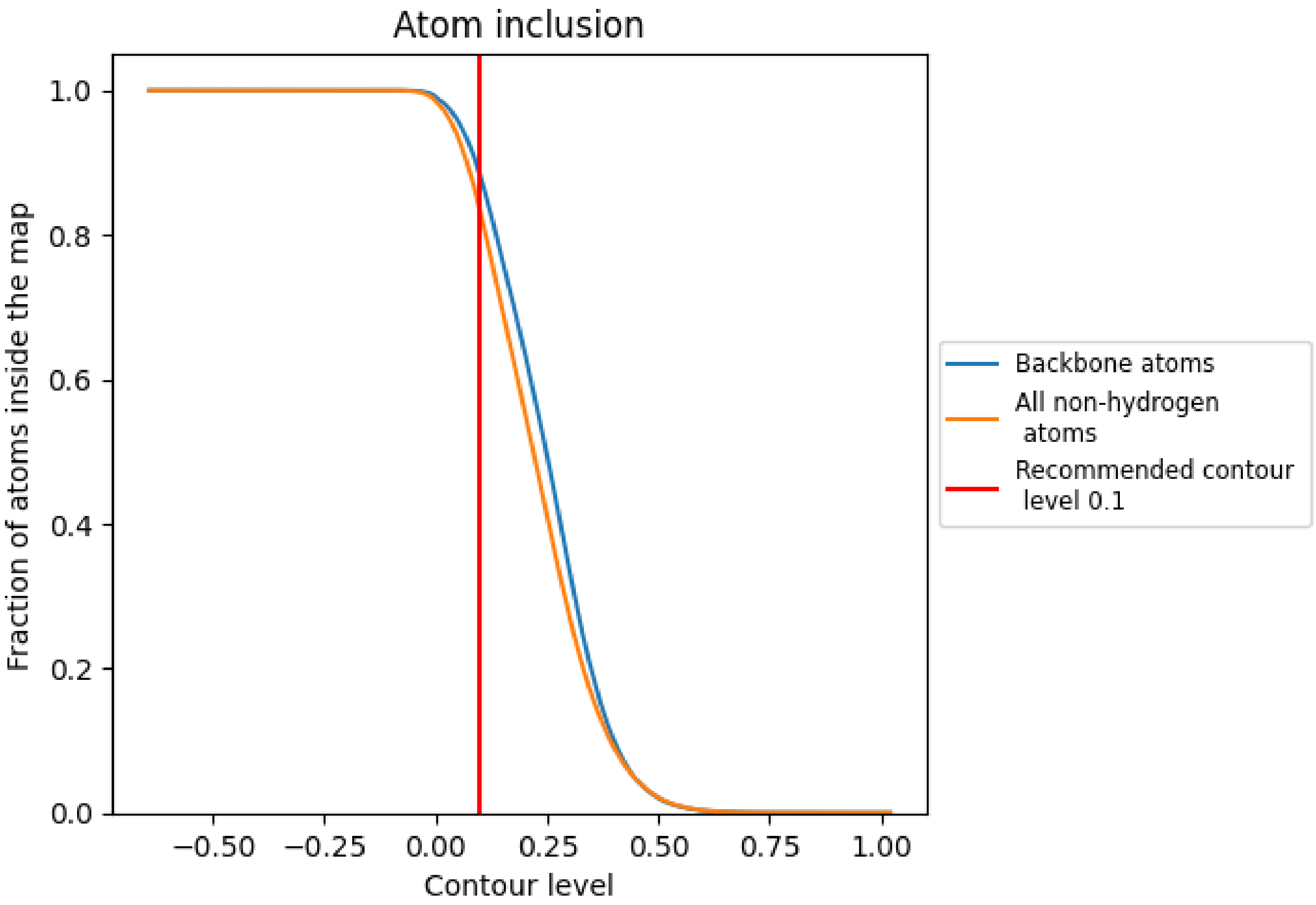
9.3 Atom inclusion mapped to coordinate model ⓘ



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 (0.1).

9.4 Atom inclusion ⓘ



At the recommended contour level, 88% of all backbone atoms, 83% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8321	0.4600
5	0.8791	0.4610
7	0.9300	0.4640
8	0.9164	0.4870
A	0.8162	0.5030
B	0.8606	0.5040
C	0.8541	0.5080
D	0.7774	0.4220
E	0.7699	0.4440
F	0.8599	0.5080
G	0.7917	0.4370
H	0.8094	0.4780
I	0.7879	0.4720
J	0.7019	0.3630
L	0.8338	0.4890
M	0.8430	0.4840
N	0.8132	0.5010
O	0.8653	0.5110
P	0.8182	0.5010
Q	0.8516	0.5180
R	0.8170	0.4810
S	0.8479	0.5050
T	0.8161	0.4920
U	0.7242	0.4450
V	0.8224	0.4870
W	0.8257	0.4880
X	0.8122	0.4890
Y	0.8168	0.4890
Z	0.7703	0.4300
a	0.8573	0.5030
b	0.7633	0.4570
c	0.7298	0.4050
d	0.7666	0.4720
e	0.8482	0.5200
f	0.8758	0.5270

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Chain	Atom inclusion	Q-score
g	0.7979	0.4900
h	0.8126	0.4970
i	0.7446	0.4320
j	0.8826	0.5260
k	0.6924	0.4240
l	0.8361	0.5070
m	0.7847	0.4820
o	0.6490	0.4210
p	0.8015	0.4720
q	0.0521	0.0480
x	0.6007	0.3600
y	0.5160	0.3680
z	0.1490	0.1330