Full wwPDB EM Validation Report ⓘ

Jun 5, 2023 – 05:01 pm BST

PDB ID	:	7PKQ
EMDB ID	:	EMD-13477
Title	:	Small subunit of the Chlamydomonas reinhardtii mitoribosome
Authors	:	Waltz, F.; Soufari, H.; Hashem, Y.
Deposited on	:	2021-08-26
Resolution	:	4.20 Å(reported)

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

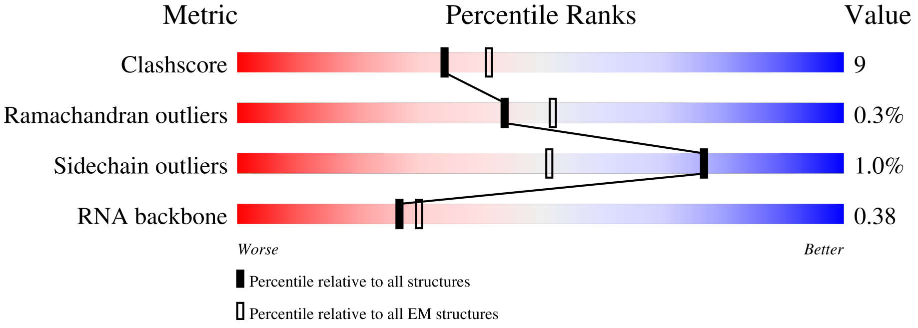
EMDB validation analysis	:	0.0.1.dev50
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance

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

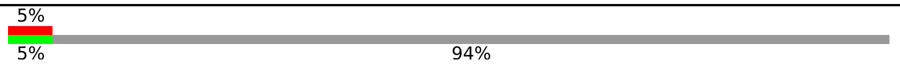
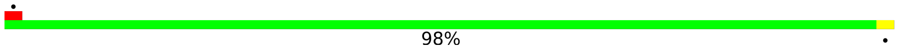
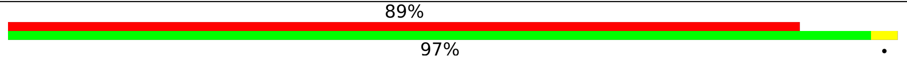
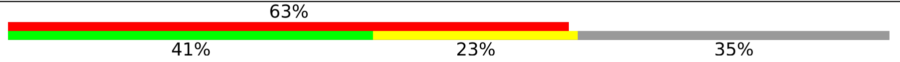
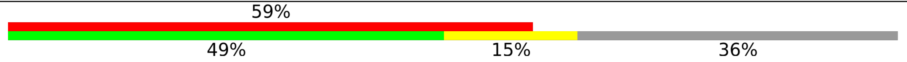
The reported resolution of this entry is 4.20 Å.

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)
Clashscore	158937	4297
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	B	883	
2	C	999	
3	D	425	
4	K	186	
5	L	271	
5	M	271	
5	N	271	

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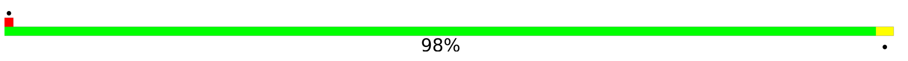
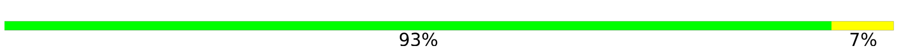
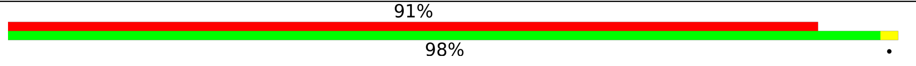
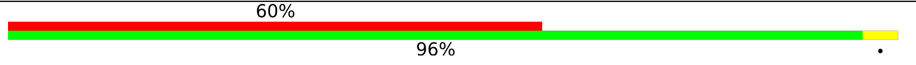
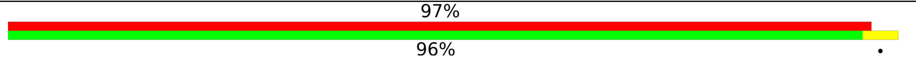
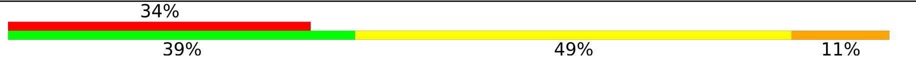
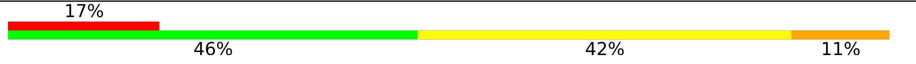
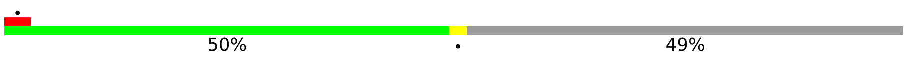
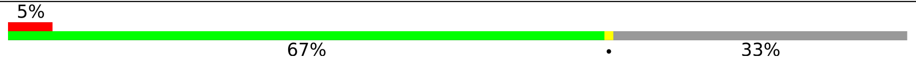
Mol	Chain	Length	Quality of chain
6	O	516	
7	P	416	
8	U	33	
9	V	152	
10	W	54	
11	X	81	
12	Y	108	
13	Z	571	
14	d	415	
15	f	122	
16	p	88	
17	r	356	
18	w	193	
19	1	101	
20	4	415	
21	2	213	
22	3	393	
23	a	253	
24	b	530	
25	e	368	
26	o	319	
27	z	133	
28	v	190	
29	q	220	
30	l	128	

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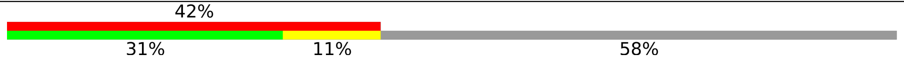
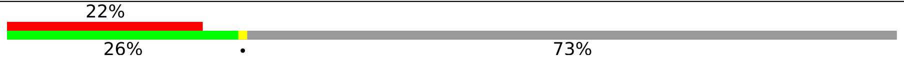
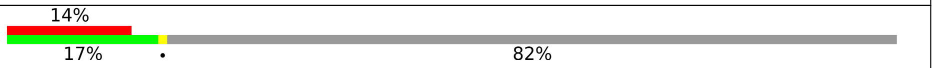
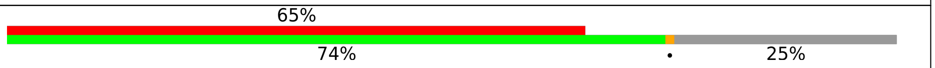
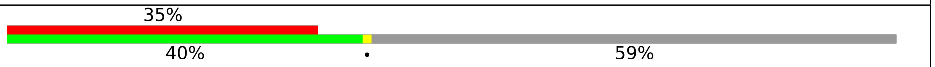
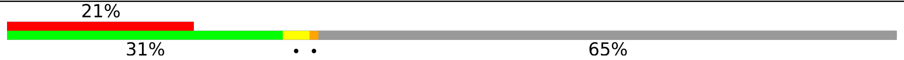
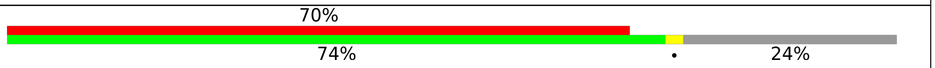
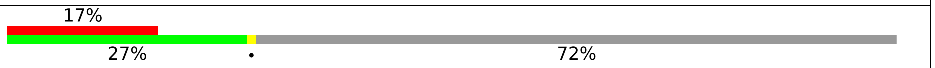
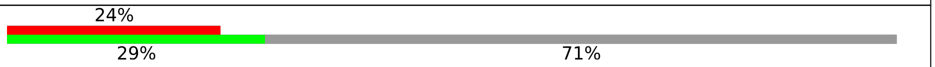
Mol	Chain	Length	Quality of chain
31	h	412	
32	k	233	
33	j	612	
34	m	124	
35	n	112	
36	u	136	
37	s	116	
38	g	324	
39	i	446	
40	x	485	
41	c	490	
42	y	209	

2 Entry composition (i)

There are 42 unique types of molecules in this entry. The entry contains 70313 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called mS35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	53	386	235	81	69	1	0	0

- Molecule 2 is a protein called mS45.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	369	2766	1742	518	503	3	0	0

- Molecule 3 is a protein called mS45-insert.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	D	425	2125	1275	425	425	0	0

- Molecule 4 is a protein called mS31/46.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	K	186	930	558	186	186	0	0

- Molecule 5 is a protein called mS105.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	L	175	1373	861	226	284	2	0	0
5	M	174	1370	862	225	281	2	0	0
5	N	195	1479	926	247	304	2	0	0

- Molecule 6 is a protein called mS106.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	O	236	1710	1069	327	309	5	0	0

- Molecule 7 is a protein called mS107.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	P	337	2601	1647	492	456	6	0	0

- Molecule 8 is a protein called Unk1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	U	33	165	99	33	33	0	0

- Molecule 9 is a protein called Unk2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	V	152	760	456	152	152	0	0

- Molecule 10 is a protein called Unk3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	W	54	270	162	54	54	0	0

- Molecule 11 is a protein called Unk4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	X	81	405	243	81	81	0	0

- Molecule 12 is a protein called Unk5.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	Y	108	540	324	108	108	0	0

- Molecule 13 is a protein called Unk6.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	Z	571	2855	1713	571	571	0	0

- Molecule 14 is a protein called uS4m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	d	129	923	581	173	162	7	0	0

- Molecule 15 is a protein called Mitochondrial ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	f	103	824	533	145	142	4	0	0

- Molecule 16 is a protein called bS16m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	p	79	627	395	117	113	2	0	0

- Molecule 17 is a protein called bS18m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	r	56	459	295	93	70	1	0	0

- Molecule 18 is a protein called mS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	w	155	1245	768	252	224	1	0	0

- Molecule 19 is a RNA chain called S1 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
19	1	93	1986	886	352	655	93	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	52	A	-	insertion	GB 12503
1	53	C	-	insertion	GB 12503

- Molecule 20 is a RNA chain called S4 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
20	4	415	8811	3946	1532	2918	415	0	0

- Molecule 21 is a RNA chain called S2 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
21	2	213	4533	2024	798	1498	213	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	66	U	G	conflict	GB 12503
2	67	U	A	conflict	GB 12503
2	68	U	C	conflict	GB 12503
2	69	U	G	conflict	GB 12503
2	70	U	C	conflict	GB 12503
2	71	U	C	conflict	GB 12503
2	72	U	A	conflict	GB 12503
2	73	U	A	conflict	GB 12503
2	75	U	A	conflict	GB 12503

- Molecule 22 is a RNA chain called S3 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
22	3	393	8405	3759	1534	2719	393	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	?	-	U	deletion	GB 12503
3	?	-	G	deletion	GB 12503
3	?	-	U	deletion	GB 12503
3	?	-	A	deletion	GB 12503
3	?	-	A	deletion	GB 12503
3	?	-	U	deletion	GB 12503

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Chain	Residue	Modelled	Actual	Comment	Reference
3	?	-	G	deletion	GB 12503
3	?	-	C	deletion	GB 12503
3	251	G	A	conflict	GB 12503
3	?	-	U	deletion	GB 12503
3	?	-	U	deletion	GB 12503
3	?	-	U	deletion	GB 12503
3	?	-	C	deletion	GB 12503
3	?	-	A	deletion	GB 12503

- Molecule 23 is a protein called bS1m.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	a	212	Total 1562	C 965	N 301	O 291	S 5	0	0

- Molecule 24 is a protein called uS2m.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	b	241	Total 1824	C 1153	N 341	O 322	S 8	0	0

- Molecule 25 is a protein called S5 DRBM domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	e	176	Total 1403	C 882	N 275	O 238	S 8	0	0

- Molecule 26 is a protein called uS15m.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	o	163	Total 1284	C 802	N 249	O 228	S 5	0	0

- Molecule 27 is a protein called mS34.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	z	85	Total 667	C 427	N 118	O 122	0	0

- Molecule 28 is a protein called mS23.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	v	128	Total 1003	C 632	N 189	O 180	S 2	0	0

- Molecule 29 is a protein called uS17m.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	q	147	Total 1128	C 709	N 217	O 201	S 1	0	0

- Molecule 30 is a protein called uS12m.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	l	106	Total 805	C 501	N 160	O 140	S 4	0	0

- Molecule 31 is a protein called uS8m.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	h	351	Total 2711	C 1709	N 504	O 484	S 14	0	0

- Molecule 32 is a protein called uS11m.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	k	99	Total 729	C 458	N 130	O 141	0	0

- Molecule 33 is a protein called Ribosomal_S10 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	j	164	Total 1211	C 765	N 222	O 219	S 5	0	0

- Molecule 34 is a protein called Mitochondrial ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	m	89	Total 685	C 430	N 128	O 126	S 1	0	0

- Molecule 35 is a protein called Mitochondrial ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	n	97	Total 779	C 479	N 163	O 133	S 4	0	0

- Molecule 36 is a protein called Plastid-specific ribosomal protein 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	u	24	Total 199	C 120	N 45	O 34	0	0

- Molecule 37 is a protein called uS19m.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	s	87	Total 678	C 438	N 120	O 117	S 3	0	0

- Molecule 38 is a protein called uS7m,Ribosomal_S7 domain-containing protein,Ribosomal_ S7 domain-containing protein,Ribosomal_S7 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	g	132	Total 909	C 561	N 179	O 165	S 4	0	0

- Molecule 39 is a protein called 30S ribosomal protein S9, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	154	Total 1019	C 622	N 198	O 194	S 5	0	0

- Molecule 40 is a protein called mS29.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	x	368	Total 2647	C 1661	N 490	O 490	S 6	0	0

- Molecule 41 is a protein called Ribosomal_S3_C domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	c	135	Total 1012	C 643	N 186	O 181	S 2	0	0

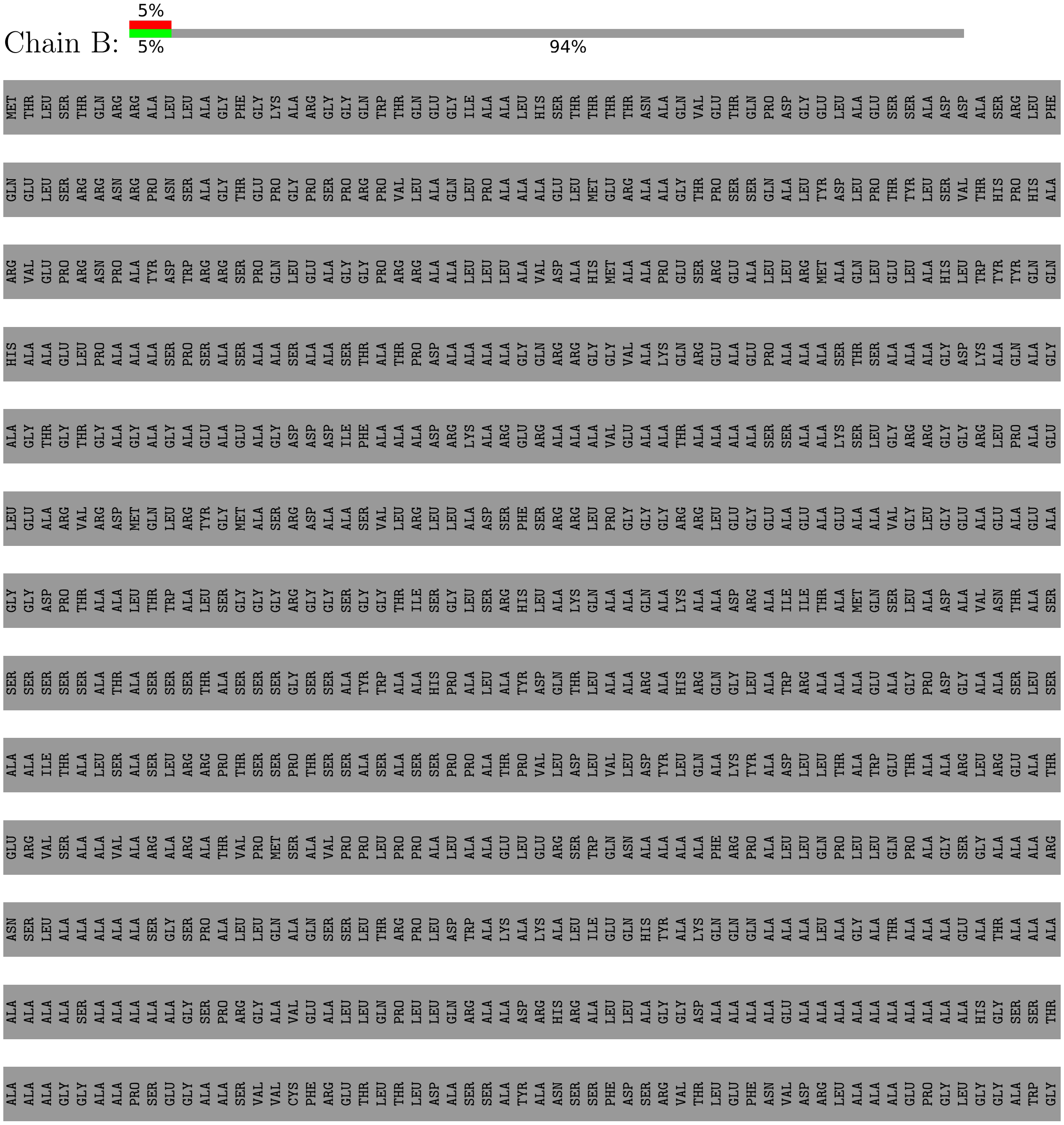
- Molecule 42 is a protein called mS33.

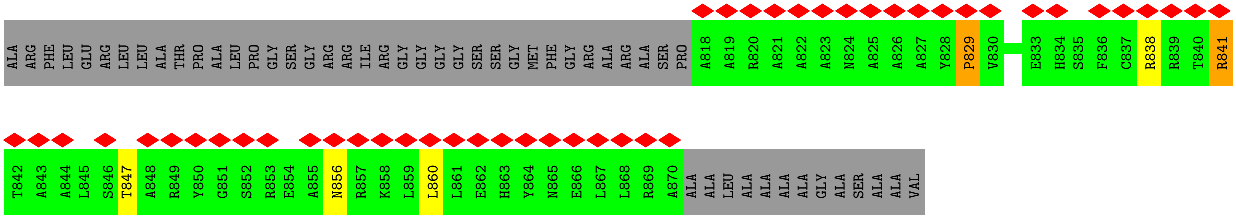
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	y	61	510	319	101	88	2	0	0

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.

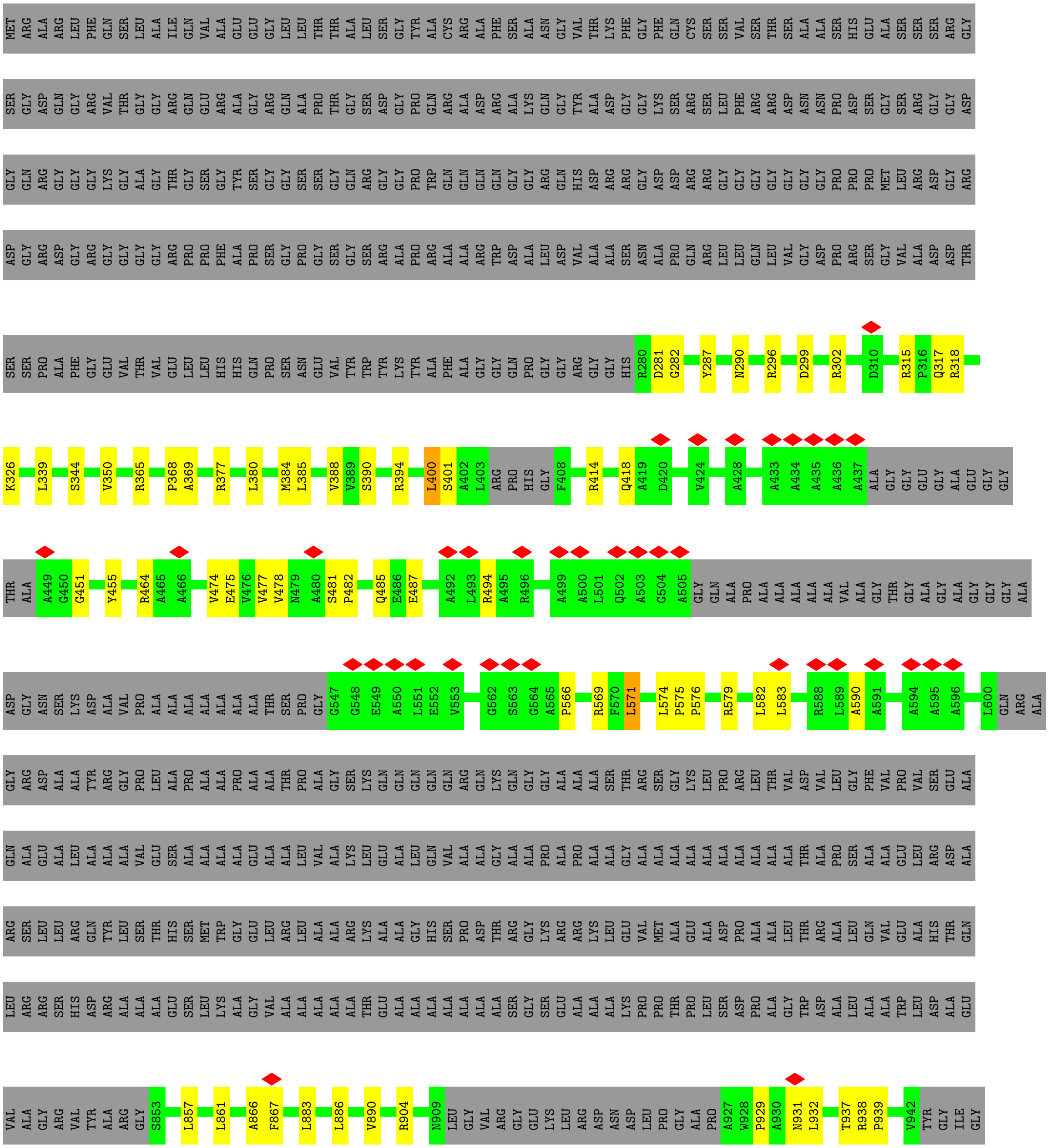
- Molecule 1: mS35

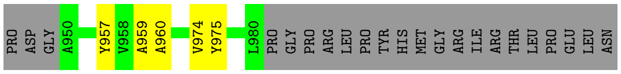




- Molecule 2: mS45

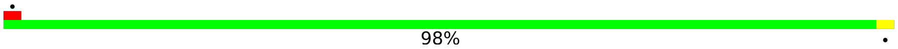
Chain C:

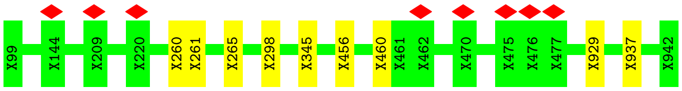




- Molecule 3: mS45-insert

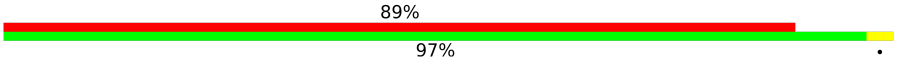
Chain D:

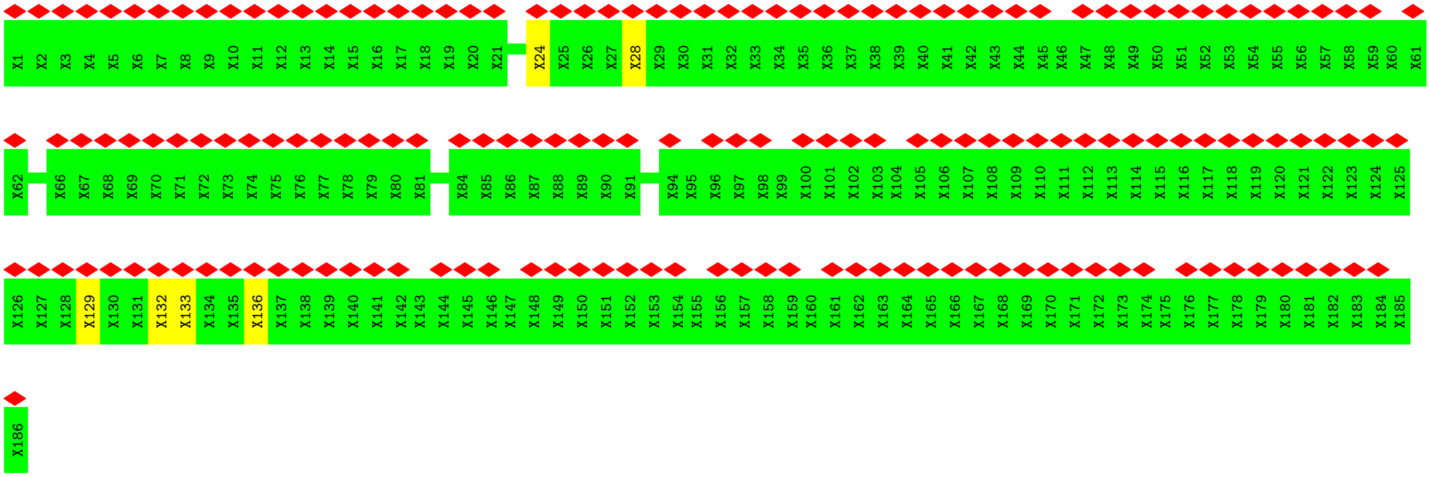




- Molecule 4: mS31/46

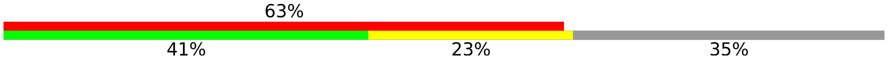
Chain K:

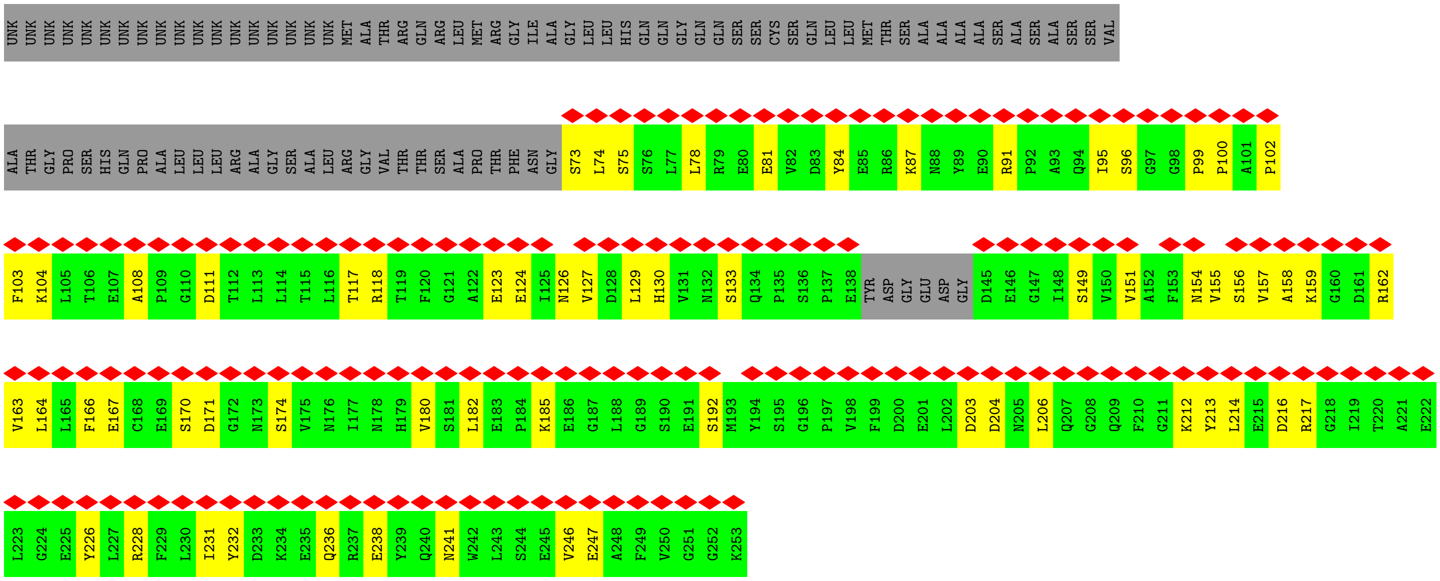




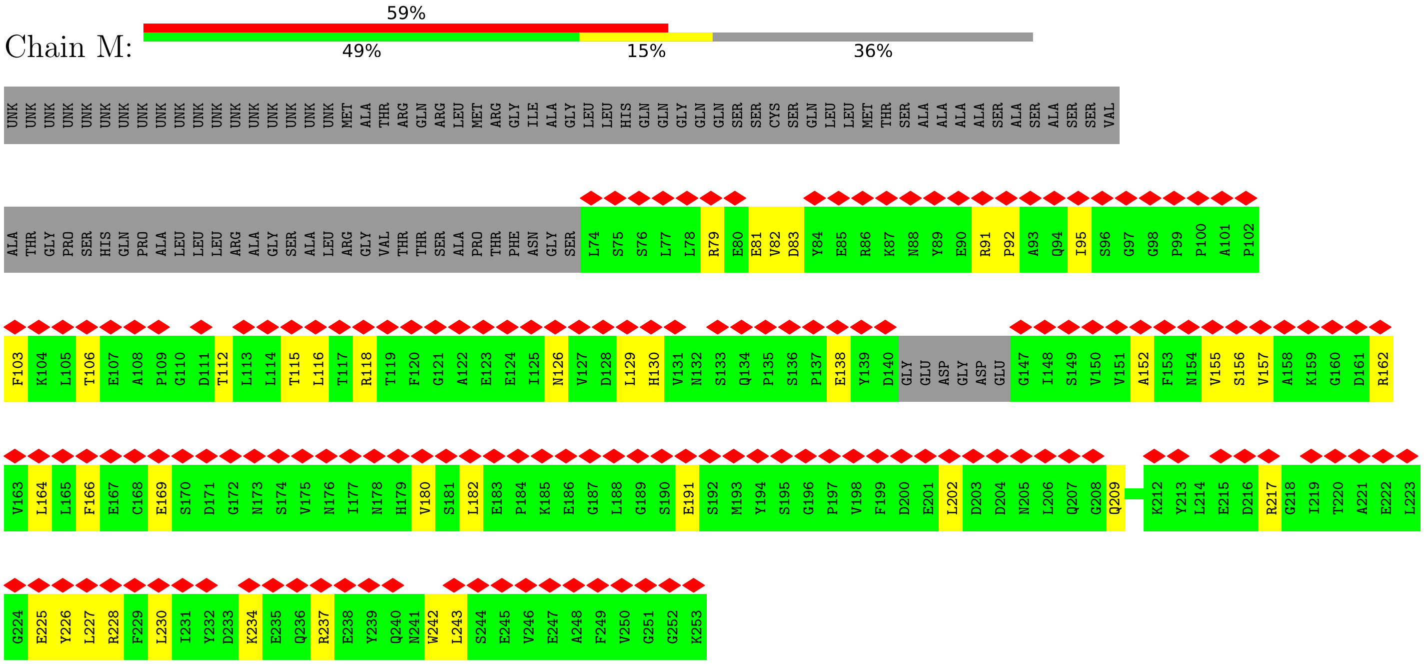
- Molecule 5: mS105

Chain L:

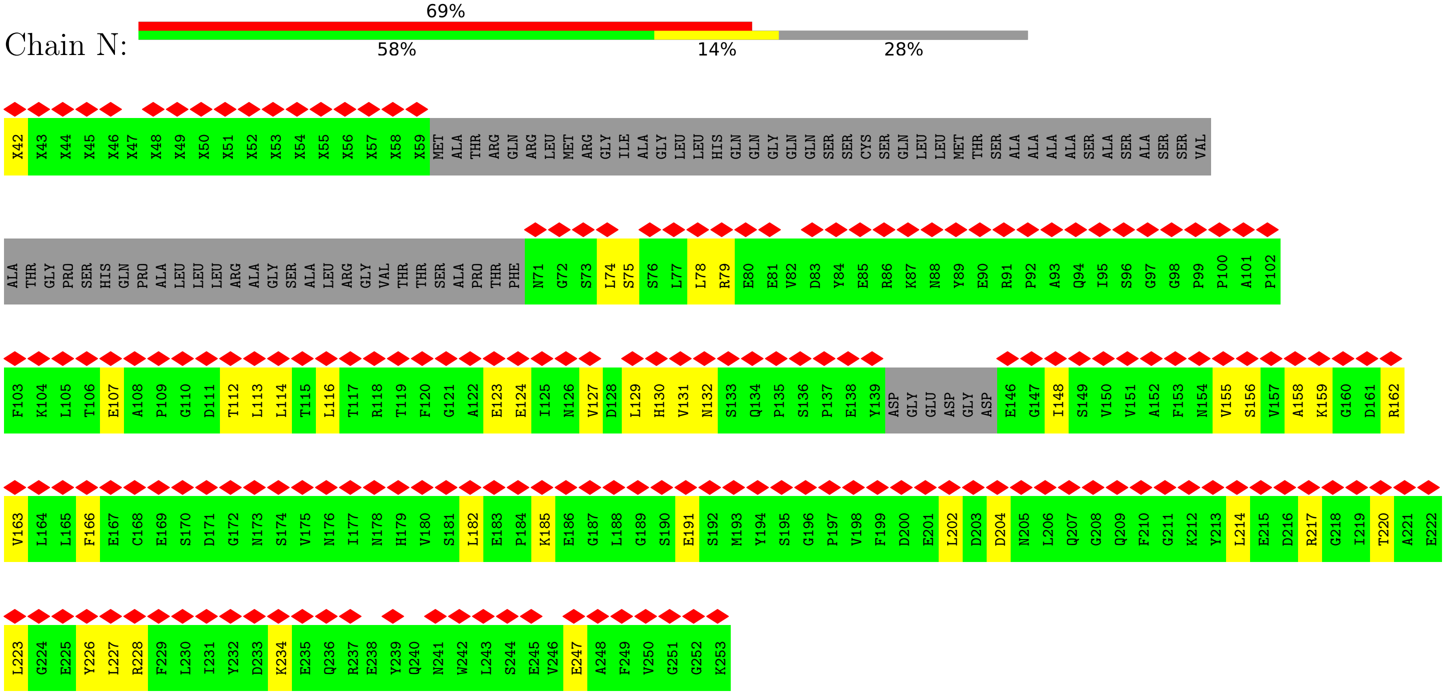




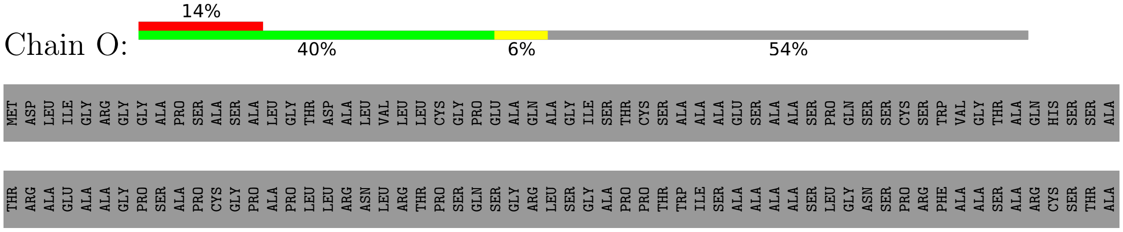
- Molecule 5: mS105

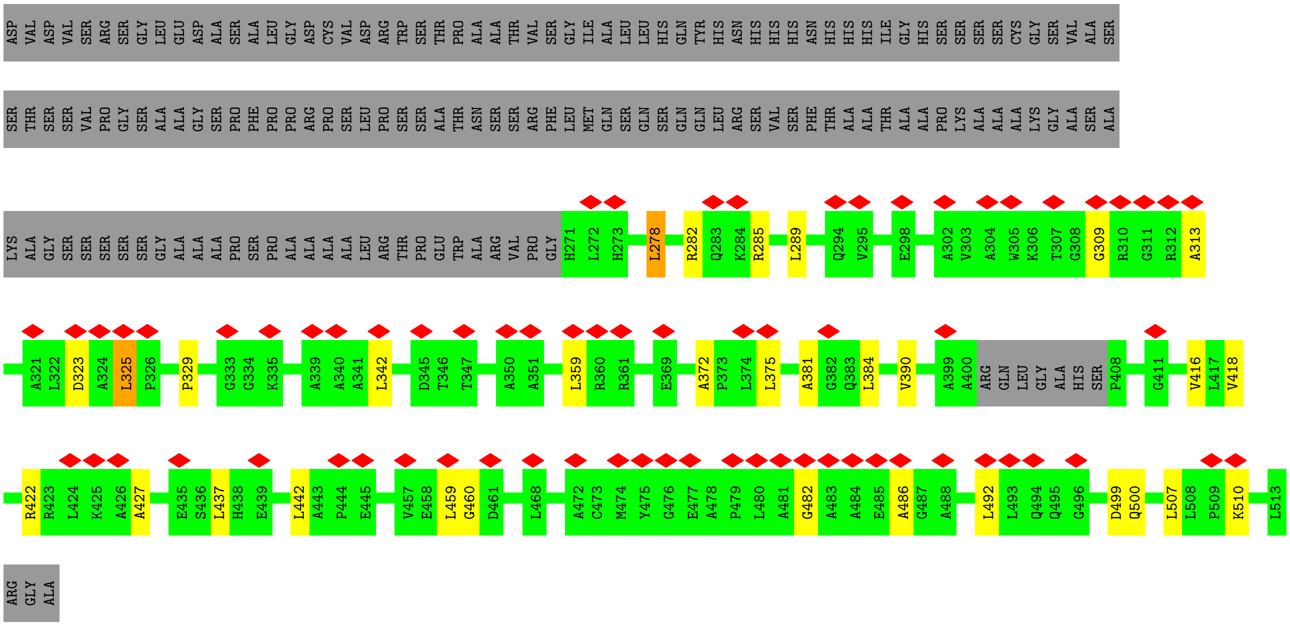


- Molecule 5: mS105

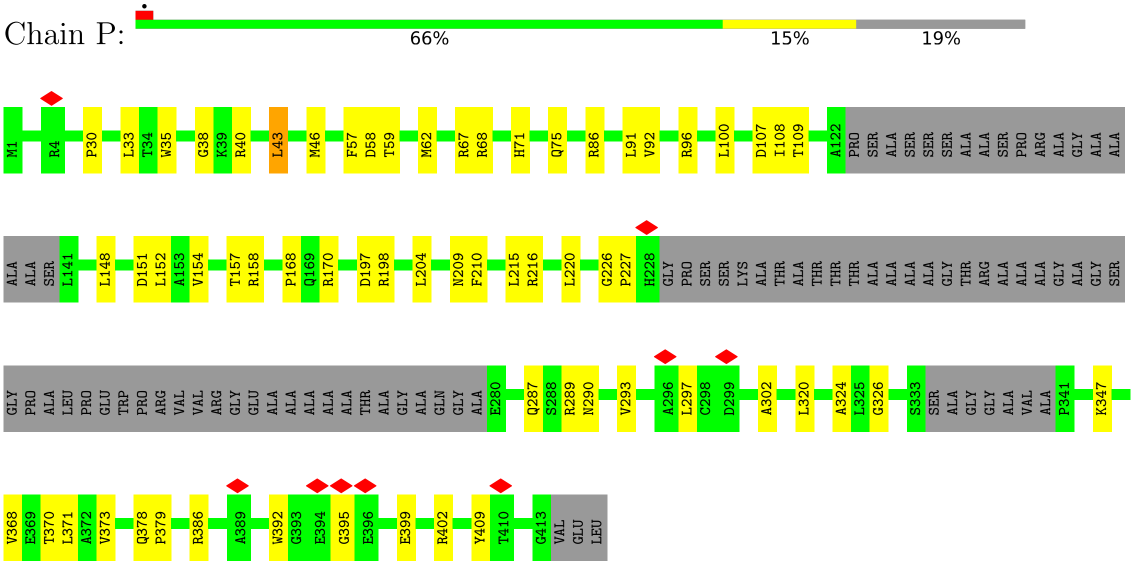


- Molecule 6: mS106

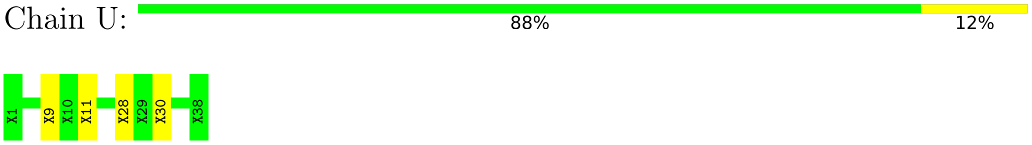




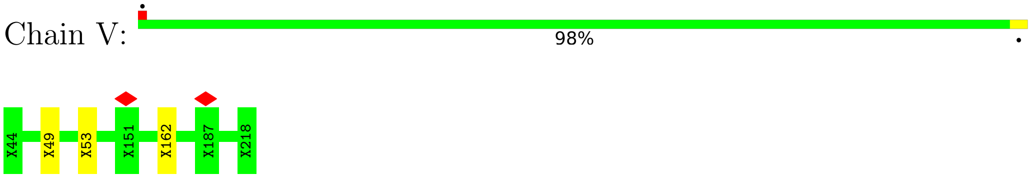
- Molecule 7: mS107



- Molecule 8: Unk1

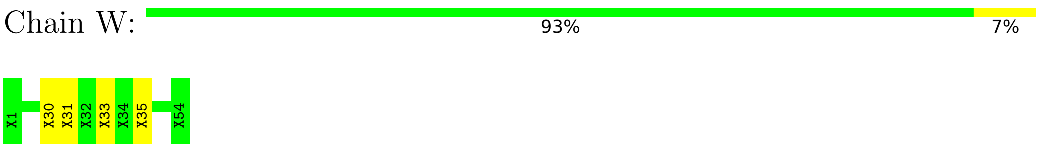


- Molecule 9: Unk2



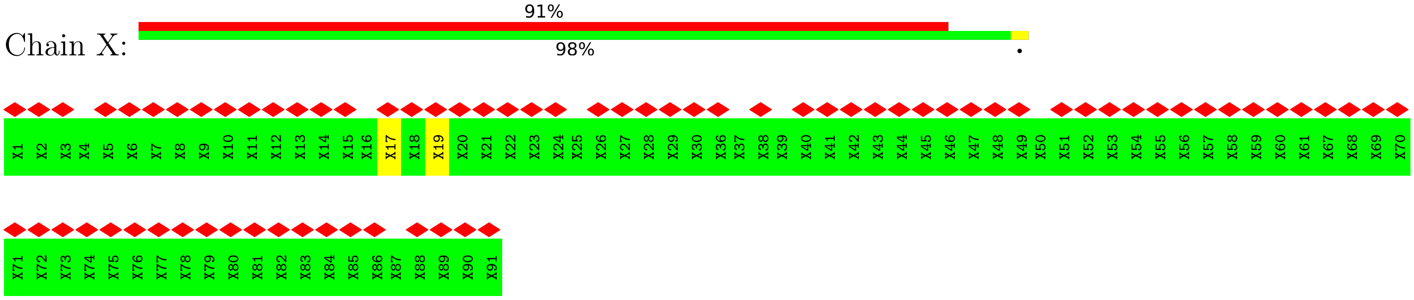
- Molecule 10: Unk3

Chain W:



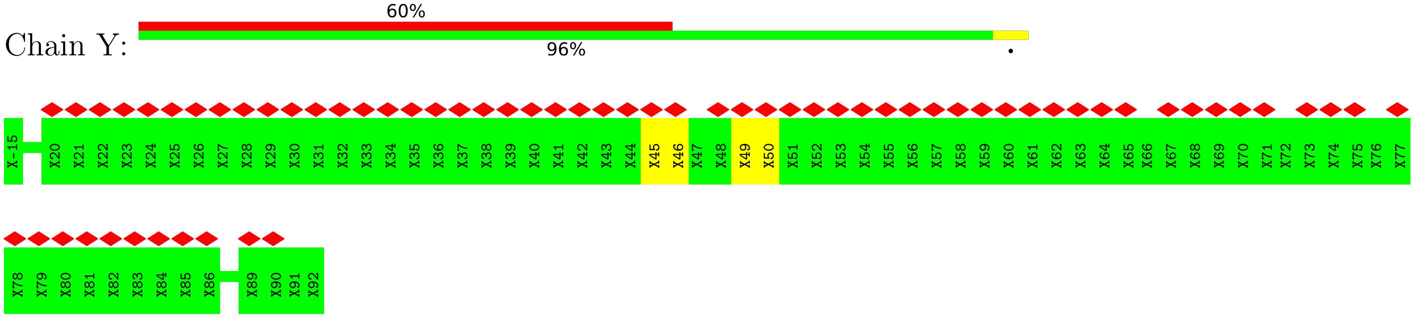
- Molecule 11: Unk4

Chain X:



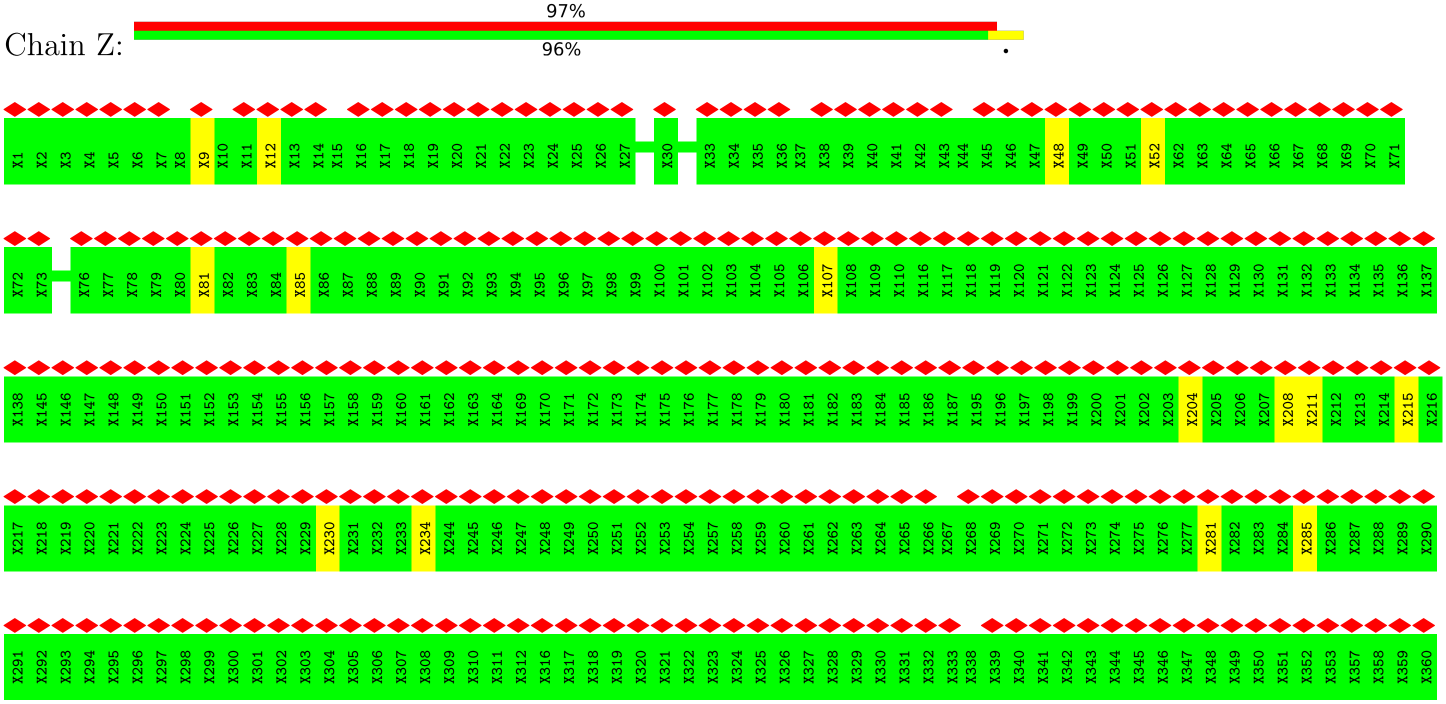
- Molecule 12: Unk5

Chain Y:



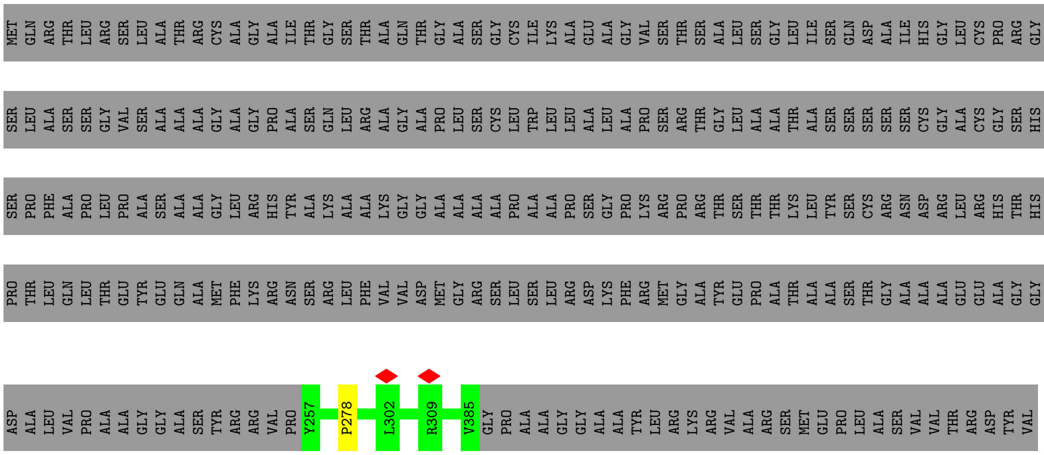
- Molecule 13: Unk6

Chain Z:



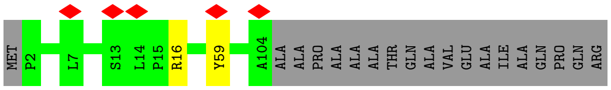
- Molecule 14: uS4m

Chain d:



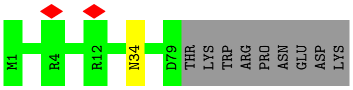
- Molecule 15: Mitochondrial ribosomal protein S6

Chain f:

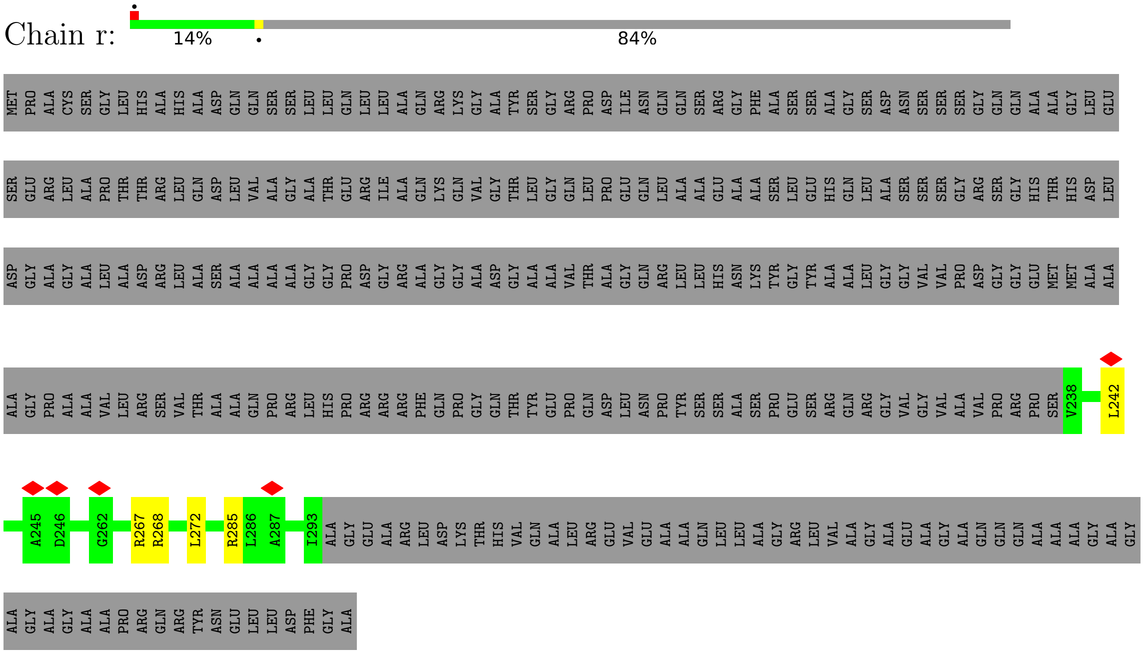


- Molecule 16: bS16m

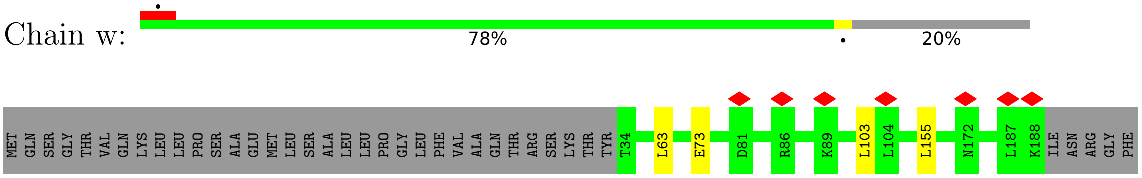
Chain p:



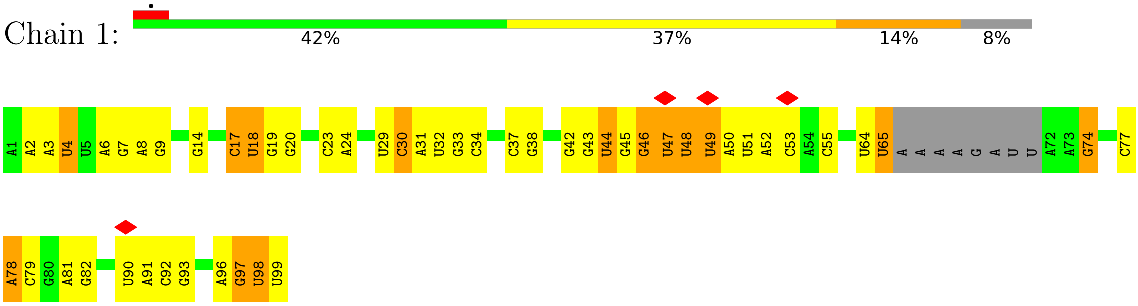
- Molecule 17: bS18m



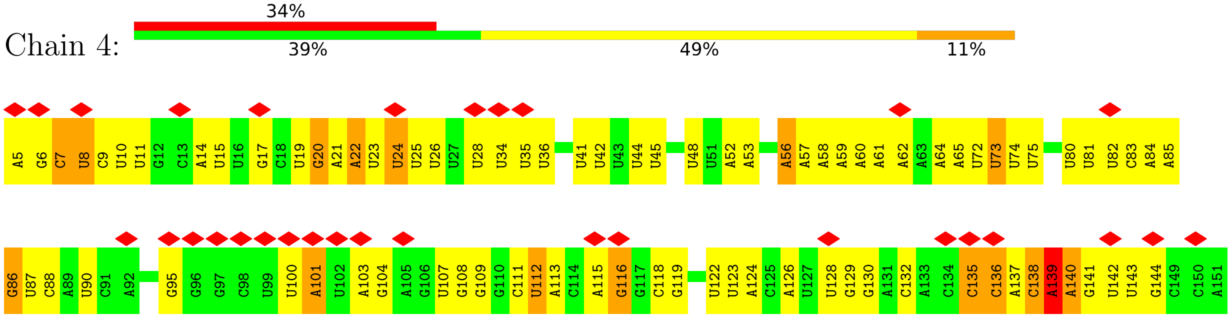
- Molecule 18: mS26

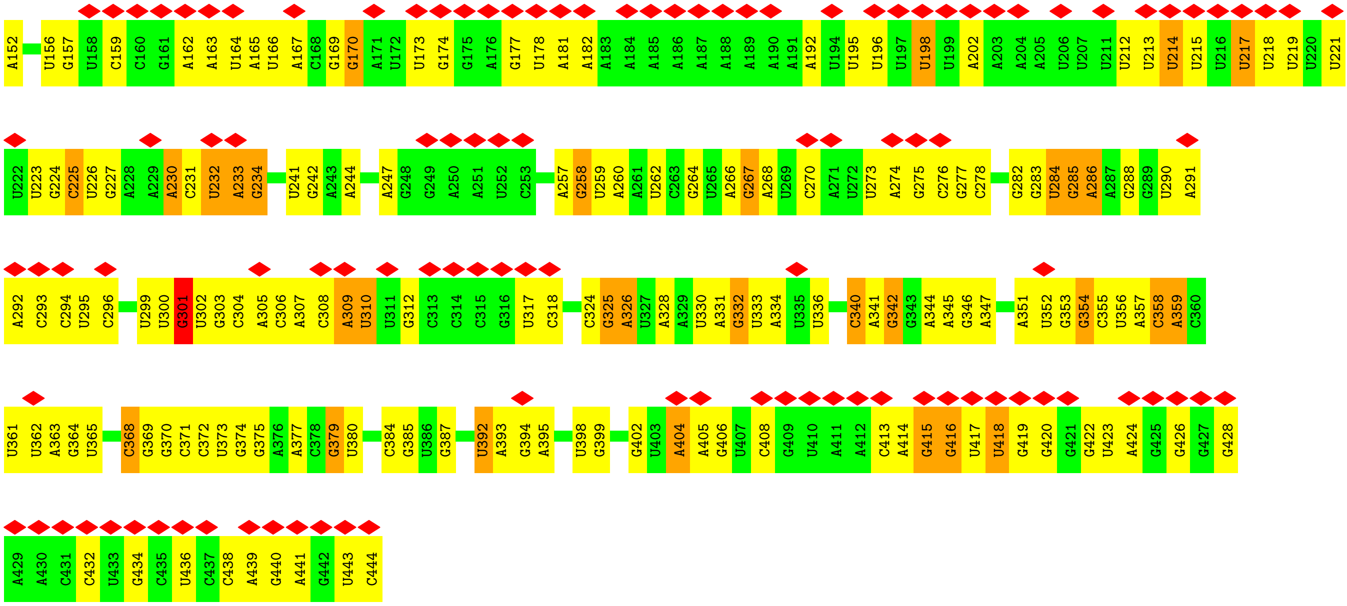


- Molecule 19: S1 rRNA



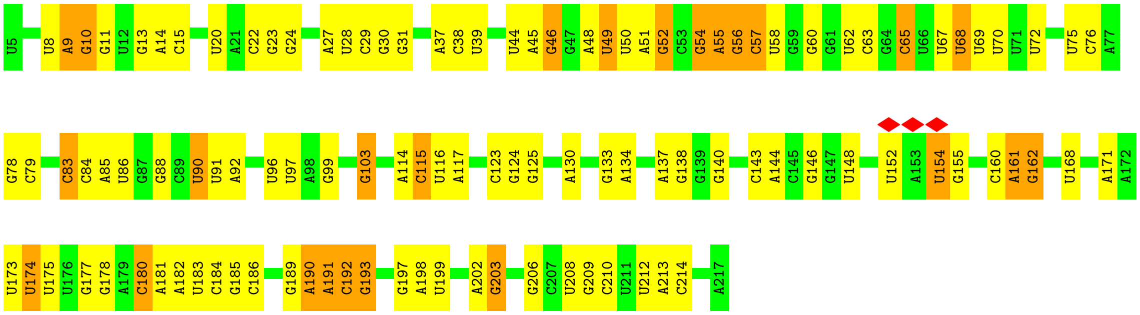
- Molecule 20: S4 rRNA





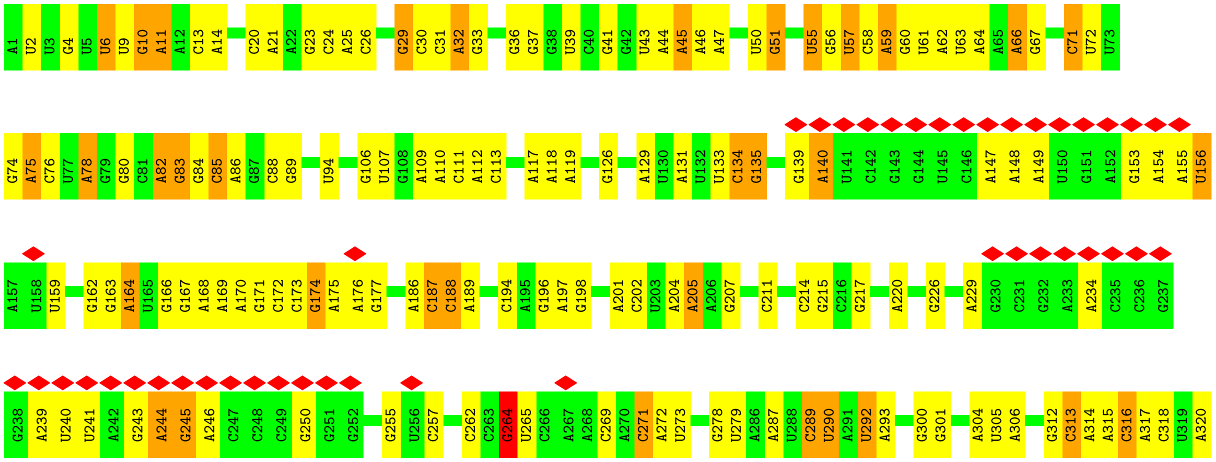
- Molecule 21: S2 rRNA

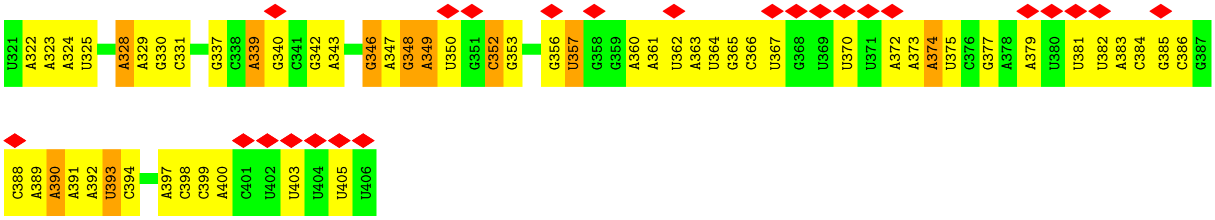
Chain 2:



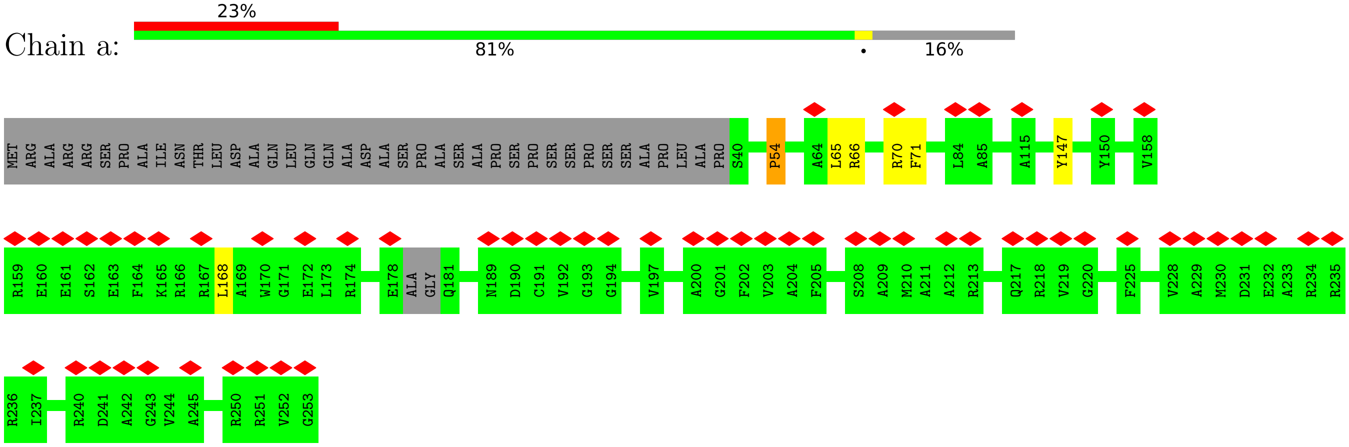
- Molecule 22: S3 rRNA

Chain 3:

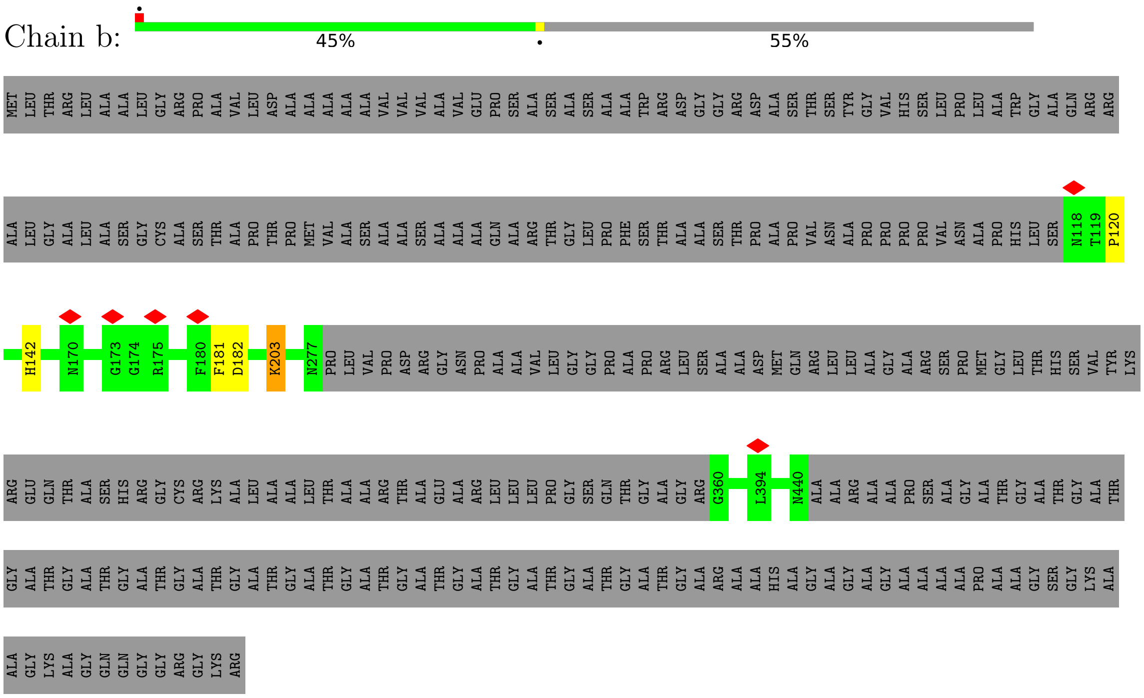




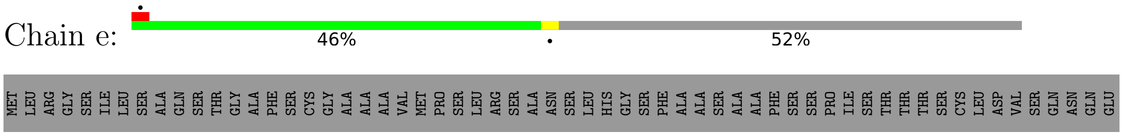
• Molecule 23: bS1m

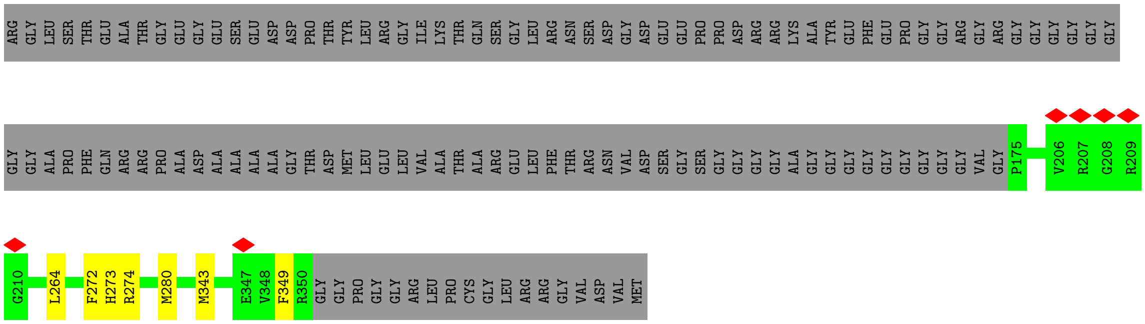


• Molecule 24: uS2m



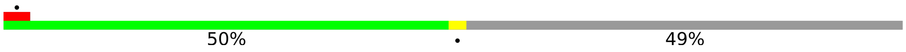
• Molecule 25: S5 DRBM domain-containing protein

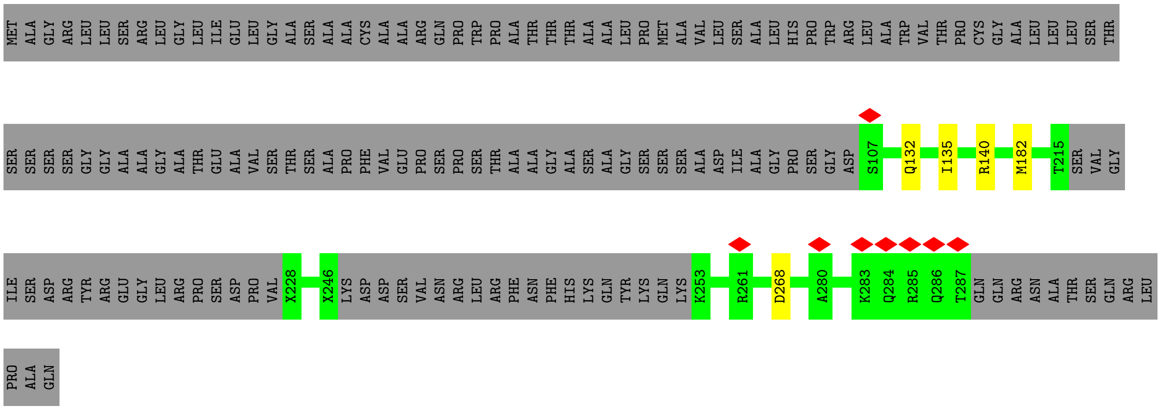




- Molecule 26: uS15m

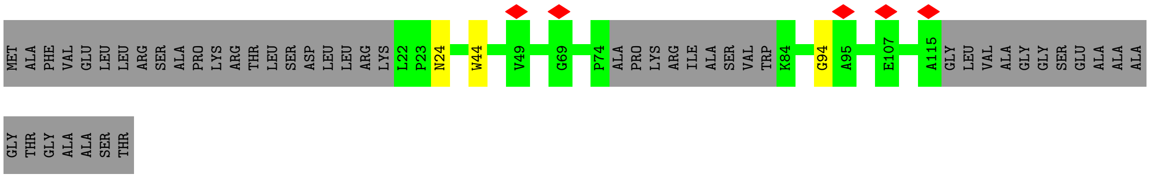
Chain o:





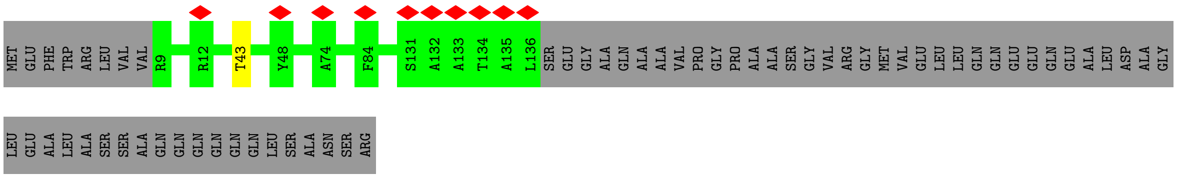
- Molecule 27: mS34

Chain z:



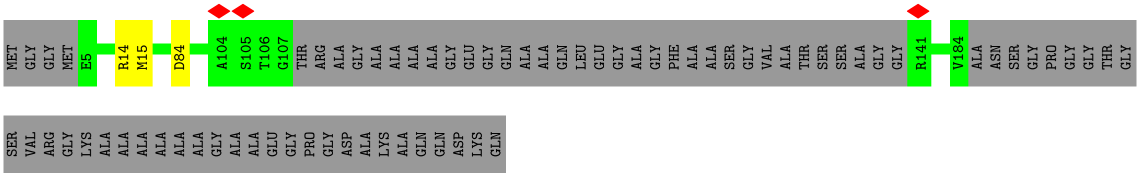
- Molecule 28: mS23

Chain v:

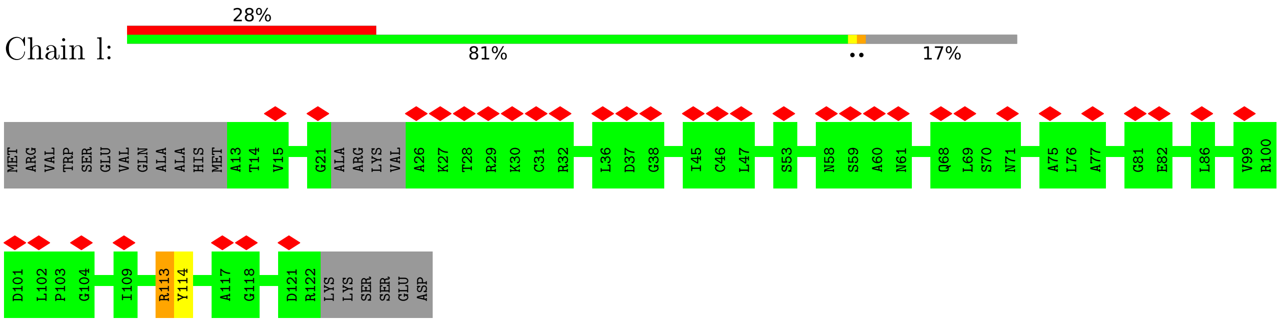


- Molecule 29: uS17m

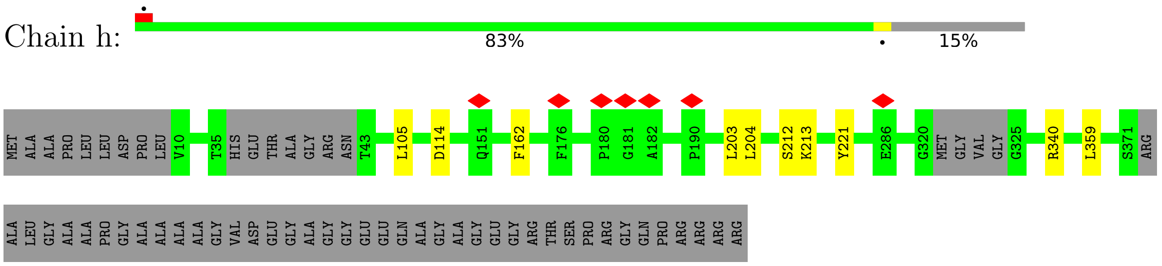
Chain q:



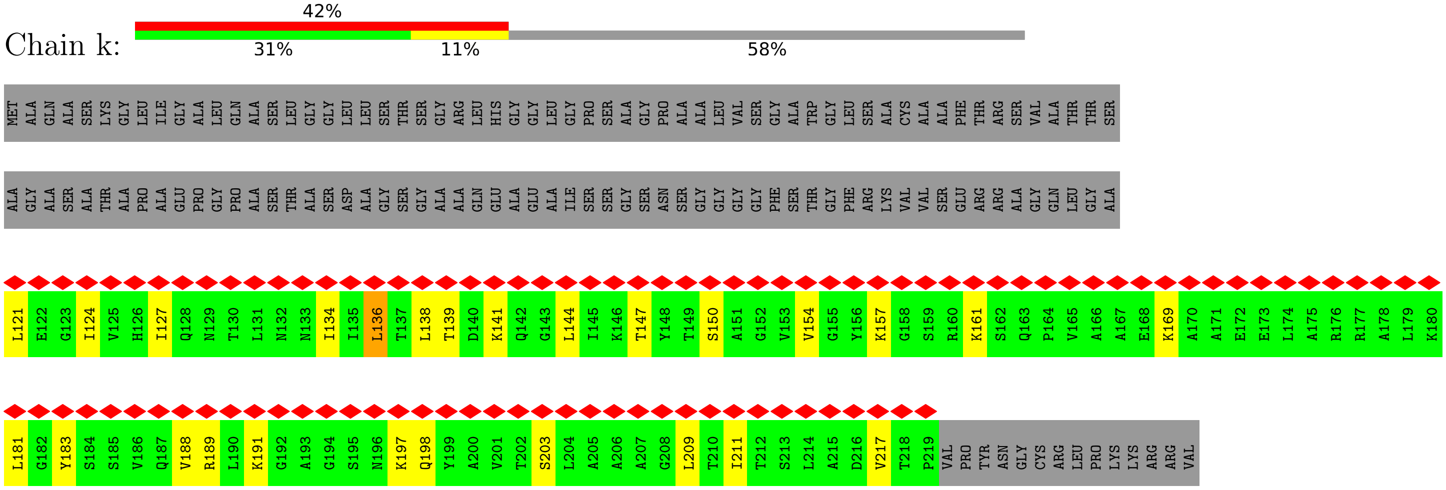
- Molecule 30: uS12m



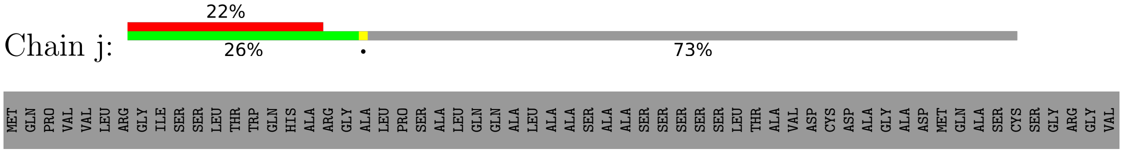
- Molecule 31: uS8m

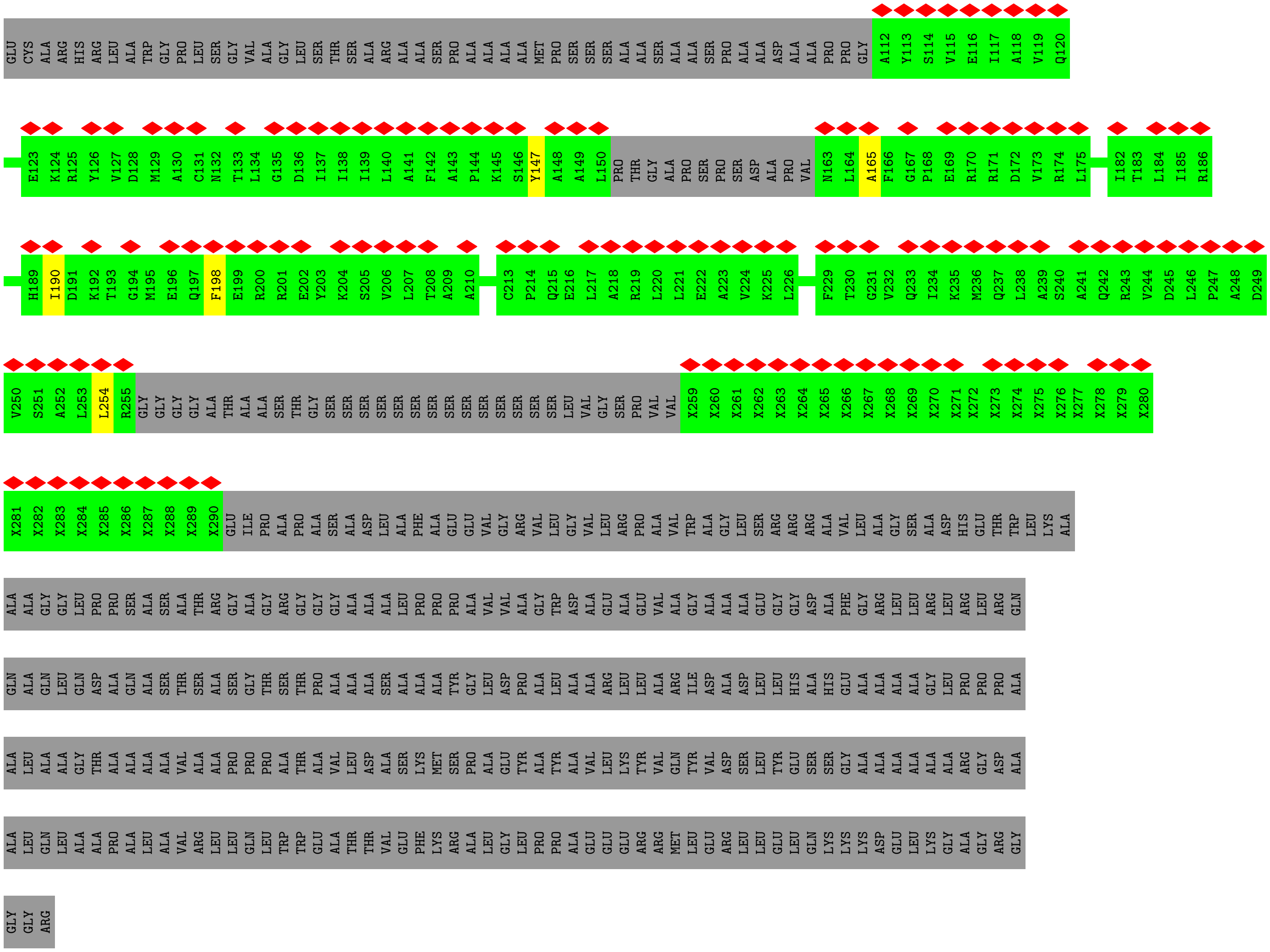


- Molecule 32: uS11m

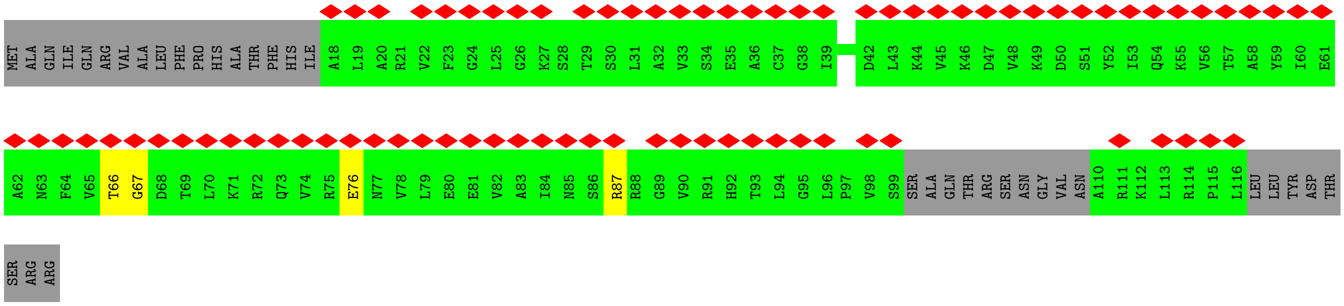


- Molecule 33: Ribosomal_S10 domain-containing protein

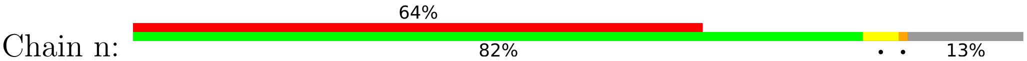


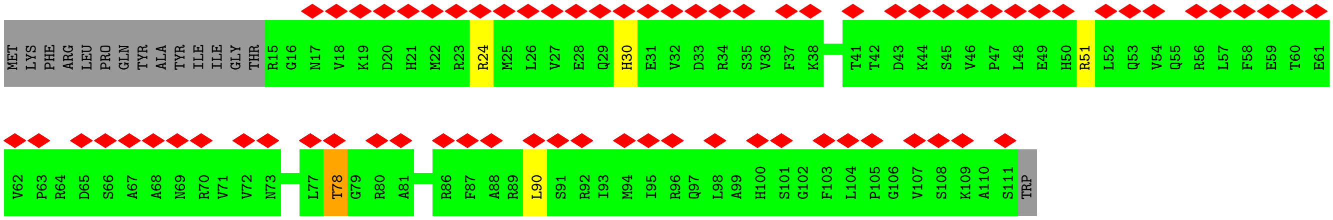


- Molecule 34: Mitochondrial ribosomal protein S13



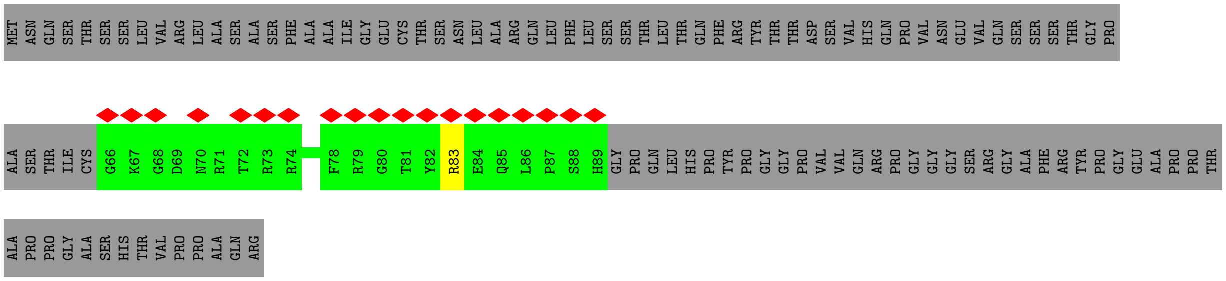
- Molecule 35: Mitochondrial ribosomal protein S14





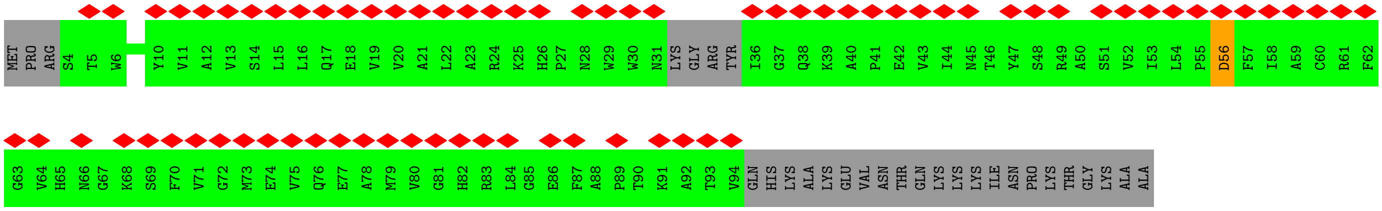
- Molecule 36: Plastid-specific ribosomal protein 4

Chain u:



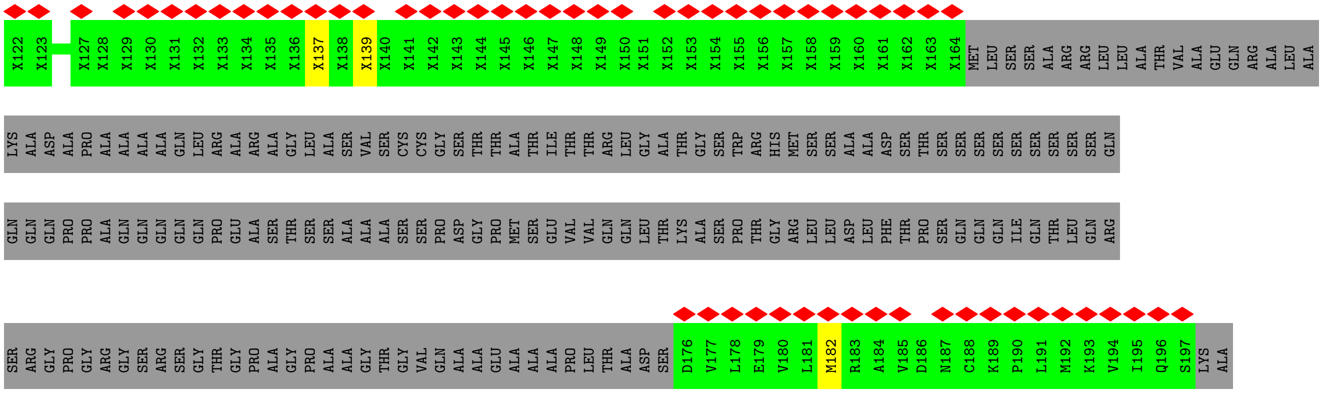
- Molecule 37: uS19m

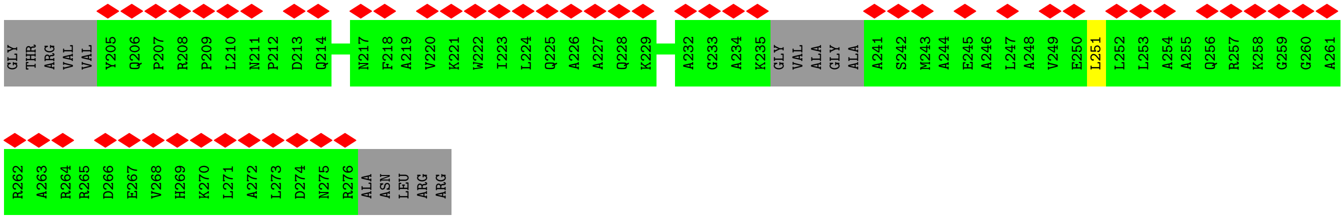
Chain s:



- Molecule 38: uS7m,Ribosomal_S7 domain-containing protein,Ribosomal_S7 domain-containing protein,Ribosomal_S7 domain-containing protein

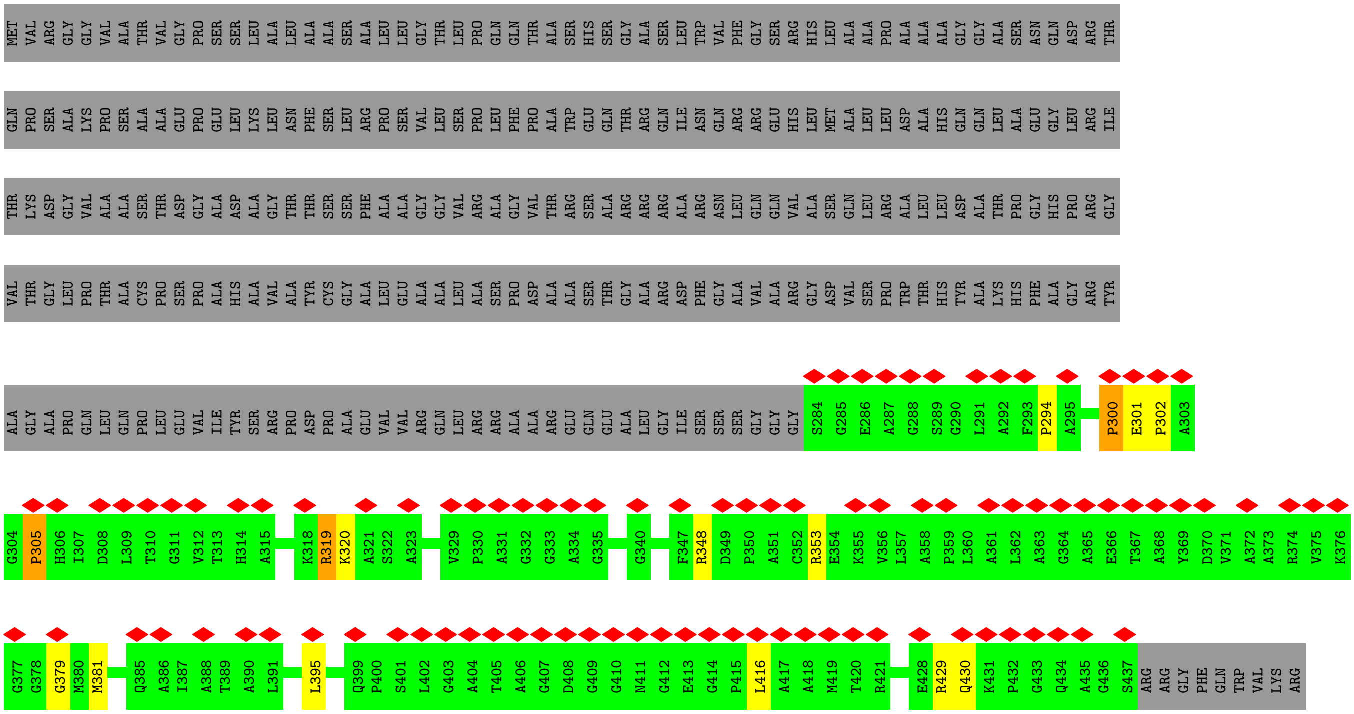
Chain g:





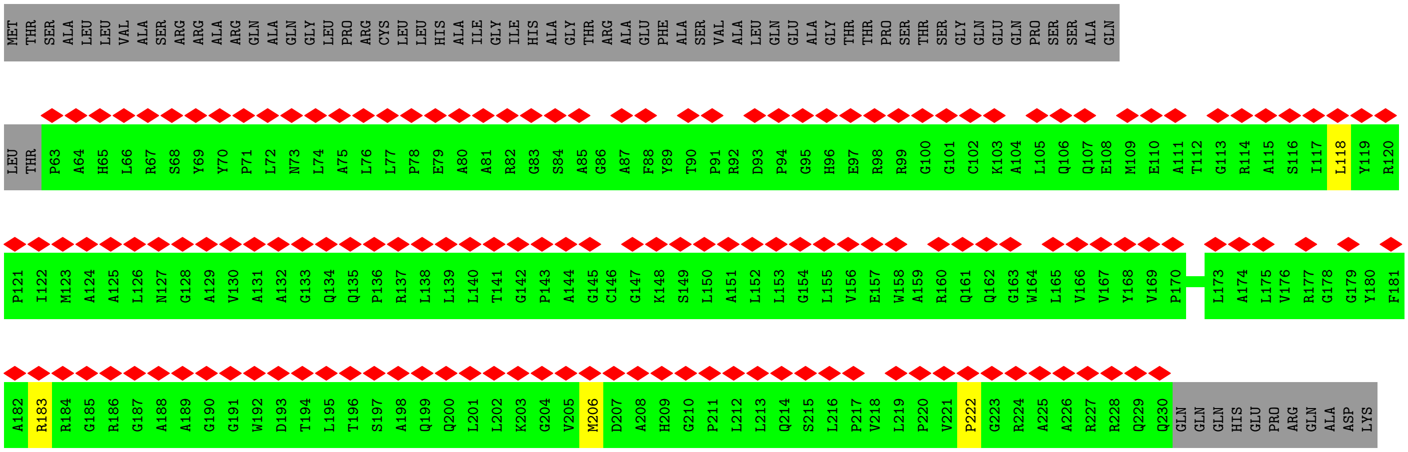
- Molecule 39: 30S ribosomal protein S9, chloroplastic

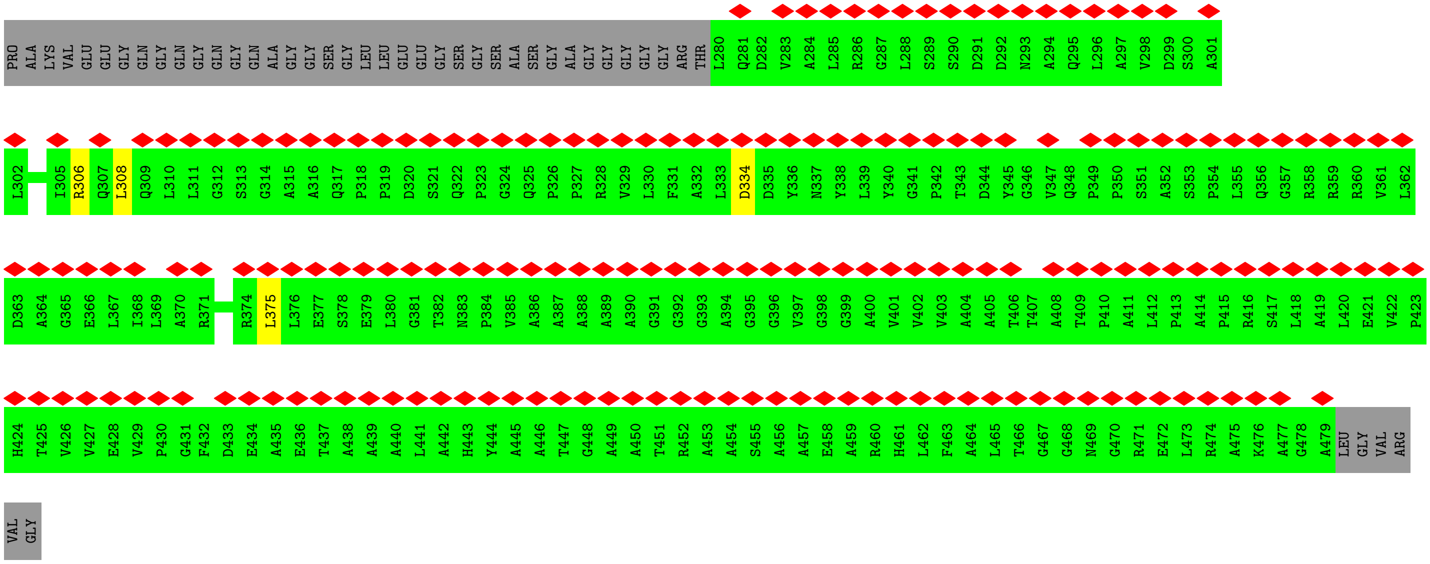
Chain i:



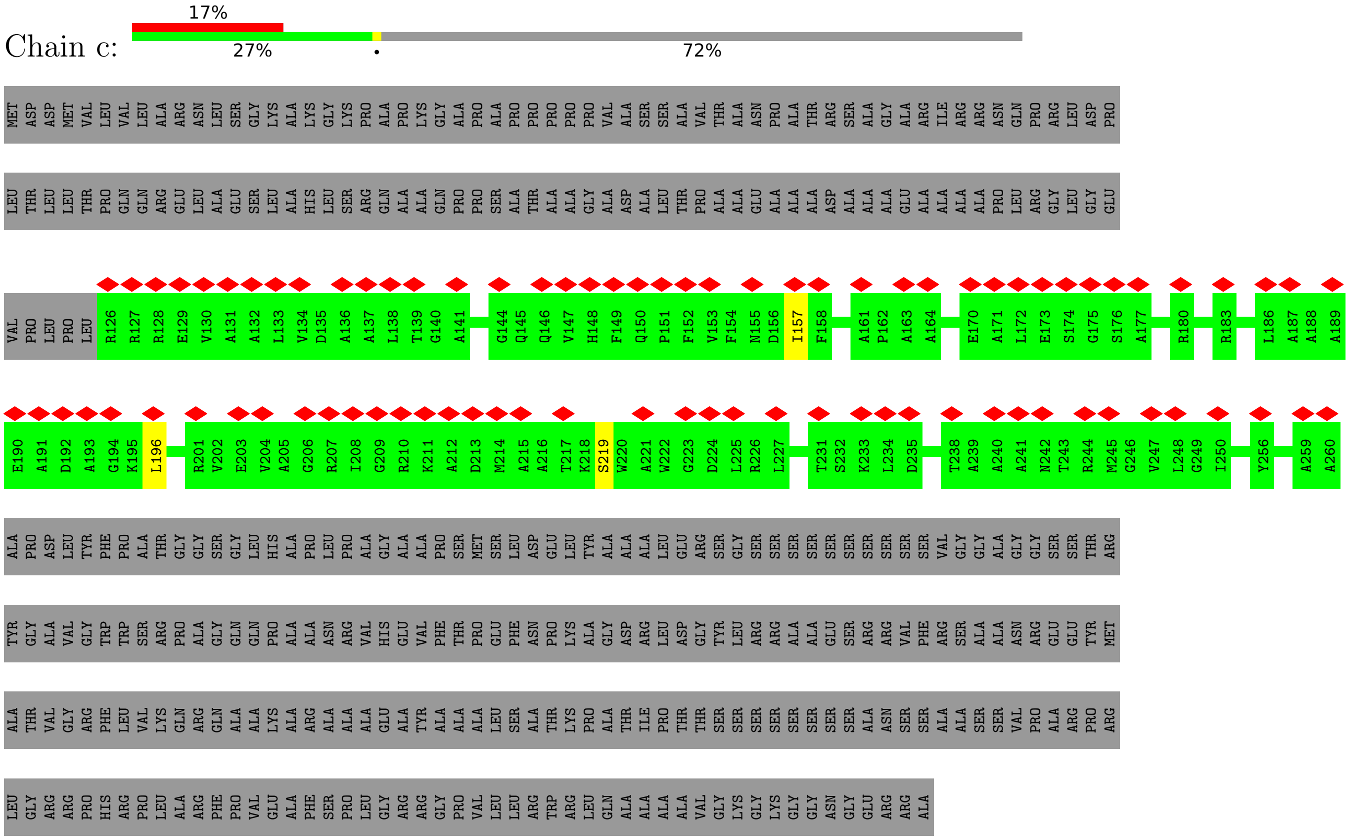
- Molecule 40: mS29

Chain x:

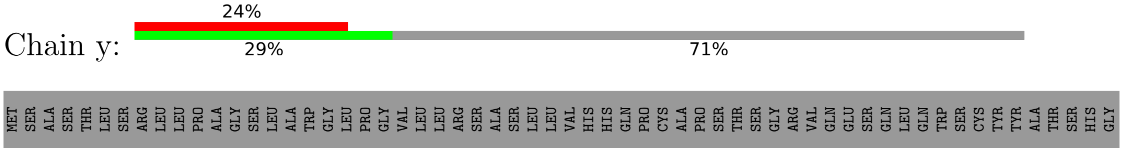


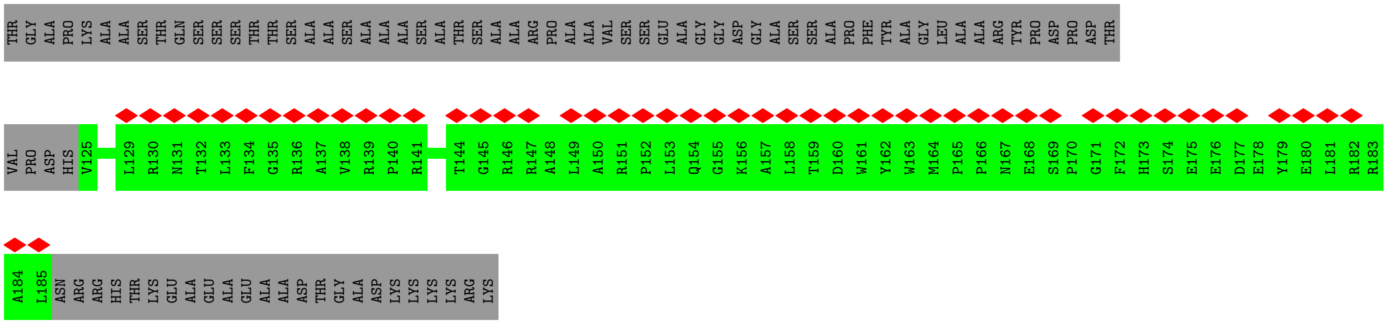


- Molecule 41: Ribosomal_S3_C domain-containing protein



- Molecule 42: mS33




THR GLY ALA PRO LYS ALA ALA SER THR GLN SER SER SER THR THR SER ALA ALA SER ALA ALA ALA SER ALA THR SER ALA ALA ARG PRO ALA ALA VAL SER SER GLU ALA GLY GLY ASP GLY ALA SER SER ALA PRO PHE TYR ALA GLY LEU ALA ALA ARG TYR PRO ASP PRO ASP THR
VAL PRO ASP HIS V125 L129 R130 N131 T132 L133 F134 G135 R136 A137 V138 R139 P140 R141 T144 G145 R146 R147 A148 L149 A150 R151 P152 L153 Q154 G155 K156 A157 L158 T159 D160 W161 Y162 W163 M164 P165 P166 N167 E168 S169 P170 G171 F172 H173 S174 E175 E176 D177 E178 Y179 E180 L181 R182 R183
A184 L185 ASN ARG ARG HIS THR LYS GLU ALA GLU ALA GLU ALA ALA ASP THR GLY ALA ASP LYS LYS LYS LYS ARG LYS

4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	40131	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose $(e^-/\text{Å}^2)$	45	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.082	Depositor
Minimum map value	-0.044	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	406.8, 406.8, 406.8	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.13, 1.13, 1.13	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	B	0.62	0/390	0.81	1/526 (0.2%)
2	C	0.38	0/2806	0.74	3/3811 (0.1%)
5	L	0.41	0/1399	0.69	1/1893 (0.1%)
5	M	0.44	0/1397	0.75	2/1891 (0.1%)
5	N	0.41	0/1416	0.75	4/1916 (0.2%)
6	O	0.33	0/1737	0.70	3/2357 (0.1%)
7	P	0.34	0/2647	0.67	3/3590 (0.1%)
14	d	0.61	0/934	0.87	1/1262 (0.1%)
15	f	0.65	0/845	0.89	0/1144
16	p	0.63	0/647	0.97	1/880 (0.1%)
17	r	0.40	0/469	1.05	2/633 (0.3%)
18	w	0.42	0/1263	0.79	4/1698 (0.2%)
19	1	0.48	0/2219	0.98	6/3455 (0.2%)
20	4	0.54	0/9843	0.97	12/15307 (0.1%)
21	2	0.47	0/5065	0.96	6/7891 (0.1%)
22	3	0.51	0/9410	0.98	24/14662 (0.2%)
23	a	0.37	0/1584	0.78	7/2146 (0.3%)
24	b	0.63	0/1865	0.91	4/2541 (0.2%)
25	e	0.50	0/1436	0.87	4/1941 (0.2%)
26	o	0.48	0/1209	0.90	4/1628 (0.2%)
27	z	0.39	0/687	0.75	0/935
28	v	0.40	0/1020	0.76	0/1380
29	q	0.47	0/1145	0.73	2/1549 (0.1%)
30	l	0.35	0/814	0.75	1/1088 (0.1%)
31	h	0.46	0/2764	0.82	9/3749 (0.2%)
32	k	0.43	0/735	0.82	2/994 (0.2%)
33	j	0.61	0/1068	0.87	1/1442 (0.1%)
34	m	0.58	0/690	0.97	2/926 (0.2%)
35	n	0.61	0/790	0.98	2/1059 (0.2%)
36	u	0.57	0/202	0.92	0/266
37	s	0.64	0/696	0.89	1/945 (0.1%)
38	g	0.50	0/700	0.94	2/938 (0.2%)
39	i	0.60	0/1031	1.03	10/1398 (0.7%)
40	x	0.49	0/2700	0.79	9/3682 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
41	c	0.55	0/1032	0.86	2/1399 (0.1%)
42	y	0.60	0/524	0.83	0/708
All	All	0.49	0/65179	0.89	135/93630 (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
2	C	0	6
6	O	0	1
13	Z	0	4
23	a	0	1
25	e	0	2
26	o	0	1
27	z	0	3
28	v	0	1
29	q	0	1
30	l	0	1
31	h	0	2
33	j	0	4
38	g	0	2
39	i	0	4
41	c	0	1
All	All	0	34

There are no bond length outliers.

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	204	ASP	CB-CG-OD1	9.48	126.83	118.30
22	3	6	U	N1-C2-O2	9.42	129.40	122.80
22	3	6	U	N3-C2-O2	-9.41	115.62	122.20
40	x	375	LEU	CB-CG-CD2	-9.38	95.05	111.00
34	m	87	ARG	CG-CD-NE	-9.26	92.35	111.80
22	3	6	U	C2-N1-C1'	9.18	128.71	117.70
26	o	135	ILE	CG1-CB-CG2	-8.74	92.17	111.40
2	C	861	LEU	CA-CB-CG	8.22	134.21	115.30
17	r	242	LEU	CA-CB-CG	8.16	134.07	115.30
29	q	84	ASP	CB-CG-OD1	7.95	125.45	118.30
40	x	183	ARG	NE-CZ-NH1	7.71	124.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	h	213	LYS	CA-CB-CG	7.71	130.35	113.40
39	i	429	ARG	CG-CD-NE	7.59	127.73	111.80
23	a	66	ARG	NE-CZ-NH2	7.48	124.04	120.30
5	L	204	ASP	CB-CG-OD1	7.45	125.01	118.30
31	h	114	ASP	CB-CG-OD1	7.23	124.81	118.30
16	p	34	ASN	N-CA-C	-7.04	91.98	111.00
23	a	65	LEU	CB-CG-CD2	-7.03	99.05	111.00
40	x	118	LEU	CB-CG-CD2	-6.93	99.21	111.00
22	3	188	C	C2-N1-C1'	6.93	126.42	118.80
20	4	223	U	C2-N1-C1'	6.85	125.92	117.70
39	i	429	ARG	CB-CG-CD	-6.85	93.79	111.60
39	i	381	MET	CB-CG-SD	-6.75	92.14	112.40
22	3	290	U	C2-N1-C1'	6.71	125.75	117.70
26	o	268	ASP	CB-CG-OD1	6.69	124.32	118.30
39	i	305	PRO	N-CA-CB	6.60	111.22	103.30
21	2	154	U	C2-N1-C1'	6.57	125.58	117.70
22	3	290	U	N1-C1'-C2'	6.55	122.52	114.00
41	c	157	ILE	CG1-CB-CG2	-6.55	96.99	111.40
7	P	91	LEU	CB-CG-CD2	6.54	122.12	111.00
24	b	181	PHE	CB-CA-C	-6.48	97.44	110.40
21	2	183	U	C2-N1-C1'	6.47	125.46	117.70
22	3	289	C	C2-N1-C1'	6.46	125.91	118.80
22	3	171	G	C4-N9-C1'	6.44	134.88	126.50
41	c	196	LEU	CA-CB-CG	6.43	130.10	115.30
25	e	264	LEU	CA-CB-CG	-6.43	100.50	115.30
32	k	209	LEU	N-CA-C	-6.43	93.64	111.00
20	4	223	U	N1-C1'-C2'	6.39	122.30	114.00
29	q	15	MET	CB-CG-SD	-6.37	93.30	112.40
40	x	334	ASP	CB-CG-OD1	6.35	124.02	118.30
40	x	222	PRO	N-CA-CB	6.26	110.82	103.30
19	1	4	U	C2-N1-C1'	6.25	125.20	117.70
5	N	214	LEU	CA-CB-CG	6.22	129.60	115.30
6	O	278	LEU	CA-CB-CG	6.15	129.44	115.30
24	b	120	PRO	N-CA-CB	6.15	110.67	103.30
22	3	264	G	N3-C4-N9	-6.14	122.32	126.00
1	B	829	PRO	N-CA-CB	6.02	110.53	103.30
6	O	325	LEU	CA-CB-CG	5.97	129.03	115.30
22	3	71	C	C2-N1-C1'	5.96	125.36	118.80
31	h	340	ARG	NE-CZ-NH1	5.93	123.27	120.30
18	w	103	LEU	CA-CB-CG	5.89	128.85	115.30
5	M	202	LEU	CA-CB-CG	5.84	128.74	115.30
20	4	170	G	O4'-C1'-N9	5.84	112.88	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	3	188	C	C6-N1-C1’	-5.82	113.81	120.80
19	1	97	G	N3-C4-N9	-5.80	122.52	126.00
22	3	6	U	C6-N1-C1’	-5.79	113.10	121.20
5	M	83	ASP	CB-CG-OD1	5.78	123.50	118.30
23	a	54	PRO	N-CA-CB	5.77	110.22	103.30
23	a	147	TYR	C-N-CA	5.77	136.11	121.70
14	d	278	PRO	N-CA-CB	5.76	110.22	103.30
20	4	139	A	C2’-C3’-O3’	5.76	122.92	113.70
20	4	342	G	C4-N9-C1’	5.75	133.98	126.50
22	3	264	G	C4-N9-C1’	-5.71	119.08	126.50
22	3	171	G	C8-N9-C1’	-5.71	119.58	127.00
35	n	78	THR	N-CA-CB	5.69	121.11	110.30
30	l	113	ARG	C-N-CA	5.69	135.91	121.70
39	i	416	LEU	CA-CB-CG	5.68	128.38	115.30
23	a	70	ARG	NE-CZ-NH2	-5.68	117.46	120.30
39	i	320	LYS	N-CA-C	-5.68	95.67	111.00
40	x	306	ARG	NE-CZ-NH1	-5.67	117.47	120.30
39	i	302	PRO	N-CA-CB	5.66	110.09	103.30
22	3	318	C	C2-N1-C1’	5.65	125.01	118.80
2	C	400	LEU	CA-CB-CG	5.64	128.28	115.30
7	P	43	LEU	CA-CB-CG	5.60	128.17	115.30
6	O	342	LEU	CA-CB-CG	5.56	128.08	115.30
22	3	264	G	C8-N9-C1’	5.54	134.21	127.00
25	e	274	ARG	NE-CZ-NH2	-5.54	117.53	120.30
32	k	136	LEU	CA-CB-CG	5.53	128.01	115.30
26	o	132	GLN	CA-CB-CG	5.52	125.55	113.40
24	b	203	LYS	CB-CA-C	5.52	121.44	110.40
20	4	325	G	C4-N9-C1’	5.52	133.68	126.50
31	h	203	LEU	CA-CB-CG	5.51	127.97	115.30
39	i	294	PRO	N-CA-CB	5.49	109.89	103.30
19	1	44	U	C2’-C3’-O3’	5.48	122.47	113.70
39	i	300	PRO	N-CA-CB	5.47	109.86	103.30
20	4	223	U	C6-N1-C1’	-5.46	113.55	121.20
18	w	63	LEU	CA-CB-CG	5.46	127.85	115.30
38	g	251	LEU	CA-CB-CG	5.46	127.85	115.30
35	n	30	HIS	N-CA-C	-5.45	96.27	111.00
19	1	43	G	C4-N9-C1’	5.42	133.55	126.50
5	N	113	LEU	CA-CB-CG	5.39	127.70	115.30
25	e	343	MET	CA-CB-CG	5.39	122.46	113.30
39	i	395	LEU	CB-CG-CD2	-5.39	101.84	111.00
20	4	139	A	P-O3’-C3’	5.38	126.16	119.70
21	2	44	U	C2-N1-C1’	5.36	124.14	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	168	LEU	CA-CB-CG	5.36	127.64	115.30
19	1	4	U	N1-C1'-C2'	5.36	120.96	114.00
34	m	76	GLU	N-CA-CB	5.34	120.22	110.60
20	4	301	G	O4'-C1'-N9	5.34	112.47	108.20
22	3	289	C	C6-N1-C1'	-5.33	114.40	120.80
18	w	155	LEU	CA-CB-CG	5.31	127.50	115.30
22	3	75	A	C4-N9-C1'	5.30	135.85	126.30
22	3	357	U	C2-N1-C1'	5.29	124.05	117.70
31	h	204	LEU	CA-CB-CG	5.29	127.47	115.30
5	N	202	LEU	CA-CB-CG	5.28	127.45	115.30
37	s	56	ASP	CB-CA-C	5.26	120.93	110.40
22	3	187	C	C2-N1-C1'	5.26	124.59	118.80
20	4	20	G	N7-C8-N9	5.25	115.72	113.10
31	h	204	LEU	CB-CG-CD2	-5.24	102.09	111.00
21	2	183	U	C6-N1-C1'	-5.22	113.89	121.20
18	w	73	GLU	N-CA-CB	5.21	119.98	110.60
22	3	75	A	C8-N9-C1'	-5.20	118.35	127.70
21	2	83	C	C2-N1-C1'	5.19	124.51	118.80
31	h	162	PHE	CB-CG-CD1	5.19	124.43	120.80
2	C	571	LEU	CA-CB-CG	5.17	127.20	115.30
22	3	71	C	O4'-C1'-N1	5.17	112.34	108.20
40	x	183	ARG	NE-CZ-NH2	-5.16	117.72	120.30
19	1	17	C	C2-N1-C1'	5.16	124.47	118.80
31	h	105	LEU	CA-CB-CG	5.14	127.13	115.30
24	b	182	ASP	N-CA-CB	5.14	119.86	110.60
25	e	280	MET	CG-SD-CE	-5.14	91.98	100.20
26	o	182	MET	CB-CG-SD	5.13	127.78	112.40
23	a	70	ARG	NE-CZ-NH1	5.11	122.86	120.30
33	j	254	LEU	CA-CB-CG	5.10	127.04	115.30
40	x	206	MET	CA-CB-CG	5.10	121.97	113.30
20	4	354	G	C4-N9-C1'	5.10	133.12	126.50
20	4	217	U	N1-C1'-C2'	5.08	120.60	114.00
22	3	71	C	C6-N1-C1'	-5.08	114.71	120.80
22	3	393	U	C2-N1-C1'	5.07	123.79	117.70
38	g	182	MET	CB-CG-SD	5.07	127.61	112.40
17	r	272	LEU	CA-CB-CG	5.07	126.96	115.30
31	h	359	LEU	CA-CB-CG	5.07	126.96	115.30
40	x	308	LEU	CB-CG-CD2	5.05	119.58	111.00
21	2	154	U	C6-N1-C1'	-5.04	114.15	121.20
7	P	62	MET	CB-CG-SD	5.01	127.43	112.40

There are no chirality outliers.

All (34) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	401	SER	Peptide
2	C	866	ALA	Peptide
2	C	867	PHE	Peptide
2	C	929	PRO	Peptide
2	C	931	ASN	Peptide
2	C	932	LEU	Peptide
6	O	323	ASP	Peptide
13	Z	107	UNK	Peptide
13	Z	12	UNK	Peptide
13	Z	477	UNK	Peptide
13	Z	9	UNK	Peptide
23	a	71	PHE	Peptide
41	c	219	SER	Peptide
25	e	272	PHE	Peptide
25	e	349	PHE	Peptide
38	g	137	UNK	Peptide
38	g	139	UNK	Peptide
31	h	212	SER	Peptide
31	h	221	TYR	Peptide
39	i	319	ARG	Peptide
39	i	348	ARG	Peptide
39	i	379	GLY	Peptide
39	i	430	GLN	Peptide
33	j	147	TYR	Peptide
33	j	165	ALA	Peptide
33	j	190	ILE	Peptide
33	j	198	PHE	Peptide
30	l	113	ARG	Peptide
26	o	140	ARG	Peptide
29	q	14	ARG	Peptide
28	v	43	THR	Peptide
27	z	24	ASN	Peptide
27	z	44	TRP	Peptide
27	z	94	GLY	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	386	0	364	4	0
2	C	2766	0	2848	38	0
3	D	2125	0	461	7	0
4	K	930	0	193	3	0
5	L	1373	0	1304	41	0
5	M	1370	0	1302	25	0
5	N	1479	0	1339	28	0
6	O	1710	0	1751	19	0
7	P	2601	0	2693	42	0
8	U	165	0	38	3	0
9	V	760	0	169	6	0
10	W	270	0	67	2	0
11	X	405	0	93	1	0
12	Y	540	0	114	2	0
13	Z	2855	0	640	8	0
14	d	923	0	891	0	0
15	f	824	0	831	0	0
16	p	627	0	610	0	0
17	r	459	0	490	0	0
18	w	1245	0	1212	0	0
19	1	1986	0	1000	20	0
20	4	8811	0	4439	91	0
21	2	4533	0	2289	45	0
22	3	8405	0	4237	85	0
23	a	1562	0	1533	0	0
24	b	1824	0	1798	0	0
25	e	1403	0	1415	0	0
26	o	1284	0	1233	0	0
27	z	667	0	645	0	0
28	v	1003	0	1039	0	0
29	q	1128	0	1171	0	0
30	l	805	0	859	0	0
31	h	2711	0	2759	0	0
32	k	729	0	773	0	0
33	j	1211	0	1120	0	0
34	m	685	0	729	0	0
35	n	779	0	806	0	0
36	u	199	0	199	0	0
37	s	678	0	677	0	0
38	g	909	0	774	0	0
39	i	1019	0	976	0	0
40	x	2647	0	2649	0	0
41	c	1012	0	1013	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	y	510	0	499	0	0
All	All	70313	0	52042	426	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (426) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:162:UNK:CB	20:4:48:U:C2'	2.19	1.20
20:4:299:U:H3	22:3:343:A:H61	1.09	0.98
9:V:162:UNK:CB	20:4:48:U:O2'	2.12	0.97
9:V:162:UNK:CB	20:4:48:U:H2'	1.91	0.96
20:4:138:C:H42	20:4:152:A:N6	1.63	0.96
20:4:138:C:N4	20:4:152:A:H62	1.66	0.93
21:2:180:C:N4	21:2:198:A:H62	1.67	0.92
21:2:180:C:H42	21:2:198:A:H62	0.94	0.91
20:4:345:A:H62	20:4:379:G:H21	1.19	0.89
9:V:162:UNK:CB	20:4:48:U:C3'	2.50	0.89
21:2:180:C:H42	21:2:198:A:N6	1.74	0.85
20:4:259:U:H3	20:4:286:A:H62	1.20	0.84
20:4:101:A:H62	22:3:405:U:H3	1.24	0.84
19:1:19:G:H21	22:3:328:A:H62	1.23	0.83
20:4:345:A:H62	20:4:379:G:N2	1.77	0.81
22:3:126:G:H1	22:3:170:A:H2	1.27	0.80
9:V:162:UNK:CB	20:4:48:U:H3'	2.12	0.79
4:K:129:UNK:O	4:K:133:UNK:N	2.16	0.78
22:3:126:G:N1	22:3:170:A:C2	2.49	0.78
20:4:345:A:N6	20:4:379:G:H21	1.82	0.77
6:O:482:GLY:O	6:O:486:ALA:HB3	1.84	0.77
22:3:32:A:H62	22:3:41:G:N2	1.88	0.71
20:4:259:U:H2'	20:4:260:A:H8	1.56	0.70
20:4:138:C:H42	20:4:152:A:H62	0.82	0.70
5:M:155:VAL:HB	5:M:166:PHE:HB2	1.75	0.69
19:1:19:G:N2	22:3:328:A:H62	1.91	0.68
5:M:126:ASN:HB2	5:M:156:SER:HB2	1.74	0.68
2:C:377:ARG:NH1	3:D:345:UNK:O	2.28	0.67
5:N:163:VAL:HG23	5:N:185:LYS:HG2	1.76	0.66
7:P:158:ARG:HH22	20:4:359:A:H4'	1.60	0.66
5:N:129:LEU:HD11	5:N:227:LEU:HD22	1.79	0.65
5:N:112:THR:HB	5:N:131:VAL:H	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:566:PRO:HA	2:C:569:ARG:HD2	1.78	0.64
22:3:32:A:N6	22:3:41:G:H21	1.96	0.64
6:O:507:LEU:HD23	6:O:510:LYS:HD3	1.80	0.63
21:2:9:A:H61	21:2:30:G:H1	1.45	0.63
5:L:123:GLU:HG2	5:L:159:LYS:HD3	1.81	0.63
20:4:19:U:H2'	20:4:20:G:H8	1.65	0.62
20:4:392:U:H2'	20:4:393:A:H8	1.64	0.62
2:C:904:ARG:HH22	2:C:974:VAL:HG22	1.65	0.62
20:4:260:A:H61	20:4:285:G:H1'	1.64	0.61
21:2:130:A:H61	21:2:140:G:H1	1.48	0.61
22:3:167:G:H2'	22:3:168:A:H8	1.66	0.61
5:N:155:VAL:HB	5:N:166:PHE:HB2	1.82	0.61
5:N:123:GLU:OE2	5:N:217:ARG:NH2	2.33	0.60
5:N:162:ARG:HD2	5:N:182:LEU:HD11	1.84	0.60
5:L:157:VAL:HB	5:L:164:LEU:HB3	1.83	0.60
19:1:19:G:H21	22:3:328:A:N6	1.98	0.60
22:3:131:A:N1	22:3:166:G:N2	2.50	0.60
6:O:309:GLY:O	6:O:313:ALA:HB2	2.03	0.59
7:P:226:GLY:HA2	7:P:290:ASN:HD22	1.67	0.59
20:4:259:U:H3	20:4:286:A:N6	1.96	0.59
5:M:157:VAL:HB	5:M:164:LEU:HB2	1.85	0.59
7:P:386:ARG:NH2	7:P:409:TYR:OH	2.36	0.59
8:U:28:UNK:O	8:U:30:UNK:N	2.36	0.59
5:N:148:ILE:O	5:N:228:ARG:NH1	2.36	0.58
22:3:32:A:N6	22:3:41:G:N2	2.50	0.58
7:P:38:GLY:O	7:P:68:ARG:NH2	2.36	0.58
20:4:332:G:H1	20:4:392:U:H3	1.51	0.58
19:1:46:G:H3'	19:1:47:U:H4'	1.84	0.58
5:L:154:ASN:HA	5:L:167:GLU:HA	1.84	0.58
10:W:33:UNK:C	10:W:35:UNK:N	2.61	0.58
2:C:315:ARG:NH2	2:C:317:GLN:OE1	2.36	0.58
22:3:243:G:N7	22:3:244:A:N6	2.52	0.58
5:N:114:LEU:HD11	5:N:234:LYS:HE2	1.86	0.57
5:N:124:GLU:HB3	5:N:158:ALA:HB3	1.86	0.57
13:Z:204:UNK:O	13:Z:208:UNK:N	2.37	0.57
20:4:104:G:H1	22:3:403:U:H3	1.51	0.57
2:C:365:ARG:HE	2:C:369:ALA:HA	1.70	0.57
20:4:336:U:H3	20:4:387:G:H1	1.53	0.57
1:B:847:THR:HB	1:B:856:ASN:HB3	1.86	0.57
22:3:126:G:N1	22:3:170:A:H2	1.94	0.56
7:P:216:ARG:HD3	7:P:320:LEU:HD23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:395:GLY:H	7:P:399:GLU:HG2	1.70	0.56
22:3:305:U:H2’	22:3:306:A:H8	1.71	0.56
22:3:360:A:H2’	22:3:361:A:C8	2.41	0.56
2:C:380:LEU:O	2:C:384:MET:HB3	2.06	0.55
22:3:312:G:N2	22:3:315:A:OP2	2.40	0.55
13:Z:281:UNK:O	13:Z:285:UNK:N	2.40	0.55
5:L:130:HIS:NE2	5:N:191:GLU:OE1	2.36	0.55
7:P:40:ARG:HH12	21:2:63:C:H5’	1.70	0.55
22:3:239:A:N6	22:3:245:G:OP2	2.40	0.55
7:P:220:LEU:HD21	7:P:320:LEU:HG	1.89	0.55
21:2:56:G:O6	21:2:85:A:N6	2.40	0.55
2:C:281:ASP:OD1	2:C:281:ASP:N	2.40	0.54
20:4:259:U:C2	20:4:286:A:N6	2.68	0.54
20:4:129:G:H2’	20:4:130:G:H8	1.71	0.54
7:P:33:LEU:HD22	7:P:57:PHE:HE1	1.73	0.54
7:P:326:GLY:HA3	7:P:370:THR:HG22	1.90	0.54
7:P:30:PRO:HA	7:P:33:LEU:HD12	1.88	0.54
19:1:65:U:O2	19:1:74:G:N2	2.41	0.54
20:4:169:G:H21	20:4:244:A:H62	1.54	0.54
20:4:347:A:O2’	20:4:377:A:N6	2.40	0.54
22:3:126:G:O6	22:3:170:A:N1	2.41	0.54
13:Z:498:UNK:O	13:Z:502:UNK:N	2.41	0.54
20:4:232:U:H3’	20:4:233:A:H2’	1.90	0.54
20:4:267:G:H2’	20:4:268:A:C8	2.43	0.54
5:L:162:ARG:HH21	5:L:182:LEU:HG	1.73	0.53
20:4:258:G:N2	20:4:286:A:OP2	2.41	0.53
22:3:58:C:H4’	22:3:60:G:H4’	1.89	0.53
1:B:847:THR:HB	1:B:856:ASN:HD22	1.74	0.53
20:4:21:A:H2’	20:4:22:A:C4	2.44	0.53
20:4:300:U:H2’	20:4:301:G:C8	2.43	0.53
6:O:460:GLY:HA2	6:O:492:LEU:HD11	1.90	0.53
22:3:36:G:H2’	22:3:37:G:H8	1.72	0.53
2:C:365:ARG:NH2	2:C:368:PRO:O	2.40	0.53
5:L:192:SER:O	5:M:112:THR:OG1	2.26	0.53
22:3:106:G:N2	22:3:205:A:N1	2.56	0.53
22:3:316:C:H2’	22:3:317:A:H8	1.73	0.53
5:L:124:GLU:HB3	5:L:158:ALA:HB3	1.91	0.53
7:P:71:HIS:NE2	7:P:75:GLN:OE1	2.42	0.53
22:3:118:A:H1’	22:3:186:A:H5’	1.90	0.53
22:3:346:G:H2’	22:3:347:A:C8	2.44	0.53
20:4:336:U:O2	20:4:387:G:N2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:O:285:ARG:HH12	6:O:289:LEU:HG	1.74	0.52
7:P:368:VAL:HA	7:P:371:LEU:HD12	1.92	0.52
2:C:482:PRO:HA	2:C:485:GLN:HG2	1.91	0.52
7:P:197:ASP:OD1	7:P:289:ARG:NH1	2.43	0.52
5:L:126:ASN:HB2	5:L:156:SER:HB2	1.90	0.52
5:L:163:VAL:HG23	5:L:185:LYS:HA	1.90	0.52
2:C:478:VAL:O	2:C:485:GLN:NE2	2.33	0.52
20:4:259:U:H2’	20:4:260:A:C8	2.39	0.52
20:4:19:U:H2’	20:4:20:G:C8	2.44	0.52
2:C:481:SER:O	2:C:485:GLN:NE2	2.38	0.52
19:1:98:U:H3	21:2:38:C:H42	1.58	0.51
7:P:108:ILE:HD12	7:P:152:LEU:HD22	1.92	0.51
5:M:209:GLN:HB3	5:N:74:LEU:HD13	1.91	0.51
22:3:366:C:OP1	22:3:386:C:N4	2.37	0.51
20:4:118:C:H2’	20:4:119:G:H8	1.75	0.51
7:P:227:PRO:O	7:P:287:GLN:NE2	2.44	0.51
13:Z:230:UNK:O	13:Z:234:UNK:N	2.43	0.51
21:2:103:G:H22	21:2:115:C:H5’	1.74	0.51
22:3:262:C:H1’	22:3:313:C:H41	1.76	0.51
6:O:381:ALA:HA	6:O:384:LEU:HD12	1.93	0.51
22:3:29:G:H22	22:3:45:A:H5’	1.75	0.51
9:V:49:UNK:O	9:V:53:UNK:N	2.44	0.51
7:P:96:ARG:HA	7:P:100:LEU:HD12	1.91	0.51
19:1:82:G:H1’	21:2:162:G:H5’	1.93	0.51
20:4:135:C:H2’	20:4:136:C:H4’	1.93	0.51
5:L:74:LEU:O	5:L:78:LEU:HB2	2.11	0.50
5:M:226:TYR:O	5:M:230:LEU:HB2	2.11	0.50
7:P:59:THR:HG21	7:P:108:ILE:HD13	1.92	0.50
5:L:84:TYR:HA	5:L:87:LYS:HE3	1.94	0.50
21:2:192:C:H5”	21:2:193:G:H5”	1.93	0.50
5:L:73:SER:OG	5:L:74:LEU:N	2.45	0.50
19:1:19:G:H2’	19:1:20:G:H8	1.75	0.50
2:C:939:PRO:HB3	2:C:960:ALA:HA	1.93	0.50
5:M:118:ARG:NH1	5:M:217:ARG:O	2.44	0.50
7:P:157:THR:OG1	7:P:198:ARG:NH1	2.44	0.50
20:4:116:G:H1	22:3:367:U:H3	1.59	0.50
22:3:66:A:H2’	22:3:67:G:C8	2.47	0.50
5:L:212:LYS:O	5:L:216:ASP:CB	2.60	0.50
5:M:225:GLU:OE1	5:M:228:ARG:NH2	2.44	0.50
3:D:261:UNK:HA	3:D:265:UNK:HA	1.94	0.50
5:L:91:ARG:NH2	5:L:95:ILE:O	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:106:THR:O	5:M:115:THR:OG1	2.29	0.50
20:4:230:A:O2’	20:4:234:G:N7	2.41	0.50
20:4:310:U:O2	20:4:415:G:N2	2.45	0.50
2:C:282:GLY:O	2:C:318:ARG:NH1	2.45	0.49
5:L:130:HIS:HB3	5:L:133:SER:HB2	1.94	0.49
22:3:66:A:H2’	22:3:67:G:H8	1.76	0.49
21:2:57:C:O2’	21:2:88:G:N2	2.45	0.49
22:3:57:U:O2’	22:3:61:U:OP1	2.30	0.49
2:C:494:ARG:HH22	2:C:574:LEU:HA	1.76	0.49
5:L:149:SER:HA	5:L:228:ARG:HH21	1.78	0.49
5:L:166:PHE:HE1	5:L:180:VAL:HG23	1.77	0.49
7:P:109:THR:HG21	7:P:170:ARG:HG3	1.94	0.49
19:1:48:U:H4’	19:1:49:U:H5”	1.93	0.49
5:L:213:TYR:O	5:L:217:ARG:NH1	2.40	0.49
5:N:107:GLU:OE1	5:N:234:LYS:NZ	2.43	0.49
5:M:191:GLU:O	5:N:130:HIS:NE2	2.40	0.49
20:4:10:U:H3	20:4:95:G:H1	1.59	0.49
20:4:282:G:H2’	20:4:283:G:H8	1.77	0.49
20:4:303:G:O6	22:3:339:A:N6	2.45	0.49
13:Z:508:UNK:O	13:Z:512:UNK:N	2.46	0.48
20:4:7:C:O2’	20:4:103:A:OP1	2.31	0.48
20:4:178:U:O2’	20:4:181:A:O4’	2.30	0.48
22:3:362:U:H2’	22:3:363:A:H8	1.77	0.48
6:O:278:LEU:O	6:O:282:ARG:CB	2.61	0.48
3:D:456:UNK:O	3:D:460:UNK:N	2.47	0.48
5:N:116:LEU:HB2	5:N:127:VAL:HB	1.94	0.48
7:P:289:ARG:NH2	7:P:290:ASN:OD1	2.46	0.48
22:3:140:A:H2	22:3:153:G:H21	1.62	0.48
1:B:847:THR:HG22	1:B:860:LEU:HD13	1.96	0.48
2:C:350:VAL:HG12	3:D:298:UNK:O	2.14	0.48
12:Y:46:UNK:O	12:Y:50:UNK:CB	2.61	0.48
20:4:57:A:H2’	20:4:58:A:H8	1.79	0.48
20:4:325:G:H3’	20:4:326:A:H8	1.79	0.48
5:L:91:ARG:HH12	5:L:96:SER:HA	1.79	0.48
11:X:17:UNK:O	11:X:19:UNK:N	2.46	0.48
5:L:78:LEU:HD22	5:L:247:GLU:HB2	1.95	0.48
20:4:415:G:N3	20:4:416:G:N2	2.62	0.48
21:2:143:C:H2’	21:2:144:A:H8	1.79	0.48
21:2:84:C:H2’	21:2:85:A:C8	2.49	0.47
22:3:364:U:H2’	22:3:365:G:H8	1.79	0.47
5:M:138:GLU:OE1	5:N:42:UNK:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:75:SER:HA	5:N:78:LEU:HD12	1.95	0.47
13:Z:211:UNK:O	13:Z:215:UNK:N	2.47	0.47
22:3:111:C:H2'	22:3:112:A:H8	1.79	0.47
22:3:348:G:N3	22:3:352:C:N4	2.59	0.47
19:1:19:G:H5'	22:3:85:C:H42	1.80	0.47
19:1:30:C:N4	21:2:174:U:O4'	2.47	0.47
21:2:190:A:H3'	21:2:191:A:H8	1.80	0.47
22:3:24:C:H2'	22:3:25:A:H8	1.78	0.47
22:3:372:A:H2'	22:3:373:A:C8	2.49	0.47
5:L:127:VAL:HG22	5:L:155:VAL:HG22	1.96	0.47
5:N:159:LYS:HD2	5:N:162:ARG:HH22	1.79	0.47
2:C:339:LEU:HD22	2:C:344:SER:HA	1.96	0.47
2:C:583:LEU:HD22	2:C:590:ALA:HB2	1.97	0.47
7:P:59:THR:HB	7:P:107:ASP:HB3	1.96	0.47
20:4:107:U:H2'	20:4:108:G:C8	2.49	0.47
21:2:184:C:H2'	21:2:185:G:C8	2.49	0.47
22:3:162:G:H2'	22:3:163:G:H8	1.80	0.47
2:C:290:ASN:OD1	2:C:326:LYS:NZ	2.33	0.47
5:N:220:THR:HG23	5:N:223:LEU:H	1.79	0.47
6:O:372:ALA:HA	6:O:375:LEU:HG	1.96	0.47
20:4:5:A:H2'	20:4:6:G:C8	2.50	0.47
21:2:60:G:N1	21:2:84:C:O2	2.48	0.47
21:2:45:A:H2'	21:2:46:G:C8	2.50	0.47
22:3:214:C:H2'	22:3:215:G:C8	2.50	0.47
2:C:296:ARG:NH1	3:D:929:UNK:O	2.47	0.46
5:L:151:VAL:O	5:L:170:SER:N	2.38	0.46
20:4:59:A:H2'	20:4:60:A:H8	1.80	0.46
2:C:571:LEU:HA	2:C:574:LEU:HD12	1.97	0.46
5:L:212:LYS:O	5:L:216:ASP:HB2	2.16	0.46
7:P:168:PRO:HB3	7:P:210:PHE:CD1	2.50	0.46
20:4:8:U:H4'	20:4:9:C:H5"	1.97	0.46
20:4:328:A:C6	20:4:394:G:C6	3.03	0.46
21:2:52:G:N1	21:2:90:U:O2	2.48	0.46
21:2:184:C:H2'	21:2:185:G:H8	1.80	0.46
20:4:57:A:H2'	20:4:58:A:C8	2.50	0.46
21:2:130:A:N6	21:2:140:G:H1	2.13	0.46
7:P:209:ASN:OD1	21:2:10:G:N2	2.47	0.46
19:1:23:C:H2'	19:1:24:A:C8	2.50	0.46
22:3:24:C:H2'	22:3:25:A:C8	2.51	0.46
21:2:54:G:H5"	21:2:55:A:H5'	1.97	0.46
22:3:82:A:H4'	22:3:271:C:H2'	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:129:LEU:HD23	5:M:227:LEU:HD23	1.97	0.46
20:4:340:C:H2'	20:4:341:A:H8	1.79	0.46
4:K:132:UNK:O	4:K:136:UNK:N	2.48	0.46
5:L:104:LYS:N	5:L:117:THR:O	2.44	0.46
5:M:92:PRO:HG2	5:M:95:ILE:HG12	1.98	0.46
7:P:168:PRO:HD2	21:2:30:G:H5'	1.98	0.46
22:3:163:G:H2'	22:3:164:A:H8	1.81	0.46
5:L:81:GLU:HA	5:L:84:TYR:HB3	1.98	0.46
21:2:28:U:H2'	21:2:29:C:C6	2.51	0.46
22:3:399:C:H2'	22:3:400:A:H8	1.81	0.46
19:1:78:A:H61	21:2:133:G:H1'	1.81	0.45
6:O:375:LEU:HD11	6:O:416:VAL:HG23	1.98	0.45
19:1:23:C:H2'	19:1:24:A:H8	1.81	0.45
21:2:23:G:H2'	21:2:24:G:H8	1.81	0.45
22:3:364:U:H2'	22:3:365:G:C8	2.51	0.45
5:L:100:PRO:O	5:L:103:PHE:N	2.49	0.45
7:P:67:ARG:HD2	21:2:69:U:P	2.56	0.45
20:4:404:A:O2'	20:4:405:A:O4'	2.32	0.45
22:3:301:G:H1	22:3:325:U:H3	1.64	0.45
6:O:427:ALA:HB2	6:O:459:LEU:HD23	1.97	0.45
5:N:130:HIS:HE1	5:N:132:ASN:HB2	1.81	0.45
6:O:309:GLY:O	6:O:313:ALA:CB	2.63	0.45
20:4:156:U:H2'	20:4:157:G:H8	1.82	0.45
22:3:399:C:H2'	22:3:400:A:C8	2.51	0.45
2:C:287:TYR:HA	2:C:290:ASN:HD22	1.82	0.45
5:L:232:TYR:O	5:L:236:GLN:OE1	2.35	0.45
2:C:299:ASP:OD1	2:C:302:ARG:N	2.40	0.45
2:C:475:GLU:HA	2:C:478:VAL:HG22	1.97	0.45
6:O:278:LEU:O	6:O:282:ARG:HB2	2.16	0.45
22:3:173:C:H3'	22:3:174:G:H2'	1.98	0.45
5:N:159:LYS:HB3	5:N:162:ARG:HH12	1.80	0.45
6:O:289:LEU:HD23	6:O:289:LEU:HA	1.89	0.45
1:B:838:ARG:HE	1:B:841:ARG:HH11	1.65	0.45
5:M:166:PHE:HE1	5:M:180:VAL:HG13	1.82	0.45
22:3:82:A:H3'	22:3:83:G:H8	1.80	0.45
20:4:173:U:H2'	20:4:174:G:C8	2.52	0.45
2:C:400:LEU:HD11	2:C:487:GLU:HG2	1.98	0.44
5:M:112:THR:OG1	5:M:130:HIS:NE2	2.50	0.44
5:N:114:LEU:HB2	5:N:129:LEU:HB2	1.99	0.44
19:1:8:A:H2'	19:1:9:G:H8	1.82	0.44
20:4:60:A:H2'	20:4:61:A:C8	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:4:306:C:O2	20:4:309:A:O2’	2.34	0.44
21:2:181:A:H2’	21:2:182:A:H8	1.82	0.44
5:L:151:VAL:N	5:L:170:SER:O	2.47	0.44
7:P:302:ALA:O	7:P:347:LYS:NZ	2.42	0.44
20:4:398:U:H2’	20:4:399:G:H8	1.81	0.44
5:N:158:ALA:HB1	5:N:185:LYS:HE2	1.98	0.44
6:O:418:VAL:HG12	6:O:422:ARG:HH12	1.82	0.44
20:4:139:A:H2’	20:4:140:A:C8	2.52	0.44
22:3:366:C:H2’	22:3:367:U:H6	1.83	0.44
2:C:418:GLN:HG2	2:C:464:ARG:HG2	1.99	0.44
5:M:91:ARG:HA	5:M:91:ARG:HD3	4.57	0.44
5:N:116:LEU:HD11	5:N:226:TYR:HE2	1.83	0.44
13:Z:48:UNK:O	13:Z:52:UNK:N	2.51	0.44
21:2:143:C:H2’	21:2:144:A:C8	2.53	0.44
22:3:347:A:H2’	22:3:349:A:H8	1.81	0.44
2:C:957:TYR:HE1	2:C:959:ALA:HB2	1.82	0.44
7:P:35:TRP:CZ3	21:2:65:C:H5”	2.52	0.44
22:3:36:G:H2’	22:3:37:G:C8	2.52	0.44
5:L:102:PRO:HD2	5:L:118:ARG:HD2	2.00	0.44
22:3:126:G:C6	22:3:170:A:N1	2.86	0.44
22:3:133:U:O2	22:3:163:G:N2	2.48	0.44
20:4:22:A:H2’	20:4:24:U:H3	1.82	0.44
22:3:365:G:N3	22:3:384:C:O2’	2.47	0.44
2:C:575:PRO:HA	2:C:576:PRO:HD3	1.86	0.44
8:U:9:UNK:C	8:U:11:UNK:N	2.81	0.44
8:U:28:UNK:C	8:U:30:UNK:N	2.81	0.44
5:M:152:ALA:HA	5:M:169:GLU:HA	2.00	0.44
19:1:18:U:O3’	22:3:85:C:N4	2.51	0.44
20:4:17:G:H1	20:4:87:U:H3	1.64	0.44
20:4:259:U:O4	20:4:286:A:N7	2.50	0.44
20:4:358:C:H42	20:4:368:C:H41	1.65	0.44
7:P:204:LEU:HD21	7:P:293:VAL:HG22	1.98	0.43
20:4:262:U:H3	20:4:283:G:H1	1.65	0.43
22:3:361:A:H2’	22:3:362:U:C6	2.53	0.43
2:C:975:TYR:HE2	3:D:937:UNK:CB	2.31	0.43
5:L:75:SER:OG	5:L:247:GLU:OE1	2.36	0.43
20:4:111:C:H5”	20:4:112:U:H5”	1.99	0.43
22:3:13:C:H2’	22:3:14:A:C8	2.53	0.43
22:3:197:A:H2’	22:3:198:G:H8	1.83	0.43
2:C:474:VAL:HA	2:C:477:VAL:HG12	1.99	0.43
7:P:151:ASP:HA	7:P:154:VAL:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:3:328:A:H2'	22:3:329:A:C8	2.53	0.43
12:Y:45:UNK:O	12:Y:49:UNK:N	2.51	0.43
19:1:92:C:H2'	19:1:93:G:H8	1.84	0.43
20:4:152:A:N1	20:4:283:G:H1'	2.33	0.43
5:M:103:PHE:HB3	5:M:116:LEU:HD22	2.01	0.43
20:4:101:A:N6	22:3:405:U:H3	2.05	0.43
20:4:260:A:N6	20:4:285:G:H1'	2.31	0.43
20:4:273:U:H3'	22:3:390:A:H61	1.82	0.43
20:4:398:U:H2'	20:4:399:G:C8	2.54	0.43
21:2:177:G:H2'	21:2:178:G:H8	1.83	0.43
22:3:169:A:H2'	22:3:170:A:C8	2.54	0.43
6:O:437:LEU:HB3	6:O:442:LEU:HB2	2.00	0.43
7:P:370:THR:HA	7:P:373:VAL:HG12	2.00	0.43
22:3:140:A:N6	22:3:156:U:O2	2.47	0.43
3:D:260:UNK:O	3:D:265:UNK:N	2.52	0.43
2:C:385:LEU:HA	2:C:388:VAL:HG22	2.01	0.43
5:L:95:ILE:HA	5:L:226:TYR:CE1	2.54	0.43
6:O:325:LEU:HD11	6:O:329:PRO:HD3	2.00	0.43
6:O:499:ASP:OD1	6:O:500:GLN:N	2.51	0.43
21:2:49:U:O4	22:3:320:A:H1'	2.18	0.43
5:L:99:PRO:HA	5:L:100:PRO:HD3	1.84	0.43
21:2:96:U:H2'	21:2:97:U:H6	1.83	0.42
20:4:198:U:N3	20:4:202:A:C6	2.87	0.42
22:3:370:U:H3	22:3:374:A:H2	1.66	0.42
5:N:79:ARG:NH2	5:N:247:GLU:OE1	2.53	0.42
7:P:92:VAL:HG13	7:P:148:LEU:HD22	2.01	0.42
7:P:158:ARG:NH1	20:4:359:A:O3'	2.51	0.42
22:3:196:G:H2'	22:3:197:A:H8	1.84	0.42
5:L:129:LEU:HD13	5:L:231:ILE:HB	2.00	0.42
5:L:214:LEU:HD23	5:L:214:LEU:HA	1.91	0.42
20:4:122:U:H2'	20:4:123:U:C6	2.54	0.42
20:4:214:U:H2'	20:4:215:U:C6	2.54	0.42
2:C:937:THR:OG1	2:C:938:ARG:N	2.52	0.42
5:L:203:ASP:HB3	5:L:206:LEU:HG	2.02	0.42
19:1:30:C:H41	21:2:174:U:H5'	1.85	0.42
20:4:11:U:O2'	20:4:14:A:OP2	2.36	0.42
22:3:55:U:H2'	22:3:56:G:H8	1.84	0.42
5:L:104:LYS:O	5:L:117:THR:N	2.49	0.42
5:M:242:TRP:HE3	5:M:243:LEU:HD22	1.85	0.42
20:4:5:A:H2'	20:4:6:G:H8	1.84	0.42
2:C:883:LEU:HA	2:C:883:LEU:HD23	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:238:GLU:OE1	5:L:241:ASN:ND2	2.46	0.42
20:4:173:U:H2'	20:4:174:G:H8	1.85	0.42
20:4:284:U:H3'	20:4:285:G:C8	2.54	0.42
20:4:356:U:O2	20:4:370:G:C2	2.73	0.42
2:C:886:LEU:O	2:C:890:VAL:HB	2.20	0.42
21:2:30:G:H2'	21:2:31:G:H8	1.85	0.42
21:2:123:C:H2'	21:2:124:G:C8	2.54	0.42
22:3:163:G:H2'	22:3:164:A:C8	2.54	0.42
5:L:171:ASP:OD1	5:L:174:SER:N	2.53	0.41
5:M:79:ARG:HH22	5:M:82:VAL:HG11	1.85	0.41
22:3:11:A:N6	22:3:59:A:O4'	2.53	0.41
5:N:156:SER:HB2	5:N:163:VAL:HG11	2.01	0.41
7:P:58:ASP:OD1	7:P:58:ASP:N	2.46	0.41
13:Z:81:UNK:O	13:Z:85:UNK:N	2.52	0.41
20:4:129:G:H2'	20:4:130:G:C8	2.53	0.41
5:L:108:ALA:HB3	5:L:111:ASP:HB2	2.02	0.41
7:P:378:GLN:HA	7:P:379:PRO:HD3	1.93	0.41
20:4:59:A:H2'	20:4:60:A:C8	2.55	0.41
22:3:75:A:O2'	22:3:78:A:O2'	2.32	0.41
5:M:79:ARG:HH12	5:M:82:VAL:HG21	1.84	0.41
19:1:97:G:H1	21:2:39:U:H3	1.68	0.41
21:2:174:U:H1'	21:2:203:G:H22	1.85	0.41
21:2:198:A:H3'	21:2:199:U:H6	1.84	0.41
22:3:63:U:H2'	22:3:64:A:H8	1.85	0.41
7:P:67:ARG:HD2	21:2:69:U:OP1	2.19	0.41
22:3:362:U:H2'	22:3:363:A:C8	2.54	0.41
5:L:206:LEU:HD11	5:M:81:GLU:HG3	2.02	0.41
5:M:162:ARG:HE	5:M:182:LEU:HD21	1.85	0.41
20:4:418:U:O2'	20:4:419:G:O4'	2.38	0.41
22:3:134:C:N4	22:3:135:G:O6	2.54	0.41
22:3:217:G:H2'	22:3:264:G:N2	2.36	0.41
5:N:127:VAL:HG13	5:N:155:VAL:HG22	2.03	0.41
7:P:43:LEU:HA	7:P:46:MET:HG3	2.02	0.41
7:P:392:TRP:O	7:P:402:ARG:NH2	2.41	0.41
20:4:56:A:H2'	20:4:57:A:H8	1.86	0.41
20:4:225:C:H2'	20:4:226:U:C6	2.55	0.41
22:3:71:C:H4'	22:3:72:U:H3'	2.03	0.41
5:M:234:LYS:HZ2	5:M:237:ARG:HH12	1.69	0.41
22:3:348:G:H1'	22:3:352:C:H42	1.86	0.41
2:C:390:SER:O	2:C:394:ARG:HG2	2.20	0.41
5:M:106:THR:OG1	5:M:115:THR:OG1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:75:SER:OG	5:N:247:GLU:OE1	2.39	0.41
6:O:282:ARG:HA	6:O:285:ARG:HB2	2.02	0.41
7:P:220:LEU:HD22	7:P:324:ALA:HB2	2.03	0.41
20:4:72:U:H2'	20:4:73:U:C5	2.56	0.41
20:4:419:G:H2'	20:4:420:G:C8	2.56	0.41
22:3:50:U:H2'	22:3:51:G:C8	2.55	0.41
2:C:571:LEU:O	2:C:579:ARG:NE	2.54	0.41
21:2:68:U:O2'	21:2:69:U:O5'	2.39	0.40
19:1:82:G:N3	21:2:161:A:O2'	2.54	0.40
20:4:86:G:H2'	20:4:87:U:C6	2.55	0.40
2:C:582:LEU:HD23	2:C:582:LEU:HA	1.92	0.40
7:P:35:TRP:HZ3	21:2:65:C:H5"	1.86	0.40
7:P:38:GLY:HA2	7:P:68:ARG:HE	1.86	0.40
10:W:30:UNK:O	10:W:31:UNK:CB	2.69	0.40
22:3:10:G:H1'	22:3:11:A:H2'	2.04	0.40
22:3:292:U:H2'	22:3:293:A:C8	2.57	0.40
2:C:857:LEU:HA	2:C:857:LEU:HD23	1.89	0.40
7:P:215:LEU:HD22	7:P:297:LEU:HG	2.02	0.40
20:4:394:G:O2'	20:4:395:A:O4'	2.40	0.40
22:3:62:A:H2'	22:3:63:U:C6	2.57	0.40
2:C:451:GLY:O	2:C:455:TYR:N	2.51	0.40
4:K:24:UNK:O	4:K:28:UNK:N	2.54	0.40
5:L:78:LEU:HD11	5:L:246:VAL:HG13	2.03	0.40
5:N:130:HIS:CE1	5:N:132:ASN:HB2	2.56	0.40
6:O:359:LEU:HD11	6:O:390:VAL:HG13	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	51/883 (6%)	44 (86%)	6 (12%)	1 (2%)	7 40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	355/999 (36%)	341 (96%)	14 (4%)	0	100	100
5	L	171/271 (63%)	164 (96%)	7 (4%)	0	100	100
5	M	170/271 (63%)	166 (98%)	4 (2%)	0	100	100
5	N	173/271 (64%)	172 (99%)	1 (1%)	0	100	100
6	O	232/516 (45%)	224 (97%)	8 (3%)	0	100	100
7	P	329/416 (79%)	325 (99%)	4 (1%)	0	100	100
14	d	127/415 (31%)	117 (92%)	10 (8%)	0	100	100
15	f	101/122 (83%)	96 (95%)	4 (4%)	1 (1%)	15	54
16	p	77/88 (88%)	68 (88%)	9 (12%)	0	100	100
17	r	54/356 (15%)	50 (93%)	4 (7%)	0	100	100
18	w	153/193 (79%)	139 (91%)	14 (9%)	0	100	100
23	a	208/253 (82%)	192 (92%)	15 (7%)	1 (0%)	29	68
24	b	237/530 (45%)	216 (91%)	20 (8%)	1 (0%)	34	72
25	e	174/368 (47%)	156 (90%)	17 (10%)	1 (1%)	25	64
26	o	140/319 (44%)	134 (96%)	6 (4%)	0	100	100
27	z	81/133 (61%)	73 (90%)	8 (10%)	0	100	100
28	v	126/190 (66%)	117 (93%)	9 (7%)	0	100	100
29	q	143/220 (65%)	136 (95%)	7 (5%)	0	100	100
30	l	102/128 (80%)	91 (89%)	10 (10%)	1 (1%)	15	54
31	h	345/412 (84%)	320 (93%)	25 (7%)	0	100	100
32	k	97/233 (42%)	97 (100%)	0	0	100	100
33	j	128/612 (21%)	113 (88%)	15 (12%)	0	100	100
34	m	85/124 (68%)	80 (94%)	3 (4%)	2 (2%)	6	36
35	n	95/112 (85%)	90 (95%)	4 (4%)	1 (1%)	14	52
36	u	22/136 (16%)	21 (96%)	1 (4%)	0	100	100
37	s	83/116 (72%)	75 (90%)	7 (8%)	1 (1%)	13	50
38	g	83/324 (26%)	79 (95%)	4 (5%)	0	100	100
39	i	152/446 (34%)	135 (89%)	14 (9%)	3 (2%)	7	40
40	x	364/485 (75%)	338 (93%)	26 (7%)	0	100	100
41	c	133/490 (27%)	123 (92%)	10 (8%)	0	100	100
42	y	59/209 (28%)	56 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	4850/10641 (46%)	4548 (94%)	289 (6%)	13 (0%)	44	76

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	829	PRO
15	f	59	TYR
23	a	54	PRO
30	l	114	TYR
39	i	300	PRO
34	m	67	GLY
35	n	78	THR
37	s	56	ASP
25	e	273	HIS
34	m	66	THR
39	i	305	PRO
24	b	142	HIS
39	i	301	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	31/567 (6%)	30 (97%)	1 (3%)	39	62
2	C	267/664 (40%)	266 (100%)	1 (0%)	91	94
5	L	151/207 (73%)	151 (100%)	0	100	100
5	M	150/207 (72%)	150 (100%)	0	100	100
5	N	152/207 (73%)	152 (100%)	0	100	100
6	O	155/354 (44%)	155 (100%)	0	100	100
7	P	258/296 (87%)	257 (100%)	1 (0%)	91	94
14	d	83/304 (27%)	83 (100%)	0	100	100
15	f	88/101 (87%)	87 (99%)	1 (1%)	73	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	p	65/74 (88%)	65 (100%)	0	100	100
17	r	48/248 (19%)	45 (94%)	3 (6%)	18	45
18	w	116/162 (72%)	116 (100%)	0	100	100
23	a	152/197 (77%)	152 (100%)	0	100	100
24	b	185/356 (52%)	184 (100%)	1 (0%)	88	93
25	e	145/273 (53%)	145 (100%)	0	100	100
26	o	124/243 (51%)	124 (100%)	0	100	100
27	z	66/99 (67%)	66 (100%)	0	100	100
28	v	102/148 (69%)	102 (100%)	0	100	100
29	q	113/145 (78%)	113 (100%)	0	100	100
30	l	86/105 (82%)	86 (100%)	0	100	100
31	h	280/315 (89%)	280 (100%)	0	100	100
32	k	77/161 (48%)	52 (68%)	25 (32%)	0	2
33	j	110/399 (28%)	110 (100%)	0	100	100
34	m	75/105 (71%)	75 (100%)	0	100	100
35	n	85/98 (87%)	82 (96%)	3 (4%)	36	60
36	u	20/110 (18%)	19 (95%)	1 (5%)	24	51
37	s	71/95 (75%)	71 (100%)	0	100	100
38	g	71/209 (34%)	71 (100%)	0	100	100
39	i	84/311 (27%)	82 (98%)	2 (2%)	49	69
40	x	251/336 (75%)	251 (100%)	0	100	100
41	c	92/342 (27%)	92 (100%)	0	100	100
42	y	52/159 (33%)	52 (100%)	0	100	100
All	All	3805/7597 (50%)	3766 (99%)	39 (1%)	77	86

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	841	ARG
2	C	414	ARG
7	P	86	ARG
15	f	16	ARG
17	r	267	ARG
17	r	268	ARG

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Mol	Chain	Res	Type
17	r	285	ARG
24	b	203	LYS
32	k	121	LEU
32	k	124	ILE
32	k	127	ILE
32	k	134	ILE
32	k	136	LEU
32	k	138	LEU
32	k	139	THR
32	k	141	LYS
32	k	144	LEU
32	k	147	THR
32	k	150	SER
32	k	154	VAL
32	k	157	LYS
32	k	161	LYS
32	k	169	LYS
32	k	181	LEU
32	k	183	TYR
32	k	188	VAL
32	k	189	ARG
32	k	191	LYS
32	k	197	LYS
32	k	198	GLN
32	k	203	SER
32	k	211	ILE
32	k	217	VAL
35	n	24	ARG
35	n	51	ARG
35	n	90	LEU
36	u	83	ARG
39	i	319	ARG
39	i	353	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
14	d	361	ASN
24	b	211	ASN
24	b	364	GLN
25	e	267	HIS
25	e	273	HIS

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Mol	Chain	Res	Type
32	k	126	HIS
32	k	129	ASN
36	u	89	HIS
37	s	17	GLN
37	s	31	ASN
38	g	196	GLN
41	c	146	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
19	1	91/101 (90%)	39 (42%)	2 (2%)
20	4	407/415 (98%)	178 (43%)	8 (1%)
21	2	212/213 (99%)	77 (36%)	0
22	3	390/393 (99%)	135 (34%)	2 (0%)
All	All	1100/1122 (98%)	429 (39%)	12 (1%)

All (429) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
19	1	2	A
19	1	3	A
19	1	4	U
19	1	6	A
19	1	7	G
19	1	14	G
19	1	17	C
19	1	18	U
19	1	29	U
19	1	30	C
19	1	31	A
19	1	32	U
19	1	33	G
19	1	34	C
19	1	37	C
19	1	38	G
19	1	42	G
19	1	44	U
19	1	45	G
19	1	46	G
19	1	47	U

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Mol	Chain	Res	Type
19	1	48	U
19	1	49	U
19	1	50	A
19	1	51	U
19	1	52	A
19	1	53	C
19	1	55	C
19	1	65	U
19	1	74	G
19	1	77	C
19	1	78	A
19	1	79	C
19	1	81	A
19	1	90	U
19	1	91	A
19	1	96	A
19	1	98	U
19	1	99	U
20	4	7	C
20	4	8	U
20	4	15	U
20	4	22	A
20	4	23	U
20	4	24	U
20	4	25	U
20	4	26	U
20	4	28	U
20	4	35	U
20	4	36	U
20	4	41	U
20	4	42	U
20	4	44	U
20	4	45	U
20	4	52	A
20	4	53	A
20	4	56	A
20	4	62	A
20	4	64	A
20	4	65	A
20	4	73	U
20	4	74	U
20	4	75	U

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Mol	Chain	Res	Type
20	4	80	U
20	4	81	U
20	4	82	U
20	4	83	C
20	4	84	A
20	4	85	A
20	4	86	G
20	4	88	C
20	4	90	U
20	4	100	U
20	4	101	A
20	4	109	G
20	4	112	U
20	4	113	A
20	4	115	A
20	4	116	G
20	4	124	A
20	4	126	A
20	4	128	U
20	4	132	C
20	4	135	C
20	4	136	C
20	4	137	A
20	4	138	C
20	4	139	A
20	4	140	A
20	4	141	G
20	4	142	U
20	4	143	U
20	4	144	G
20	4	159	C
20	4	162	A
20	4	163	A
20	4	164	U
20	4	165	A
20	4	166	U
20	4	167	A
20	4	170	G
20	4	177	G
20	4	182	A
20	4	192	A
20	4	195	U

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Mol	Chain	Res	Type
20	4	196	U
20	4	198	U
20	4	212	U
20	4	213	U
20	4	214	U
20	4	217	U
20	4	218	U
20	4	219	U
20	4	221	U
20	4	224	G
20	4	225	C
20	4	227	G
20	4	230	A
20	4	231	C
20	4	232	U
20	4	233	A
20	4	234	G
20	4	241	U
20	4	242	G
20	4	247	A
20	4	257	A
20	4	258	G
20	4	264	G
20	4	266	A
20	4	267	G
20	4	270	C
20	4	274	A
20	4	275	G
20	4	276	C
20	4	277	G
20	4	278	C
20	4	284	U
20	4	285	G
20	4	286	A
20	4	288	G
20	4	290	U
20	4	291	A
20	4	292	A
20	4	293	C
20	4	294	C
20	4	296	C
20	4	301	G

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Mol	Chain	Res	Type
20	4	302	U
20	4	304	C
20	4	305	A
20	4	307	A
20	4	308	C
20	4	309	A
20	4	310	U
20	4	312	G
20	4	317	U
20	4	318	C
20	4	324	C
20	4	326	A
20	4	330	U
20	4	331	A
20	4	332	G
20	4	333	U
20	4	334	A
20	4	340	C
20	4	342	G
20	4	344	A
20	4	346	G
20	4	351	A
20	4	352	U
20	4	353	G
20	4	354	G
20	4	355	C
20	4	357	A
20	4	358	C
20	4	359	A
20	4	361	U
20	4	362	U
20	4	363	A
20	4	364	G
20	4	365	U
20	4	368	C
20	4	369	G
20	4	371	C
20	4	372	C
20	4	373	U
20	4	374	G
20	4	375	G
20	4	379	G

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Mol	Chain	Res	Type
20	4	380	U
20	4	384	C
20	4	385	G
20	4	392	U
20	4	402	G
20	4	404	A
20	4	406	G
20	4	408	C
20	4	413	C
20	4	414	A
20	4	415	G
20	4	416	G
20	4	417	U
20	4	418	U
20	4	422	G
20	4	423	U
20	4	424	A
20	4	426	G
20	4	428	G
20	4	432	C
20	4	434	G
20	4	436	U
20	4	438	C
20	4	439	A
20	4	440	G
20	4	441	A
20	4	443	U
20	4	444	C
21	2	8	U
21	2	9	A
21	2	10	G
21	2	11	G
21	2	13	G
21	2	14	A
21	2	15	C
21	2	20	U
21	2	22	C
21	2	27	A
21	2	37	A
21	2	46	G
21	2	48	A
21	2	49	U

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Mol	Chain	Res	Type
21	2	50	U
21	2	51	A
21	2	52	G
21	2	54	G
21	2	55	A
21	2	56	G
21	2	57	C
21	2	58	U
21	2	62	U
21	2	65	C
21	2	67	U
21	2	68	U
21	2	70	U
21	2	72	U
21	2	75	U
21	2	76	C
21	2	78	G
21	2	79	C
21	2	83	C
21	2	86	U
21	2	90	U
21	2	91	U
21	2	92	A
21	2	99	G
21	2	103	G
21	2	114	A
21	2	115	C
21	2	116	U
21	2	117	A
21	2	125	G
21	2	134	A
21	2	137	A
21	2	138	G
21	2	146	G
21	2	148	U
21	2	152	U
21	2	154	U
21	2	155	G
21	2	160	C
21	2	161	A
21	2	162	G
21	2	168	U

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Mol	Chain	Res	Type
21	2	171	A
21	2	173	U
21	2	174	U
21	2	175	U
21	2	180	C
21	2	186	C
21	2	189	G
21	2	190	A
21	2	191	A
21	2	192	C
21	2	193	G
21	2	197	G
21	2	202	A
21	2	203	G
21	2	206	G
21	2	208	U
21	2	209	G
21	2	210	C
21	2	212	U
21	2	213	A
21	2	214	C
22	3	2	U
22	3	4	G
22	3	6	U
22	3	9	U
22	3	10	G
22	3	11	A
22	3	20	C
22	3	21	A
22	3	23	G
22	3	26	C
22	3	29	G
22	3	30	C
22	3	31	C
22	3	32	A
22	3	33	G
22	3	39	U
22	3	43	U
22	3	44	A
22	3	45	A
22	3	47	A
22	3	51	G

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Mol	Chain	Res	Type
22	3	55	U
22	3	57	U
22	3	59	A
22	3	66	A
22	3	74	G
22	3	76	C
22	3	78	A
22	3	80	G
22	3	82	A
22	3	83	G
22	3	84	G
22	3	85	C
22	3	86	A
22	3	88	C
22	3	89	G
22	3	94	U
22	3	107	U
22	3	109	A
22	3	110	A
22	3	113	C
22	3	117	A
22	3	119	A
22	3	129	A
22	3	134	C
22	3	135	G
22	3	139	G
22	3	140	A
22	3	147	A
22	3	148	A
22	3	149	A
22	3	154	A
22	3	155	A
22	3	156	U
22	3	159	U
22	3	164	A
22	3	172	C
22	3	174	G
22	3	175	A
22	3	176	A
22	3	177	G
22	3	187	C
22	3	188	C

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Mol	Chain	Res	Type
22	3	189	A
22	3	194	C
22	3	201	A
22	3	202	C
22	3	204	A
22	3	205	A
22	3	207	G
22	3	211	C
22	3	220	A
22	3	226	G
22	3	229	A
22	3	234	A
22	3	240	U
22	3	241	U
22	3	244	A
22	3	245	G
22	3	246	A
22	3	250	G
22	3	255	G
22	3	257	C
22	3	264	G
22	3	265	U
22	3	269	C
22	3	271	C
22	3	272	A
22	3	273	U
22	3	278	G
22	3	279	U
22	3	287	A
22	3	289	C
22	3	290	U
22	3	292	U
22	3	300	G
22	3	304	A
22	3	313	C
22	3	314	A
22	3	316	C
22	3	322	A
22	3	323	A
22	3	324	A
22	3	328	A
22	3	330	G

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Mol	Chain	Res	Type
22	3	331	C
22	3	337	G
22	3	339	A
22	3	340	G
22	3	342	G
22	3	346	G
22	3	348	G
22	3	349	A
22	3	350	U
22	3	352	C
22	3	353	G
22	3	356	G
22	3	357	U
22	3	374	A
22	3	375	U
22	3	377	G
22	3	379	A
22	3	381	U
22	3	382	U
22	3	383	A
22	3	385	G
22	3	388	C
22	3	389	A
22	3	390	A
22	3	391	A
22	3	392	A
22	3	393	U
22	3	394	C
22	3	397	A
22	3	398	C

All (12) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
19	1	44	U
19	1	64	U
20	4	34	U
20	4	139	A
20	4	165	A
20	4	166	U
20	4	230	A
20	4	274	A

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Mol	Chain	Res	Type
20	4	290	U
20	4	295	U
22	3	46	A
22	3	339	A

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	Z	18
20	4	8
3	D	7
9	V	5
11	X	2
22	3	2
8	U	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Z	608:UNK	C	652:UNK	N	59.09
1	V	85:UNK	C	87:UNK	N	51.40

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	V	194:UNK	C	206:UNK	N	47.06
1	Z	432:UNK	C	437:UNK	N	41.45
1	D	287:UNK	C	294:UNK	N	40.99
1	D	847:UNK	C	917:UNK	N	33.62
1	Z	312:UNK	C	316:UNK	N	31.86
1	Z	563:UNK	C	572:UNK	N	29.94
1	Z	52:UNK	C	62:UNK	N	29.83
1	V	149:UNK	C	151:UNK	N	27.09
1	X	61:UNK	C	67:UNK	N	26.04
1	Z	208:UNK	C	211:UNK	N	25.14
1	V	114:UNK	C	122:UNK	N	22.23
1	D	503:UNK	C	825:UNK	N	21.02
1	Z	234:UNK	C	244:UNK	N	20.95
1	Z	353:UNK	C	357:UNK	N	19.30
1	4	144:G	O3'	149:C	P	18.74
1	D	477:UNK	C	486:UNK	N	18.19
1	Z	277:UNK	C	281:UNK	N	17.65
1	X	30:UNK	C	36:UNK	N	17.30
1	Z	333:UNK	C	338:UNK	N	16.38
1	4	48:U	O3'	51:U	P	15.62
1	Z	138:UNK	C	145:UNK	N	14.83
1	Z	110:UNK	C	116:UNK	N	14.60
1	Z	254:UNK	C	257:UNK	N	14.41
1	D	212:UNK	C	217:UNK	N	13.12
1	3	100:U	O3'	106:G	P	12.55
1	D	160:UNK	C	166:UNK	N	12.12
1	4	199:U	O3'	202:A	P	11.13
1	D	369:UNK	C	376:UNK	N	11.07
1	Z	502:UNK	C	507:UNK	N	11.01
1	V	133:UNK	C	137:UNK	N	9.48
1	4	207:U	O3'	211:U	P	9.36
1	Z	187:UNK	C	195:UNK	N	8.89
1	Z	380:UNK	C	384:UNK	N	8.44
1	Z	164:UNK	C	169:UNK	N	7.72
1	3	279:U	O3'	286:A	P	7.37
1	4	28:U	O3'	34:U	P	7.28
1	Z	480:UNK	C	486:UNK	N	6.01
1	U	22:UNK	C	28:UNK	N	5.69
1	4	178:U	O3'	181:A	P	5.51
1	4	65:A	O3'	72:U	P	5.35
1	4	192:A	O3'	194:U	P	4.93

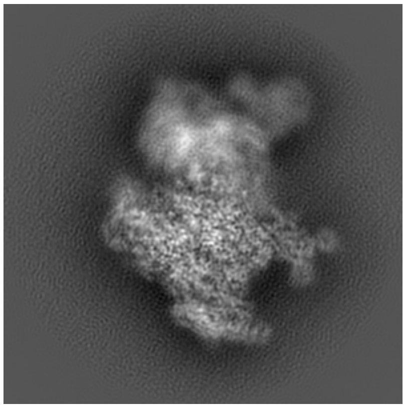
6 Map visualisation

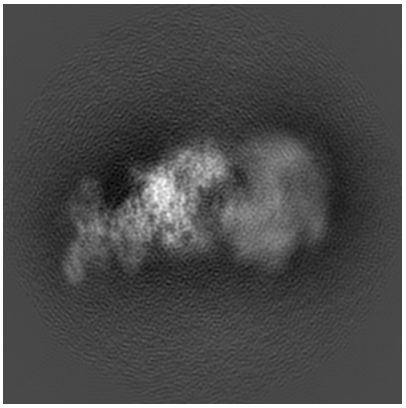
This section contains visualisations of the EMDB entry EMD-13477. These allow visual inspection of the internal detail of the map and identification of artifacts.

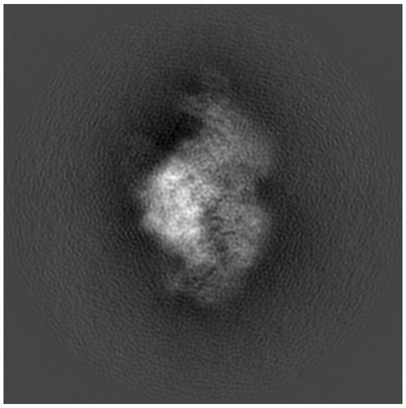
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

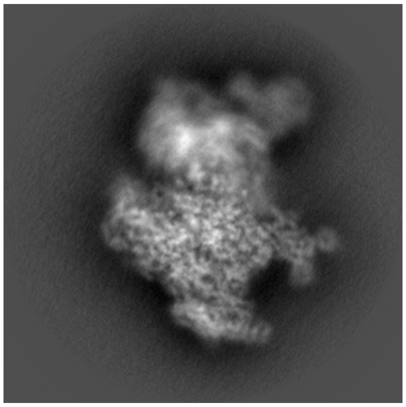
6.1.1 Primary map

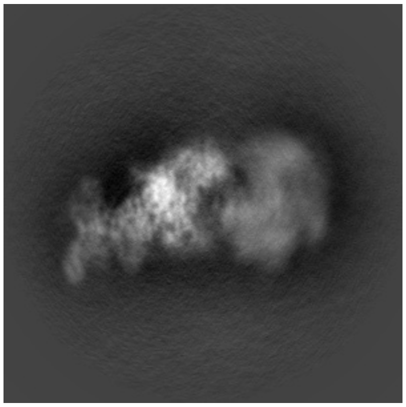

X

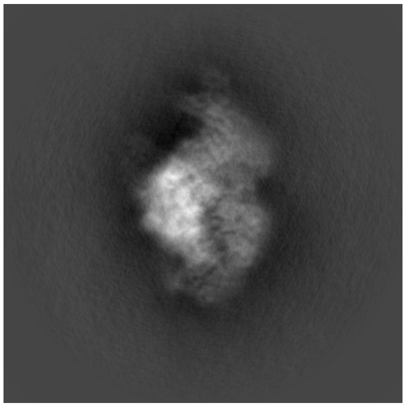

Y


Z

6.1.2 Raw map


X

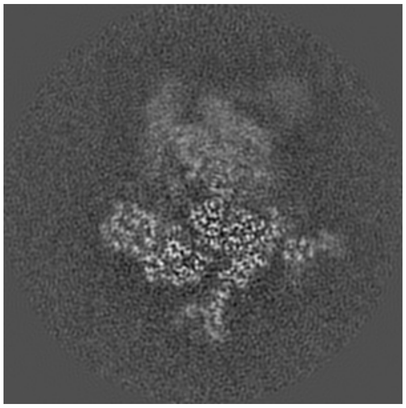

Y


Z

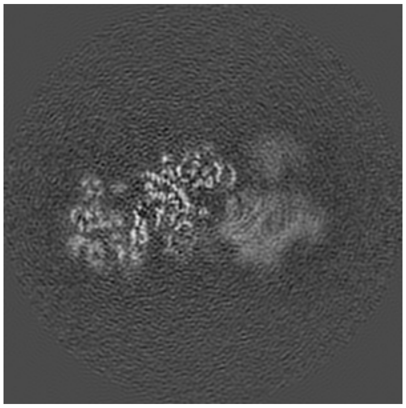
The images above show the map projected in three orthogonal directions.

6.2 Central slices

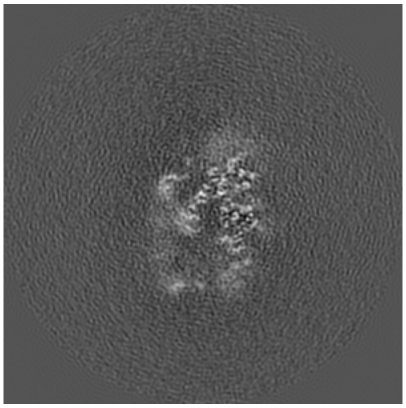
6.2.1 Primary map



X Index: 180

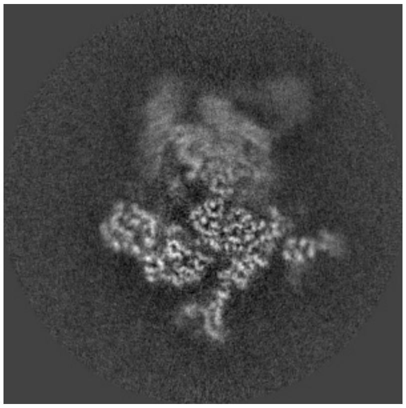


Y Index: 180

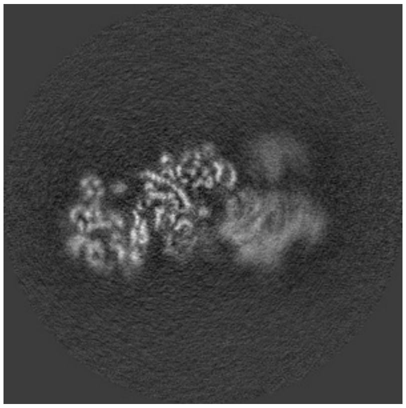


Z Index: 180

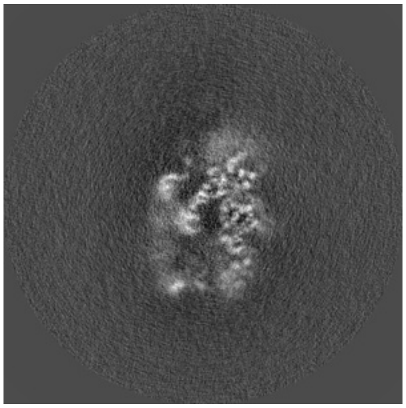
6.2.2 Raw map



X Index: 180



Y Index: 180

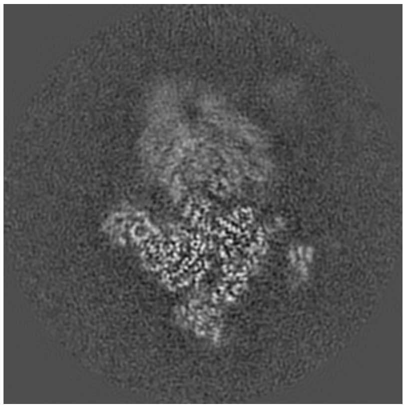


Z Index: 180

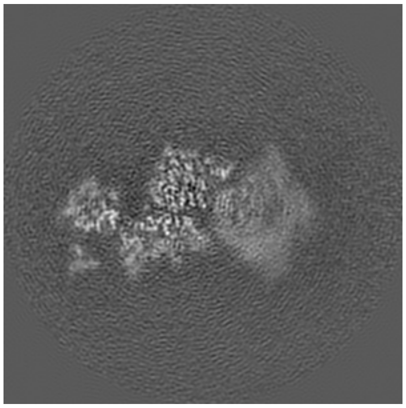
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

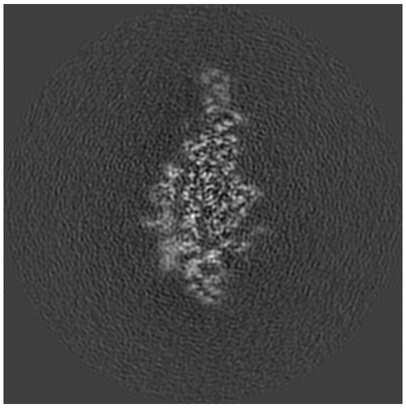
6.3.1 Primary map



X Index: 173

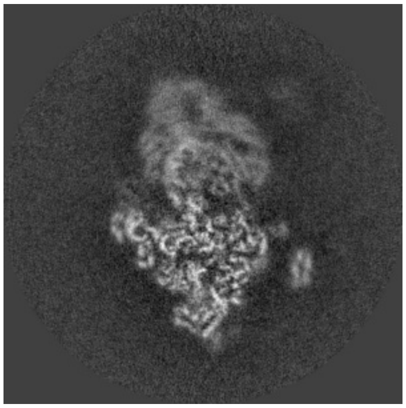


Y Index: 190

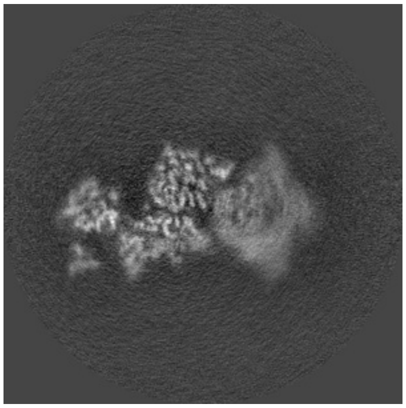


Z Index: 149

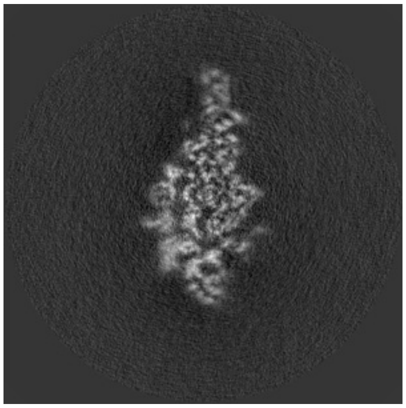
6.3.2 Raw map



X Index: 168



Y Index: 190

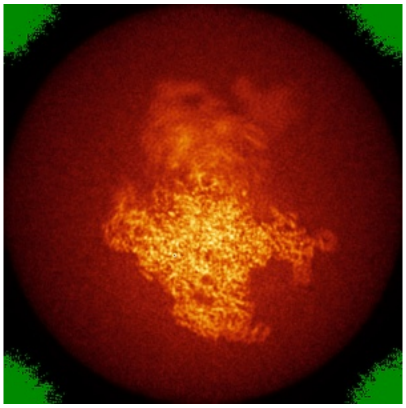


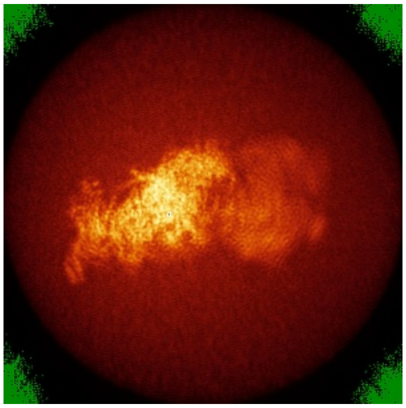
Z Index: 149

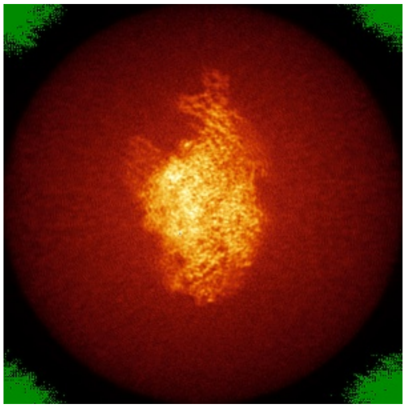
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color)

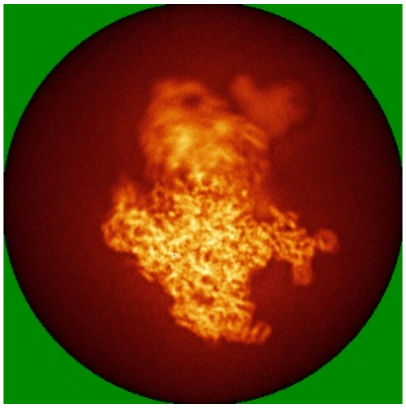
6.4.1 Primary map

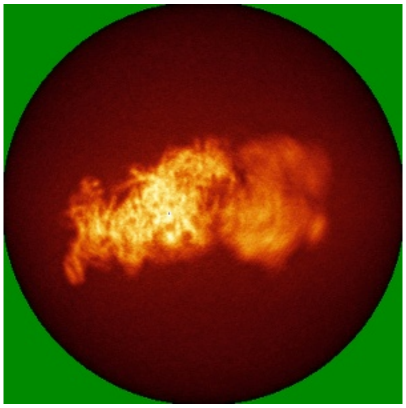

X

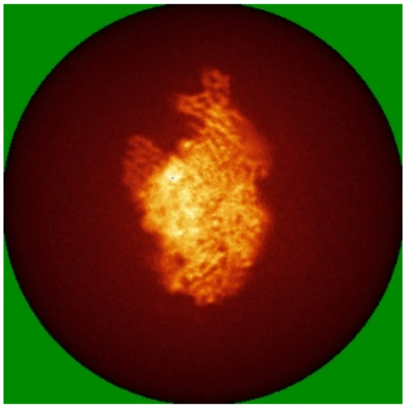

Y


Z

6.4.2 Raw map


X


Y


Z

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

6.5 Orthogonal surface views

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

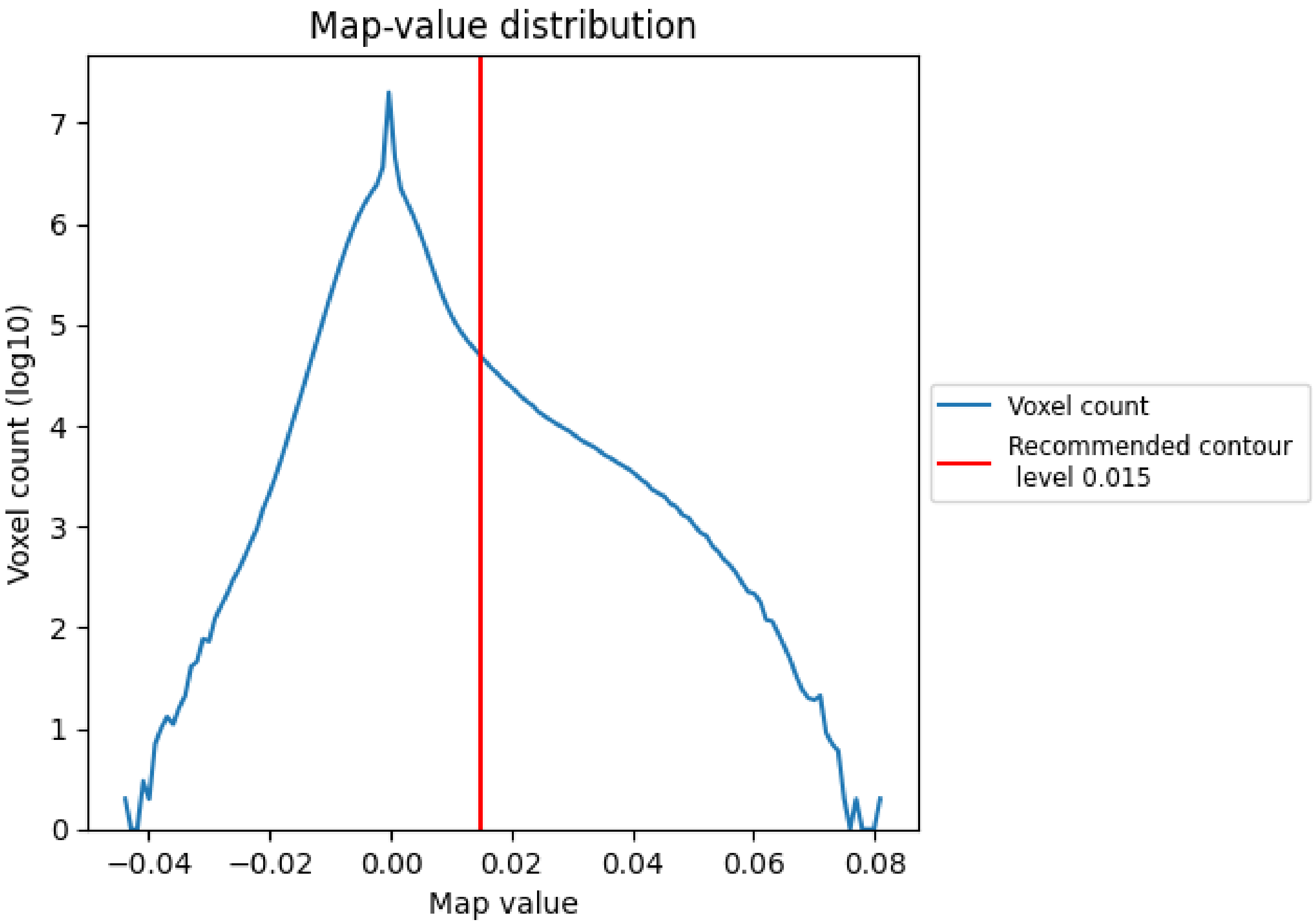
6.6 Mask visualisation

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

7 Map analysis ⓘ

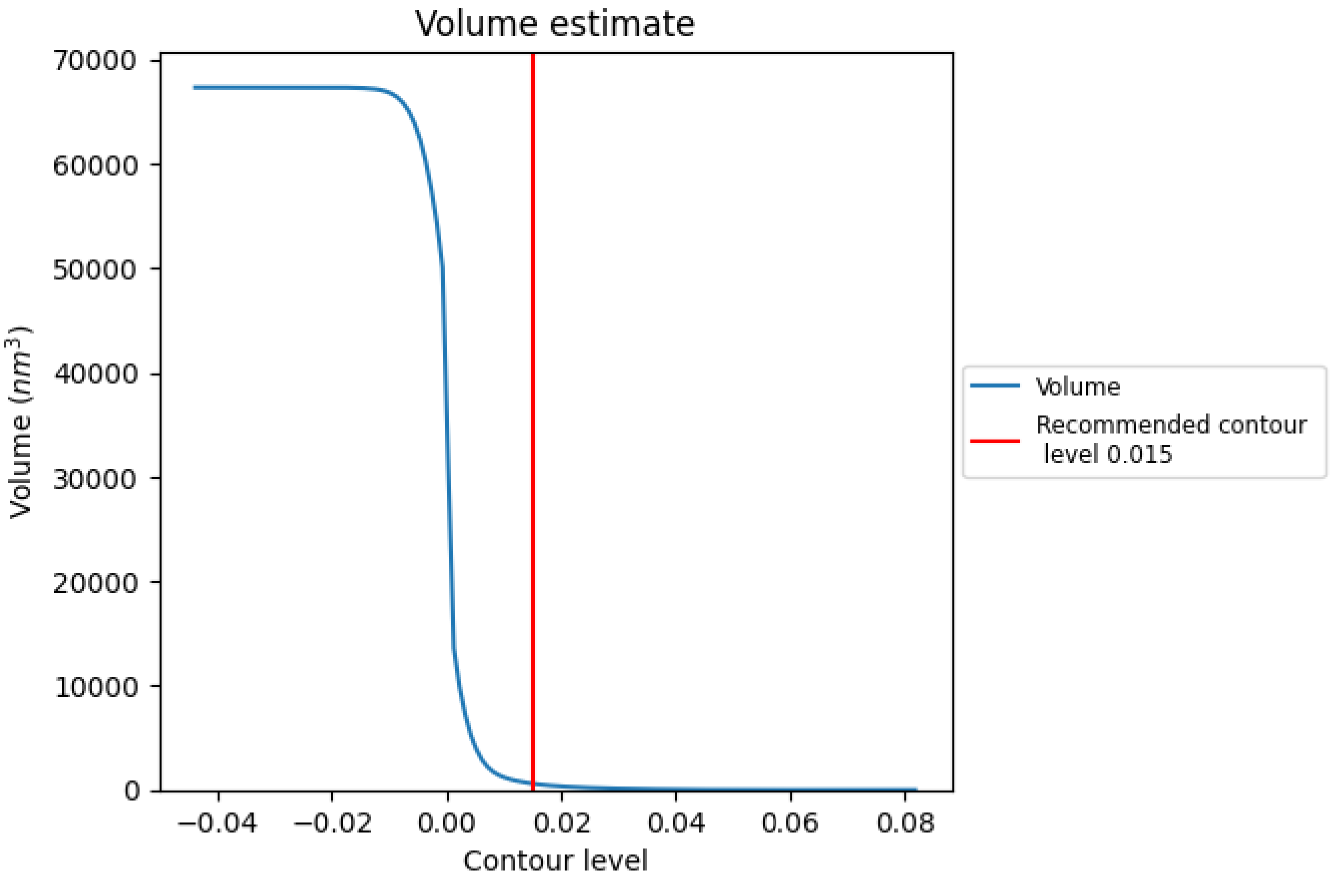
This section contains the results of statistical analysis of the map.

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.

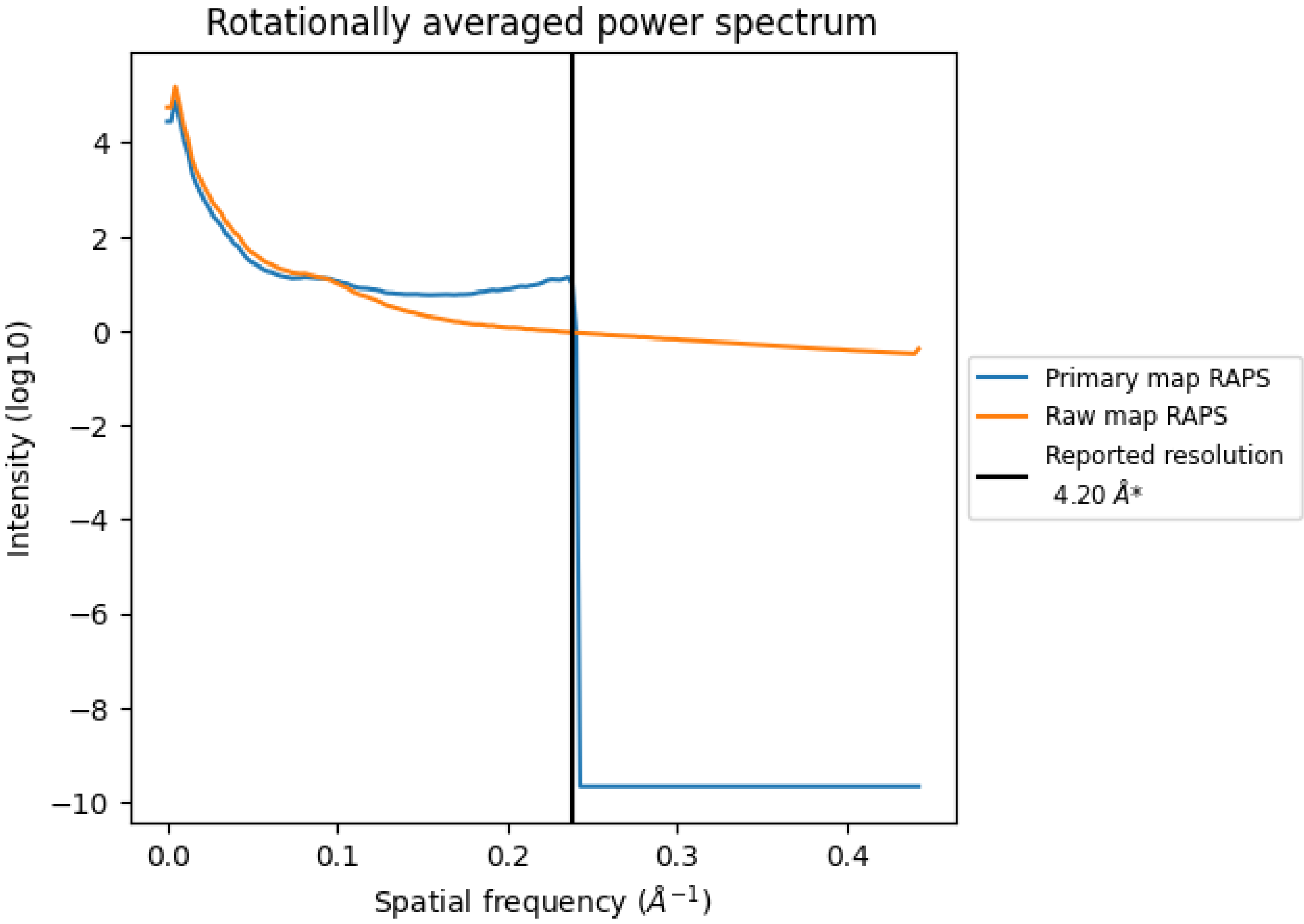
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 611 nm^3; this corresponds to an approximate mass of 552 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 ⓘ

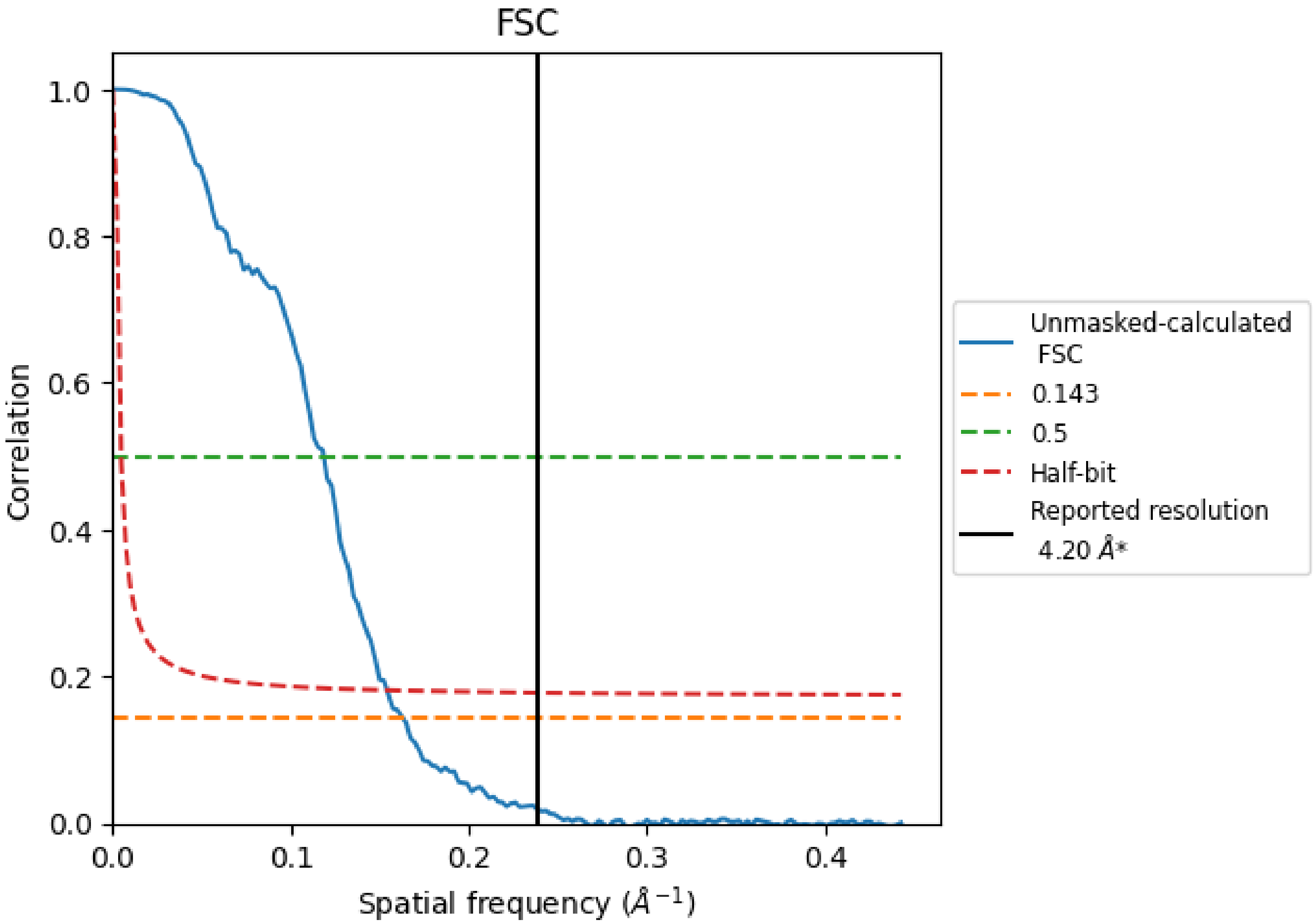


*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

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 0.238 $Å^{-1}$

8.2 Resolution estimates ⓘ

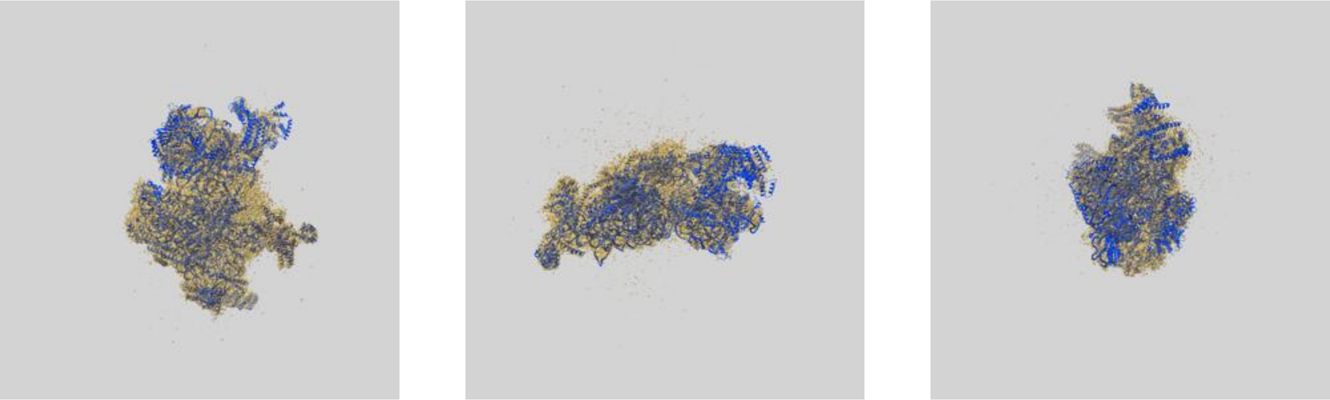
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.13	8.44	6.49

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.13 differs from the reported value 4.2 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13477 and PDB model 7PKQ. Per-residue inclusion information can be found in section 3 on page 13.

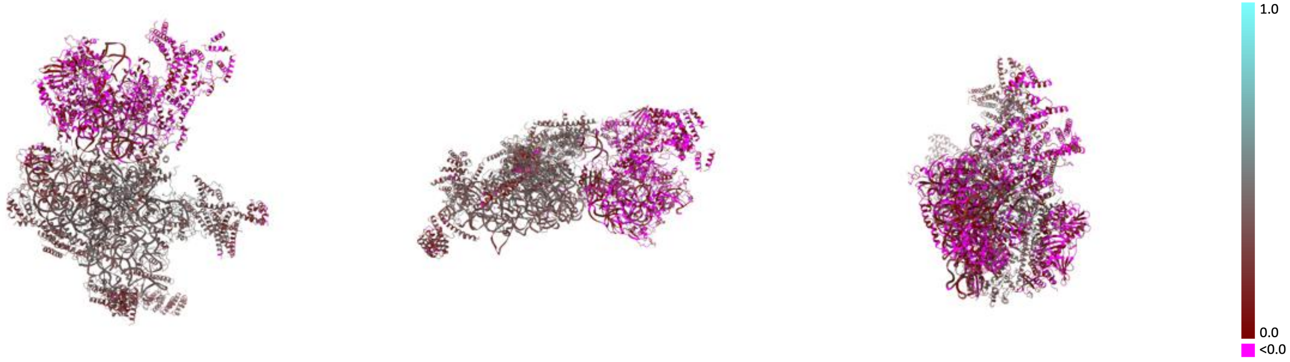
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.015 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.

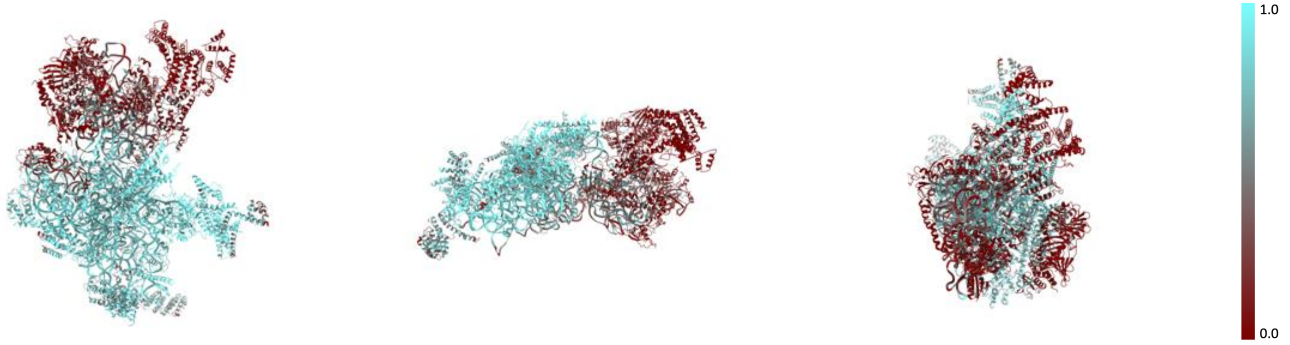
9.2 Q-score mapped to coordinate model ⓘ



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.

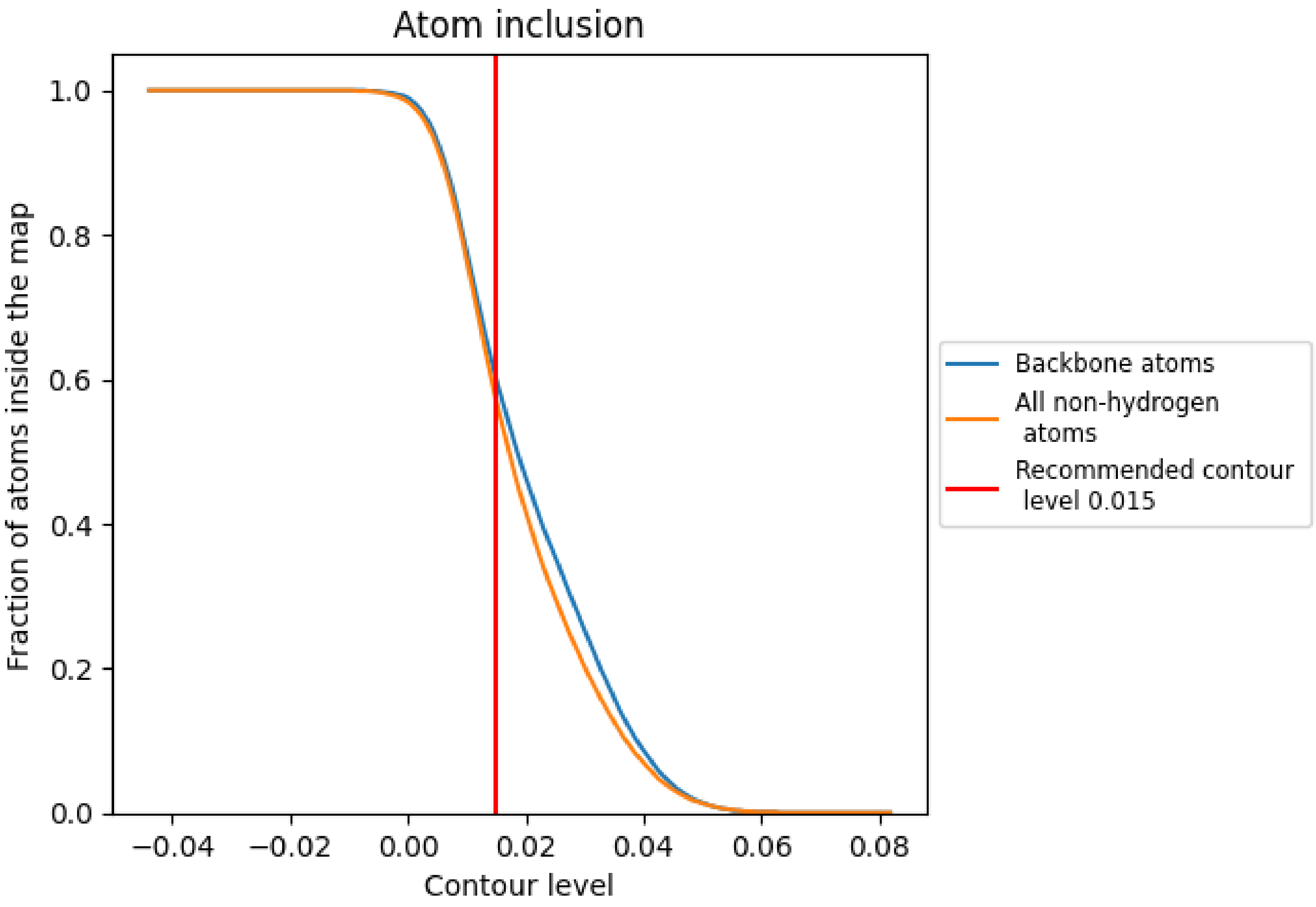
9.3 Atom inclusion mapped to coordinate model ⓘ



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 (0.015).

9.4 Atom inclusion ⓘ



At the recommended contour level, 60% of all backbone atoms, 57% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5710	0.2310
1	0.8810	0.3540
2	0.9110	0.3690
3	0.7290	0.2880
4	0.5200	0.1300
B	0.1950	0.0660
C	0.7330	0.3360
D	0.9320	0.3970
K	0.1620	0.0320
L	0.0760	0.0090
M	0.1230	0.0240
N	0.0640	0.0210
O	0.5260	0.2440
P	0.7770	0.3220
U	0.9270	0.4520
V	0.9410	0.4120
W	0.9110	0.4700
X	0.1730	0.0620
Y	0.3960	0.1550
Z	0.0570	0.0200
a	0.5790	0.2910
b	0.7600	0.3630
c	0.3550	0.1170
d	0.8110	0.3920
e	0.7760	0.4110
f	0.7620	0.3340
g	0.2090	0.0470
h	0.8100	0.4020
i	0.3450	0.0510
j	0.2500	0.0620
k	0.0280	0.1500
l	0.5140	0.3440
m	0.1180	-0.0010
n	0.2750	0.0470
o	0.7820	0.3540

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Chain	Atom inclusion	Q-score
p	🟦 0.8100	🟫 0.3480
q	🟦 0.8170	🟫 0.3840
r	🟦 0.7390	🟫 0.3070
s	🟥 0.1260	🟥 0.0060
u	🟫 0.2390	🟪 -0.0540
v	🟦 0.7310	🟫 0.3520
w	🟦 0.7940	🟫 0.3490
x	🟥 0.1280	🟥 0.0260
y	🟫 0.2260	🟥 0.0240
z	🟦 0.7600	🟫 0.3430