Full wwPDB EM Validation Report ⓘ

Jun 9, 2025 – 02:16 pm BST

PDB ID	:	9HCG / pdb_00009hcg
EMDB ID	:	EMD-52048
Title	:	Mouse mitoribosome large subunit assembly intermediate bound to NSUN4, METRF4, MRM2, GTPBP7 and MALSU1-L0R8F8-mt-ACP complex, State D (SAMC knock-out)
Authors	:	Singh, V.; Freyer, C.; Amunts, A.; Wredenberg, A.
Deposited on	:	2024-11-08
Resolution	:	2.91 Å(reported)

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

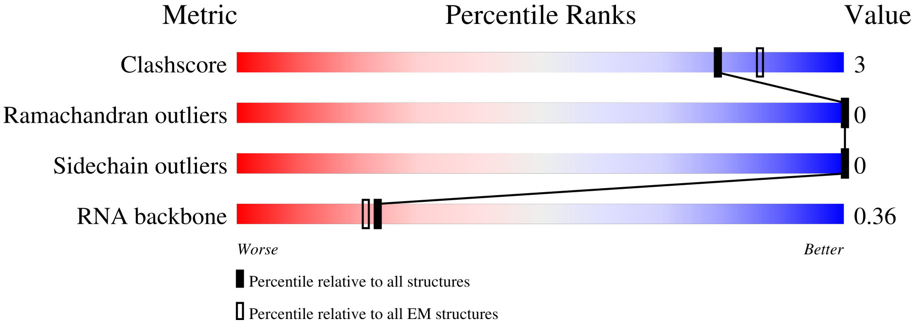
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance

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

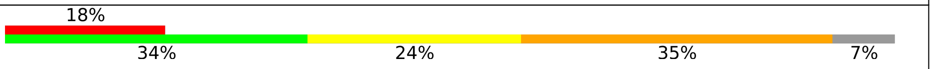
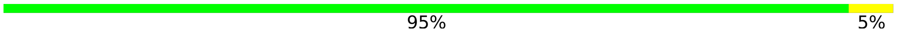
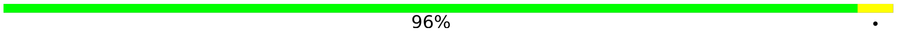
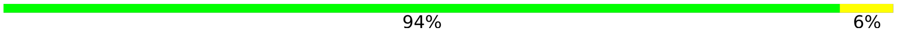
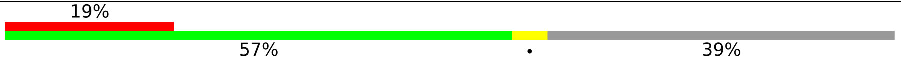
The reported resolution of this entry is 2.91 Å.

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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	A	1584	
2	B	68	
3	D	246	
4	E	308	
5	F	250	
6	H	95	
7	I	262	

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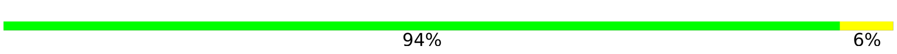
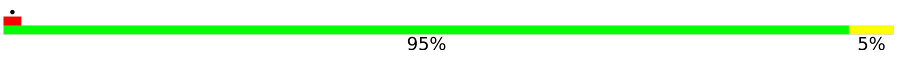
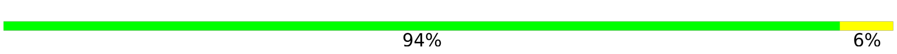
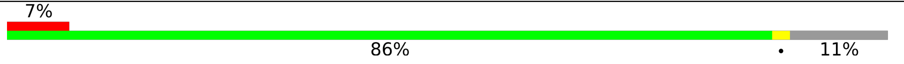
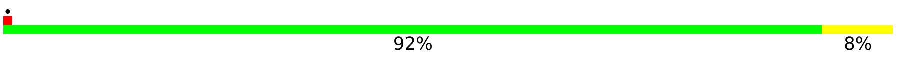
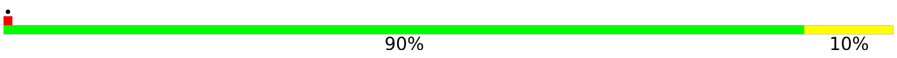
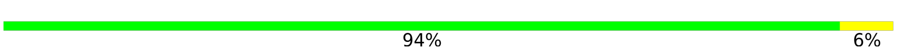
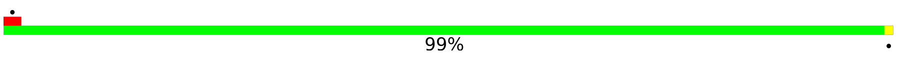
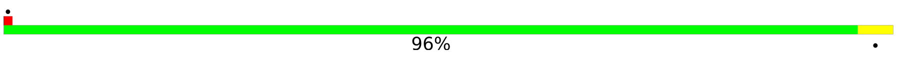
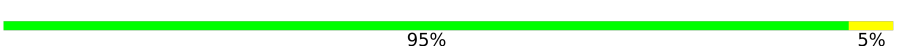
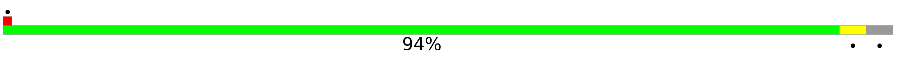
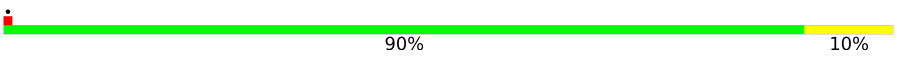
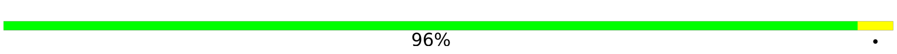
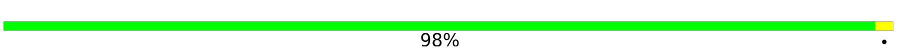
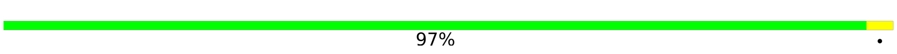
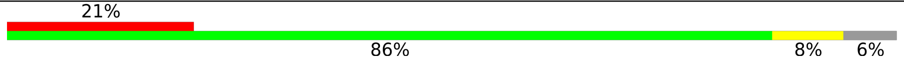
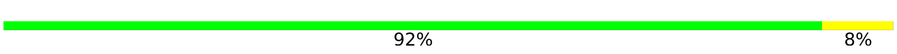
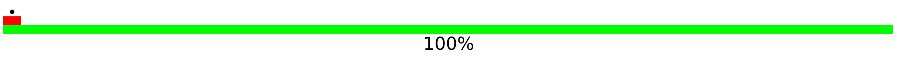
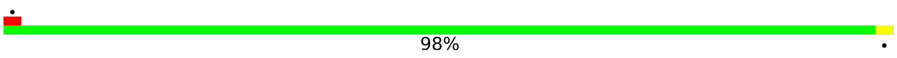
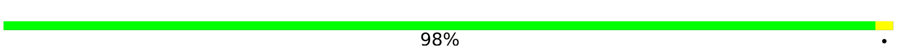
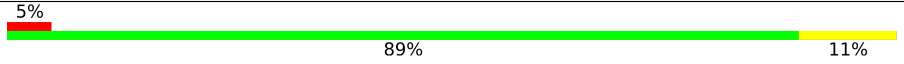
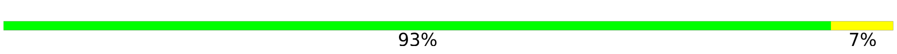
Mol	Chain	Length	Quality of chain
8	J	175	
9	K	177	
10	L	115	
11	M	287	
12	N	222	
13	O	153	
14	P	141	
15	Q	217	
16	R	140	
17	S	159	
18	T	166	
19	U	145	
20	V	207	
21	W	100	
22	X	242	
23	Y	176	
24	Z	121	
25	x	345	
26	0	108	
27	1	52	
28	2	46	
29	3	95	
30	4	37	
31	6	335	
32	7	292	

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Mol	Chain	Length	Quality of chain
33	b	148	93% 7%
34	c	290	92%
35	d	306	62% 8% 30%
36	e	283	58% 62% 6% 32%
37	f	128	59% 73% 8% 19%
38	g	132	95% 5%
39	h	110	86% 14%
40	i	97	98%
41	j	121	72% 5% 23%
42	k	118	9% 66% 5% 29%
43	o	78	97%
44	p	153	87% 7% 7%
45	q	135	97%
46	r	196	77% 20%
47	s	384	95%
48	u	125	12% 93% 7%
49	v	69	12% 94% 6%
50	w	79	80% 95% 5%
51	5	394	98%
52	8	70	56% 96%
53	9	135	89% 10%
54	a	142	7% 67% 6% 27%
55	m	127	28% 31% 5% 65%
56	z	326	10% 13% 85%
57	l	135	38% 56% 39%

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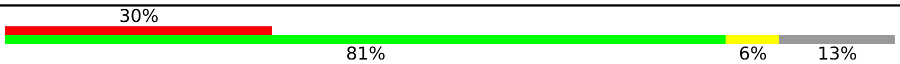
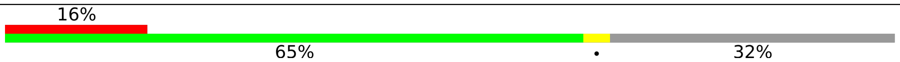
Mol	Chain	Length	Quality of chain
58	t	246	
59	y	346	

2 Entry composition (i)

There are 64 unique types of molecules in this entry. The entry contains 198354 atoms, of which 91682 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 16S rRNA (1584-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
1	A	1447	46288	13812	15535	5537	9957	1447	0	0

- Molecule 2 is a RNA chain called tRNA-Phe (68-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
2	B	63	2024	604	678	247	432	63	0	0

- Molecule 3 is a protein called Large ribosomal subunit protein uL2m.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	D	227	3598	1105	1830	349	305	9	0	0

- Molecule 4 is a protein called Large ribosomal subunit protein uL3m.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	E	308	4900	1577	2441	432	442	8	0	0

- Molecule 5 is a protein called Large ribosomal subunit protein uL4m.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	F	250	4030	1286	2025	364	349	6	0	0

- Molecule 6 is a protein called Large ribosomal subunit protein bL9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
6	H	95	1593	492	814	150	137	0	0

- Molecule 7 is a protein called Large ribosomal subunit protein uL10m.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	I	161	Total	C	H	N	O	S	0	0
			2700	851	1393	235	214	7		

- Molecule 8 is a protein called Large ribosomal subunit protein uL11m.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	J	175	Total	C	H	N	O	S	0	0
			2720	846	1394	234	243	3		

- Molecule 9 is a protein called Large ribosomal subunit protein uL13m.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	K	177	Total	C	H	N	O	S	0	0
			2893	927	1444	262	253	7		

- Molecule 10 is a protein called Large ribosomal subunit protein uL14m.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	L	115	Total	C	H	N	O	S	0	0
			1837	560	944	174	155	4		

- Molecule 11 is a protein called Large ribosomal subunit protein uL15m.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	M	287	Total	C	H	N	O	S	0	0
			4692	1475	2377	428	406	6		

- Molecule 12 is a protein called Large ribosomal subunit protein uL16m.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	N	197	Total	C	H	N	O	S	0	0
			3240	1045	1626	285	274	10		

- Molecule 13 is a protein called Large ribosomal subunit protein bL17m.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	O	153	Total	C	H	N	O	S	0	0
			2541	795	1282	240	219	5		

- Molecule 14 is a protein called Large ribosomal subunit protein uL18m.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
14	P	141	2302	725	1148	221	203	5	0	0

- Molecule 15 is a protein called Large ribosomal subunit protein bL19m.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
15	Q	217	3612	1150	1822	309	322	9	0	0

- Molecule 16 is a protein called Large ribosomal subunit protein bL20m.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
16	R	140	2385	738	1224	233	187	3	0	0

- Molecule 17 is a protein called Large ribosomal subunit protein bL21m.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
17	S	159	2673	840	1372	233	226	2	0	0

- Molecule 18 is a protein called Large ribosomal subunit protein uL22m.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
18	T	166	2771	871	1402	256	234	8	0	0

- Molecule 19 is a protein called Large ribosomal subunit protein uL23m.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
19	U	127	2109	675	1057	196	178	3	0	0

- Molecule 20 is a protein called Large ribosomal subunit protein uL24m.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
20	V	201	3295	1043	1643	305	298	6	0	0

- Molecule 21 is a protein called Large ribosomal subunit protein bL27m.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	W	100	Total 1603	C 515	H 809	N 141	O 135	S 3	0	0

- Molecule 22 is a protein called Large ribosomal subunit protein bL28m.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	X	242	Total 4072	C 1304	H 2051	N 358	O 355	S 4	0	0

- Molecule 23 is a protein called Large ribosomal subunit protein uL29m.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	Y	176	Total 3076	C 973	H 1553	N 290	O 255	S 5	0	0

- Molecule 24 is a protein called Large ribosomal subunit protein uL30m.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	Z	121	Total 2026	C 632	H 1039	N 182	O 170	S 3	0	0

- Molecule 25 is a protein called 5-cytosine rRNA methyltransferase NSUN4.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	x	325	Total 5110	C 1626	H 2546	N 448	O 473	S 17	1	0

- Molecule 26 is a protein called Large ribosomal subunit protein bL32m.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	0	108	Total 1789	C 546	H 908	N 174	O 155	S 6	0	0

- Molecule 27 is a protein called Large ribosomal subunit protein bL33m.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	1	52	Total 900	C 278	H 472	N 80	O 70	0	0

- Molecule 28 is a protein called Large ribosomal subunit protein bL34m.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
28	2	46	787	235	407	86	58	1	0	0

- Molecule 29 is a protein called Large ribosomal subunit protein bL35m.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
29	3	95	1695	528	872	164	127	4	0	0

- Molecule 30 is a protein called Large ribosomal subunit protein bL36m.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
30	4	37	676	206	354	68	45	3	0	0

- Molecule 31 is a protein called Large ribosomal subunit protein mL38.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
31	6	313	5219	1718	2546	484	465	6	0	0

- Molecule 32 is a protein called Large ribosomal subunit protein mL39.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
32	7	292	4757	1517	2378	409	438	15	0	0

- Molecule 33 is a protein called Large ribosomal subunit protein mL43.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
33	b	148	2376	731	1195	234	214	2	0	0

- Molecule 34 is a protein called Large ribosomal subunit protein mL44.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
34	c	280	4516	1444	2262	391	411	8	0	0

- Molecule 35 is a protein called Large ribosomal subunit protein mL45.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	d	213	Total	C	H	N	O	S	0	0
			3502	1129	1742	312	309	10		

- Molecule 36 is a protein called Large ribosomal subunit protein mL46.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	e	193	Total	C	H	N	O	S	0	0
			3174	1013	1598	278	279	6		

- Molecule 37 is a protein called Large ribosomal subunit protein mL48.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	f	104	Total	C	H	N	O	S	0	0
			1674	533	836	141	160	4		

- Molecule 38 is a protein called Large ribosomal subunit protein mL49.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	g	132	Total	C	H	N	O	S	0	0
			2184	709	1094	187	192	2		

- Molecule 39 is a protein called Large ribosomal subunit protein mL50.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	h	110	Total	C	H	N	O	S	0	0
			1739	552	867	156	160	4		

- Molecule 40 is a protein called Large ribosomal subunit protein mL51.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	i	97	Total	C	H	N	O	S	0	0
			1685	540	854	161	128	2		

- Molecule 41 is a protein called Large ribosomal subunit protein mL52.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	j	93	Total	C	H	N	O	S	0	0
			1512	467	768	145	130	2		

- Molecule 42 is a protein called Large ribosomal subunit protein mL53.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
42	k	84	1316	408	659	120	124	5	0	0

- Molecule 43 is a protein called Large ribosomal subunit protein mL63.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
43	o	78	1263	402	623	118	116	4	0	0

- Molecule 44 is a protein called Large ribosomal subunit protein mL62.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
44	p	143	2352	729	1185	216	218	4	0	0

- Molecule 45 is a protein called Large ribosomal subunit protein mL64.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
45	q	135	2253	703	1123	223	199	5	0	0

- Molecule 46 is a protein called Large ribosomal subunit protein mL66.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
46	r	157	2606	812	1331	242	210	11	0	0

- Molecule 47 is a protein called Large ribosomal subunit protein mL65.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
47	s	377	6103	1938	3058	555	540	12	0	0

- Molecule 48 is a protein called Mitochondrial assembly of ribosomal large subunit protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
48	u	125	2041	659	1012	170	191	9	0	0

- Molecule 49 is a protein called Predicted gene, 55359.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
49	v	69	1189	374	603	112	99	1	0	0

- Molecule 50 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
50	w	79	1277	410	640	95	127	5	0	0

- Molecule 51 is a protein called Large ribosomal subunit protein mL37.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
51	5	394	6468	2081	3243	564	571	9	0	0

- Molecule 52 is a protein called Large ribosomal subunit protein mL40.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
52	8	70	1163	368	574	102	117	2	0	0

- Molecule 53 is a protein called Large ribosomal subunit protein mL41.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
53	9	122	1973	635	990	167	179	2	0	0

- Molecule 54 is a protein called Large ribosomal subunit protein mL42.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
54	a	103	1703	542	843	156	159	3	0	0

- Molecule 55 is a protein called Large ribosomal subunit protein mL55.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
55	m	45	769	233	395	77	61	3	0	0

- Molecule 56 is a protein called Mitochondrial ribosome-associated GTPase 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
56	z	48	800	247	415	73	64	1	0	0

- Molecule 57 is a protein called Large ribosomal subunit protein mL54.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
57	l	82	1358	432	677	121	126	2	0	0

- Molecule 58 is a protein called rRNA methyltransferase 2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
58	t	214	3350	1048	1695	299	300	8	0	0

- Molecule 59 is a protein called Transcription termination factor 4, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
59	y	237	3938	1238	1995	345	351	9	0	0

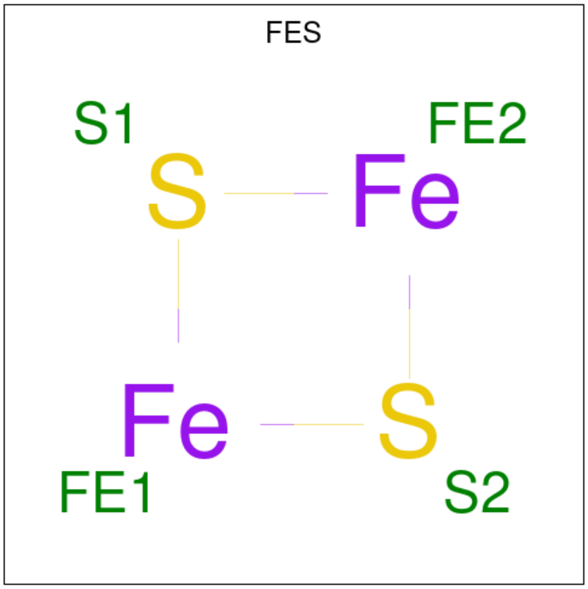
- Molecule 60 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
60	A	101	101	101	0
60	E	1	1	1	0
60	M	1	1	1	0
60	O	1	1	1	0
60	6	1	1	1	0

- Molecule 61 is ZINC ION (CCD ID: ZN) (formula: Zn).

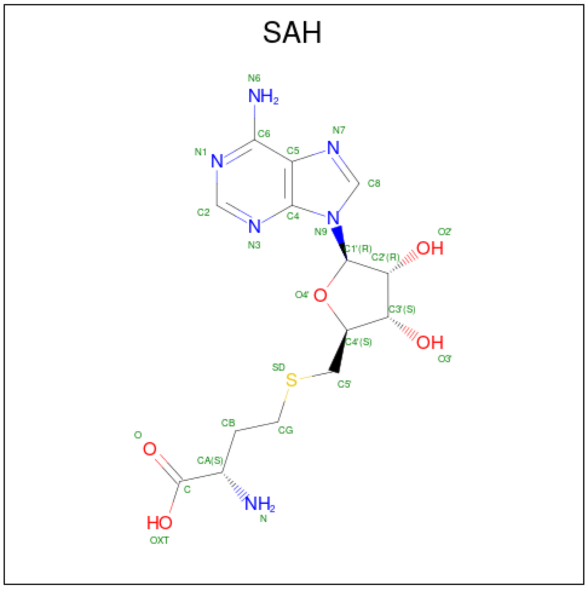
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
61	0	1	1	1	0
61	4	1	1	1	0

- Molecule 62 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
62	r	1	4	2	2	0

- Molecule 63 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	S	
63	t	1	45	14	19	6	5	1	0

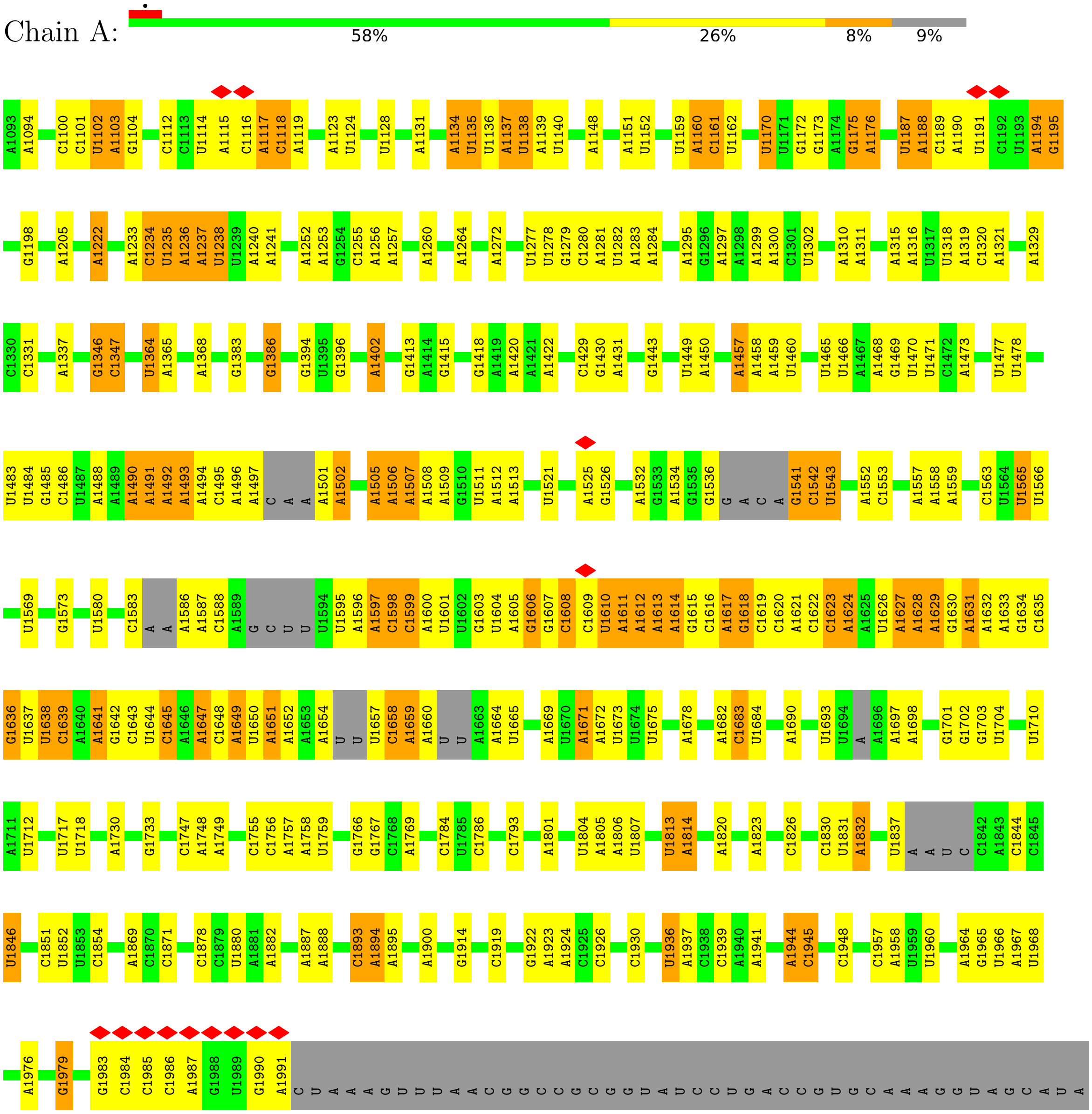
- Molecule 64 is water.

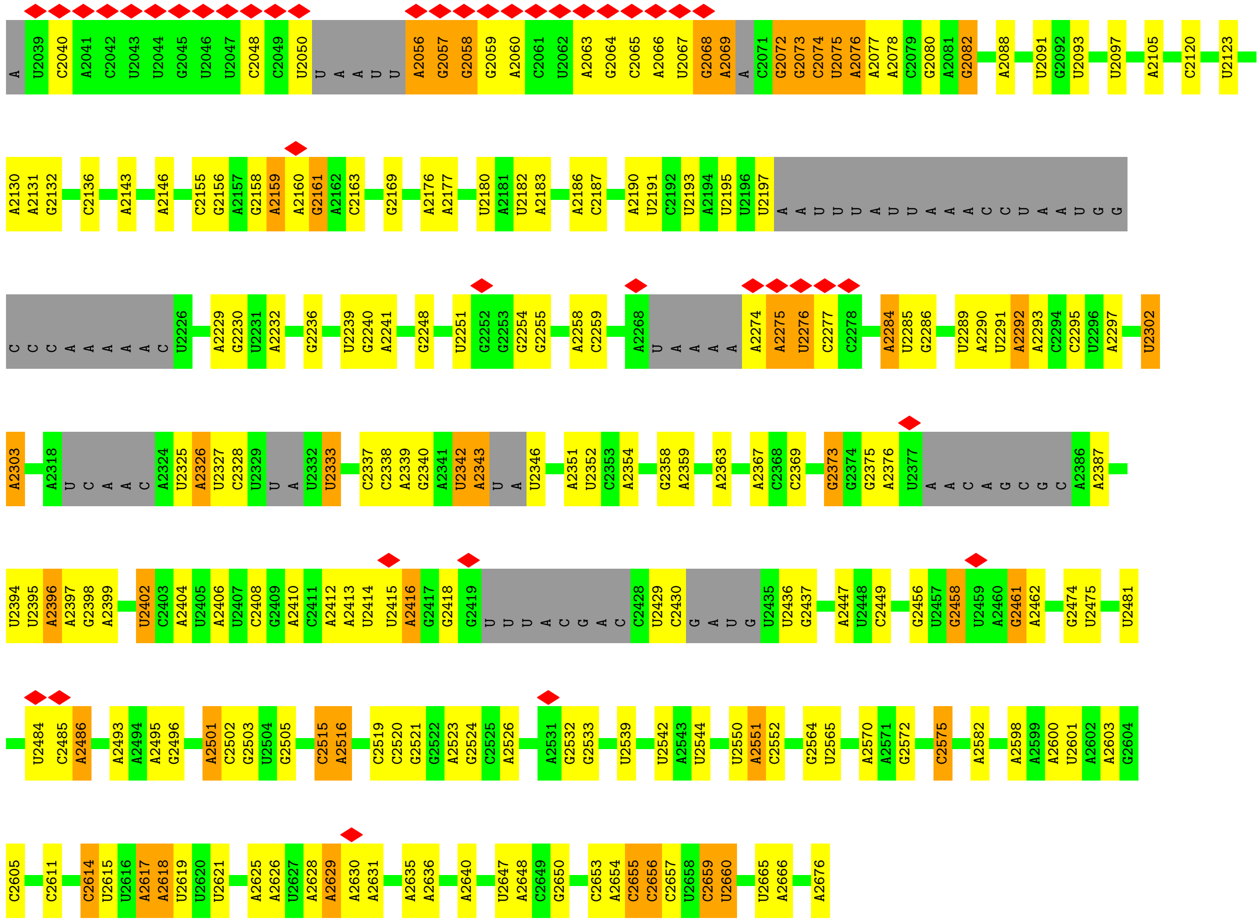
Mol	Chain	Residues	Atoms	AltConf
64	A	1	Total O 1 1	0

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.

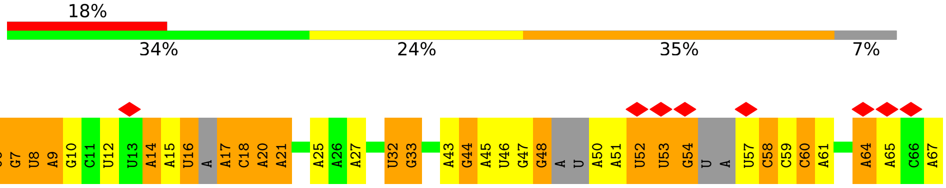
- Molecule 1: 16S rRNA (1584-MER)





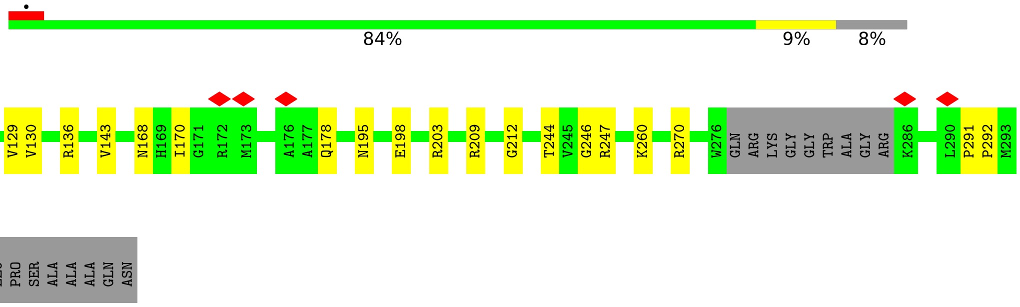
- Molecule 2: tRNA-Phe (68-MER)

Chain B:



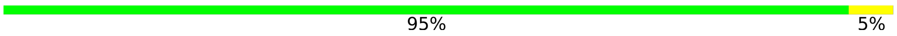
- Molecule 3: Large ribosomal subunit protein uL2m

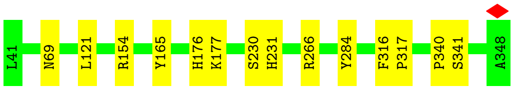
Chain D:



- Molecule 4: Large ribosomal subunit protein uL3m

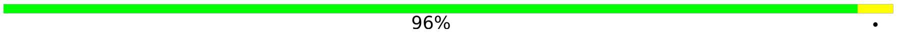
Chain E:

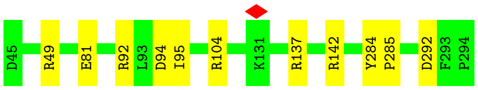




- Molecule 5: Large ribosomal subunit protein uL4m

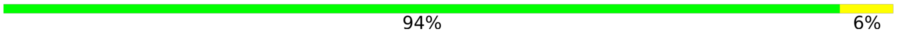
Chain F:

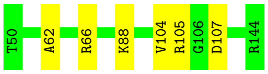




- Molecule 6: Large ribosomal subunit protein bL9m

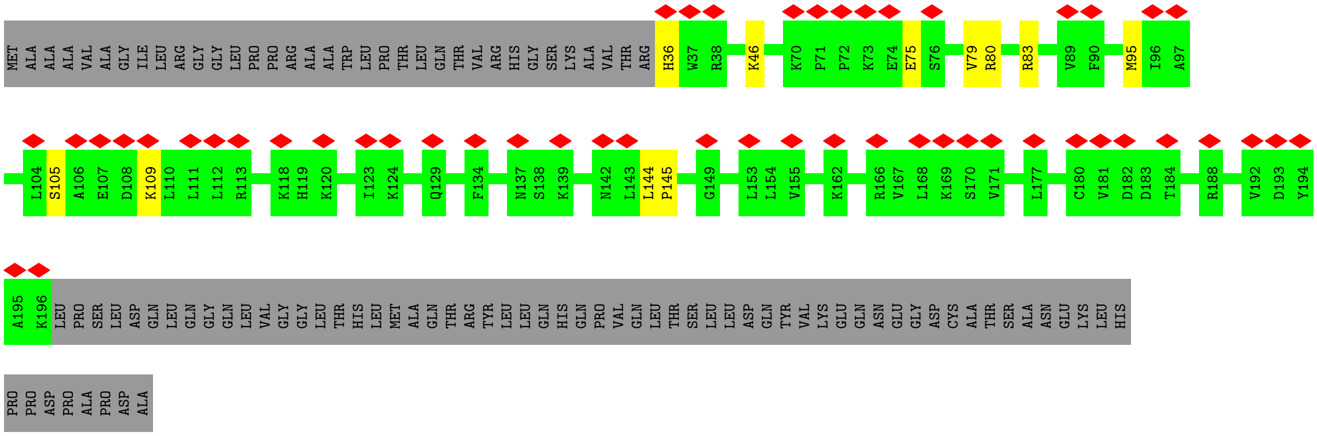
Chain H:





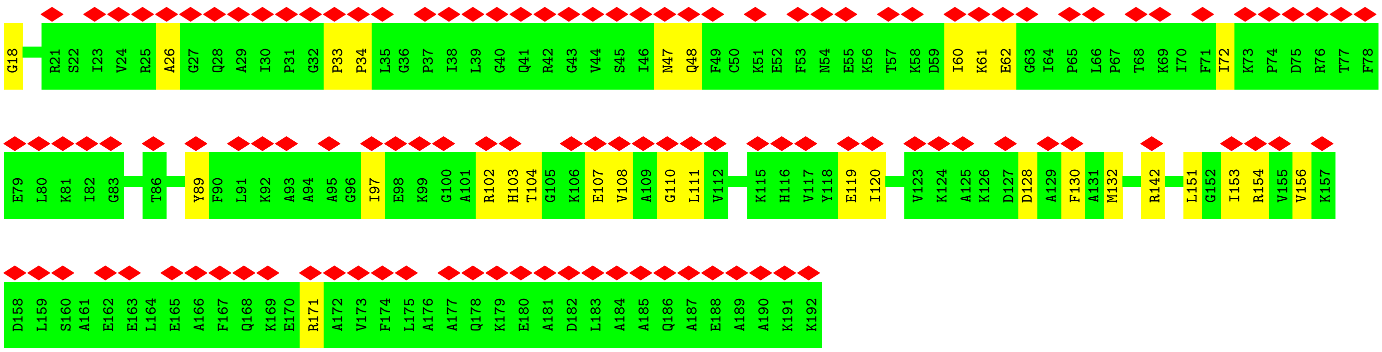
- Molecule 7: Large ribosomal subunit protein uL10m

Chain I:



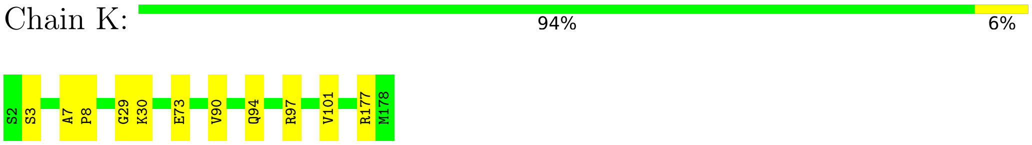
- Molecule 8: Large ribosomal subunit protein uL11m

Chain J:



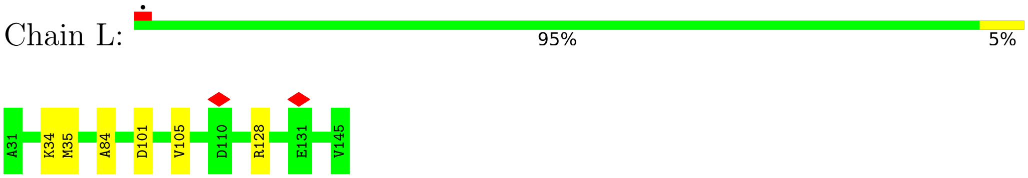
- Molecule 9: Large ribosomal subunit protein uL13m

Chain K:



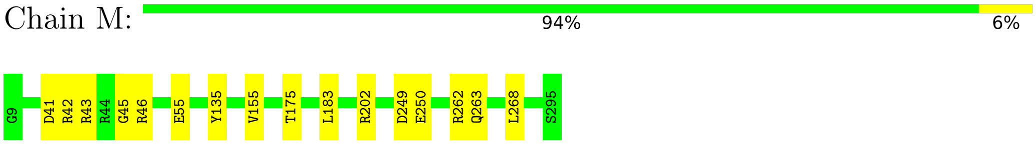
- Molecule 10: Large ribosomal subunit protein uL14m

Chain L:



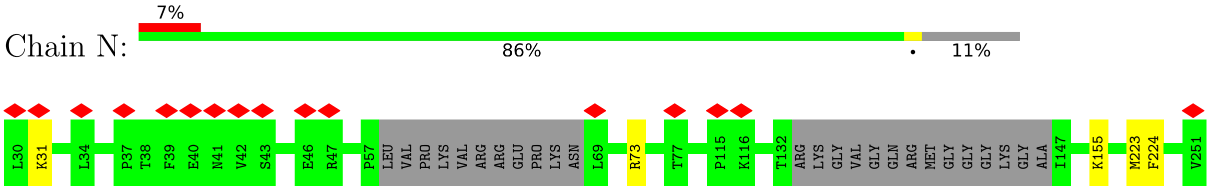
- Molecule 11: Large ribosomal subunit protein uL15m

Chain M:



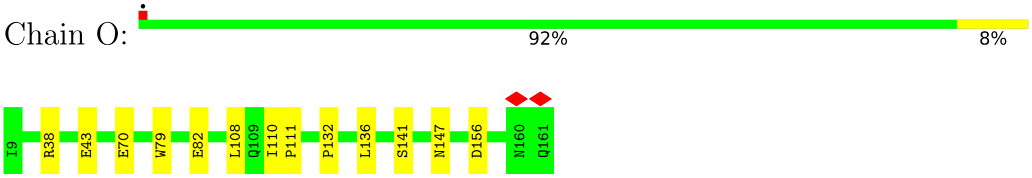
- Molecule 12: Large ribosomal subunit protein uL16m

Chain N:



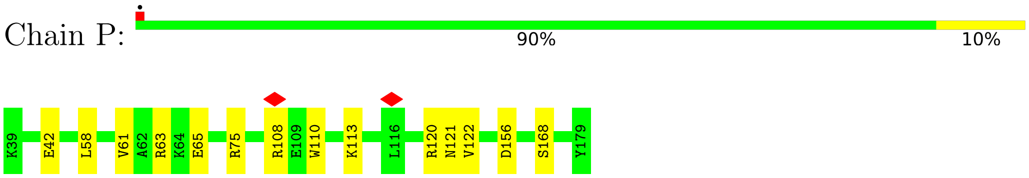
- Molecule 13: Large ribosomal subunit protein bL17m

Chain O:



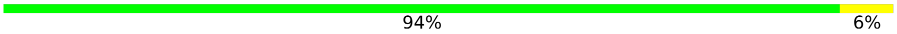
- Molecule 14: Large ribosomal subunit protein uL18m

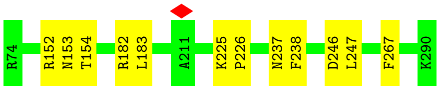
Chain P:



- Molecule 15: Large ribosomal subunit protein bL19m

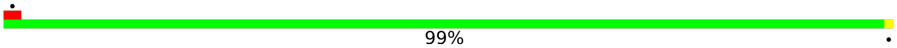
Chain Q:

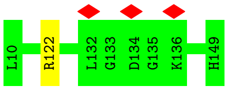




- Molecule 16: Large ribosomal subunit protein bL20m

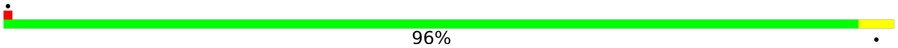
Chain R:

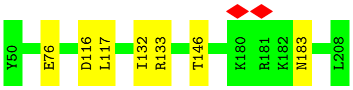




- Molecule 17: Large ribosomal subunit protein bL21m

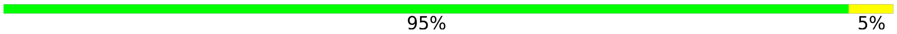
Chain S:





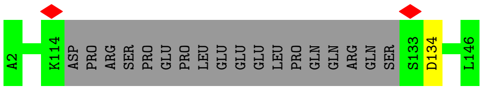
- Molecule 18: Large ribosomal subunit protein uL22m

Chain T:



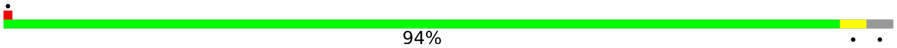
- Molecule 19: Large ribosomal subunit protein uL23m

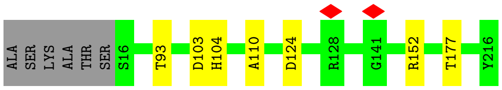
Chain U:



- Molecule 20: Large ribosomal subunit protein uL24m

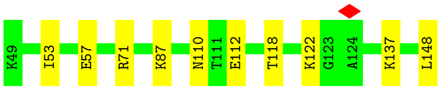
Chain V:





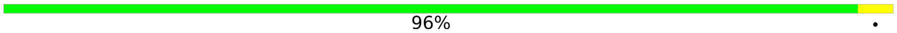
- Molecule 21: Large ribosomal subunit protein bL27m

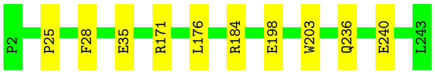
Chain W:



- Molecule 22: Large ribosomal subunit protein bL28m

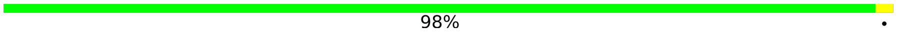
Chain X:





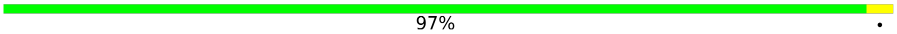
- Molecule 23: Large ribosomal subunit protein uL29m

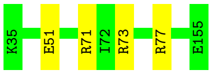
Chain Y:



- Molecule 24: Large ribosomal subunit protein uL30m

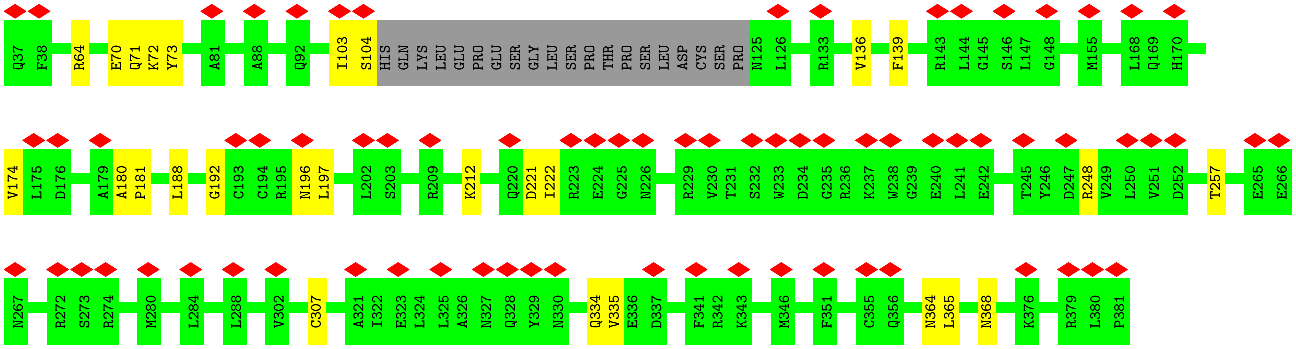
Chain Z:





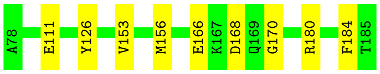
- Molecule 25: 5-cytosine rRNA methyltransferase NSUN4

Chain x:



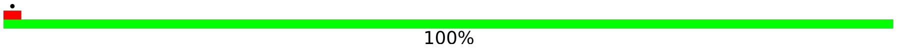
- Molecule 26: Large ribosomal subunit protein bL32m

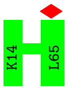
Chain 0:



- Molecule 27: Large ribosomal subunit protein bL33m

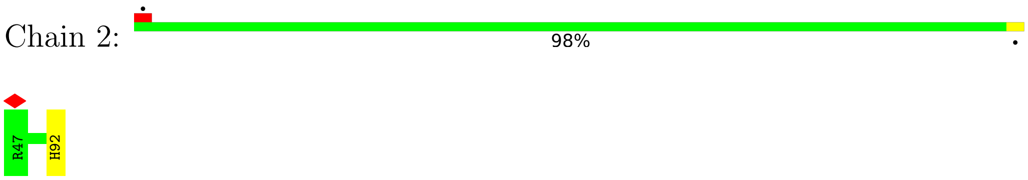
Chain 1:





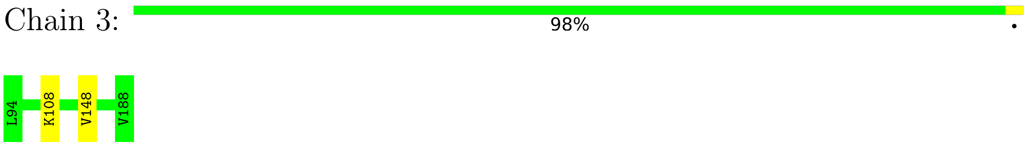
- Molecule 28: Large ribosomal subunit protein bL34m

Chain 2:



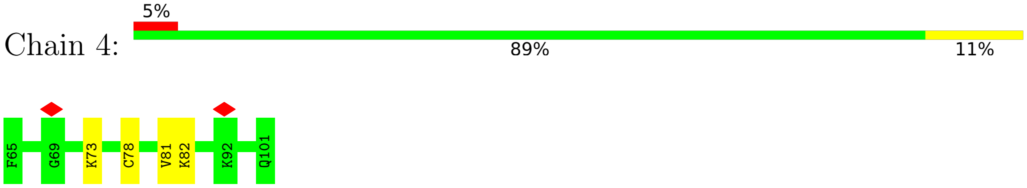
- Molecule 29: Large ribosomal subunit protein bL35m

Chain 3:



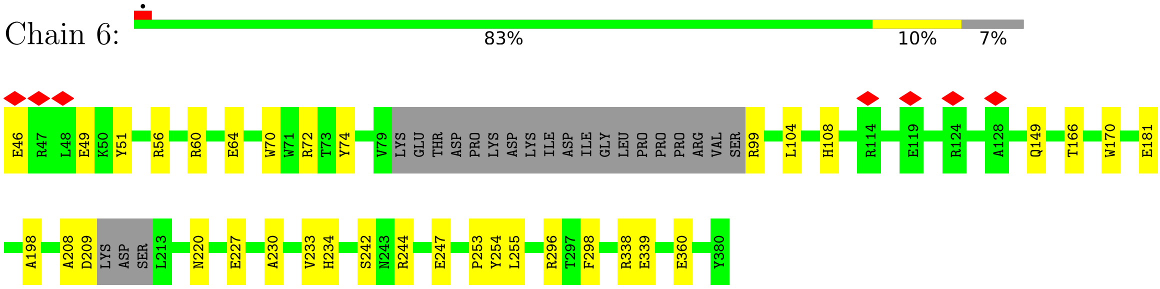
- Molecule 30: Large ribosomal subunit protein bL36m

Chain 4:



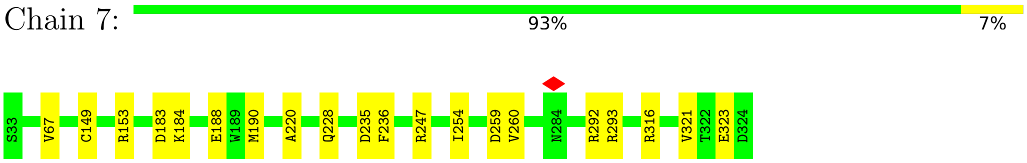
- Molecule 31: Large ribosomal subunit protein mL38

Chain 6:



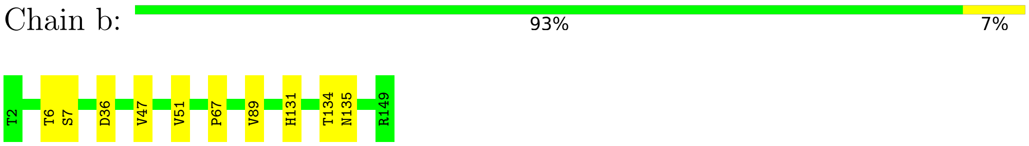
- Molecule 32: Large ribosomal subunit protein mL39

Chain 7:



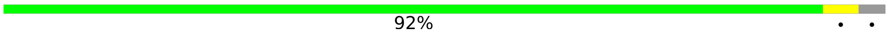
- Molecule 33: Large ribosomal subunit protein mL43

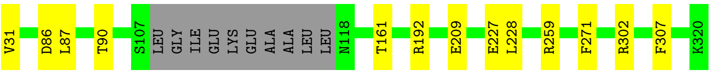
Chain b:



- Molecule 34: Large ribosomal subunit protein mL44

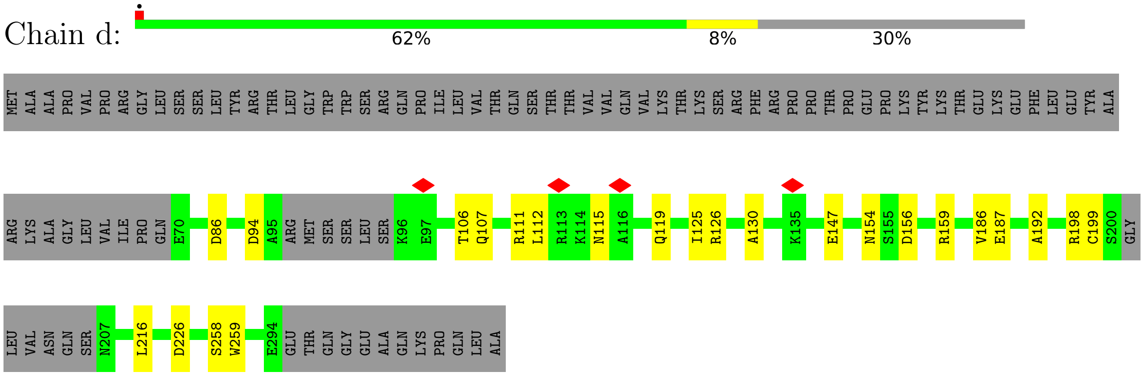
Chain c:





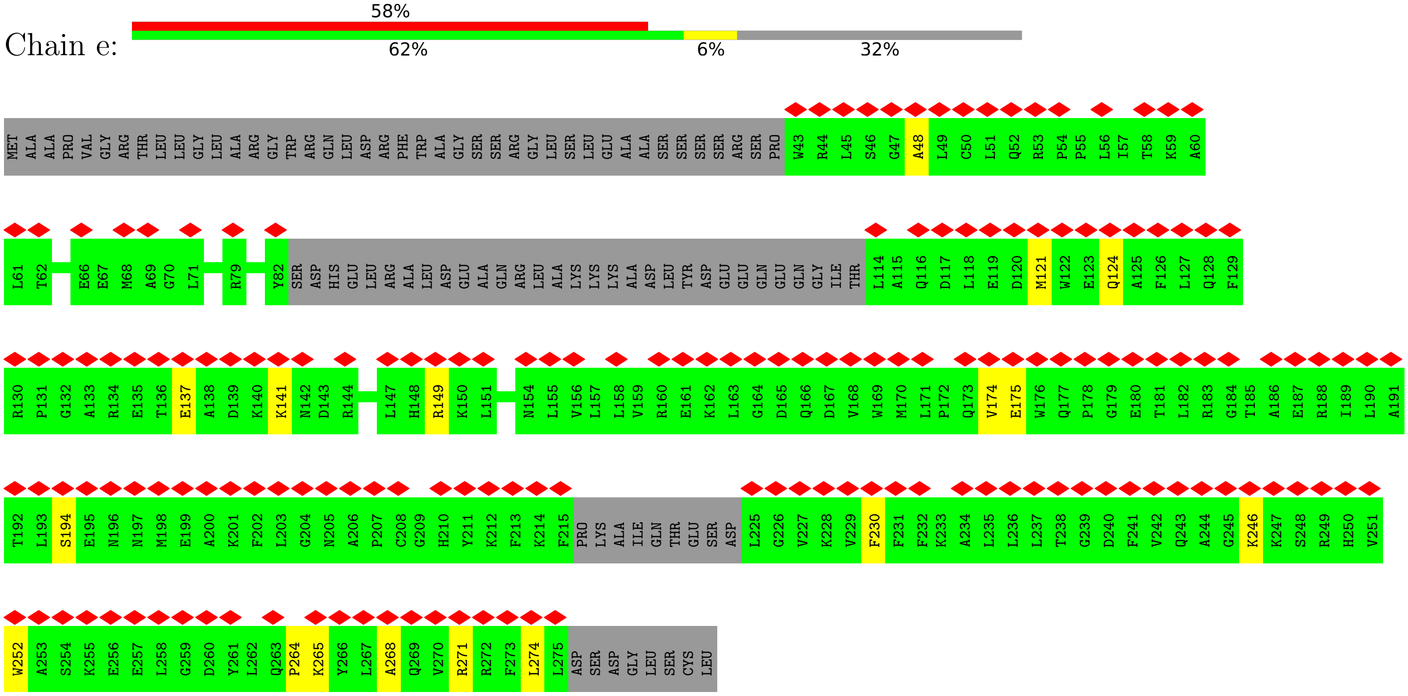
- Molecule 35: Large ribosomal subunit protein mL45

Chain d:



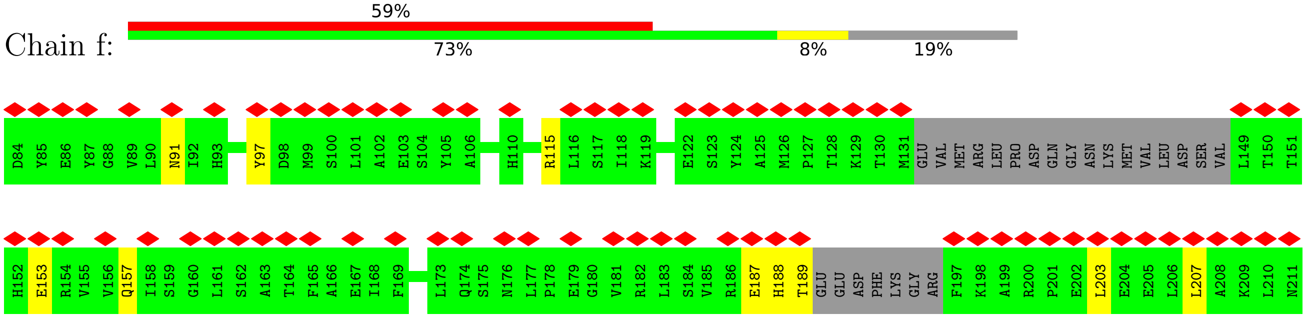
- Molecule 36: Large ribosomal subunit protein mL46

Chain e:



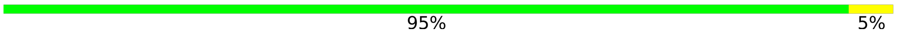
- Molecule 37: Large ribosomal subunit protein mL48

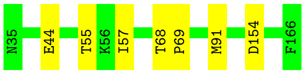
Chain f:



- Molecule 38: Large ribosomal subunit protein mL49

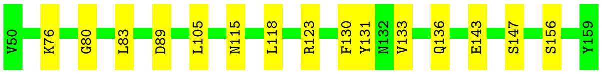
Chain g:





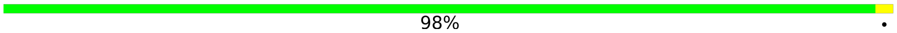
- Molecule 39: Large ribosomal subunit protein mL50

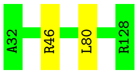
Chain h:



- Molecule 40: Large ribosomal subunit protein mL51

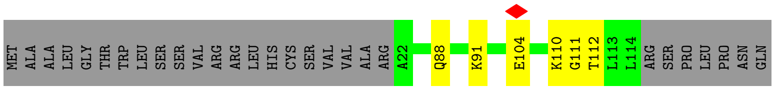
Chain i:





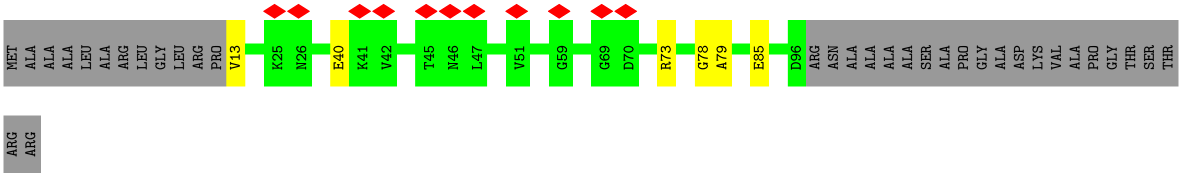
- Molecule 41: Large ribosomal subunit protein mL52

Chain j:



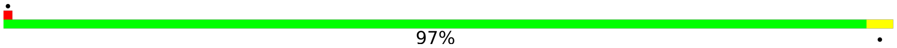
- Molecule 42: Large ribosomal subunit protein mL53

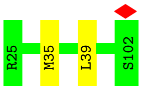
Chain k:



- Molecule 43: Large ribosomal subunit protein mL63

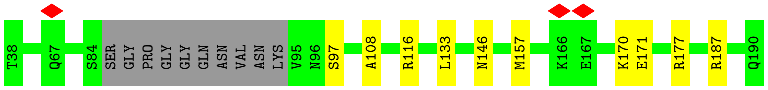
Chain o:





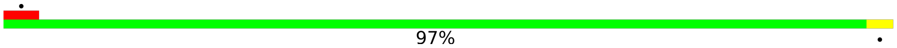
- Molecule 44: Large ribosomal subunit protein mL62

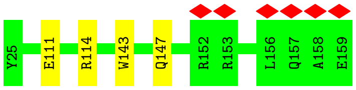
Chain p:



- Molecule 45: Large ribosomal subunit protein mL64

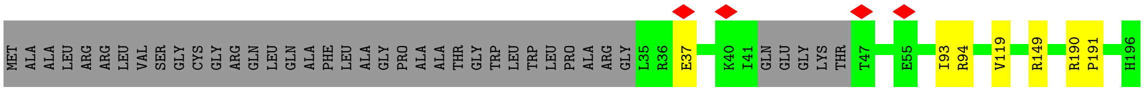
Chain q:





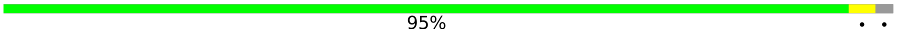
- Molecule 46: Large ribosomal subunit protein mL66

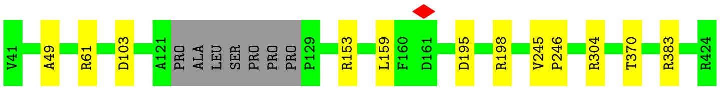
Chain r:



- Molecule 47: Large ribosomal subunit protein mL65

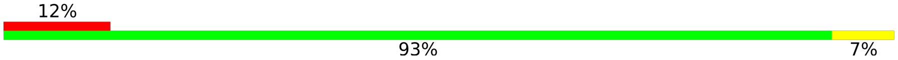
Chain s:

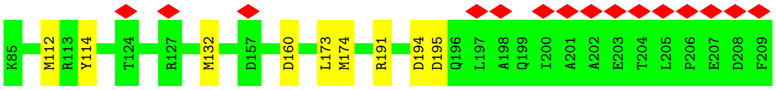




- Molecule 48: Mitochondrial assembly of ribosomal large subunit protein 1

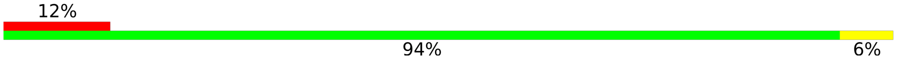
Chain u:

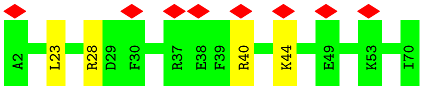




- Molecule 49: Predicted gene, 55359

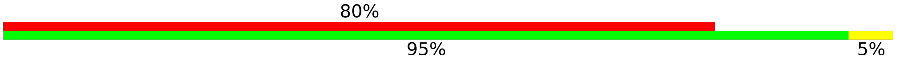
Chain v:

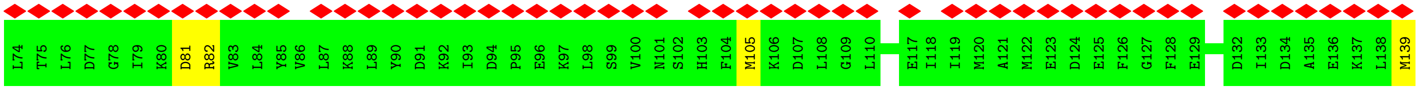


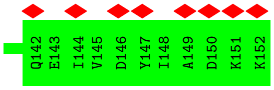


- Molecule 50: Acyl carrier protein, mitochondrial

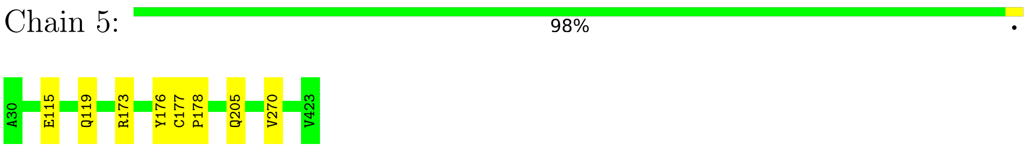
Chain w:



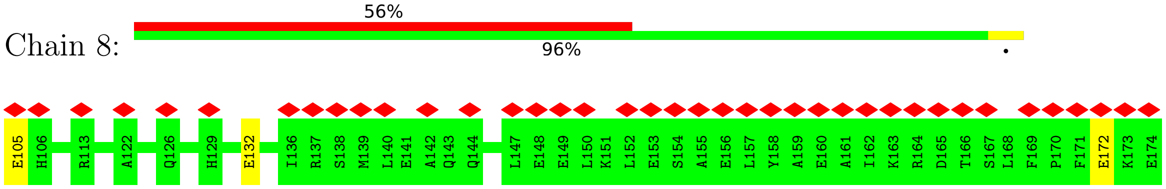




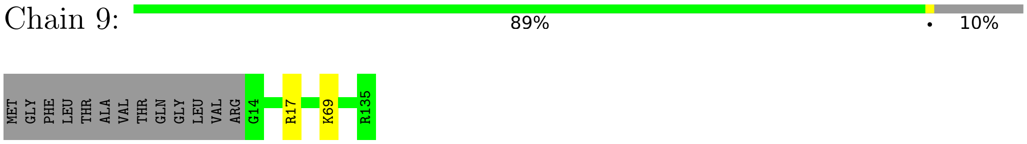
- Molecule 51: Large ribosomal subunit protein mL37



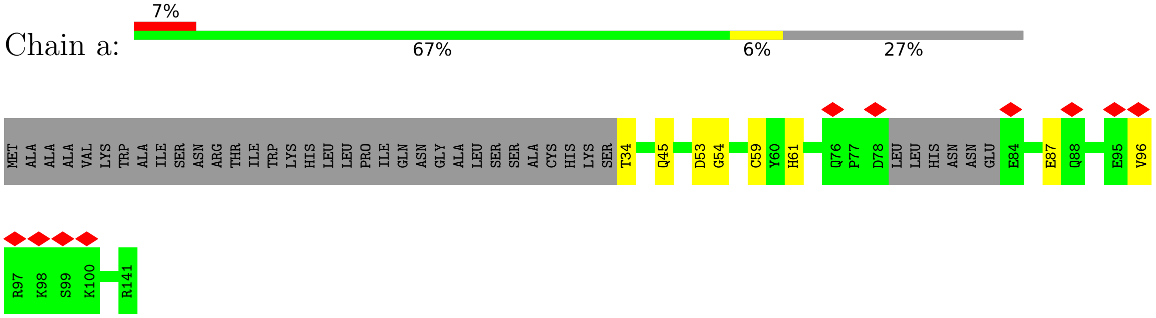
- Molecule 52: Large ribosomal subunit protein mL40



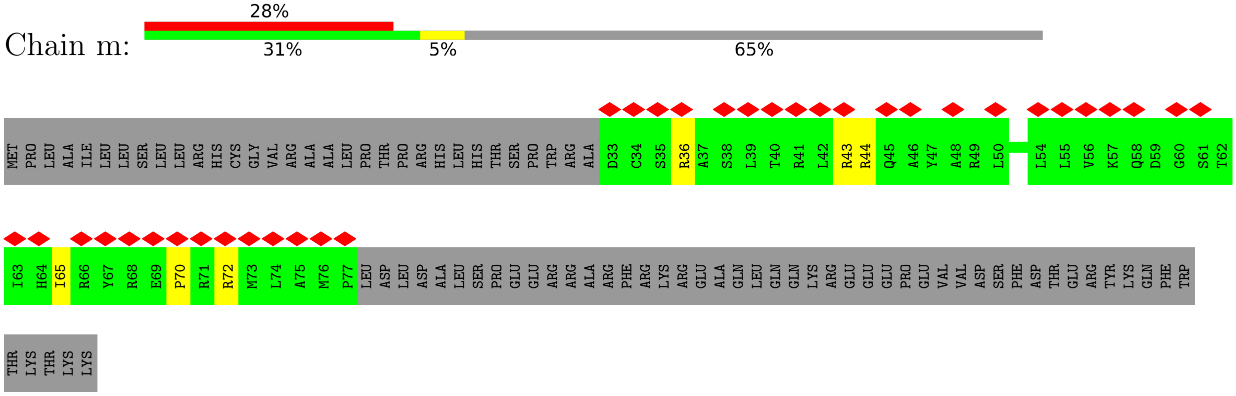
- Molecule 53: Large ribosomal subunit protein mL41



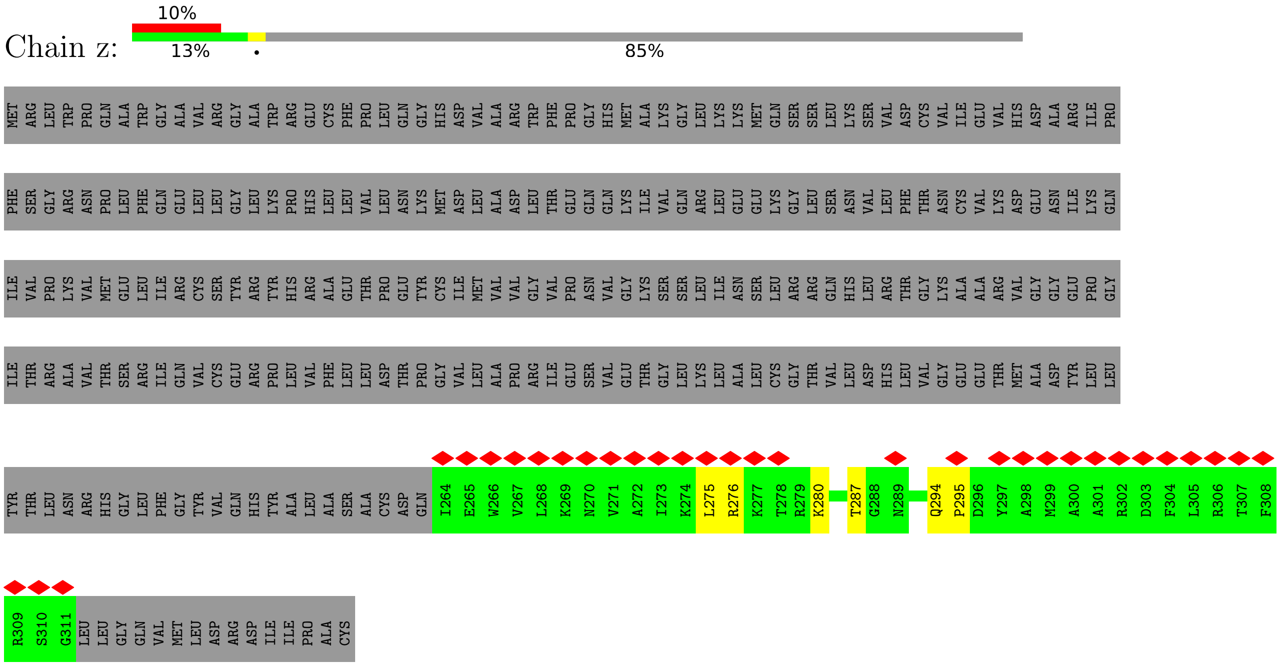
- Molecule 54: Large ribosomal subunit protein mL42



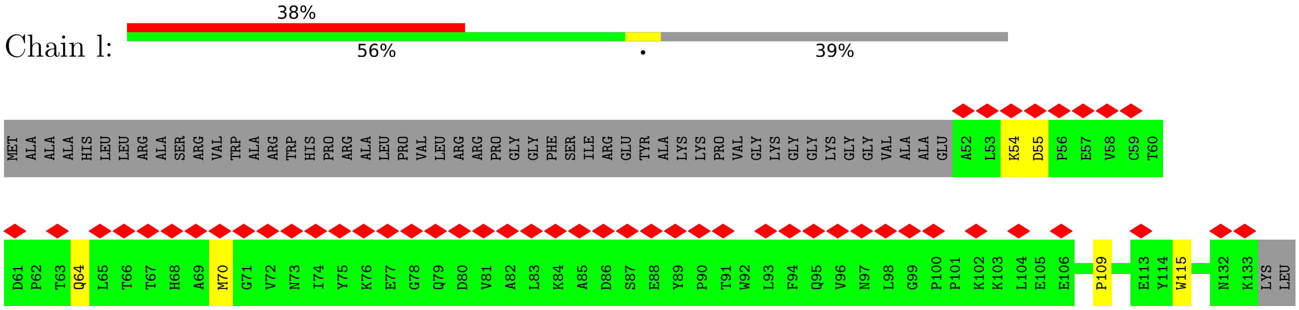
- Molecule 55: Large ribosomal subunit protein mL55



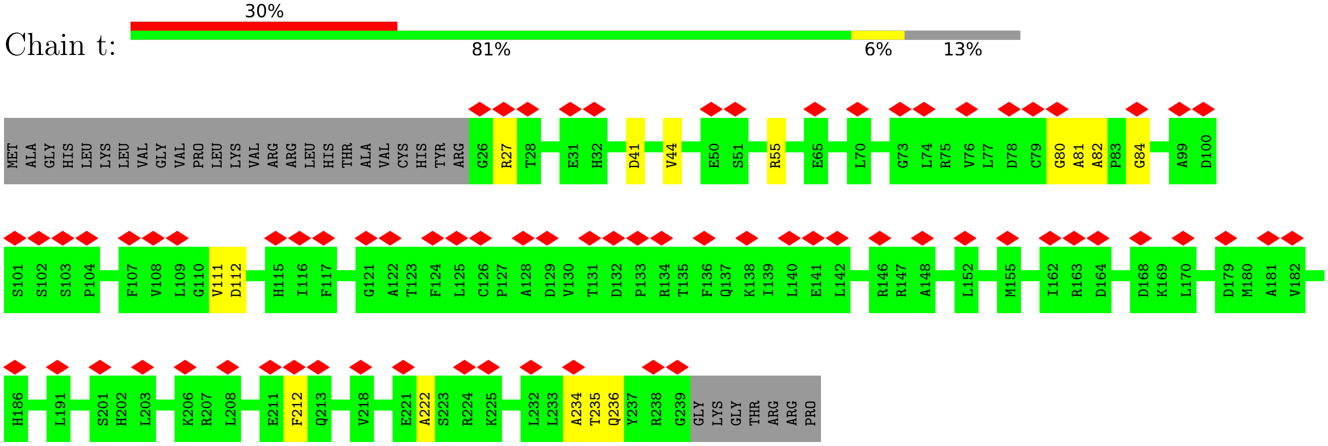
- Molecule 56: Mitochondrial ribosome-associated GTPase 1



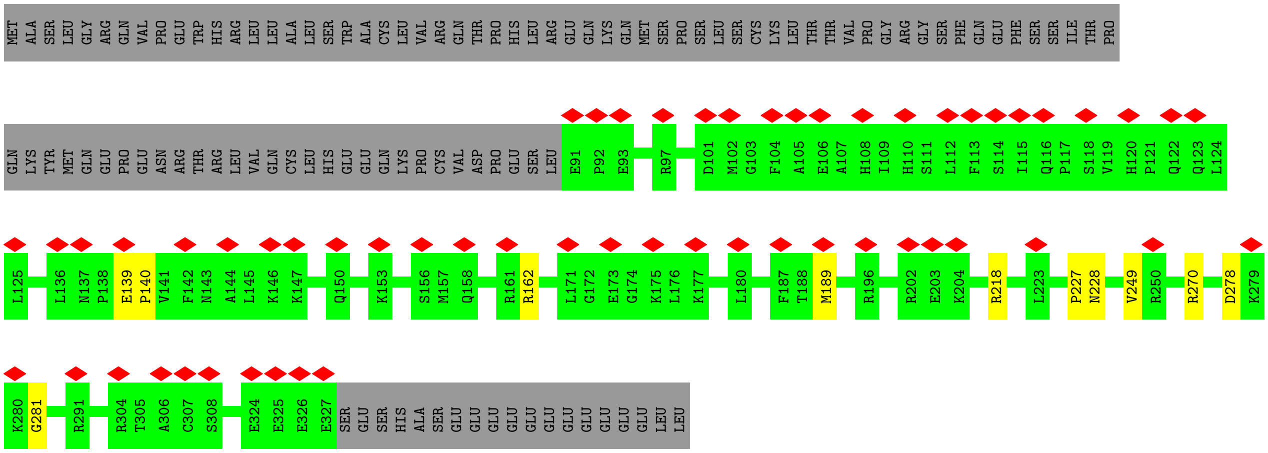
- Molecule 57: Large ribosomal subunit protein mL54



- Molecule 58: rRNA methyltransferase 2, mitochondrial



- Molecule 59: Transcription termination factor 4, mitochondrial


MET ALA SER LEU GLY ARG GLN VAL PRO GLU TRP HIS ARG LEU LEU ALA LEU SER TRP ALA CYS LEU VAL ARG GLN THR PRO HIS LEU ARG GLU GLN LYS GLN MET SER PRO SER LEU SER CYS LYS LEU THR THR VAL PRO GLY ARG GLY SER PHE GLN GLU PHE SER SER ILE THR PRO
GLN LYS TYR MET GLN GLU PRO GLU ASN ARG THR ARG LEU VAL GLN CYS LEU HIS GLU GLU GLN LYS PRO CYS VAL ASP PRO GLU SER LEU E91 P92 E93 R97 D101 M102 G103 F104 A105 E106 A107 H108 I109 H110 S111 L112 F113 S114 I115 Q116 P117 S118 V119 H120 P121 Q122 Q123 L124
L125 L136 N137 P138 E139 P140 V141 F142 N143 A144 L145 K146 K147 Q150 K153 S156 M157 Q158 R161 R162 L171 G172 E173 G174 K175 L176 K177 L180 F187 T188 M189 R196 R202 E203 K204 R218 L223 P227 N228 V249 R250 R270 D278 K279
K280 G281 R291 R304 T305 A306 C307 S308 E324 E325 E326 E327 SER GLU SER HIS ALA SER GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU LEU LEU

4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	97203	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	40	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.058	Depositor
Minimum map value	-0.021	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	456.9858, 456.9858, 456.9858	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84627, 0.84627, 0.84627	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, PSU, FES, SAH

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	A	0.14	0/34391	0.28	0/53487
2	B	0.16	0/1506	0.34	0/2337
3	D	0.10	0/1802	0.30	0/2424
4	E	0.11	0/2535	0.29	0/3443
5	F	0.12	0/2061	0.29	0/2805
6	H	0.10	0/793	0.25	0/1066
7	I	0.10	0/1339	0.24	0/1813
8	J	0.10	0/1346	0.27	0/1809
9	K	0.11	0/1491	0.26	0/2022
10	L	0.10	0/908	0.27	0/1224
11	M	0.12	0/2369	0.31	0/3197
12	N	0.08	0/1659	0.23	0/2238
13	O	0.11	0/1285	0.28	0/1732
14	P	0.10	0/1181	0.24	0/1600
15	Q	0.10	0/1832	0.27	0/2471
16	R	0.11	0/1182	0.23	0/1585
17	S	0.11	0/1328	0.29	0/1798
18	T	0.12	0/1402	0.29	0/1885
19	U	0.12	0/1080	0.28	0/1464
20	V	0.09	0/1695	0.24	0/2295
21	W	0.09	0/816	0.26	0/1105
22	X	0.10	0/2075	0.25	0/2806
23	Y	0.10	0/1561	0.23	0/2093
24	Z	0.10	0/1013	0.27	0/1368
25	x	0.11	0/2620	0.26	0/3549
26	0	0.11	0/896	0.28	0/1200
27	1	0.08	0/434	0.27	0/578
28	2	0.14	0/387	0.31	0/514
29	3	0.12	0/843	0.27	0/1122
30	4	0.10	0/328	0.26	0/430
31	6	0.10	0/2766	0.25	0/3758
32	7	0.09	0/2436	0.25	0/3300

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	b	0.11	0/1203	0.30	0/1625
34	c	0.09	0/2305	0.24	0/3117
35	d	0.10	0/1809	0.28	0/2451
36	e	0.09	0/1608	0.25	0/2165
37	f	0.08	0/851	0.26	0/1149
38	g	0.11	0/1126	0.30	0/1533
39	h	0.10	0/894	0.27	0/1216
40	i	0.12	0/855	0.28	0/1147
41	j	0.09	0/759	0.24	0/1019
42	k	0.09	0/666	0.28	0/899
43	o	0.11	0/655	0.27	0/880
44	p	0.08	0/1186	0.24	0/1592
45	q	0.09	0/1161	0.22	0/1571
46	r	0.09	0/1309	0.28	0/1767
47	s	0.11	0/3118	0.28	0/4232
48	u	0.08	0/1053	0.22	0/1425
49	v	0.08	0/596	0.25	0/795
50	w	0.10	0/646	0.30	0/869
51	5	0.10	0/3317	0.27	0/4519
52	8	0.07	0/598	0.20	0/799
53	9	0.10	0/1009	0.27	0/1358
54	a	0.10	0/884	0.28	0/1197
55	m	0.08	0/380	0.22	0/510
56	z	0.08	0/390	0.21	0/524
57	l	0.07	0/698	0.22	0/946
58	t	0.08	0/1688	0.25	0/2288
59	y	0.07	0/1980	0.20	0/2667
All	All	0.11	0/112104	0.27	0/158778

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	A	30753	15535	15557	149	0
2	B	1346	678	680	38	0
3	D	1768	1830	1830	14	0
4	E	2459	2441	2441	8	0
5	F	2005	2025	2024	8	0
6	H	779	814	814	4	0
7	I	1307	1393	1393	8	0
8	J	1326	1394	1394	20	0
9	K	1449	1444	1444	10	0
10	L	893	944	944	4	0
11	M	2315	2377	2377	13	0
12	N	1614	1626	1626	5	0
13	O	1259	1282	1282	10	0
14	P	1154	1148	1148	15	0
15	Q	1790	1822	1822	7	0
16	R	1161	1224	1224	1	0
17	S	1301	1372	1372	5	0
18	T	1369	1402	1402	6	0
19	U	1052	1057	1057	1	0
20	V	1652	1643	1643	5	0
21	W	794	809	808	9	0
22	X	2021	2051	2051	6	0
23	Y	1523	1553	1553	3	0
24	Z	987	1039	1039	3	0
25	x	2564	2546	2546	18	0
26	0	881	908	908	8	0
27	1	428	472	472	0	0
28	2	380	407	407	1	0
29	3	823	872	872	2	0
30	4	322	354	354	2	0
31	6	2673	2546	2545	28	0
32	7	2379	2378	2378	13	0
33	b	1181	1195	1195	7	0
34	c	2254	2262	2262	10	0
35	d	1760	1742	1742	14	0
36	e	1576	1598	1598	11	0
37	f	838	836	836	7	0
38	g	1090	1094	1094	5	0
39	h	872	867	867	9	0
40	i	831	854	854	2	0
41	j	744	768	768	5	0
42	k	657	659	659	5	0
43	o	640	623	623	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	p	1167	1185	1185	7	0
45	q	1130	1123	1123	2	0
46	r	1275	1331	1330	6	0
47	s	3045	3058	3057	8	0
48	u	1029	1012	1012	5	0
49	v	586	603	603	2	0
50	w	637	640	640	2	0
51	5	3225	3243	3243	5	0
52	8	589	574	574	3	0
53	9	983	990	990	2	0
54	a	860	843	843	6	0
55	m	374	395	395	5	0
56	z	385	415	415	4	0
57	l	681	677	677	4	0
58	t	1655	1695	1695	9	0
59	y	1943	1995	1995	6	0
60	6	1	0	0	0	0
60	A	101	0	0	0	0
60	E	1	0	0	0	0
60	M	1	0	0	0	0
60	O	1	0	0	0	0
61	0	1	0	0	0	0
61	4	1	0	0	0	0
62	r	4	0	0	0	0
63	t	26	19	19	0	0
64	A	1	0	0	0	0
All	All	106672	91682	91701	497	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 3.

All (497) 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)
1:A:1172:G:N2	1:A:1175:G:O2’	2.08	0.87
35:d:94:ASP:OD1	35:d:107:GLN:NE2	2.13	0.81
2:B:20:A:O4’	14:P:108:ARG:NH1	2.13	0.80
9:K:3:SER:O	34:c:302:ARG:NH1	2.14	0.79
31:6:198:ALA:O	31:6:254:TYR:OH	2.00	0.79
1:A:2551:A:O2’	4:E:266:ARG:NH1	2.15	0.79
1:A:2080:G:O2’	1:A:2082:G:OP2	2.01	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:y:162:ARG:NH2	59:y:189:MET:O	2.17	0.78
14:P:65:GLU:OE2	31:6:74:TYR:OH	2.01	0.78
2:B:21:A:OP2	14:P:113:LYS:NZ	2.18	0.77
1:A:2402:U:O4	1:A:2458:G:N2	2.17	0.77
8:J:18:GLY:N	8:J:72:ILE:O	2.17	0.77
14:P:58:LEU:O	44:p:177:ARG:NH2	2.18	0.77
1:A:1506:A:O2'	1:A:1507:A:O5'	2.03	0.76
10:L:128:ARG:NH1	48:u:114:TYR:O	2.17	0.76
25:x:70:GLU:O	25:x:368:ASN:ND2	2.19	0.76
22:X:35:GLU:N	22:X:35:GLU:OE1	2.18	0.76
1:A:1402:A:OP1	3:D:260:LYS:NZ	2.19	0.76
17:S:116:ASP:OD1	17:S:117:LEU:N	2.19	0.76
14:P:63:ARG:NH2	21:W:137:LYS:O	2.21	0.73
1:A:1195:G:N7	23:Y:230:LYS:NZ	2.36	0.73
20:V:124:ASP:OD2	20:V:152:ARG:NH2	2.22	0.73
1:A:1614:A:N6	1:A:1639:C:O2	2.22	0.72
1:A:1966:U:OP2	3:D:209:ARG:NE	2.22	0.72
49:v:23:LEU:O	49:v:28:ARG:NE	2.23	0.71
1:A:1599:C:N4	1:A:1645:C:OP2	2.23	0.71
1:A:2159:A:O2'	1:A:2161:G:OP1	2.09	0.71
18:T:127:ASN:ND2	35:d:226:ASP:OD2	2.24	0.70
1:A:1701:G:N7	11:M:43:ARG:NH2	2.39	0.70
21:W:148:LEU:O	31:6:339:GLU:N	2.25	0.69
35:d:147:GLU:OE2	35:d:159:ARG:NH2	2.25	0.69
35:d:111:ARG:O	35:d:115:ASN:N	2.25	0.69
32:7:228:GLN:OE1	32:7:228:GLN:N	2.25	0.68
1:A:1608:C:OP1	57:l:54:LYS:NZ	2.27	0.68
14:P:168:SER:O	44:p:187:ARG:NH2	2.26	0.68
1:A:1469:G:O2'	11:M:55:GLU:OE1	2.12	0.68
32:7:293:ARG:NH1	32:7:321:VAL:O	2.27	0.67
37:f:91:ASN:ND2	37:f:157:GLN:OE1	2.28	0.67
32:7:149:CYS:SG	32:7:153:ARG:NH1	2.69	0.66
1:A:2614:C:O2	9:K:97:ARG:NH2	2.27	0.66
1:A:1491:A:HO2'	1:A:1492:A:P	2.19	0.66
1:A:1636:G:O2'	1:A:1641:A:N6	2.29	0.66
31:6:60:ARG:NH2	31:6:64:GLU:OE1	2.29	0.66
57:l:64:GLN:NE2	57:l:70:MET:SD	2.69	0.66
2:B:16:U:O2'	31:6:99:ARG:NH2	2.29	0.65
32:7:190:MET:SD	32:7:292:ARG:NH2	2.68	0.65
31:6:242:SER:OG	31:6:244:ARG:NH1	2.29	0.65
1:A:1710:U:O2'	5:F:104:ARG:NH2	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:g:44:GLU:OE1	38:g:44:GLU:N	2.29	0.65
26:0:111:GLU:N	26:0:111:GLU:OE1	2.30	0.65
18:T:46:GLU:OE1	18:T:46:GLU:N	2.31	0.64
13:O:43:GLU:OE2	26:0:126:TYR:OH	2.15	0.64
55:m:70:PRO:O	55:m:72:ARG:NH1	2.30	0.64
1:A:1491:A:O2'	1:A:1492:A:OP1	2.10	0.63
44:p:108:ALA:O	44:p:116:ARG:NH1	2.31	0.63
35:d:86:ASP:OD2	35:d:198:ARG:NH1	2.31	0.63
21:W:112:GLU:OE1	21:W:112:GLU:N	2.29	0.63
12:N:73:ARG:O	12:N:155:LYS:NZ	2.31	0.63
16:R:122:ARG:NH2	17:S:76:GLU:OE2	2.31	0.63
4:E:165:TYR:OH	4:E:176:HIS:NE2	2.21	0.62
5:F:49:ARG:NH1	5:F:81:GLU:O	2.31	0.62
59:y:218:ARG:NH1	59:y:249:VAL:O	2.32	0.62
31:6:70:TRP:O	31:6:72:ARG:NH2	2.32	0.62
1:A:2656:C:O2'	1:A:2657:C:O4'	2.16	0.62
36:e:264:PRO:O	36:e:268:ALA:N	2.31	0.61
1:A:1501:A:O2'	1:A:1502:A:OP2	2.15	0.61
37:f:187:GLU:OE1	37:f:187:GLU:N	2.33	0.61
45:q:143:TRP:O	45:q:147:GLN:NE2	2.34	0.61
32:7:293:ARG:NH2	32:7:323:GLU:OE2	2.33	0.61
8:J:107:GLU:OE1	8:J:171:ARG:NH1	2.33	0.61
1:A:1299:A:O4'	1:A:1329:A:N6	2.34	0.61
1:A:2057:G:O2'	1:A:2058:G:OP1	2.19	0.61
22:X:176:LEU:O	22:X:184:ARG:NH1	2.35	0.60
1:A:1175:G:O2'	1:A:1176:A:OP2	2.14	0.60
3:D:198:GLU:OE2	3:D:203:ARG:N	2.35	0.60
18:T:72:ARG:O	18:T:167:HIS:ND1	2.34	0.60
30:4:73:LYS:NZ	30:4:78:CYS:O	2.35	0.60
1:A:1936:U:OP2	1:A:1941:A:N6	2.34	0.60
1:A:1222:A:OP1	5:F:142:ARG:NH2	2.34	0.59
2:B:5:A:H2'	2:B:6:U:C5	2.37	0.59
31:6:46:GLU:N	31:6:46:GLU:OE1	2.36	0.59
32:7:259:ASP:OD1	32:7:260:VAL:N	2.36	0.59
2:B:6:U:O2'	2:B:7:G:OP2	2.18	0.59
1:A:1418:G:OP1	3:D:270:ARG:NH2	2.35	0.59
1:A:2486:A:OP2	58:t:27:ARG:NH2	2.35	0.59
2:B:3:U:H2'	2:B:4:A:C8	2.38	0.59
31:6:104:LEU:O	31:6:108:HIS:ND1	2.36	0.58
26:0:166:GLU:OE1	26:0:166:GLU:N	2.32	0.58
1:A:2275:A:O2'	1:A:2276:U:OP1	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:6:170:TRP:NE1	41:j:112:THR:O	2.36	0.58
1:A:2395:U:O4	1:A:2396:A:N6	2.37	0.58
31:6:60:ARG:O	31:6:60:ARG:NH1	2.36	0.58
1:A:2617:A:O2'	1:A:2618:A:OP2	2.21	0.58
1:A:2068:G:H4'	1:A:2069:A:OP1	2.05	0.57
13:O:141:SER:O	13:O:147:ASN:ND2	2.37	0.57
23:Y:153:ASP:OD1	23:Y:156:ARG:NH2	2.36	0.57
1:A:1237:A:O2'	1:A:1238:U:OP1	2.17	0.57
2:B:20:A:OP1	14:P:110:TRP:N	2.35	0.56
7:I:79:VAL:O	7:I:83:ARG:N	2.34	0.56
1:A:1854:C:OP2	47:s:304:ARG:NH1	2.38	0.56
25:x:196:ASN:OD1	25:x:197:LEU:N	2.37	0.56
2:B:12:U:O2'	2:B:14:A:OP1	2.23	0.56
1:A:1102:U:O2'	1:A:1103:A:OP2	2.21	0.56
1:A:1831:U:H2'	1:A:1832:A:O4'	2.06	0.56
2:B:27:A:OP1	37:f:115:ARG:NH2	2.37	0.56
4:E:69:ASN:OD1	4:E:154:ARG:NH2	2.40	0.55
1:A:2158:G:H2'	1:A:2159:A:H4'	1.88	0.55
1:A:2191:U:OP1	6:H:88:LYS:NZ	2.36	0.55
1:A:1383:G:O2'	1:A:1386:G:O2'	2.22	0.55
1:A:1542:C:H2'	1:A:1543:U:H5'	1.89	0.55
46:r:37:GLU:OE1	46:r:37:GLU:N	2.39	0.55
1:A:1623:C:O3'	8:J:142:ARG:NH1	2.40	0.55
1:A:1893:C:O2'	1:A:1894:A:OP2	2.21	0.55
32:7:183:ASP:OD1	32:7:184:LYS:N	2.38	0.55
22:X:236:GLN:NE2	22:X:240:GLU:OE2	2.40	0.55
4:E:340:PRO:O	4:E:341:SER:OG	2.25	0.55
13:O:70:GLU:N	13:O:70:GLU:OE1	2.35	0.55
31:6:181:GLU:N	31:6:181:GLU:OE1	2.40	0.55
37:f:153:GLU:N	37:f:153:GLU:OE1	2.40	0.54
2:B:57:U:H2'	2:B:58:C:O4'	2.08	0.54
2:B:20:A:O5'	14:P:108:ARG:NH1	2.41	0.54
7:I:95:MET:SD	7:I:95:MET:N	2.79	0.54
24:Z:71:ARG:NH1	24:Z:73:ARG:O	2.37	0.54
36:e:268:ALA:O	36:e:271:ARG:NH1	2.41	0.54
8:J:104:THR:O	8:J:154:ARG:NH2	2.41	0.54
1:A:1846:U:O2'	51:5:270:VAL:O	2.25	0.54
1:A:2068:G:O2'	1:A:2069:A:O5'	2.23	0.54
14:P:61:VAL:HG12	14:P:61:VAL:O	2.07	0.54
35:d:154:ASN:ND2	35:d:156:ASP:OD2	2.40	0.54
1:A:1505:A:H1'	1:A:1506:A:OP2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:x:180:ALA:HB3	25:x:181:PRO:CD	2.37	0.54
47:s:195:ASP:OD1	47:s:198:ARG:NH2	2.41	0.54
2:B:60:C:H2'	2:B:61:A:C8	2.43	0.54
14:P:121:ASN:OD1	14:P:122:VAL:N	2.41	0.53
34:c:209:GLU:OE1	34:c:209:GLU:N	2.38	0.53
2:B:14:A:N1	2:B:21:A:O2'	2.40	0.53
34:c:161:THR:O	34:c:192:ARG:NH2	2.38	0.53
2:B:43:A:H2'	2:B:44:G:O4'	2.08	0.53
39:h:89:ASP:O	39:h:123:ARG:NH1	2.41	0.53
8:J:89:TYR:OH	57:l:55:ASP:OD2	2.22	0.53
31:6:227:GLU:OE1	31:6:230:ALA:N	2.42	0.53
36:e:194:SER:O	36:e:246:LYS:NZ	2.41	0.53
44:p:97:SER:O	44:p:146:ASN:ND2	2.42	0.53
1:A:2653:C:OP1	4:E:177:LYS:NZ	2.40	0.53
2:B:25:A:OP1	31:6:56:ARG:NH2	2.40	0.53
31:6:233:VAL:O	31:6:296:ARG:NH1	2.40	0.53
2:B:64:A:O2'	36:e:265:LYS:NZ	2.42	0.53
11:M:263:GLN:NE2	11:M:268:LEU:O	2.41	0.52
33:b:89:VAL:HG12	33:b:89:VAL:O	2.08	0.52
35:d:186:VAL:HG22	35:d:187:GLU:H	1.74	0.52
56:z:294:GLN:NE2	56:z:295:PRO:O	2.43	0.52
25:x:221:ASP:OD1	25:x:222:ILE:N	2.39	0.52
1:A:1137:A:O2'	1:A:1138:U:OP1	2.26	0.52
1:A:1647:A:O5'	12:N:31:LYS:NZ	2.39	0.52
36:e:121:MET:O	36:e:124:GLN:NE2	2.43	0.52
1:A:1712:U:OP2	40:i:46:ARG:NH1	2.36	0.52
1:A:1965:G:OP1	3:D:136:ARG:NH2	2.42	0.52
12:N:224:PHE:CE2	43:o:35:MET:HG3	2.44	0.52
2:B:20:A:HO2'	2:B:21:A:P	2.32	0.52
1:A:1187:U:O2'	1:A:1188:A:OP1	2.28	0.52
1:A:1493:A:O2'	21:W:57:GLU:OE1	2.28	0.52
1:A:1607:G:N2	8:J:102:ARG:O	2.32	0.52
1:A:2057:G:HO2'	1:A:2058:G:P	2.33	0.51
7:I:105:SER:O	7:I:109:LYS:N	2.43	0.51
1:A:1813:U:O2'	1:A:1814:A:O5'	2.26	0.51
7:I:75:GLU:O	7:I:80:ARG:NH2	2.43	0.51
3:D:195:ASN:ND2	3:D:246:GLY:O	2.44	0.51
1:A:1506:A:O2'	1:A:1507:A:P	2.68	0.51
31:6:220:ASN:OD1	31:6:234:HIS:NE2	2.42	0.51
1:A:1235:U:H1'	1:A:1236:A:OP2	2.10	0.51
1:A:2072:G:O2'	1:A:2073:G:OP1	2.24	0.51

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:A:1160:A:O2'	1:A:1161:C:P	2.69	0.51
1:A:1172:G:H22	1:A:1175:G:HO2'	1.59	0.51
1:A:2075:U:O2'	1:A:2076:A:H2'	2.11	0.51
2:B:2:U:H3'	2:B:3:U:H6	1.76	0.51
41:j:104:GLU:OE1	41:j:104:GLU:N	2.44	0.51
13:O:38:ARG:NH2	13:O:82:GLU:OE1	2.37	0.51
1:A:2073:G:H3'	1:A:2074:C:H5"	1.94	0.50
8:J:108:VAL:CG2	8:J:111:LEU:HD11	2.41	0.50
21:W:118:THR:OG1	31:6:51:TYR:O	2.26	0.50
55:m:43:ARG:O	55:m:44:ARG:NE	2.44	0.50
2:B:20:A:O2'	2:B:21:A:OP1	2.27	0.50
4:E:316:PHE:HB3	4:E:317:PRO:HD3	1.93	0.50
2:B:7:G:N2	2:B:60:C:N3	2.60	0.50
8:J:60:ILE:HG13	8:J:61:LYS:H	1.76	0.50
58:t:41:ASP:OD2	58:t:44:VAL:N	2.40	0.50
45:q:111:GLU:OE1	45:q:114:ARG:NH2	2.36	0.49
14:P:42:GLU:OE2	31:6:338:ARG:NH1	2.45	0.49
52:8:105:GLU:OE1	52:8:105:GLU:N	2.46	0.49
11:M:202:ARG:NH1	11:M:263:GLN:O	2.44	0.49
35:d:115:ASN:O	35:d:119:GLN:N	2.28	0.49
1:A:1588:C:N4	1:A:1658:C:N3	2.61	0.49
29:3:148:VAL:CG1	31:6:360:GLU:HA	2.43	0.49
31:6:208:ALA:O	31:6:209:ASP:CB	2.61	0.49
39:h:76:LYS:O	39:h:80:GLY:N	2.40	0.49
58:t:55:ARG:NH2	58:t:222:ALA:O	2.45	0.49
26:0:180:ARG:HD2	26:0:184:PHE:HD2	1.77	0.49
9:K:73:GLU:N	9:K:73:GLU:OE1	2.46	0.49
1:A:2284:A:N3	1:A:2333:U:N3	2.61	0.48
3:D:125:GLU:HB3	3:D:143:VAL:HG22	1.95	0.48
1:A:1137:A:HO2'	1:A:1138:U:P	2.36	0.48
8:J:128:ASP:OD2	8:J:132:MET:N	2.46	0.48
25:x:73:TYR:O	25:x:139:PHE:HE2	1.96	0.48
1:A:1364:U:H2'	1:A:1365:A:O4'	2.13	0.48
5:F:94:ASP:OD1	5:F:94:ASP:N	2.45	0.48
11:M:202:ARG:O	11:M:262:ARG:NE	2.46	0.48
1:A:1658:C:H2'	1:A:1659:A:O4'	2.14	0.48
11:M:155:VAL:O	11:M:175:THR:HA	2.13	0.48
52:8:172:GLU:OE1	52:8:172:GLU:N	2.47	0.48
34:c:227:GLU:OE2	34:c:302:ARG:NE	2.42	0.48
35:d:106:THR:OG1	35:d:107:GLN:N	2.44	0.48
39:h:105:LEU:HD13	39:h:131:TYR:HE2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:292:ASP:OD1	38:g:55:THR:HG22	2.14	0.48
18:T:190:ALA:O	18:T:194:ILE:HD12	2.13	0.48
31:6:233:VAL:HG23	31:6:298:PHE:CD1	2.49	0.48
12:N:224:PHE:CZ	43:o:39:LEU:HG	2.49	0.48
13:O:156:ASP:OD2	32:7:316:ARG:NH2	2.47	0.48
31:6:247:GLU:OE1	31:6:247:GLU:N	2.47	0.48
10:L:84:ALA:HB1	10:L:105:VAL:HG22	1.95	0.47
1:A:2057:G:O2’	1:A:2058:G:P	2.71	0.47
3:D:178:GLN:N	3:D:178:GLN:OE1	2.47	0.47
6:H:104:VAL:HG13	6:H:105:ARG:N	2.30	0.47
37:f:97:TYR:CE2	55:m:65:ILE:HG22	2.50	0.47
1:A:1610:U:N3	1:A:1613:A:OP2	2.47	0.47
1:A:2501:A:H4’	1:A:2501:A:OP2	2.14	0.47
3:D:212:GLY:O	3:D:247:ARG:NH2	2.47	0.47
9:K:90:VAL:HG22	9:K:94:GLN:HB2	1.96	0.47
2:B:59:C:H2’	2:B:60:C:N1	2.29	0.47
8:J:130:PHE:O	8:J:132:MET:N	2.42	0.47
41:j:112:THR:O	41:j:112:THR:HG22	2.14	0.47
57:l:109:PRO:O	57:l:115:TRP:NE1	2.47	0.47
1:A:1944:A:O2’	1:A:1945:C:OP1	2.29	0.47
48:u:132:MET:HE2	48:u:173:LEU:HD21	1.97	0.47
39:h:136:GLN:N	39:h:136:GLN:OE1	2.47	0.47
47:s:49:ALA:O	47:s:61:ARG:NH1	2.47	0.47
1:A:2326:A:OP1	1:A:2326:A:H3’	2.14	0.47
9:K:73:GLU:OE2	46:r:149:ARG:NH2	2.44	0.47
31:6:208:ALA:O	31:6:209:ASP:HB2	2.15	0.47
58:t:235:THR:HG22	58:t:236:GLN:N	2.30	0.47
21:W:122:LYS:N	31:6:49:GLU:O	2.48	0.46
22:X:28:PHE:CE1	22:X:203:TRP:HB2	2.50	0.46
34:c:87:LEU:O	34:c:90:THR:OG1	2.30	0.46
17:S:132:ILE:HG22	17:S:133:ARG:N	2.30	0.46
1:A:1604:U:H1’	1:A:1606:G:OP2	2.16	0.46
50:w:105:MET:HG2	50:w:139:MET:CE	2.45	0.46
1:A:1604:U:O4	1:A:1631:A:N6	2.44	0.46
37:f:188:HIS:O	37:f:189:THR:C	2.58	0.46
58:t:235:THR:HG22	58:t:236:GLN:H	1.79	0.46
8:J:103:HIS:O	8:J:104:THR:OG1	2.33	0.46
11:M:135:TYR:HA	11:M:183:LEU:HD22	1.97	0.46
1:A:1597:A:H2’	1:A:1597:A:N3	2.31	0.46
1:A:1237:A:HO2’	1:A:1238:U:P	2.36	0.46
1:A:2629:A:N3	1:A:2629:A:H2’	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:N:223:MET:O	12:N:224:PHE:HB2	2.14	0.46
25:x:257:THR:HG23	25:x:257:THR:O	2.16	0.46
25:x:136:VAL:HG12	25:x:136:VAL:O	2.16	0.45
40:i:80:LEU:HD12	40:i:80:LEU:O	2.16	0.45
1:A:1506:A:O2’	1:A:1507:A:O4’	2.33	0.45
1:A:1565:U:H5”	1:A:1565:U:H6	1.81	0.45
1:A:2429:U:H2’	1:A:2430:C:C5	2.52	0.45
34:c:31:VAL:HG13	34:c:31:VAL:O	2.16	0.45
48:u:112:MET:SD	48:u:191:ARG:NE	2.89	0.45
1:A:1457:A:OP1	1:A:1457:A:H4’	2.13	0.45
1:A:1683:C:C2’	1:A:1683:C:O2	2.64	0.45
8:J:47:ASN:OD1	8:J:48:GLN:N	2.49	0.45
1:A:1598:C:O2’	1:A:1649:A:N1	2.50	0.45
1:A:2302:U:HO2’	1:A:2303:A:P	2.40	0.45
1:A:2342:U:H4’	1:A:2343:A:OP1	2.17	0.45
2:B:9:A:C8	2:B:44:G:H2’	2.51	0.45
6:H:62:ALA:O	6:H:66:ARG:NH1	2.50	0.45
9:K:177:ARG:NH1	42:k:85:GLU:OE2	2.50	0.45
42:k:13:VAL:O	42:k:13:VAL:HG13	2.16	0.45
46:r:93:ILE:HG22	46:r:94:ARG:O	2.17	0.45
58:t:81:ALA:O	58:t:84:GLY:N	2.49	0.45
1:A:1134:A:N7	23:Y:197:ASN:ND2	2.64	0.45
1:A:1563:C:OP2	24:Z:77:ARG:NH1	2.50	0.45
1:A:2575:C:H4’	1:A:2575:C:OP1	2.17	0.45
50:w:81:ASP:OD1	50:w:82:ARG:N	2.49	0.45
11:M:249:ASP:OD1	11:M:250:GLU:N	2.50	0.45
13:O:110:ILE:HG23	13:O:111:PRO:HD2	1.99	0.45
25:x:364:ASN:OD1	25:x:365:LEU:N	2.50	0.45
32:7:254:ILE:O	32:7:254:ILE:HG13	2.17	0.45
33:b:36:ASP:OD1	33:b:36:ASP:N	2.48	0.45
1:A:1622:C:O2’	1:A:1631:A:O5’	2.31	0.45
1:A:1960:U:H2’	1:A:1960:U:O2	2.17	0.45
1:A:2292:A:N3	1:A:2292:A:H2’	2.31	0.45
1:A:2655:C:H4’	1:A:2656:C:OP2	2.17	0.45
25:x:334:GLN:NE2	25:x:335:VAL:O	2.50	0.45
11:M:41:ASP:O	11:M:45:GLY:N	2.49	0.44
49:v:40:ARG:O	49:v:44:LYS:HG2	2.17	0.44
1:A:1170:U:O4	29:3:108:LYS:NZ	2.50	0.44
1:A:1621:A:H2’	1:A:1622:C:O4’	2.18	0.44
2:B:6:U:O2’	2:B:7:G:P	2.75	0.44
4:E:230:SER:O	4:E:231:HIS:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:284:TYR:HB2	5:F:285:PRO:CD	2.47	0.44
8:J:111:LEU:HD23	8:J:156:VAL:HB	1.99	0.44
25:x:71:GLN:NE2	25:x:72:LYS:O	2.50	0.44
51:5:173:ARG:HA	51:5:176:TYR:CE1	2.52	0.44
1:A:1234:C:H3’	1:A:1235:U:C5’	2.47	0.44
35:d:258:SER:OG	35:d:259:TRP:N	2.51	0.44
38:g:68:THR:CG2	38:g:69:PRO:HD2	2.47	0.44
59:y:227:PRO:O	59:y:228:ASN:HB2	2.17	0.44
1:A:1830:C:H2’	1:A:1831:U:C1’	2.47	0.44
1:A:2416:A:OP2	7:I:36:HIS:NE2	2.50	0.44
9:K:101:VAL:HG12	9:K:101:VAL:O	2.17	0.44
24:Z:51:GLU:OE1	24:Z:51:GLU:N	2.45	0.44
47:s:245:VAL:HG22	47:s:246:PRO:HD2	1.98	0.44
1:A:1893:C:H1’	1:A:1894:A:OP2	2.18	0.44
20:V:93:THR:HG21	20:V:110:ALA:HB1	2.00	0.44
33:b:6:THR:HG22	33:b:7:SER:N	2.33	0.44
47:s:370:THR:CG2	47:s:383:ARG:HB2	2.48	0.44
54:a:34:THR:HG22	54:a:34:THR:O	2.18	0.44
2:B:8:U:O2’	2:B:46:U:O4’	2.34	0.44
32:7:188:GLU:OE1	32:7:188:GLU:N	2.49	0.44
1:A:2626:A:OP1	46:r:94:ARG:NH2	2.49	0.44
32:7:67:VAL:O	32:7:67:VAL:HG22	2.18	0.44
2:B:20:A:N3	2:B:20:A:H3’	2.33	0.44
31:6:233:VAL:HG23	31:6:298:PHE:CE1	2.53	0.44
2:B:6:U:C4	2:B:7:G:C6	3.06	0.43
3:D:195:ASN:OD1	3:D:244:THR:HG23	2.18	0.43
6:H:107:ASP:OD1	6:H:107:ASP:N	2.44	0.43
13:O:108:LEU:HD11	13:O:136:LEU:HD22	2.00	0.43
56:z:287:THR:HG22	56:z:287:THR:O	2.18	0.43
1:A:1628:A:O2’	1:A:1629:A:H5’	2.18	0.43
1:A:1671:A:O3’	9:K:29:GLY:HA3	2.19	0.43
1:A:1187:U:O2	1:A:1187:U:H2’	2.17	0.43
1:A:1541:G:O2’	1:A:1542:C:OP1	2.30	0.43
1:A:2659:C:H4’	1:A:2660:U:OP1	2.19	0.43
15:Q:246:ASP:OD1	15:Q:247:LEU:N	2.51	0.43
21:W:110:ASN:OD1	21:W:110:ASN:O	2.36	0.43
25:x:174:VAL:HA	25:x:248:ARG:O	2.18	0.43
1:A:1134:A:H1’	1:A:1135:U:H5’	2.00	0.43
1:A:1234:C:O2’	1:A:1235:U:H5”	2.19	0.43
1:A:1431:A:H2’	1:A:1431:A:N3	2.34	0.43
1:A:2056:A:H4’	1:A:2057:G:OP1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:e:271:ARG:HA	36:e:274:LEU:HB2	2.00	0.43
59:y:139:GLU:HB2	59:y:140:PRO:HD3	2.00	0.43
59:y:278:ASP:OD1	59:y:281:GLY:N	2.51	0.43
1:A:1611:A:N6	1:A:1638:U:O2	2.52	0.43
52:8:132:GLU:OE2	55:m:36:ARG:NE	2.52	0.43
1:A:1960:U:O2	1:A:1960:U:C2’	2.67	0.43
1:A:2461:G:N2	1:A:2572:G:O2’	2.50	0.43
13:O:79:TRP:NE1	15:Q:267:PHE:O	2.38	0.43
20:V:103:ASP:OD1	20:V:104:HIS:N	2.49	0.43
1:A:2337:C:H2’	1:A:2338:C:O4’	2.19	0.43
36:e:149:ARG:NH1	36:e:252:TRP:O	2.52	0.43
54:a:45:GLN:O	54:a:61:HIS:HA	2.18	0.43
8:J:33:PRO:N	8:J:34:PRO:CD	2.82	0.43
8:J:108:VAL:HG23	8:J:154:ARG:HB2	2.01	0.43
30:4:81:VAL:HG12	30:4:82:LYS:N	2.34	0.43
31:6:149:GLN:NE2	31:6:166:THR:OG1	2.50	0.43
42:k:73:ARG:H	42:k:73:ARG:HD3	1.84	0.43
20:V:93:THR:CG2	20:V:110:ALA:HB1	2.49	0.43
25:x:103:ILE:O	25:x:104:SER:C	2.62	0.43
1:A:1490:A:N6	1:A:1491:A:N1	2.67	0.42
3:D:112:PHE:CZ	3:D:168:ASN:HB2	2.54	0.42
8:J:97:ILE:HD13	8:J:153:ILE:HD13	2.01	0.42
15:Q:225:LYS:HB3	15:Q:226:PRO:CD	2.49	0.42
36:e:48:ALA:N	36:e:230:PHE:O	2.52	0.42
47:s:153:ARG:NH1	51:5:205:GLN:O	2.49	0.42
2:B:4:A:H2’	2:B:5:A:H4’	2.00	0.42
2:B:32:U:H2’	2:B:33:G:H4’	2.02	0.42
11:M:46:ARG:HD2	11:M:46:ARG:N	2.35	0.42
35:d:126:ARG:O	35:d:130:ALA:N	2.52	0.42
48:u:194:ASP:OD1	48:u:195:ASP:N	2.52	0.42
1:A:1610:U:C4	1:A:1613:A:OP2	2.72	0.42
1:A:1611:A:H3’	1:A:1612:A:C8	2.54	0.42
1:A:2302:U:C2’	1:A:2303:A:O5’	2.66	0.42
32:7:235:ASP:OD1	32:7:236:PHE:N	2.52	0.42
3:D:129:VAL:HG12	3:D:130:VAL:N	2.34	0.42
14:P:120:ARG:CG	14:P:120:ARG:O	2.68	0.42
25:x:180:ALA:CB	25:x:181:PRO:CD	2.97	0.42
1:A:1657:U:O3’	1:A:1658:C:O4’	2.37	0.42
54:a:96:VAL:O	54:a:96:VAL:HG13	2.20	0.42
1:A:1477:U:H2’	1:A:1478:U:C6	2.54	0.42
1:A:1541:G:H2’	1:A:1542:C:O4’	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:52:U:H1'	2:B:53:U:O4'	2.19	0.42
7:I:105:SER:N	42:k:40:GLU:OE2	2.51	0.42
28:2:92:HIS:CE1	53:9:17:ARG:HG2	2.55	0.42
47:s:159:LEU:HD23	47:s:159:LEU:O	2.19	0.42
11:M:135:TYR:HA	11:M:183:LEU:CD2	2.49	0.42
13:O:132:PRO:HA	26:0:184:PHE:CE1	2.55	0.42
1:A:1614:A:N7	1:A:1639:C:O2'	2.52	0.42
1:A:1936:U:H5	1:A:1941:A:N7	2.18	0.42
1:A:2286:G:O2'	25:x:212:LYS:NZ	2.42	0.42
2:B:3:U:C2	2:B:65:A:C2	3.07	0.42
4:E:121:LEU:HD22	4:E:284:TYR:CE1	2.55	0.42
21:W:71:ARG:O	21:W:87:LYS:NZ	2.43	0.42
36:e:137:GLU:O	36:e:141:LYS:HE3	2.20	0.42
47:s:103:ASP:OD1	47:s:103:ASP:N	2.52	0.42
1:A:1610:U:H5'	1:A:1611:A:H5"	2.01	0.42
1:A:1617:A:H2'	1:A:1618:G:O4'	2.20	0.42
1:A:1895:A:N6	1:A:2105:A:O2'	2.53	0.42
1:A:2515:C:H2'	1:A:2516:A:H5'	2.02	0.42
8:J:110:GLY:C	8:J:111:LEU:HD12	2.44	0.42
21:W:53:ILE:HG13	21:W:53:ILE:O	2.20	0.42
22:X:25:PRO:HB2	22:X:28:PHE:CD2	2.55	0.42
38:g:154:ASP:OD1	38:g:154:ASP:N	2.53	0.42
1:A:1672:A:O3'	9:K:30:LYS:NZ	2.53	0.41
1:A:2077:A:H2'	1:A:2078:A:O4'	2.20	0.41
1:A:2088:A:O2'	56:z:280:LYS:O	2.37	0.41
33:b:134:THR:O	33:b:135:ASN:HB2	2.20	0.41
35:d:192:ALA:HB2	35:d:216:LEU:HD23	2.02	0.41
36:e:174:VAL:CG1	36:e:175:GLU:N	2.83	0.41
48:u:160:ASP:O	48:u:174:MET:HA	2.19	0.41
1:A:1979:G:N1	1:A:2074:C:O2	2.53	0.41
7:I:144:LEU:N	7:I:145:PRO:HD2	2.35	0.41
14:P:75:ARG:O	14:P:75:ARG:HG2	2.19	0.41
33:b:131:HIS:CE1	33:b:134:THR:HG23	2.56	0.41
58:t:212:PHE:HD2	58:t:234:ALA:CB	2.33	0.41
19:U:134:ASP:OD1	19:U:134:ASP:N	2.53	0.41
33:b:67:PRO:HD2	39:h:156:SER:O	2.21	0.41
39:h:115:ASN:HA	39:h:118:LEU:HD13	2.02	0.41
39:h:130:PHE:O	39:h:133:VAL:HG22	2.20	0.41
51:5:115:GLU:HB2	51:5:119:GLN:HB2	2.03	0.41
1:A:1501:A:HO2'	1:A:1502:A:P	2.38	0.41
1:A:1607:G:O4'	8:J:151:LEU:HD23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1786:C:OP1	18:T:165:TYR:OH	2.38	0.41
1:A:1194:A:C2’	1:A:1195:G:O5’	2.68	0.41
2:B:4:A:H2’	2:B:5:A:C4’	2.51	0.41
2:B:18:C:O2’	14:P:108:ARG:NH1	2.53	0.41
11:M:42:ARG:NH2	17:S:183:ASN:ND2	2.68	0.41
26:0:156:MET:HE1	26:0:168:ASP:OD1	2.19	0.41
34:c:86:ASP:N	34:c:86:ASP:OD1	2.53	0.41
44:p:170:LYS:O	44:p:171:GLU:HG2	2.21	0.41
7:I:46:LYS:HE2	43:o:35:MET:HE3	2.03	0.41
20:V:177:THR:CG2	53:9:69:LYS:H	2.34	0.41
25:x:180:ALA:HB3	25:x:181:PRO:HD3	2.01	0.41
51:5:177:CYS:HB3	51:5:178:PRO:HD3	2.01	0.41
1:A:1627:A:OP1	1:A:1628:A:N6	2.53	0.41
2:B:8:U:H2’	2:B:45:A:N3	2.35	0.41
2:B:32:U:N3	55:m:43:ARG:O	2.54	0.41
34:c:228:LEU:HB2	34:c:307:PHE:CD2	2.56	0.41
34:c:307:PHE:CD2	34:c:307:PHE:O	2.74	0.41
35:d:112:LEU:HA	35:d:115:ASN:OD1	2.21	0.41
36:e:174:VAL:HG12	36:e:175:GLU:N	2.36	0.41
2:B:15:A:O2’	2:B:17:A:N7	2.54	0.41
2:B:48:G:N2	2:B:59:C:H1’	2.35	0.41
2:B:57:U:H2’	2:B:58:C:C1’	2.51	0.41
13:O:110:ILE:CG2	13:O:111:PRO:HD2	2.50	0.41
15:Q:182:ARG:HG3	15:Q:183:LEU:H	1.85	0.41
41:j:110:LYS:HG2	41:j:111:GLY:H	1.86	0.41
44:p:170:LYS:O	44:p:170:LYS:HG2	2.21	0.41
1:A:1346:G:H4’	1:A:1347:C:OP2	2.21	0.41
1:A:2373:G:OP1	5:F:137:ARG:NH1	2.44	0.41
1:A:2617:A:O2’	1:A:2618:A:C8	2.74	0.41
15:Q:153:ASN:OD1	15:Q:154:THR:N	2.49	0.41
15:Q:237:ASN:OD1	15:Q:238:PHE:N	2.54	0.41
18:T:191:LYS:NZ	54:a:87:GLU:OE2	2.54	0.41
22:X:171:ARG:NE	22:X:198:GLU:OE2	2.45	0.41
26:0:153:VAL:HG21	26:0:170:GLY:O	2.21	0.41
31:6:234:HIS:ND1	31:6:255:LEU:O	2.54	0.41
32:7:220:ALA:N	32:7:247:ARG:O	2.54	0.41
33:b:47:VAL:O	33:b:51:VAL:HG12	2.21	0.41
35:d:125:ILE:HD11	35:d:199:CYS:SG	2.61	0.41
38:g:57:ILE:HD13	38:g:91:MET:HE2	2.03	0.41
58:t:82:ALA:N	58:t:112:ASP:OD2	2.53	0.41
8:J:119:GLU:OE2	8:J:120:ILE:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:7:ALA:HB3	9:K:8:PRO:HD3	2.03	0.41
14:P:156:ASP:OD1	14:P:156:ASP:N	2.53	0.41
42:k:78:GLY:O	42:k:79:ALA:C	2.64	0.41
1:A:1597:A:H4’	1:A:1598:C:OP2	2.21	0.40
5:F:92:ARG:HE	5:F:95:ILE:CD1	2.34	0.40
8:J:26:ALA:HB3	8:J:62:GLU:HA	2.03	0.40
10:L:101:ASP:OD2	15:Q:152:ARG:NH2	2.54	0.40
11:M:42:ARG:CZ	11:M:46:ARG:HH21	2.34	0.40
25:x:64:ARG:NH1	59:y:270:ARG:O	2.49	0.40
25:x:188:LEU:O	25:x:192:GLY:N	2.52	0.40
46:r:93:ILE:HD11	46:r:119:VAL:HG21	2.03	0.40
58:t:80:GLY:N	58:t:111:VAL:O	2.54	0.40
1:A:1597:A:N6	1:A:1651:A:C5	2.89	0.40
1:A:1603:G:N2	1:A:1624:A:O4’	2.54	0.40
1:A:1608:C:H6	1:A:1608:C:OP2	2.04	0.40
3:D:170:ILE:O	3:D:170:ILE:HG23	2.21	0.40
3:D:291:PRO:N	3:D:292:PRO:CD	2.85	0.40
10:L:34:LYS:O	10:L:35:MET:HB2	2.21	0.40
25:x:257:THR:HA	25:x:307:CYS:SG	2.61	0.40
1:A:1944:A:O2’	1:A:1945:C:P	2.78	0.40
1:A:2406:A:O2’	1:A:2456:G:N2	2.54	0.40
34:c:259:ARG:HB2	34:c:271:PHE:HB2	2.03	0.40
41:j:88:GLN:O	41:j:91:LYS:HG2	2.21	0.40
44:p:133:LEU:HD21	44:p:157:MET:HE1	2.02	0.40
46:r:190:ARG:CG	46:r:191:PRO:HD2	2.51	0.40
54:a:53:ASP:OD1	54:a:54:GLY:N	2.55	0.40
1:A:1117:A:O2’	1:A:1118:C:P	2.79	0.40
1:A:1506:A:O2’	1:A:1507:A:C5’	2.69	0.40
1:A:2346:U:O2	1:A:2346:U:O4’	2.39	0.40
17:S:146:THR:OG1	54:a:59:CYS:HB2	2.21	0.40
37:f:203:LEU:O	37:f:207:LEU:HG	2.20	0.40
39:h:143:GLU:O	39:h:147:SER:OG	2.39	0.40
56:z:275:LEU:O	56:z:276:ARG:HB2	2.22	0.40
1:A:1236:A:H2’	1:A:1237:A:O4’	2.21	0.40
1:A:1629:A:N3	1:A:1629:A:H2’	2.36	0.40
2:B:53:U:O2’	2:B:54:G:H2’	2.22	0.40
26:0:180:ARG:CD	26:0:184:PHE:HD2	2.34	0.40
31:6:234:HIS:O	31:6:253:PRO:O	2.40	0.40
39:h:83:LEU:O	39:h:83:LEU:HD23	2.22	0.40

There are no symmetry-related clashes.

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	
3	D	223/246 (91%)	216 (97%)	7 (3%)	0	100	100
4	E	306/308 (99%)	292 (95%)	14 (5%)	0	100	100
5	F	248/250 (99%)	244 (98%)	4 (2%)	0	100	100
6	H	93/95 (98%)	92 (99%)	1 (1%)	0	100	100
7	I	159/262 (61%)	157 (99%)	2 (1%)	0	100	100
8	J	173/175 (99%)	165 (95%)	8 (5%)	0	100	100
9	K	175/177 (99%)	169 (97%)	6 (3%)	0	100	100
10	L	113/115 (98%)	113 (100%)	0	0	100	100
11	M	285/287 (99%)	280 (98%)	5 (2%)	0	100	100
12	N	191/222 (86%)	189 (99%)	2 (1%)	0	100	100
13	O	151/153 (99%)	150 (99%)	1 (1%)	0	100	100
14	P	139/141 (99%)	139 (100%)	0	0	100	100
15	Q	215/217 (99%)	212 (99%)	3 (1%)	0	100	100
16	R	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
17	S	157/159 (99%)	151 (96%)	6 (4%)	0	100	100
18	T	164/166 (99%)	162 (99%)	2 (1%)	0	100	100
19	U	123/145 (85%)	118 (96%)	5 (4%)	0	100	100
20	V	199/207 (96%)	196 (98%)	3 (2%)	0	100	100
21	W	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
22	X	240/242 (99%)	238 (99%)	2 (1%)	0	100	100
23	Y	174/176 (99%)	173 (99%)	1 (1%)	0	100	100
24	Z	119/121 (98%)	118 (99%)	1 (1%)	0	100	100
25	x	322/345 (93%)	313 (97%)	9 (3%)	0	100	100
26	0	106/108 (98%)	105 (99%)	1 (1%)	0	100	100
27	1	50/52 (96%)	50 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	2	44/46 (96%)	44 (100%)	0	0	100	100
29	3	93/95 (98%)	92 (99%)	1 (1%)	0	100	100
30	4	35/37 (95%)	35 (100%)	0	0	100	100
31	6	307/335 (92%)	295 (96%)	12 (4%)	0	100	100
32	7	290/292 (99%)	283 (98%)	7 (2%)	0	100	100
33	b	146/148 (99%)	141 (97%)	5 (3%)	0	100	100
34	c	276/290 (95%)	271 (98%)	5 (2%)	0	100	100
35	d	207/306 (68%)	202 (98%)	5 (2%)	0	100	100
36	e	187/283 (66%)	176 (94%)	11 (6%)	0	100	100
37	f	98/128 (77%)	95 (97%)	3 (3%)	0	100	100
38	g	130/132 (98%)	126 (97%)	4 (3%)	0	100	100
39	h	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
40	i	95/97 (98%)	91 (96%)	4 (4%)	0	100	100
41	j	91/121 (75%)	89 (98%)	2 (2%)	0	100	100
42	k	82/118 (70%)	77 (94%)	5 (6%)	0	100	100
43	o	76/78 (97%)	75 (99%)	1 (1%)	0	100	100
44	p	139/153 (91%)	134 (96%)	5 (4%)	0	100	100
45	q	133/135 (98%)	132 (99%)	1 (1%)	0	100	100
46	r	153/196 (78%)	148 (97%)	5 (3%)	0	100	100
47	s	373/384 (97%)	363 (97%)	10 (3%)	0	100	100
48	u	123/125 (98%)	117 (95%)	6 (5%)	0	100	100
49	v	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
50	w	77/79 (98%)	74 (96%)	3 (4%)	0	100	100
51	5	392/394 (100%)	387 (99%)	5 (1%)	0	100	100
52	8	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
53	9	120/135 (89%)	117 (98%)	3 (2%)	0	100	100
54	a	99/142 (70%)	96 (97%)	3 (3%)	0	100	100
55	m	43/127 (34%)	42 (98%)	1 (2%)	0	100	100
56	z	46/326 (14%)	46 (100%)	0	0	100	100
57	l	80/135 (59%)	77 (96%)	3 (4%)	0	100	100
58	t	212/246 (86%)	208 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
59	y	235/346 (68%)	232 (99%)	3 (1%)	0	100	100
All	All	8986/10287 (87%)	8779 (98%)	207 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	
3	D	186/197 (94%)	186 (100%)	0	100	100
4	E	270/270 (100%)	270 (100%)	0	100	100
5	F	216/216 (100%)	216 (100%)	0	100	100
6	H	86/86 (100%)	86 (100%)	0	100	100
7	I	149/230 (65%)	149 (100%)	0	100	100
8	J	138/138 (100%)	138 (100%)	0	100	100
9	K	157/157 (100%)	157 (100%)	0	100	100
10	L	99/99 (100%)	99 (100%)	0	100	100
11	M	248/248 (100%)	248 (100%)	0	100	100
12	N	174/192 (91%)	174 (100%)	0	100	100
13	O	133/133 (100%)	133 (100%)	0	100	100
14	P	123/123 (100%)	123 (100%)	0	100	100
15	Q	197/197 (100%)	197 (100%)	0	100	100
16	R	119/119 (100%)	119 (100%)	0	100	100
17	S	145/145 (100%)	145 (100%)	0	100	100
18	T	147/147 (100%)	147 (100%)	0	100	100
19	U	114/132 (86%)	114 (100%)	0	100	100
20	V	179/183 (98%)	179 (100%)	0	100	100
21	W	84/84 (100%)	84 (100%)	0	100	100
22	X	219/219 (100%)	219 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	Y	162/162 (100%)	162 (100%)	0	100	100
24	Z	114/114 (100%)	114 (100%)	0	100	100
25	x	283/301 (94%)	283 (100%)	0	100	100
26	0	97/97 (100%)	97 (100%)	0	100	100
27	1	49/49 (100%)	49 (100%)	0	100	100
28	2	40/40 (100%)	40 (100%)	0	100	100
29	3	88/88 (100%)	88 (100%)	0	100	100
30	4	35/35 (100%)	35 (100%)	0	100	100
31	6	278/299 (93%)	278 (100%)	0	100	100
32	7	269/269 (100%)	269 (100%)	0	100	100
33	b	130/130 (100%)	130 (100%)	0	100	100
34	c	244/251 (97%)	244 (100%)	0	100	100
35	d	190/272 (70%)	190 (100%)	0	100	100
36	e	166/238 (70%)	166 (100%)	0	100	100
37	f	93/115 (81%)	93 (100%)	0	100	100
38	g	122/122 (100%)	122 (100%)	0	100	100
39	h	100/100 (100%)	100 (100%)	0	100	100
40	i	87/87 (100%)	87 (100%)	0	100	100
41	j	75/99 (76%)	75 (100%)	0	100	100
42	k	75/95 (79%)	75 (100%)	0	100	100
43	o	65/65 (100%)	65 (100%)	0	100	100
44	p	128/135 (95%)	128 (100%)	0	100	100
45	q	117/117 (100%)	117 (100%)	0	100	100
46	r	142/168 (84%)	142 (100%)	0	100	100
47	s	329/336 (98%)	329 (100%)	0	100	100
48	u	115/115 (100%)	115 (100%)	0	100	100
49	v	60/60 (100%)	60 (100%)	0	100	100
50	w	73/73 (100%)	73 (100%)	0	100	100
51	5	356/356 (100%)	356 (100%)	0	100	100
52	8	62/62 (100%)	62 (100%)	0	100	100
53	9	104/114 (91%)	104 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	a	97/129 (75%)	97 (100%)	0	100	100
55	m	40/114 (35%)	40 (100%)	0	100	100
56	z	41/280 (15%)	41 (100%)	0	100	100
57	l	75/112 (67%)	75 (100%)	0	100	100
58	t	180/206 (87%)	180 (100%)	0	100	100
59	y	220/322 (68%)	220 (100%)	0	100	100
All	All	8084/9042 (89%)	8084 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	157	ASN
3	D	255	GLN
4	E	117	HIS
4	E	139	ASN
4	E	227	GLN
4	E	233	GLN
10	L	104	ASN
11	M	218	ASN
13	O	109	GLN
13	O	161	GLN
14	P	88	HIS
17	S	192	ASN
18	T	73	GLN
18	T	204	HIS
19	U	59	GLN
19	U	82	HIS
20	V	73	GLN
21	W	62	HIS
22	X	76	GLN
22	X	77	GLN
24	Z	67	HIS
31	6	174	HIS
31	6	239	ASN
32	7	274	GLN
32	7	289	ASN
32	7	295	GLN
33	b	141	HIS

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Mol	Chain	Res	Type
34	c	139	GLN
36	e	73	GLN
37	f	188	HIS
38	g	102	HIS
40	i	65	ASN
40	i	120	HIS
41	j	30	GLN
41	j	62	GLN
46	r	131	HIS
47	s	107	GLN
47	s	226	GLN
47	s	294	HIS
47	s	414	GLN
49	v	42	ASN
49	v	54	GLN
50	w	103	HIS
51	5	65	HIS
51	5	266	GLN
51	5	385	HIS
52	8	143	GLN
53	9	50	GLN
54	a	76	GLN
56	z	289	ASN
57	l	64	GLN
57	l	97	ASN
58	t	115	HIS
58	t	236	GLN
59	y	210	GLN
59	y	322	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1428/1584 (90%)	473 (33%)	36 (2%)
2	B	61/68 (89%)	29 (47%)	4 (6%)
All	All	1489/1652 (90%)	502 (33%)	40 (2%)

All (502) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	1094	A

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Mol	Chain	Res	Type
1	A	1100	C
1	A	1101	C
1	A	1102	U
1	A	1103	A
1	A	1104	G
1	A	1112	C
1	A	1114	U
1	A	1115	A
1	A	1116	C
1	A	1117	A
1	A	1118	C
1	A	1119	A
1	A	1123	A
1	A	1124	U
1	A	1128	U
1	A	1131	A
1	A	1134	A
1	A	1135	U
1	A	1136	U
1	A	1137	A
1	A	1138	U
1	A	1139	A
1	A	1140	U
1	A	1148	A
1	A	1151	A
1	A	1152	U
1	A	1159	U
1	A	1160	A
1	A	1161	C
1	A	1162	U
1	A	1170	U
1	A	1173	G
1	A	1175	G
1	A	1176	A
1	A	1187	U
1	A	1188	A
1	A	1189	C
1	A	1190	A
1	A	1191	U
1	A	1194	A
1	A	1195	G
1	A	1198	G

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Mol	Chain	Res	Type
1	A	1205	A
1	A	1222	A
1	A	1233	A
1	A	1234	C
1	A	1235	U
1	A	1236	A
1	A	1237	A
1	A	1238	U
1	A	1240	A
1	A	1241	A
1	A	1252	A
1	A	1253	A
1	A	1255	C
1	A	1256	A
1	A	1257	A
1	A	1260	A
1	A	1264	A
1	A	1272	A
1	A	1277	U
1	A	1278	U
1	A	1279	G
1	A	1280	C
1	A	1281	A
1	A	1282	U
1	A	1283	A
1	A	1284	A
1	A	1295	A
1	A	1297	A
1	A	1300	A
1	A	1302	U
1	A	1310	A
1	A	1311	A
1	A	1315	A
1	A	1316	A
1	A	1318	U
1	A	1319	A
1	A	1320	C
1	A	1321	A
1	A	1331	C
1	A	1337	A
1	A	1346	G
1	A	1347	C

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Mol	Chain	Res	Type
1	A	1364	U
1	A	1368	A
1	A	1386	G
1	A	1394	G
1	A	1396	G
1	A	1402	A
1	A	1413	G
1	A	1415	G
1	A	1420	A
1	A	1422	A
1	A	1429	C
1	A	1430	G
1	A	1443	G
1	A	1449	U
1	A	1450	A
1	A	1457	A
1	A	1458	A
1	A	1459	A
1	A	1460	U
1	A	1465	U
1	A	1466	U
1	A	1468	A
1	A	1470	U
1	A	1471	U
1	A	1473	A
1	A	1483	U
1	A	1484	U
1	A	1485	G
1	A	1486	C
1	A	1488	A
1	A	1490	A
1	A	1491	A
1	A	1492	A
1	A	1493	A
1	A	1494	A
1	A	1495	C
1	A	1496	A
1	A	1497	A
1	A	1502	A
1	A	1505	A
1	A	1506	A
1	A	1507	A

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Mol	Chain	Res	Type
1	A	1508	A
1	A	1509	A
1	A	1511	U
1	A	1512	A
1	A	1513	A
1	A	1521	U
1	A	1525	A
1	A	1526	G
1	A	1532	A
1	A	1534	A
1	A	1536	G
1	A	1542	C
1	A	1543	U
1	A	1552	A
1	A	1553	C
1	A	1557	A
1	A	1558	A
1	A	1559	A
1	A	1565	U
1	A	1566	U
1	A	1569	U
1	A	1573	G
1	A	1580	U
1	A	1583	C
1	A	1587	A
1	A	1595	U
1	A	1596	A
1	A	1597	A
1	A	1598	C
1	A	1599	C
1	A	1600	A
1	A	1601	U
1	A	1605	A
1	A	1606	G
1	A	1608	C
1	A	1609	C
1	A	1610	U
1	A	1611	A
1	A	1612	A
1	A	1613	A
1	A	1614	A
1	A	1615	G

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Mol	Chain	Res	Type
1	A	1616	C
1	A	1617	A
1	A	1618	G
1	A	1619	C
1	A	1620	C
1	A	1623	C
1	A	1624	A
1	A	1626	U
1	A	1627	A
1	A	1628	A
1	A	1629	A
1	A	1630	G
1	A	1631	A
1	A	1632	A
1	A	1633	A
1	A	1634	G
1	A	1635	C
1	A	1636	G
1	A	1637	U
1	A	1638	U
1	A	1639	C
1	A	1641	A
1	A	1642	G
1	A	1643	C
1	A	1644	U
1	A	1645	C
1	A	1647	A
1	A	1648	C
1	A	1649	A
1	A	1650	U
1	A	1651	A
1	A	1652	A
1	A	1654	A
1	A	1658	C
1	A	1659	A
1	A	1660	A
1	A	1664	A
1	A	1665	U
1	A	1669	A
1	A	1671	A
1	A	1673	U
1	A	1675	U

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Mol	Chain	Res	Type
1	A	1678	A
1	A	1682	A
1	A	1683	C
1	A	1684	U
1	A	1690	A
1	A	1693	U
1	A	1697	A
1	A	1698	A
1	A	1702	G
1	A	1703	G
1	A	1704	U
1	A	1717	U
1	A	1718	U
1	A	1730	A
1	A	1733	G
1	A	1747	C
1	A	1748	A
1	A	1749	A
1	A	1755	C
1	A	1756	C
1	A	1757	A
1	A	1758	A
1	A	1759	U
1	A	1766	G
1	A	1767	G
1	A	1769	A
1	A	1784	C
1	A	1793	C
1	A	1801	A
1	A	1804	U
1	A	1805	A
1	A	1806	A
1	A	1807	U
1	A	1813	U
1	A	1814	A
1	A	1820	A
1	A	1823	A
1	A	1826	C
1	A	1832	A
1	A	1837	U
1	A	1844	C
1	A	1846	U

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Mol	Chain	Res	Type
1	A	1851	C
1	A	1852	U
1	A	1869	A
1	A	1871	C
1	A	1878	C
1	A	1880	U
1	A	1882	A
1	A	1887	A
1	A	1888	A
1	A	1894	A
1	A	1900	A
1	A	1914	G
1	A	1919	C
1	A	1922	G
1	A	1923	A
1	A	1924	A
1	A	1926	C
1	A	1930	C
1	A	1936	U
1	A	1937	A
1	A	1939	C
1	A	1944	A
1	A	1945	C
1	A	1948	C
1	A	1957	C
1	A	1958	A
1	A	1964	A
1	A	1967	A
1	A	1968	U
1	A	1976	A
1	A	1979	G
1	A	1983	G
1	A	1984	C
1	A	1985	C
1	A	1986	C
1	A	1987	A
1	A	1990	G
1	A	1991	A
1	A	2040	C
1	A	2048	C
1	A	2050	U
1	A	2057	G

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Mol	Chain	Res	Type
1	A	2058	G
1	A	2059	G
1	A	2060	A
1	A	2063	A
1	A	2064	G
1	A	2065	C
1	A	2066	A
1	A	2067	U
1	A	2068	G
1	A	2069	A
1	A	2072	G
1	A	2073	G
1	A	2074	C
1	A	2075	U
1	A	2076	A
1	A	2082	G
1	A	2091	U
1	A	2093	U
1	A	2097	U
1	A	2120	C
1	A	2123	U
1	A	2130	A
1	A	2131	A
1	A	2132	G
1	A	2136	C
1	A	2143	A
1	A	2146	A
1	A	2155	C
1	A	2156	G
1	A	2159	A
1	A	2160	A
1	A	2161	G
1	A	2163	C
1	A	2169	G
1	A	2176	A
1	A	2177	A
1	A	2180	U
1	A	2182	U
1	A	2183	A
1	A	2186	A
1	A	2187	C
1	A	2190	A

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Mol	Chain	Res	Type
1	A	2193	U
1	A	2195	U
1	A	2197	U
1	A	2229	A
1	A	2230	G
1	A	2232	A
1	A	2236	G
1	A	2239	U
1	A	2240	G
1	A	2241	A
1	A	2248	G
1	A	2251	U
1	A	2254	G
1	A	2255	G
1	A	2258	A
1	A	2259	C
1	A	2275	A
1	A	2276	U
1	A	2277	C
1	A	2284	A
1	A	2285	U
1	A	2289	U
1	A	2290	A
1	A	2291	U
1	A	2292	A
1	A	2293	A
1	A	2295	C
1	A	2297	A
1	A	2303	A
1	A	2325	U
1	A	2326	A
1	A	2327	U
1	A	2328	C
1	A	2333	U
1	A	2339	A
1	A	2340	G
1	A	2342	U
1	A	2343	A
1	A	2351	A
1	A	2352	U
1	A	2354	A
1	A	2358	G

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Mol	Chain	Res	Type
1	A	2359	A
1	A	2363	A
1	A	2367	A
1	A	2369	C
1	A	2373	G
1	A	2375	G
1	A	2376	A
1	A	2387	A
1	A	2394	U
1	A	2396	A
1	A	2397	A
1	A	2398	G
1	A	2399	A
1	A	2402	U
1	A	2404	A
1	A	2408	C
1	A	2410	A
1	A	2412	A
1	A	2413	A
1	A	2415	U
1	A	2416	A
1	A	2418	G
1	A	2436	U
1	A	2437	G
1	A	2447	A
1	A	2449	C
1	A	2458	G
1	A	2461	G
1	A	2462	A
1	A	2474	G
1	A	2475	U
1	A	2481	U
1	A	2484	U
1	A	2485	C
1	A	2486	A
1	A	2493	A
1	A	2495	A
1	A	2496	G
1	A	2501	A
1	A	2502	C
1	A	2503	G
1	A	2505	G

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Mol	Chain	Res	Type
1	A	2515	C
1	A	2516	A
1	A	2519	C
1	A	2520	C
1	A	2521	G
1	A	2523	A
1	A	2524	G
1	A	2526	A
1	A	2532	G
1	A	2533	G
1	A	2539	U
1	A	2542	U
1	A	2544	U
1	A	2550	U
1	A	2551	A
1	A	2552	C
1	A	2564	G
1	A	2565	U
1	A	2570	A
1	A	2575	C
1	A	2582	A
1	A	2598	A
1	A	2600	A
1	A	2601	U
1	A	2603	A
1	A	2605	C
1	A	2611	C
1	A	2614	C
1	A	2615	U
1	A	2617	A
1	A	2618	A
1	A	2619	U
1	A	2621	U
1	A	2625	A
1	A	2628	A
1	A	2629	A
1	A	2630	A
1	A	2631	A
1	A	2635	A
1	A	2636	A
1	A	2640	A
1	A	2647	U

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Mol	Chain	Res	Type
1	A	2648	A
1	A	2650	G
1	A	2654	A
1	A	2655	C
1	A	2656	C
1	A	2659	C
1	A	2660	U
1	A	2665	U
1	A	2666	A
1	A	2676	A
2	B	2	U
2	B	3	U
2	B	4	A
2	B	5	A
2	B	6	U
2	B	7	G
2	B	8	U
2	B	9	A
2	B	10	G
2	B	14	A
2	B	16	U
2	B	17	A
2	B	18	C
2	B	20	A
2	B	21	A
2	B	32	U
2	B	33	G
2	B	44	G
2	B	47	G
2	B	48	G
2	B	50	A
2	B	51	A
2	B	52	U
2	B	53	U
2	B	54	G
2	B	58	C
2	B	60	C
2	B	64	A
2	B	67	A

All (40) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1134	A
1	A	1137	A
1	A	1187	U
1	A	1188	A
1	A	1194	A
1	A	1235	U
1	A	1237	A
1	A	1458	A
1	A	1491	A
1	A	1492	A
1	A	1505	A
1	A	1541	G
1	A	1586	A
1	A	1596	A
1	A	1597	A
1	A	1683	C
1	A	1813	U
1	A	1893	C
1	A	1944	A
1	A	1967	A
1	A	2056	A
1	A	2057	G
1	A	2065	C
1	A	2066	A
1	A	2068	G
1	A	2072	G
1	A	2075	U
1	A	2159	A
1	A	2182	U
1	A	2274	A
1	A	2275	A
1	A	2302	U
1	A	2342	U
1	A	2414	U
1	A	2564	G
1	A	2659	C
2	B	5	A
2	B	20	A
2	B	48	G
2	B	52	U

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

1 non-standard protein/DNA/RNA residue is 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	PSU	A	2509	1	18,21,22	0.47	0	22,30,33	0.61	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	PSU	A	2509	1	-	2/7/25/26	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	2509	PSU	O4'-C4'-C5'-O5'
1	A	2509	PSU	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 109 ligands modelled in this entry, 107 are monoatomic - leaving 2 for Mogul analysis.

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 $\vert Z\vert > 2$ 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	$\#\vert Z\vert > 2$	Counts	RMSZ	$\#\vert Z\vert > 2$
63	SAH	t	1001	-	24,28,28	0.71	0	25,40,40	0.82	1 (4%)
62	FES	r	201	46,7	0,4,4	-	-	-		

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
63	SAH	t	1001	-	-	4/11/31/31	0/3/3/3
62	FES	r	201	46,7	-	-	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
63	t	1001	SAH	C5-C6-N6	2.39	123.99	120.35

There are no chirality outliers.

All (4) torsion outliers are listed below:

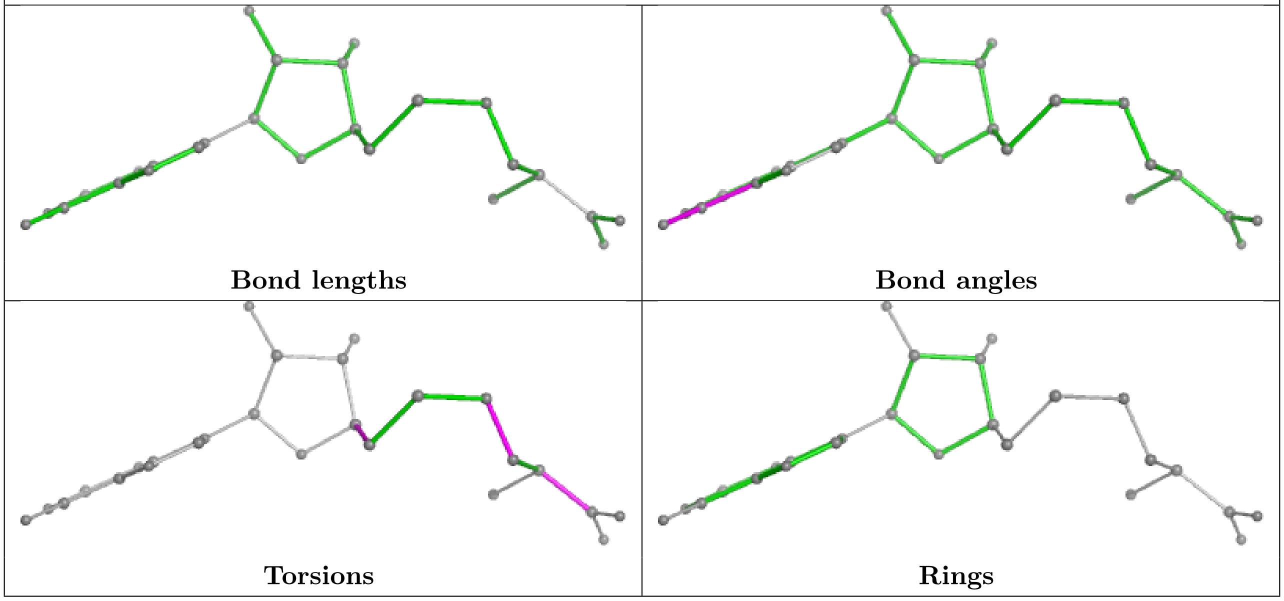
Mol	Chain	Res	Type	Atoms
63	t	1001	SAH	CA-CB-CG-SD
63	t	1001	SAH	OXT-C-CA-CB
63	t	1001	SAH	O4'-C4'-C5'-SD
63	t	1001	SAH	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand SAH t 1001



Bond lengths

Bond angles

Torsions

Rings

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
1	A	3
35	d	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	d	98:GLY	C	105:LEU	N	13.00
1	A	1192:C	O3'	1193:U	P	8.40
1	A	1191:U	O3'	1192:C	P	6.13
1	A	2251:U	O3'	2252:G	P	4.05

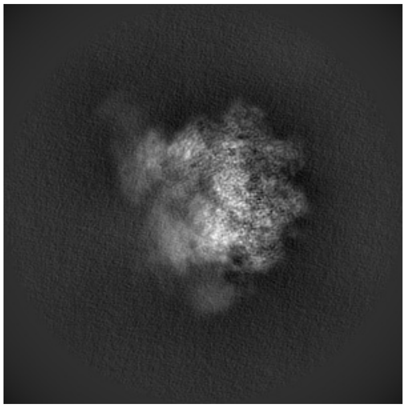
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-52048. These allow visual inspection of the internal detail of the map and identification of artifacts.

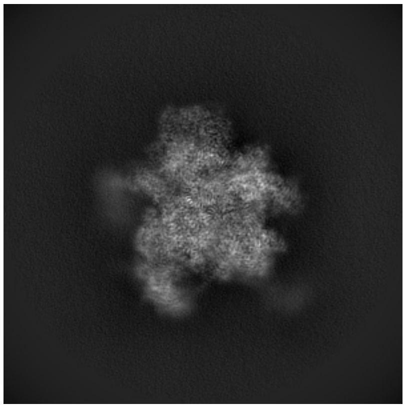
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections ⓘ

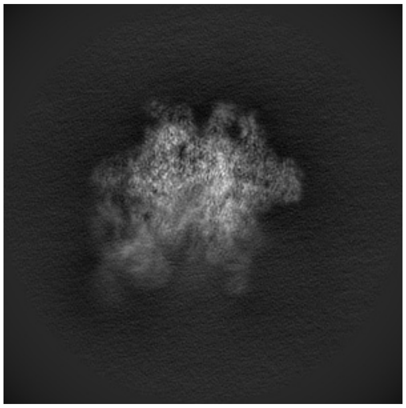
6.1.1 Primary map



X

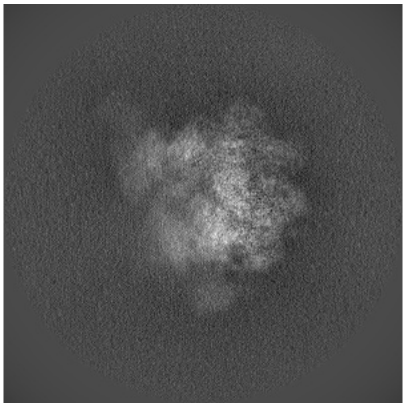


Y

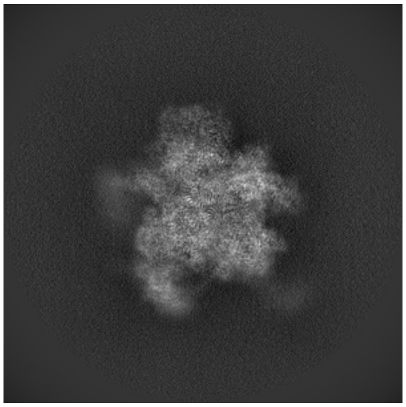


Z

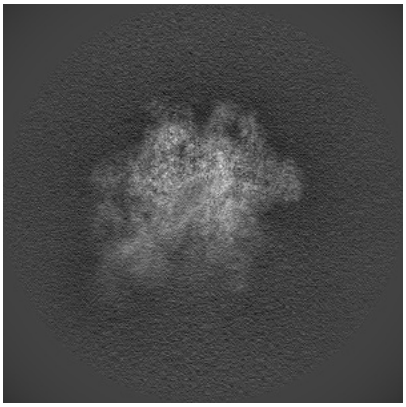
6.1.2 Raw map



X



Y

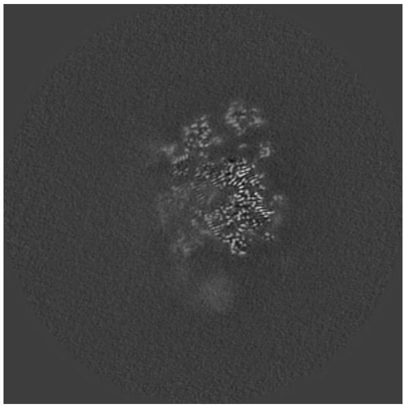


Z

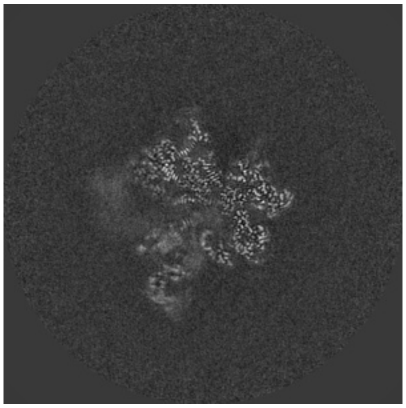
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

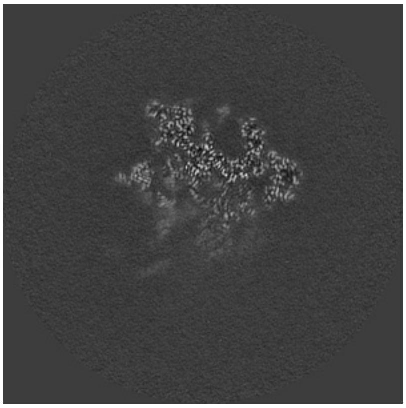
6.2.1 Primary map



X Index: 270

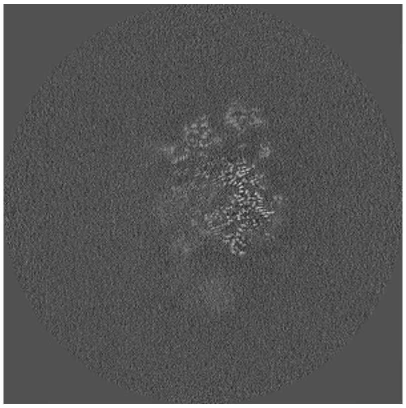


Y Index: 270

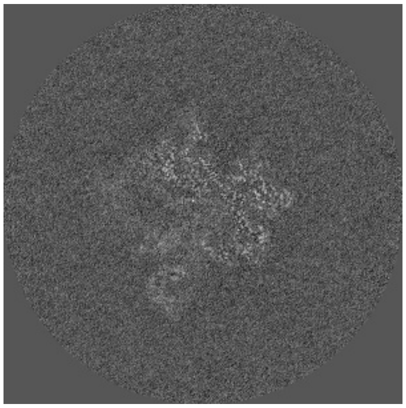


Z Index: 270

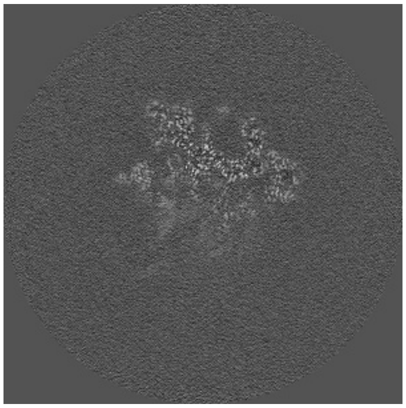
6.2.2 Raw map



X Index: 270



Y Index: 270

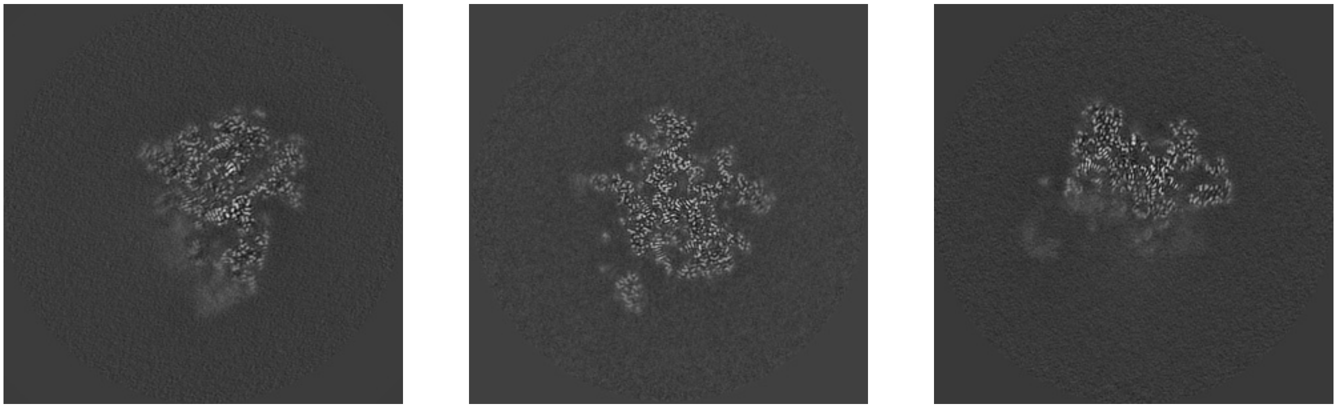


Z Index: 270

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

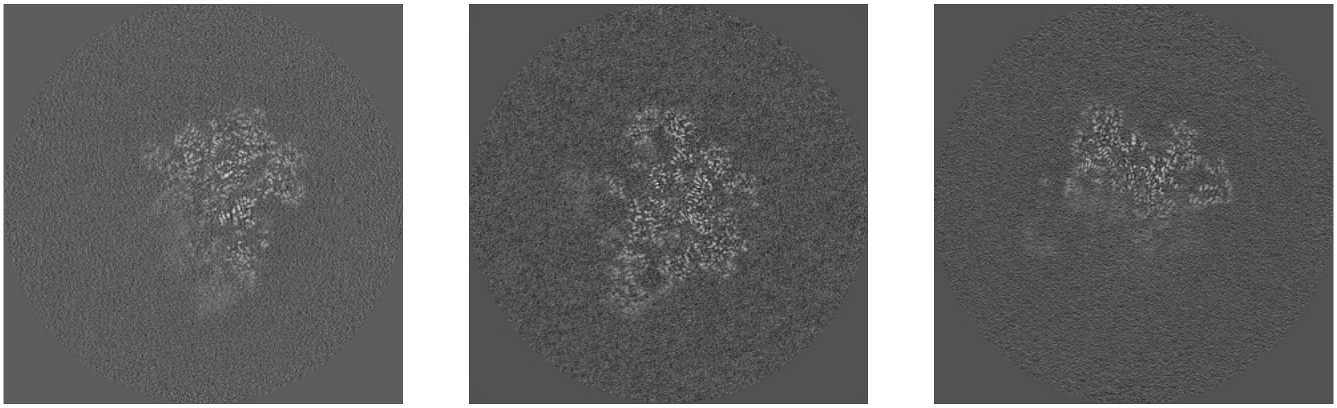
6.3 Largest variance slices ⓘ

6.3.1 Primary map



X Index: 297 Y Index: 319 Z Index: 257

6.3.2 Raw map

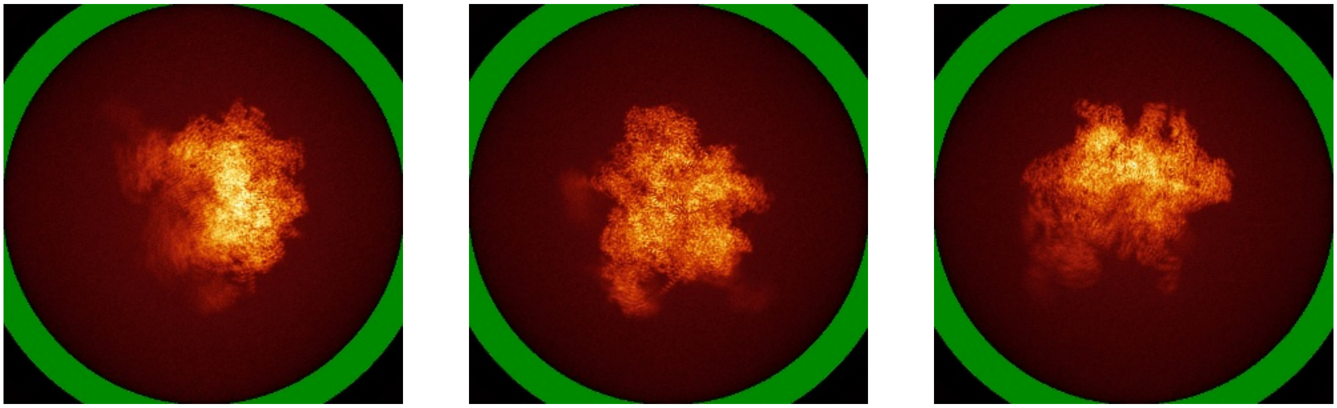


X Index: 293 Y Index: 302 Z Index: 257

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

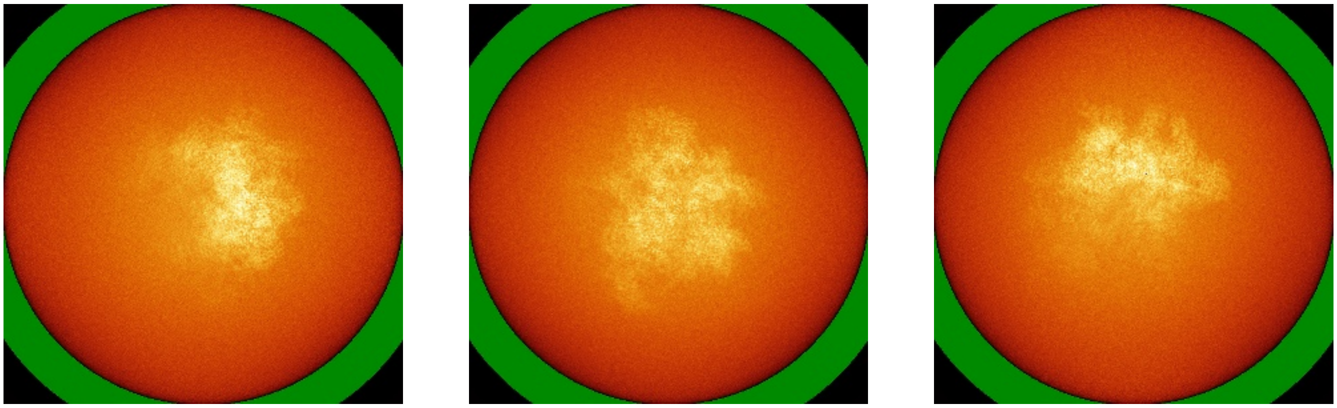
6.4 Orthogonal standard-deviation projections (False-color)

6.4.1 Primary map



X Y Z

6.4.2 Raw map

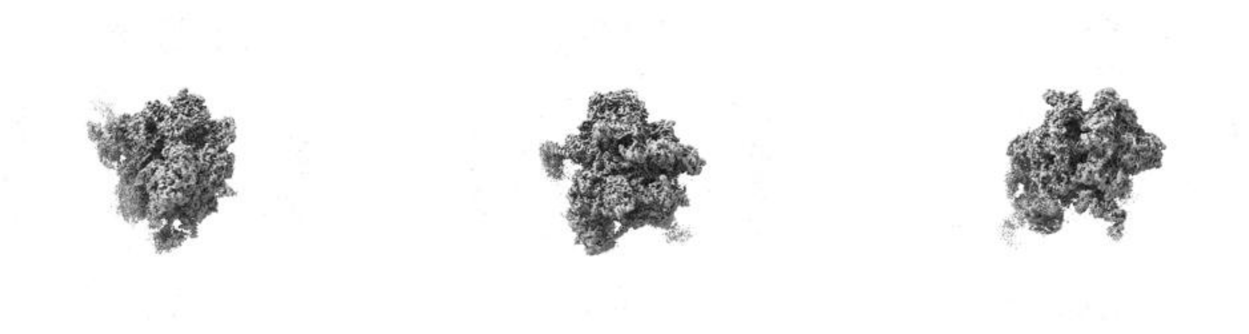


X Y Z

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 ⓘ

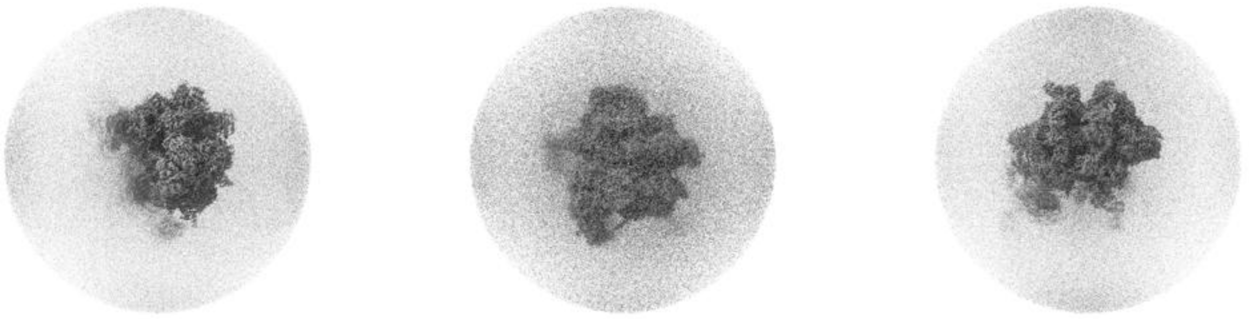
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.006. 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.

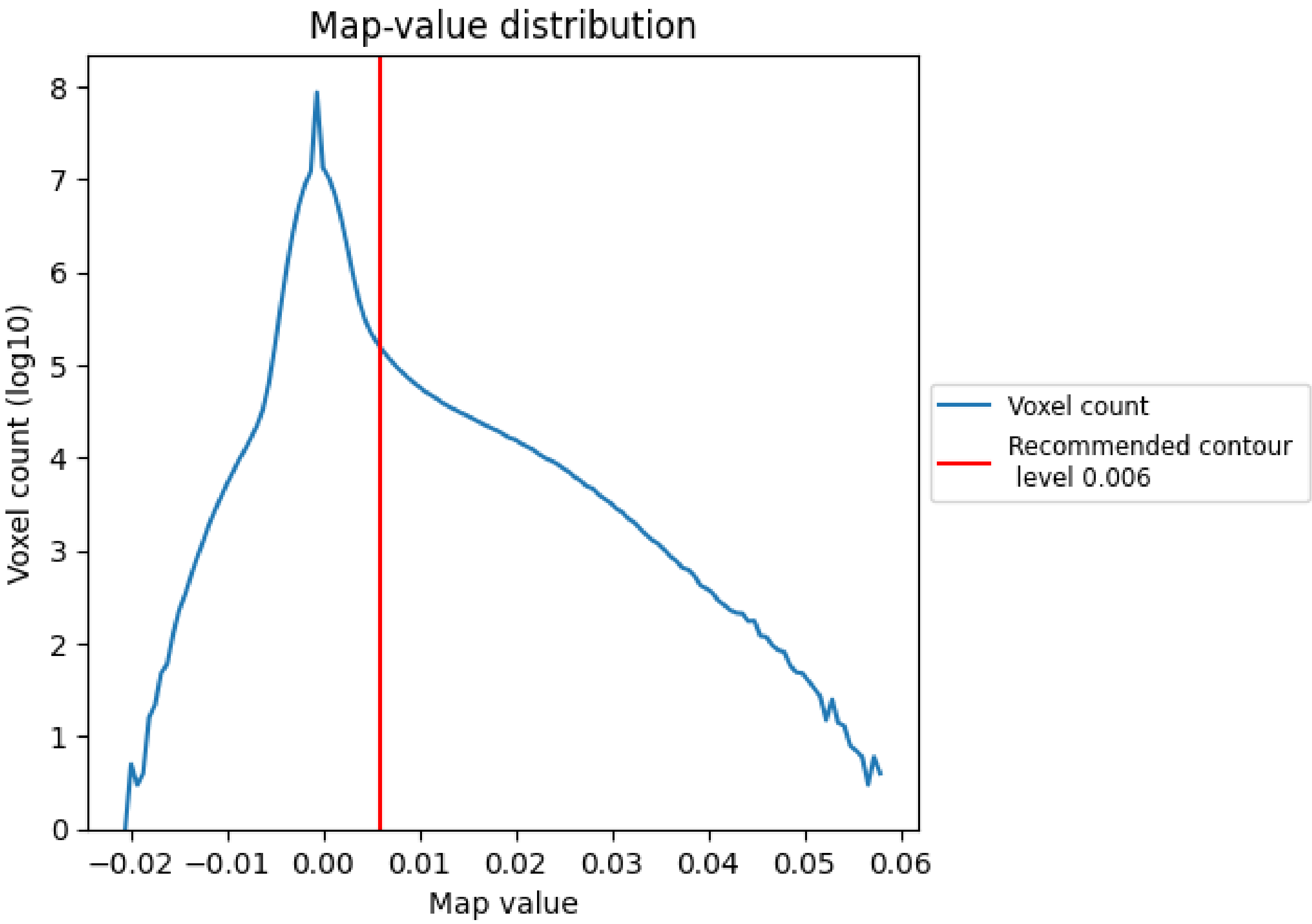
6.6 Mask visualisation ⓘ

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

7 Map analysis (i)

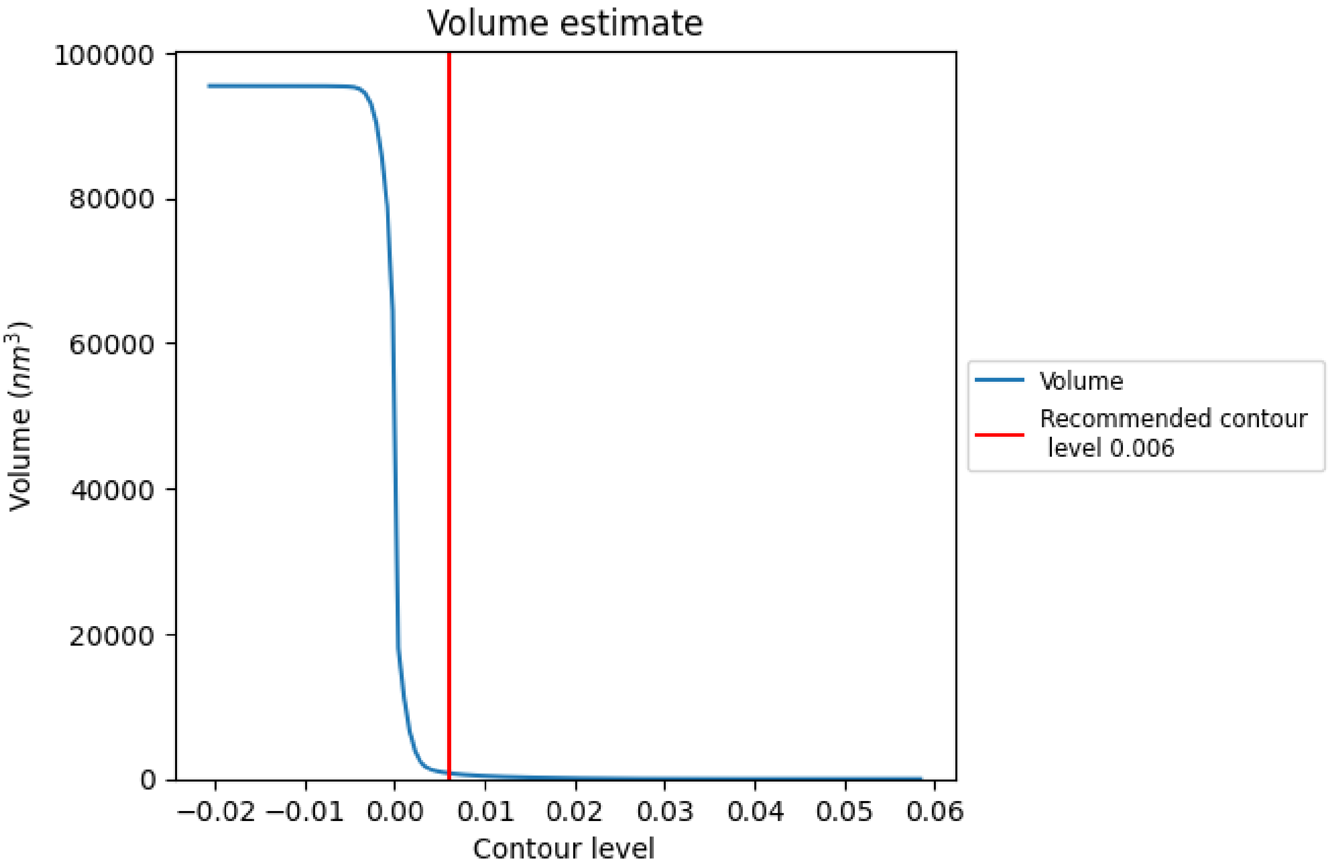
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

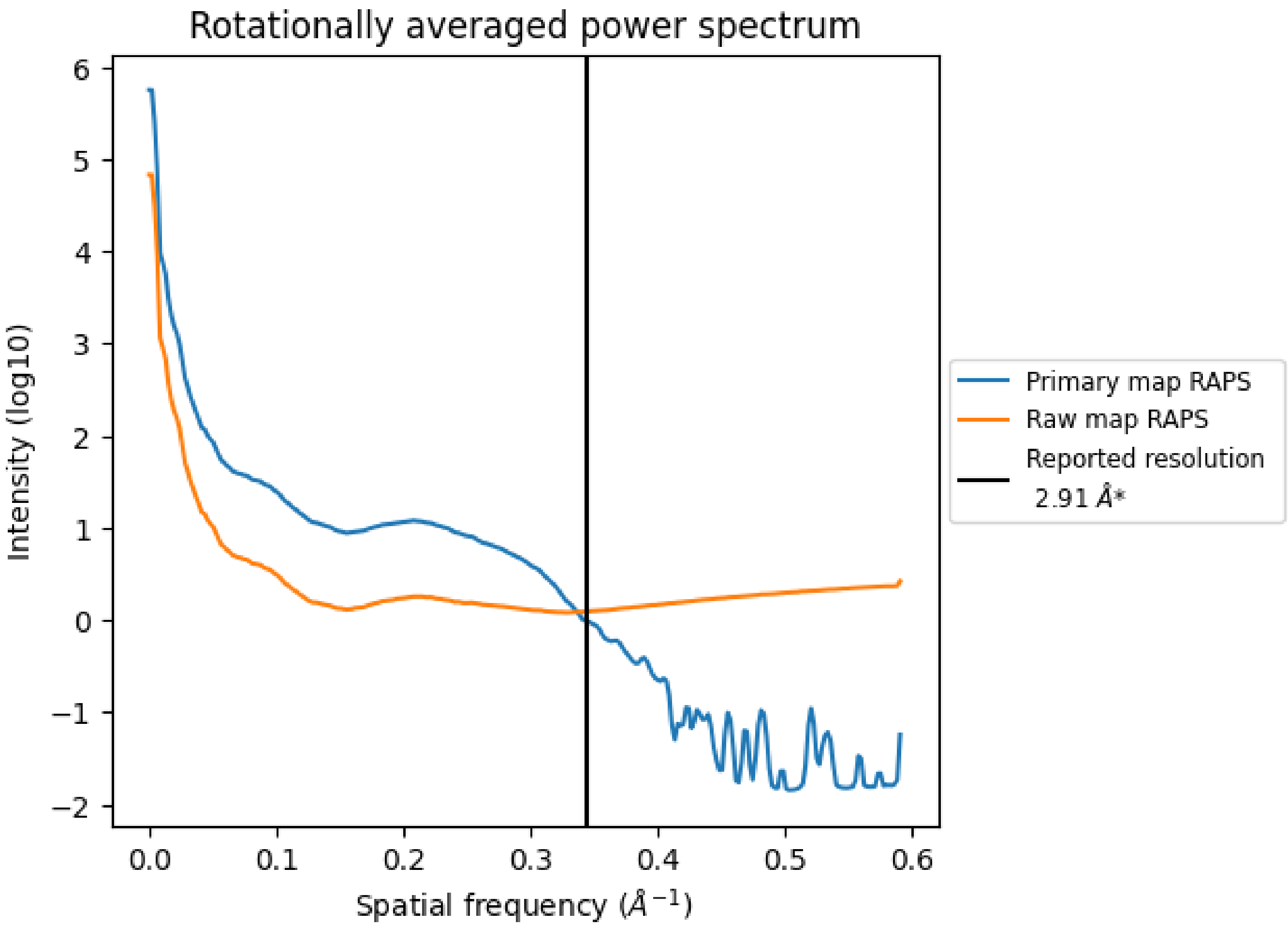
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 801 nm^3; this corresponds to an approximate mass of 724 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 ⓘ

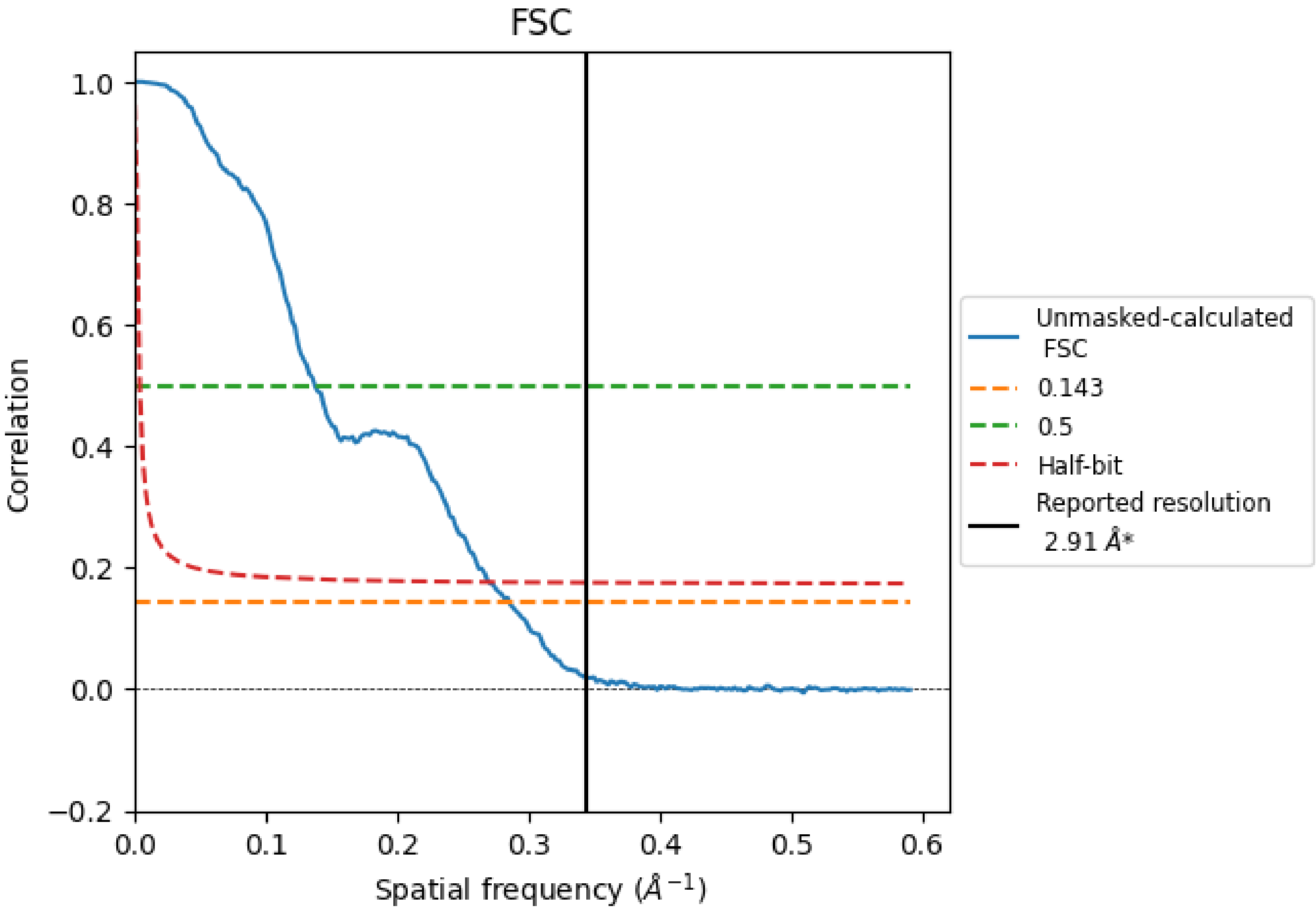


*Reported resolution corresponds to spatial frequency of 0.344 Å^{-1}

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 0.344 $Å^{-1}$

8.2 Resolution estimates ⓘ

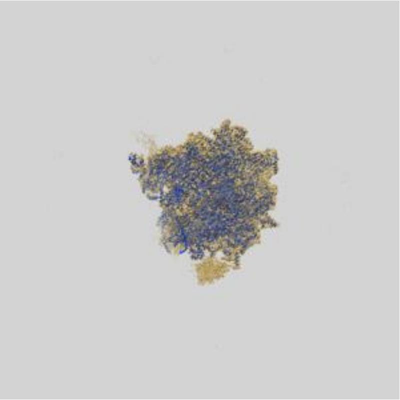
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	2.91	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.50	7.26	3.70

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.50 differs from the reported value 2.91 by more than 10 %

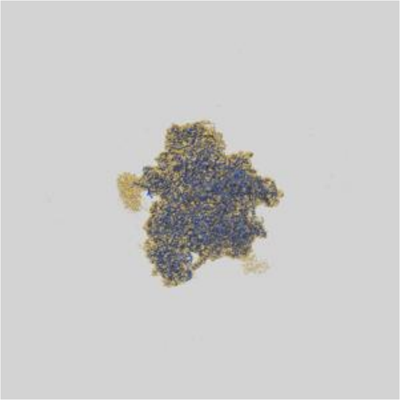
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-52048 and PDB model 9HCG. Per-residue inclusion information can be found in section 3 on page 17.

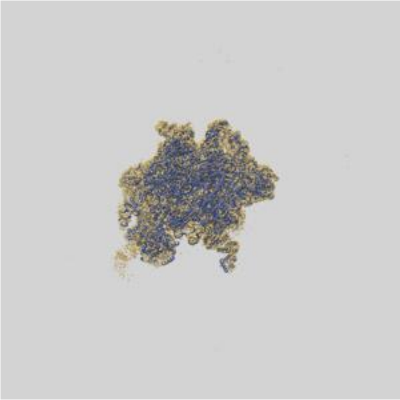
9.1 Map-model overlay



X



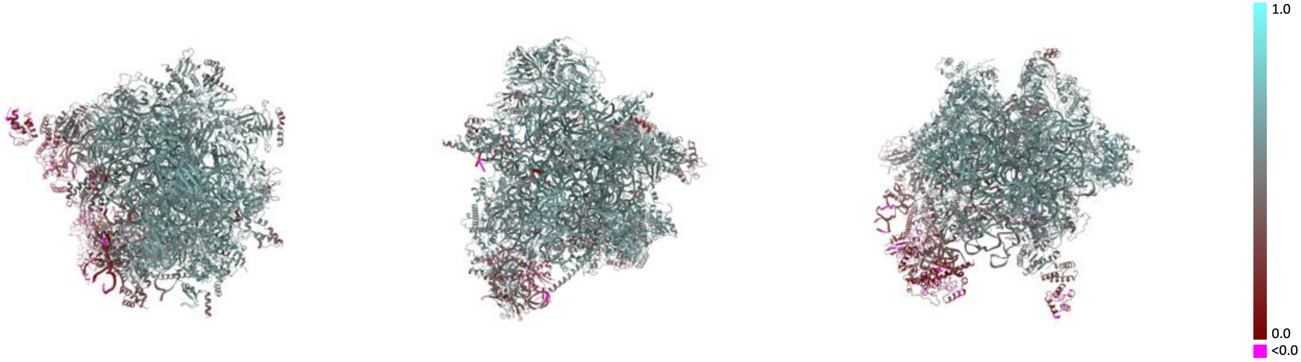
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.006 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.

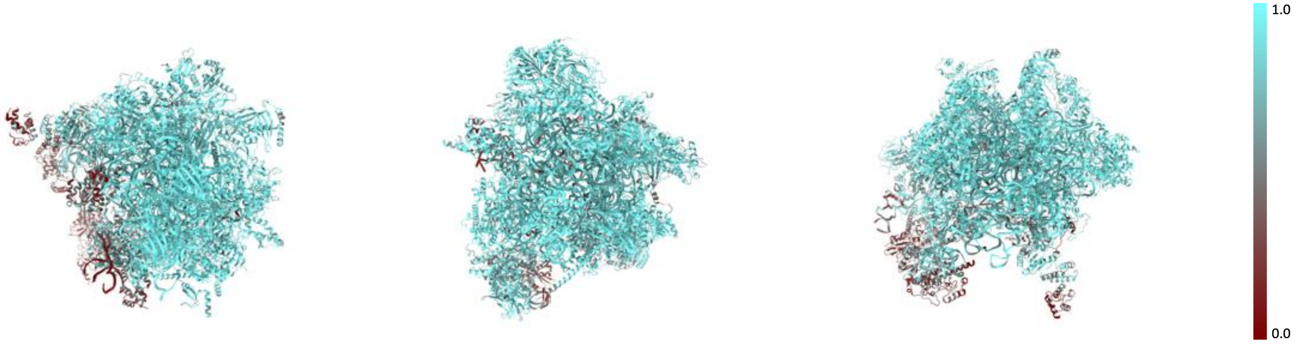
9.2 Q-score mapped to coordinate model ⓘ



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.

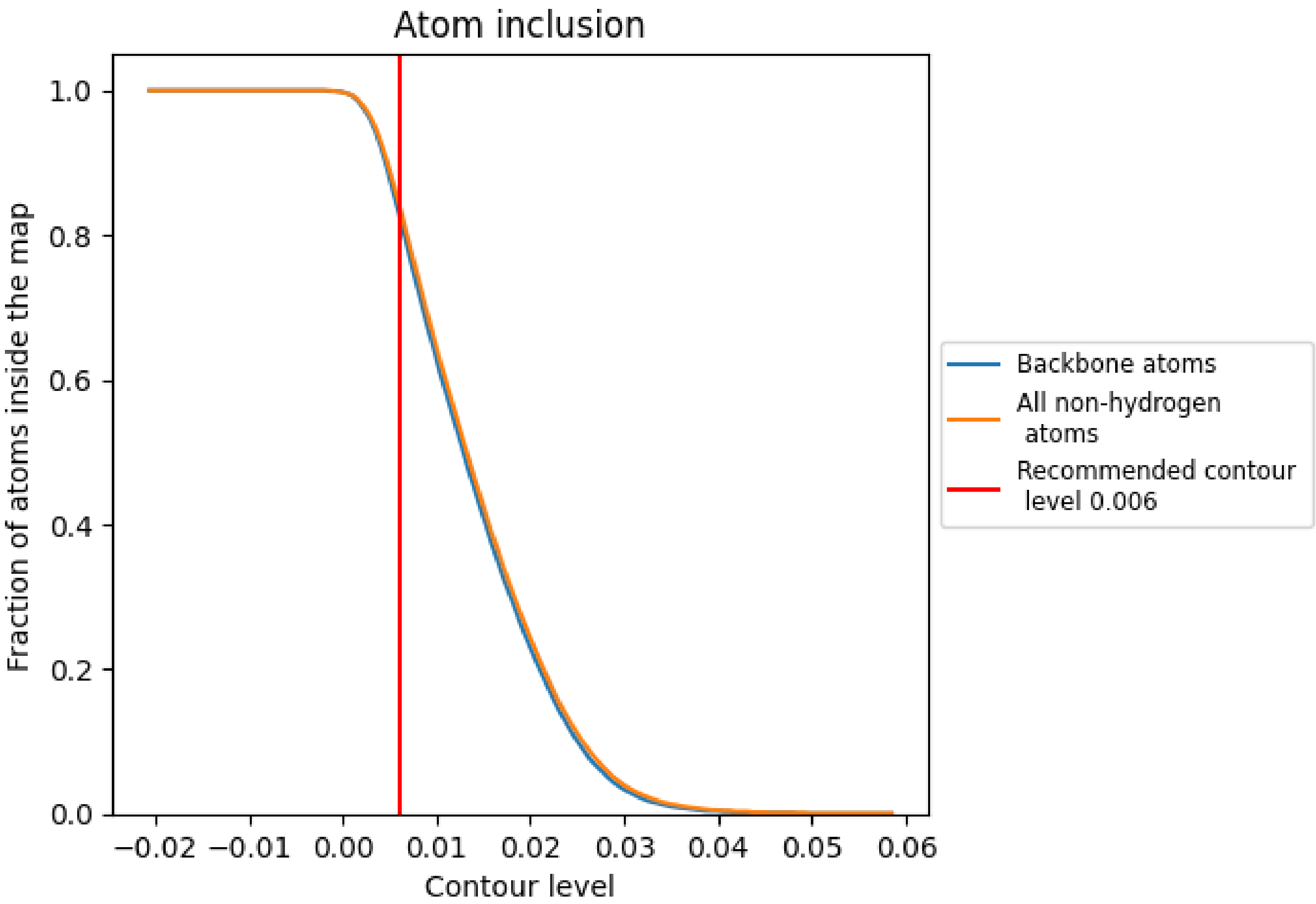
9.3 Atom inclusion mapped to coordinate model ⓘ



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 (0.006).

9.4 Atom inclusion ⓘ



At the recommended contour level, 83% of all backbone atoms, 84% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8430	0.5130
0	0.9270	0.5750
1	0.8570	0.5270
2	0.9750	0.6540
3	0.9750	0.6280
4	0.6880	0.5520
5	0.9330	0.5730
6	0.8480	0.4340
7	0.8830	0.5200
8	0.3530	0.1550
9	0.9160	0.5660
A	0.9190	0.5540
B	0.6860	0.2020
D	0.8860	0.5630
E	0.9180	0.5770
F	0.9630	0.6200
H	0.8860	0.5420
I	0.5570	0.2810
J	0.2800	0.1350
K	0.9570	0.6060
L	0.8420	0.5520
M	0.9570	0.6070
N	0.7310	0.4410
O	0.9510	0.6070
P	0.8440	0.4530
Q	0.9090	0.5560
R	0.9570	0.6180
S	0.9190	0.5770
T	0.9510	0.6260
U	0.9580	0.6170
V	0.9120	0.5610
W	0.8780	0.5190
X	0.9310	0.5880
Y	0.9470	0.6080
Z	0.9260	0.5830

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
a	0.7990	0.5530
b	0.9540	0.6150
c	0.9280	0.5720
d	0.8640	0.5140
e	0.1770	0.0840
f	0.2830	0.1700
g	0.9510	0.6000
h	0.8990	0.5270
i	0.9690	0.6480
j	0.8920	0.5350
k	0.6150	0.2780
l	0.4020	0.2350
m	0.2750	0.1290
o	0.9250	0.5890
p	0.8480	0.4900
q	0.8600	0.5060
r	0.8900	0.5310
s	0.9490	0.5960
t	0.5030	0.4410
u	0.7240	0.4490
v	0.6580	0.3320
w	0.2180	0.1060
x	0.5700	0.3350
y	0.5710	0.4080
z	0.2790	0.3260