



## Full wwPDB EM Validation Report ⓘ

Apr 22, 2025 – 02:50 pm BST

PDB ID : 9G1Z / pdb\_00009g1z  
EMDB ID : EMD-50957  
Title : Structure of Candida albicans 80S ribosome in complex with mefloquine (non-rotated state)  
Authors : Kolosova, O.; Zgadzay, Y.; Stetsenko, A.; Atamas, A.; Jenner, L.B.; Guskov, A.; Yusupov, M.  
Deposited on : 2024-07-10  
Resolution : 3.10 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev117  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
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) : 2.42

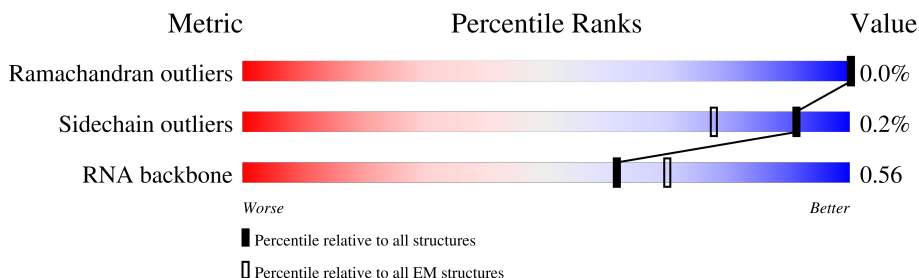
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.10 Å.

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



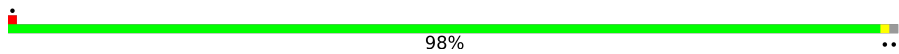


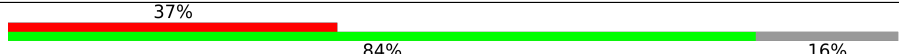
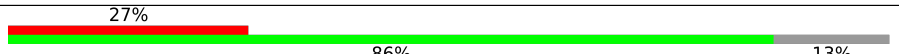

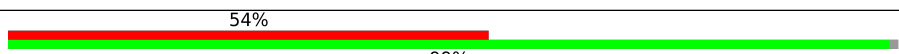


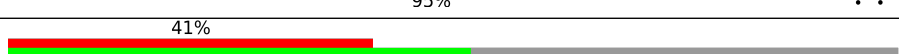
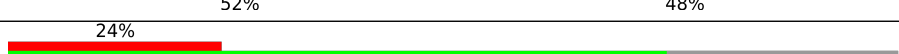

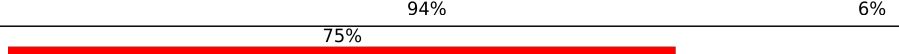
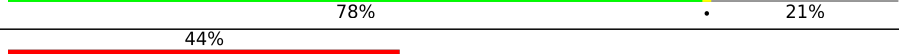


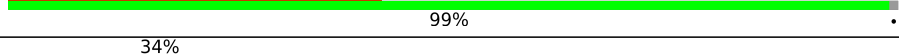
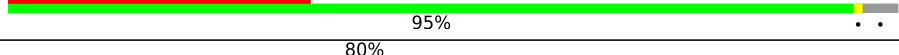

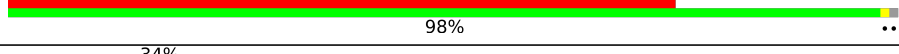

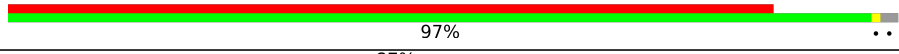
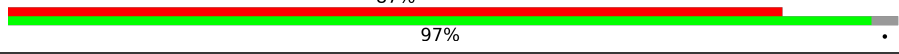


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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  $\geq 3$ , 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  $\leq 5\%$ . 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	0	172	99%
2	2	160	99%
3	3	121	93% 7%
4	4	158	84% 15%
5	5	124	56% 81% 17%
6	6	137	96%
7	7	155	40% 60%
8	8	142	85% 15%

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Mol	Chain	Length	Quality of chain
9	9	127	
10	A	1787	
11	B	261	
12	C	256	
13	D	249	
14	E	251	
15	F	262	
16	G	225	
17	H	236	
18	I	186	
19	J	206	
20	K	189	
21	L	118	
22	M	155	
23	N	143	
24	O	151	
25	P	132	
26	Q	142	
27	R	142	
28	S	137	
29	T	145	
30	U	145	
31	V	119	
32	W	87	
33	X	130	


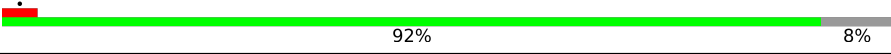
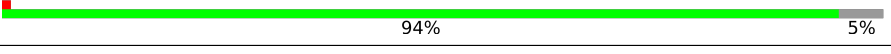
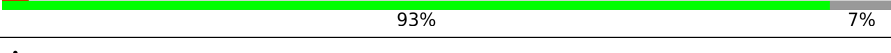
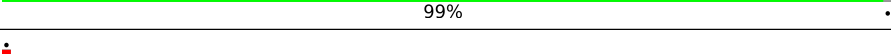
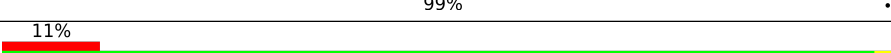
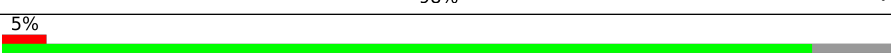
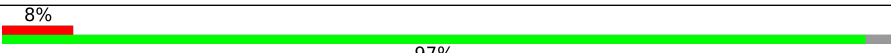
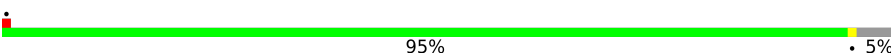
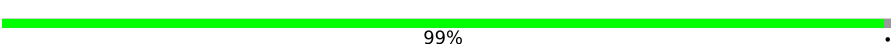
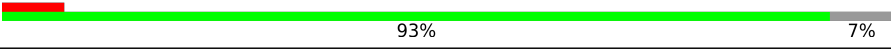
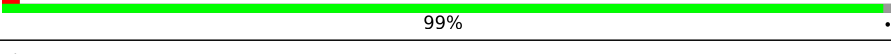
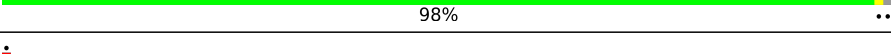
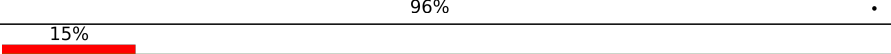
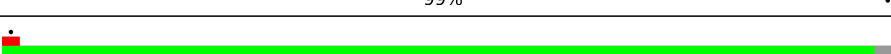
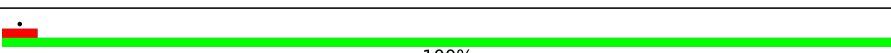
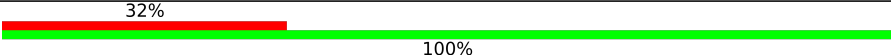
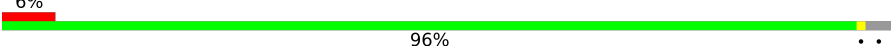
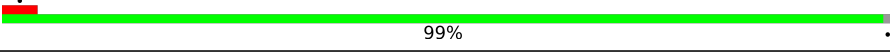


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Mol	Chain	Length	Quality of chain
34	Y	145	
35	Z	135	
36	a	105	
37	b	119	
38	c	82	
39	d	67	
40	e	56	
41	f	63	
42	g	193	
43	h	317	
44	j	254	
45	k	389	
46	l	363	
47	m	298	
48	o	241	
49	q	191	
50	s	174	
51	t	202	
52	u	131	
53	v	204	
54	w	200	
55	y	186	
56	z	190	
57	1	3359	
58	10	76	

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Mol	Chain	Length	Quality of chain
59	n	176	 88% 12%
60	p	262	 92% 8%
61	r	220	 94% 5%
62	x	185	 93% 7%
63	AA	136	 99% .
64	AB	149	 99% .
65	AC	63	 11% 98% .
66	AD	106	 5% 91% 9%
67	AE	112	 8% 97% .
68	AF	131	 95% . 5%
69	AG	107	 99% .
70	AH	121	 7% 93% 7%
71	AI	120	 99% .
72	AJ	99	 98% ..
73	AK	90	 96% .
74	AL	78	 15% 99% .
75	AM	51	 98% .
76	AN	52	 100%
77	AO	25	 32% 100%
78	AP	106	 6% 96% ..
79	AQ	92	 99% .

## 2 Entry composition [i](#)

There are 82 unique types of molecules in this entry. The entry contains 194174 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 60S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	171	Total	C	N	O	S	2	0
			1442	933	262	244	3		

- Molecule 2 is a protein called Ribosomal 60S subunit protein L21A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	159	Total	C	N	O	S	2	0
			1276	807	244	223	2		

- Molecule 3 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	121	Total	C	N	O	P	0	0
			2579	1153	463	842	121		

- Molecule 4 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	156	Total	C	N	O	P	0	0
			3313	1482	581	1094	156		

- Molecule 5 is a protein called Ribosomal 60S subunit protein L22B.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	5	103	Total	C	N	O	2	0
			848	553	139	156		

- Molecule 6 is a protein called Ribosomal 60S subunit protein L23B.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	131	Total	C	N	O	S	1	0
			986	621	186	171	8		

- Molecule 7 is a protein called Ribosomal 60S subunit protein L24A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	62	Total	C	N	O	S	0	0
			516	328	102	85	1		

- Molecule 8 is a protein called Ribosomal 60S subunit protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	121	Total	C	N	O	S	0	0
			974	622	175	176	1		

- Molecule 9 is a protein called Ribosomal 60S subunit protein L26B.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	9	126	Total	C	N	O	0	0
			989	618	190	181		

- Molecule 10 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	1635	Total	C	N	O	P	0	0
			34879	15594	6210	11440	1635		

- Molecule 11 is a protein called 40S ribosomal protein S0.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B	208	Total	C	N	O	S	0	0
			1627	1041	284	297	5		

- Molecule 12 is a protein called 40S ribosomal protein S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	C	214	Total	C	N	O	S	0	0
			1724	1094	313	313	4		

- Molecule 13 is a protein called Ribosomal 40S subunit protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	216	Total	C	N	O	S	0	0
			1620	1033	287	295	5		

- Molecule 14 is a protein called Ribosomal 40S subunit protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	E	223	Total	C	N	O	S	0	0
			1707	1087	311	305	4		

- Molecule 15 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	F	260	Total	C	N	O	S	0	0
			2055	1306	386	358	5		

- Molecule 16 is a protein called Ribosomal 40S subunit protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	G	206	Total	C	N	O	S	0	0
			1614	1008	301	301	4		

- Molecule 17 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	H	226	Total	C	N	O	S	0	0
			1820	1133	351	330	6		

- Molecule 18 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	I	96	Total	C	N	O	0	0
			780	500	144	136		

- Molecule 19 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	J	152	Total	C	N	O	S	0	0
			1216	752	248	215	1		

- Molecule 20 is a protein called Ribosomal 40S subunit protein S9B.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	K	178	Total	C	N	O	S	0	0
			1453	918	286	248	1		

- Molecule 21 is a protein called Ribosomal 40S subunit protein S10A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	L	93	Total	C	N	O	S	0	0
			783	511	129	142	1		

- Molecule 22 is a protein called Ribosomal 40S subunit protein S11A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	M	141	Total	C	N	O	S	0	0
			1129	722	212	192	3		

- Molecule 23 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	N	116	Total	C	N	O	S	0	0
			885	550	158	172	5		

- Molecule 24 is a protein called Ribosomal 40S subunit protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	O	150	Total	C	N	O	S	0	0
			1187	757	219	210	1		

- Molecule 25 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	P	127	Total	C	N	O	S	0	0
			942	579	186	174	3		

- Molecule 26 is a protein called Ribosomal 40S subunit protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Q	118	Total	C	N	O	S	0	0
			935	598	169	162	6		

- Molecule 27 is a protein called Ribosomal 40S subunit protein S16A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	R	140	Total	C	N	O	S	0	0
			1091	700	198	192	1		

- Molecule 28 is a protein called Ribosomal 40S subunit protein S17B.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	S	59	Total	C	N	O	S	0	0
			489	310	96	82	1		

- Molecule 29 is a protein called Ribosomal 40S subunit protein S18B.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	T	142	Total	C	N	O	S	0	0
			1169	733	228	205	3		

- Molecule 30 is a protein called Ribosomal 40S subunit protein S19A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	U	141	Total	C	N	O	S	0	0
			1100	689	210	200	1		

- Molecule 31 is a protein called Ribosomal 40S subunit protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	V	100	Total	C	N	O	S	0	0
			790	499	146	143	2		

- Molecule 32 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	W	87	Total	C	N	O	S	0	0
			676	415	126	133	2		

- Molecule 33 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	X	129	Total	C	N	O	S	0	0
			1032	655	191	183	3		

- Molecule 34 is a protein called Ribosomal 40S subunit protein S23B.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Y	143	Total	C	N	O	S	0	0
			1110	701	219	188	2		

- Molecule 35 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	Z	132	Total	C	N	O	0	0
			1072	670	216	186		

- Molecule 36 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	a	72	Total	C	N	O	0	0
			578	369	103	106		

- Molecule 37 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	b	100	Total	C	N	O	S	0	0
			799	494	169	130	6		

- Molecule 38 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	c	81	Total	C	N	O	S	0	0
			614	383	110	114	7		

- Molecule 39 is a protein called Ribosomal 40S subunit protein S28B.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	d	62	Total	C	N	O	S	0	0
			487	299	98	88	2		

- Molecule 40 is a protein called Ribosomal 40S subunit protein S29A.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	e	55	Total	C	N	O	S	0	0
			454	281	94	75	4		

- Molecule 41 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	f	56	Total	C	N	O	S	0	0
			444	278	89	75	2		

- Molecule 42 is a protein called Ubiquitin-ribosomal 40S subunit protein S31 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	g	70	Total	C	N	O	S	0	0
			574	362	113	93	6		

- Molecule 43 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	h	311	Total	C	N	O	S	0	0
			2398	1519	412	462	5		

- Molecule 44 is a protein called Ribosomal 60S subunit protein L2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	j	249	Total	C	N	O	S	1	0
			1894	1185	377	330	2		

- Molecule 45 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	k	386	Total	C	N	O	S	1	0
			3084	1955	584	538	7		

- Molecule 46 is a protein called Ribosomal 60S subunit protein L4B.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	l	361	Total	C	N	O	S	0	0
			2751	1729	529	490	3		

- Molecule 47 is a protein called Ribosomal 60S subunit protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	m	292	Total	C	N	O	S	0	0
			2394	1526	416	450	2		

- Molecule 48 is a protein called Ribosomal 60S subunit protein L7A.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	o	225	Total	C	N	O	S	1	0
			1819	1167	335	316	1		

- Molecule 49 is a protein called Ribosomal 60S subunit protein L9B.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	q	188	Total	C	N	O	S	0	0
			1501	948	274	275	4		

- Molecule 50 is a protein called Ribosomal 60S subunit protein L11B.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	s	170	Total	C	N	O	S	1	0
			1371	857	260	250	4		

- Molecule 51 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	t	200	Total	C	N	O	S	0	0
			1610	1009	318	283			

- Molecule 52 is a protein called Ribosomal 60S subunit protein L14B.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	u	130	Total	C	N	O	S	0	0
			1029	660	193	175	1		

- Molecule 53 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	v	203	Total	C	N	O	S	0	0
			1713	1075	356	280	2		

- Molecule 54 is a protein called Ribosomal 60S subunit protein L16A.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	w	199	Total	C	N	O	S	0	0
			1590	1025	294	269	2		

- Molecule 55 is a protein called Ribosomal 60S subunit protein L18A.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	y	185	Total	C	N	O	S	3	0
			1478	930	302	246			

- Molecule 56 is a protein called Ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	z	164	Total	C	N	O	S	1	0
			1331	829	277	222	3		

- Molecule 57 is a RNA chain called 25S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	1	3147	Total	C	N	O	P	0	0
			67271	30053	12088	21983	3147		

- Molecule 58 is a RNA chain called Endogenous tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	10	2	Total	C	N	O	P	0	0
			42	19	8	13	2		

- Molecule 59 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	n	155	Total	C	N	O		1	0
			1237	794	226	217			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
60	p	242	Total	C	N	O	S	0	0
			1875	1204	333	334	4		

- Molecule 61 is a protein called Ribosomal 60S subunit protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	r	208	Total	C	N	O	S	0	0
			1689	1069	322	291	7		

- Molecule 62 is a protein called Ribosomal 60S subunit protein L17B.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	x	172	Total	C	N	O		0	0
			1375	850	279	246			

- Molecule 63 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	AA	135	Total	C	N	O	S	0	0
			1087	705	197	183	2		

- Molecule 64 is a protein called Ribosomal 60S subunit protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	AB	148	Total	C	N	O	S	0	0
			1170	741	231	197	1		

- Molecule 65 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	AC	63	Total	C	N	O	S	1	0
			509	317	109	82	1		

- Molecule 66 is a protein called Ribosomal 60S subunit protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	AD	96	Total	C	N	O	S	0	0
			729	469	121	137	2		

- Molecule 67 is a protein called Ribosomal 60S subunit protein L31B.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	AE	109	Total	C	N	O	S	0	0
			889	562	167	158	2		

- Molecule 68 is a protein called Ribosomal 60S subunit protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	AF	125	Total	C	N	O	S	1	0
			1015	649	197	168	1		

- Molecule 69 is a protein called Ribosomal 60S subunit protein L33A.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	AG	106	Total	C	N	O	S	3	0
			867	558	166	142	1		

- Molecule 70 is a protein called Large ribosomal subunit protein eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	AH	112	Total	C	N	O	S	4	0
			913	567	188	154	4		

- Molecule 71 is a protein called Ribosomal 60S subunit protein L35A.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	AI	119	Total	C	N	O		1	0
			990	629	195	166			

- Molecule 72 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	AJ	98	Total	C	N	O	S	1	0
			772	481	158	131	2		

- Molecule 73 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	AK	86	Total	C	N	O	S	0	0
			677	413	148	110	6		

- Molecule 74 is a protein called Ribosomal 60S subunit protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	AL	77	Total	C	N	O		1	0
			623	398	116	109			

- Molecule 75 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	AM	50	Total	C	N	O		1	0
			446	280	100	66			

- Molecule 76 is a protein called Rpl40bp.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	AN	52	Total	C	N	O	S	1	0
			427	265	89	67	6		

- Molecule 77 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	AO	25	Total	C	N	O	S	0	0
			236	144	63	28	1		

- Molecule 78 is a protein called Ribosomal 60S subunit protein L42A.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	AP	103	Total	C	N	O	S	2	0
			843	533	168	137	5		

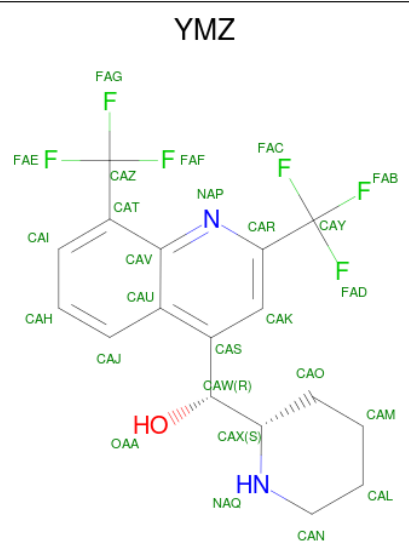
- Molecule 79 is a protein called Ribosomal 60S subunit protein L43A.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	AQ	91	Total	C	N	O	S	0	0
			698	430	140	124	4		

- Molecule 80 is ZINC ION (CCD ID: ZN) (formula: Zn).

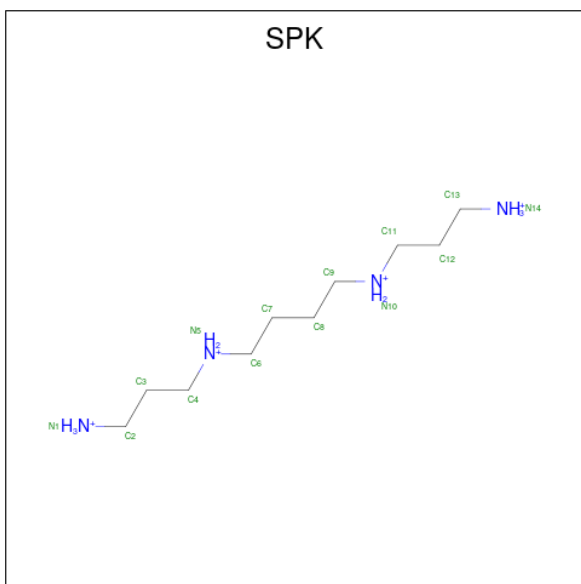
Mol	Chain	Residues	Atoms		AltConf
80	b	1	Total	Zn	0
			1	1	
80	g	1	Total	Zn	0
			1	1	
80	AH	1	Total	Zn	0
			1	1	
80	AK	1	Total	Zn	0
			1	1	
80	AN	1	Total	Zn	0
			1	1	
80	AP	1	Total	Zn	0
			1	1	
80	AQ	1	Total	Zn	0
			1	1	

- Molecule 81 is (11R,12S)- Mefloquine (CCD ID: YMZ) (formula: C<sub>17</sub>H<sub>16</sub>F<sub>6</sub>N<sub>2</sub>O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
81	j	1	Total 26	C 17	F 6	N 2	O 1	0
81	1	1	Total 26	C 17	F 6	N 2	O 1	0

- Molecule 82 is SPERMINE (FULLY PROTONATED FORM) (CCD ID: SPK) (formula:  $\text{C}_{10}\text{H}_{30}\text{N}_4$ ).

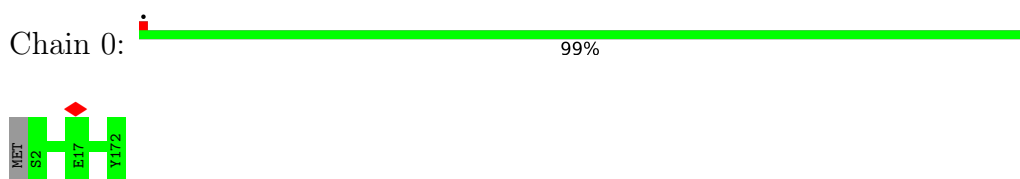


Mol	Chain	Residues	Atoms			AltConf
82	1	1	Total	C	N	0
			14	10	4	

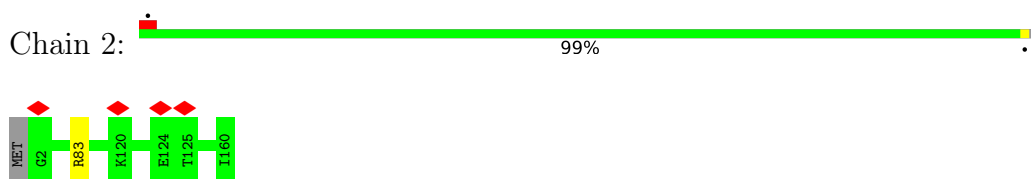
### 3 Residue-property plots [i](#)

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.

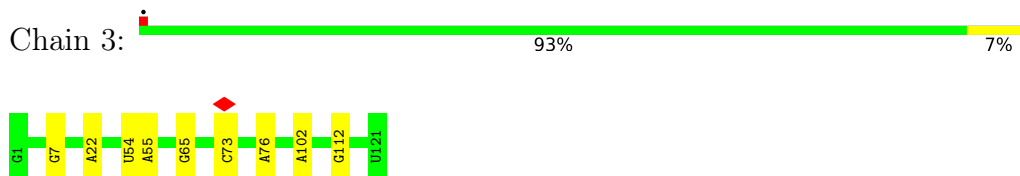
- Molecule 1: 60S ribosomal protein L20



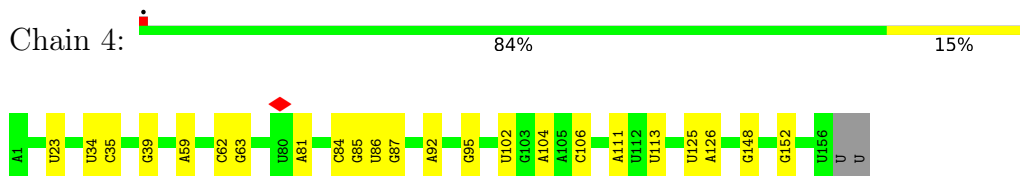
- Molecule 2: Ribosomal 60S subunit protein L21A



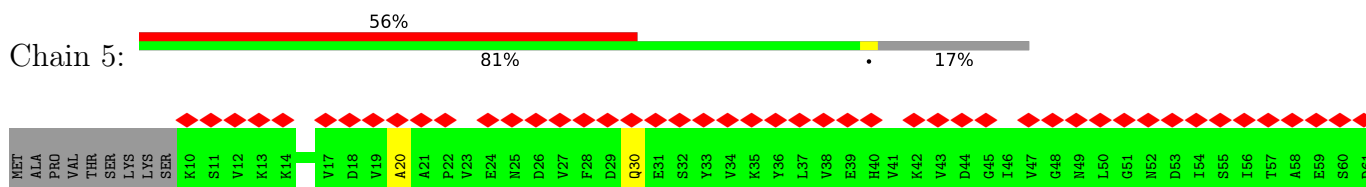
- Molecule 3: 5S rRNA



- Molecule 4: 5.8S rRNA



- Molecule 5: Ribosomal 60S subunit protein L22B





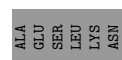
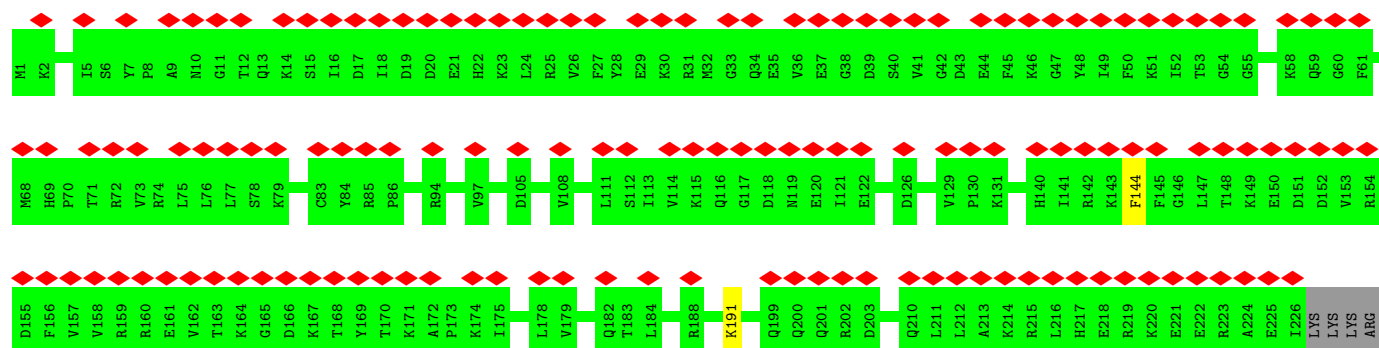




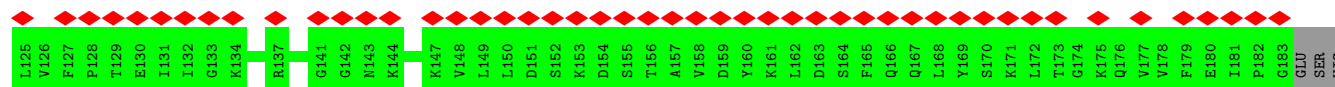
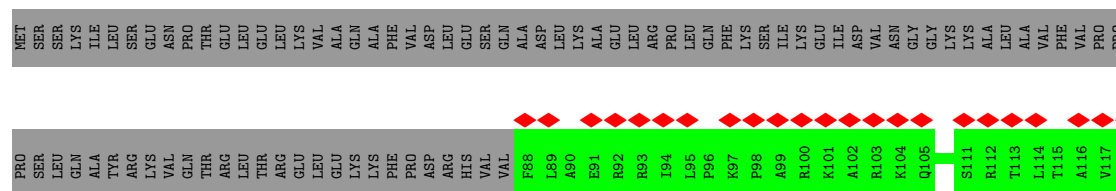
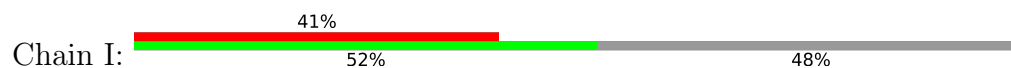




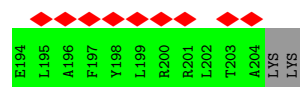
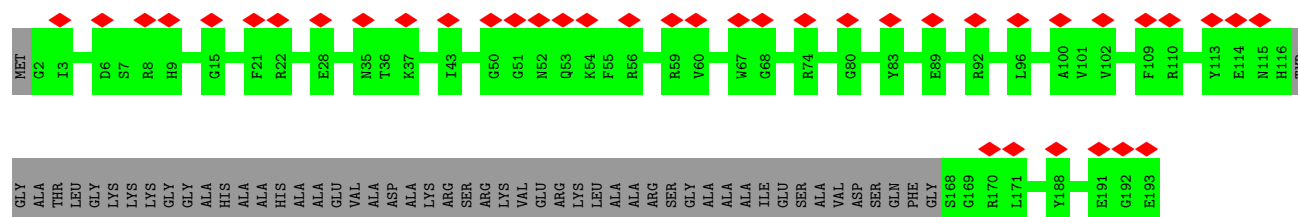
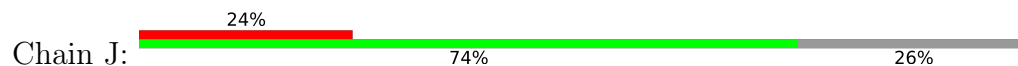
- Molecule 17: 40S ribosomal protein S6



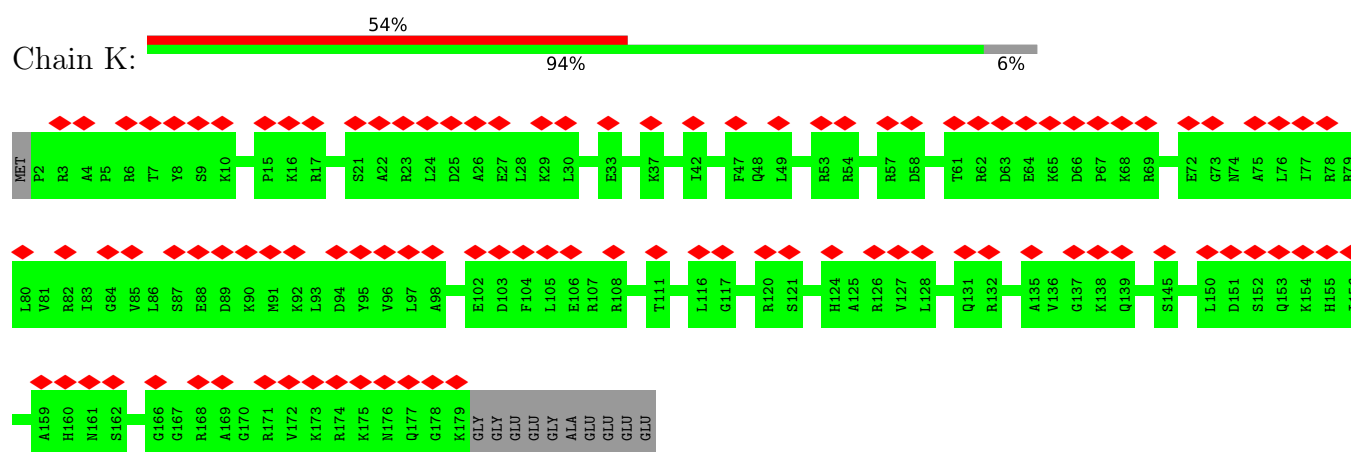
- Molecule 18: 40S ribosomal protein S7



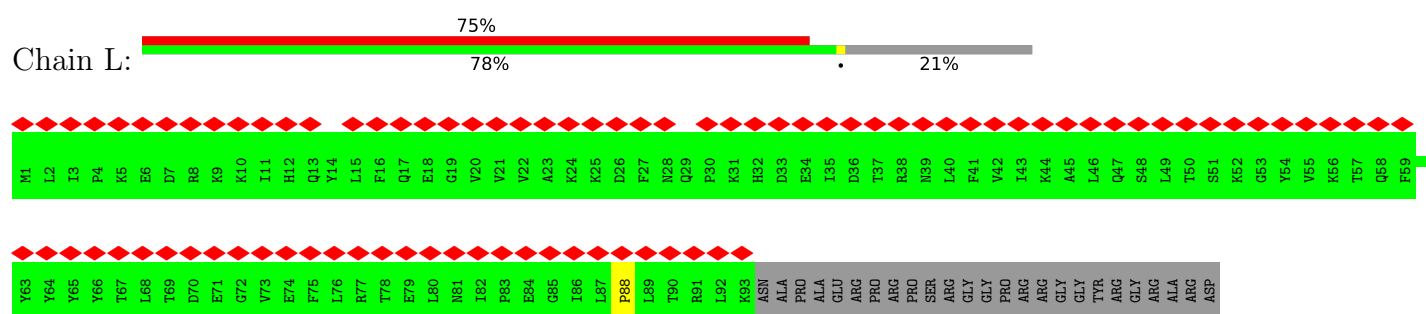
- Molecule 19: 40S ribosomal protein S8



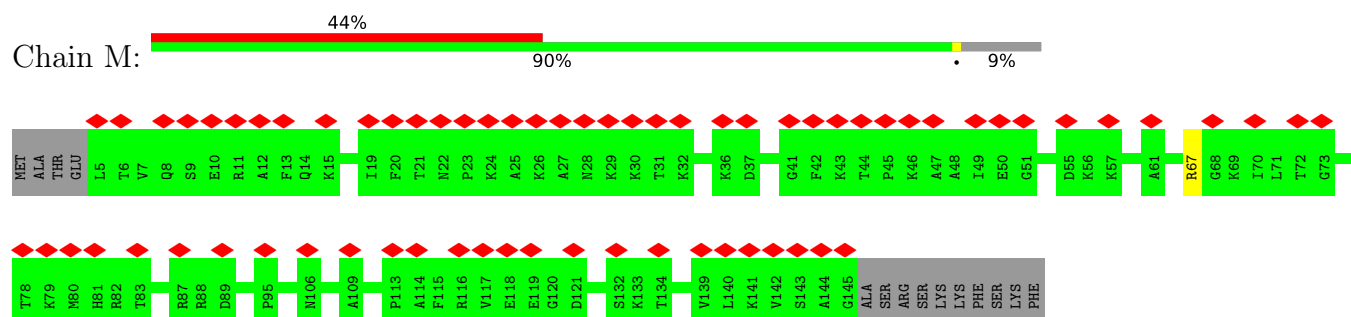
- Molecule 20: Ribosomal 40S subunit protein S9B



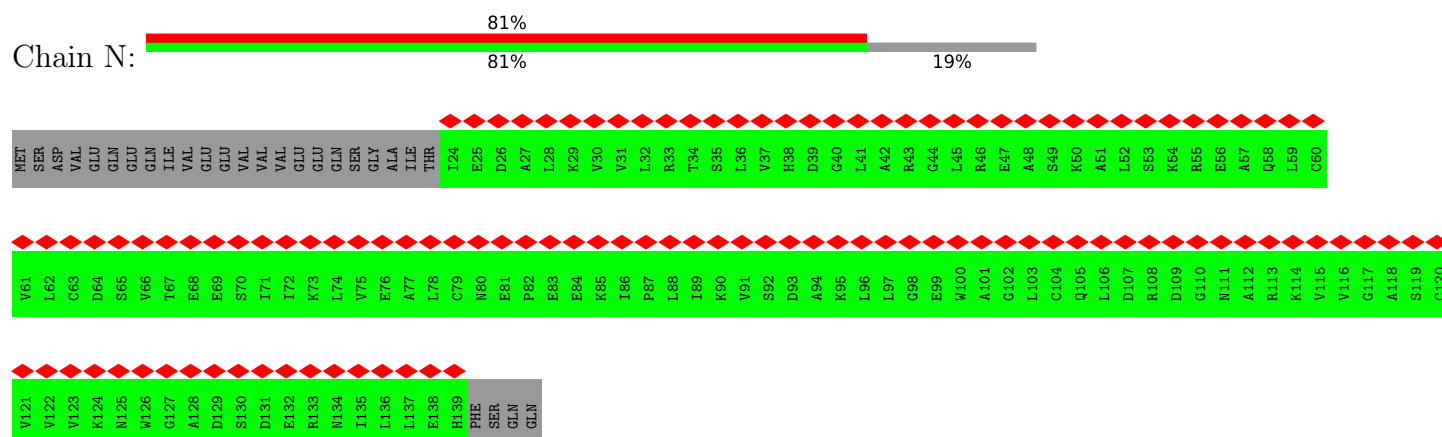
- Molecule 21: Ribosomal 40S subunit protein S10A



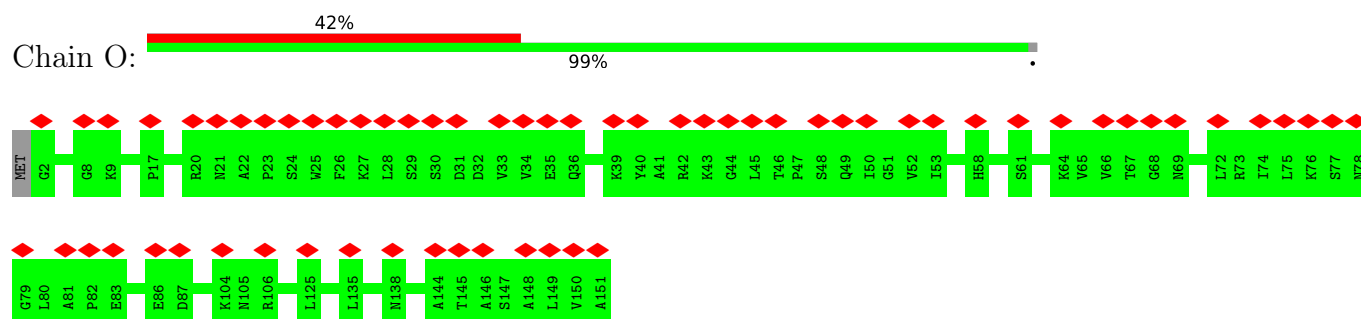
- Molecule 22: Ribosomal 40S subunit protein S11A



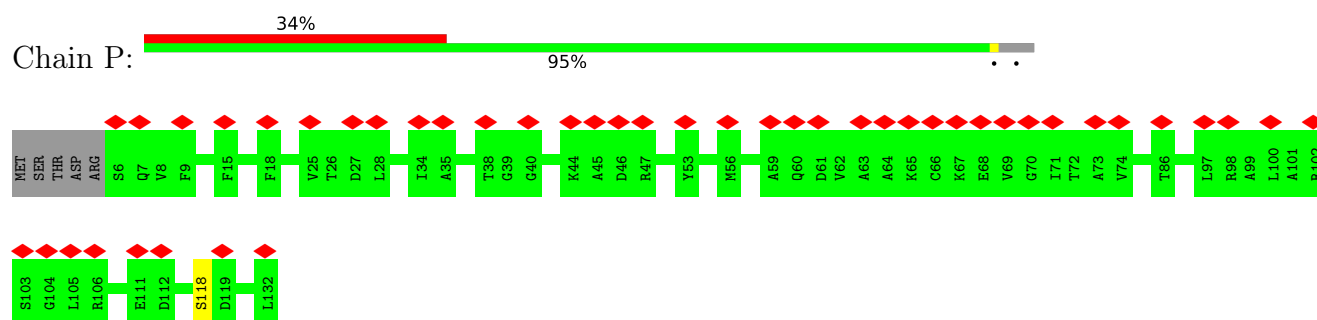
- Molecule 23: 40S ribosomal protein S12



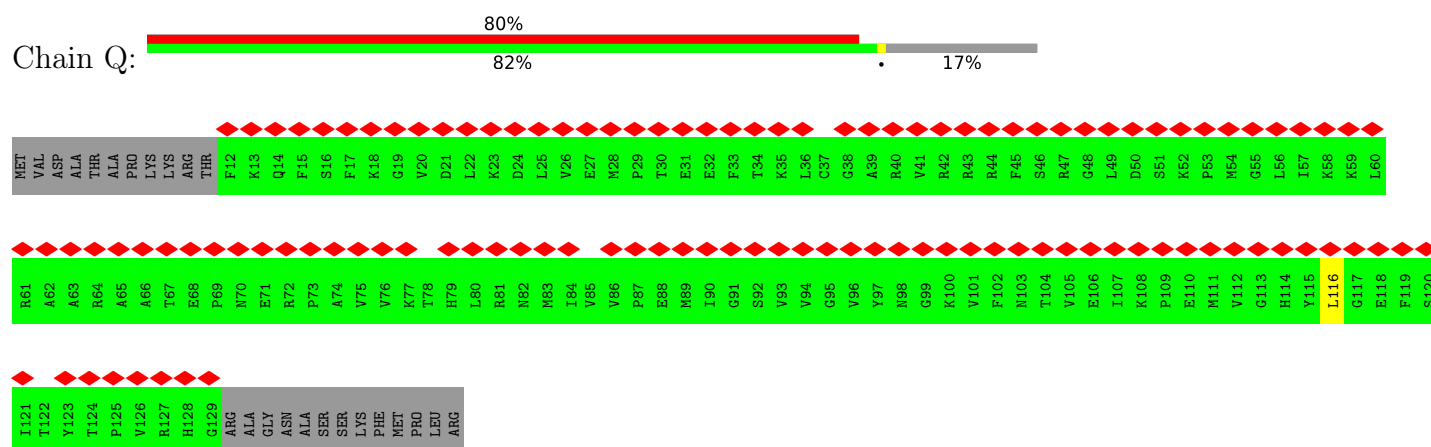
- Molecule 24: Ribosomal 40S subunit protein S13



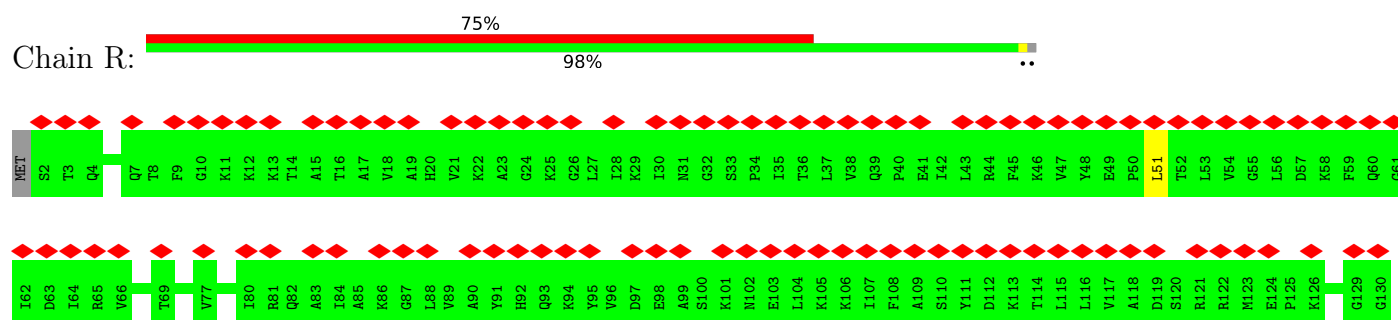
- Molecule 25: Small ribosomal subunit protein uS11

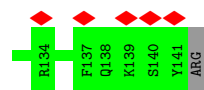


- Molecule 26: Ribosomal 40S subunit protein S15

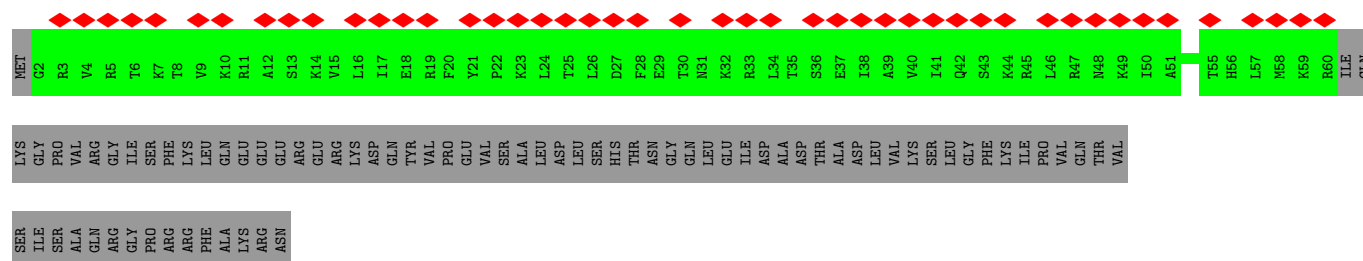


- Molecule 27: Ribosomal 40S subunit protein S16A

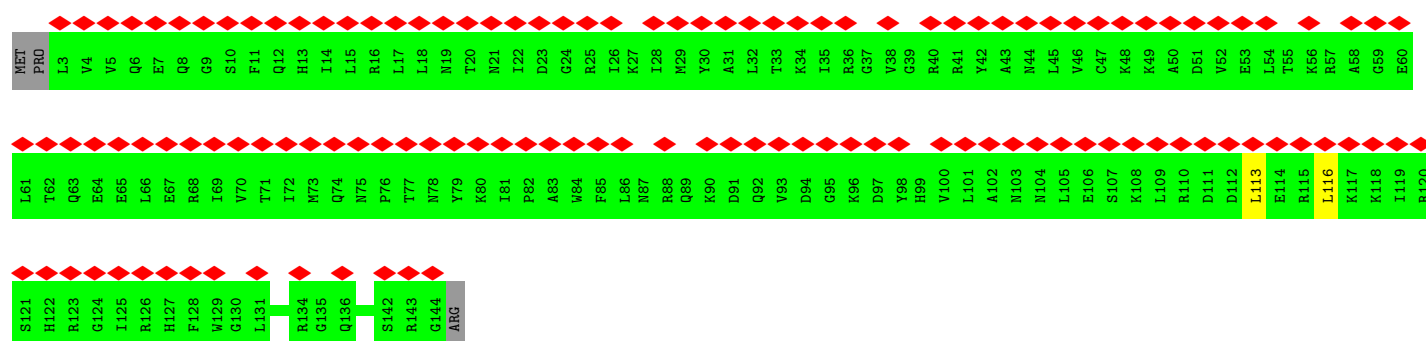
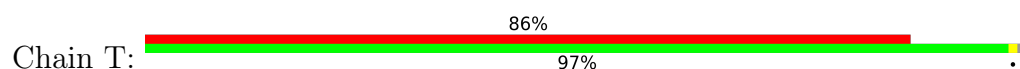




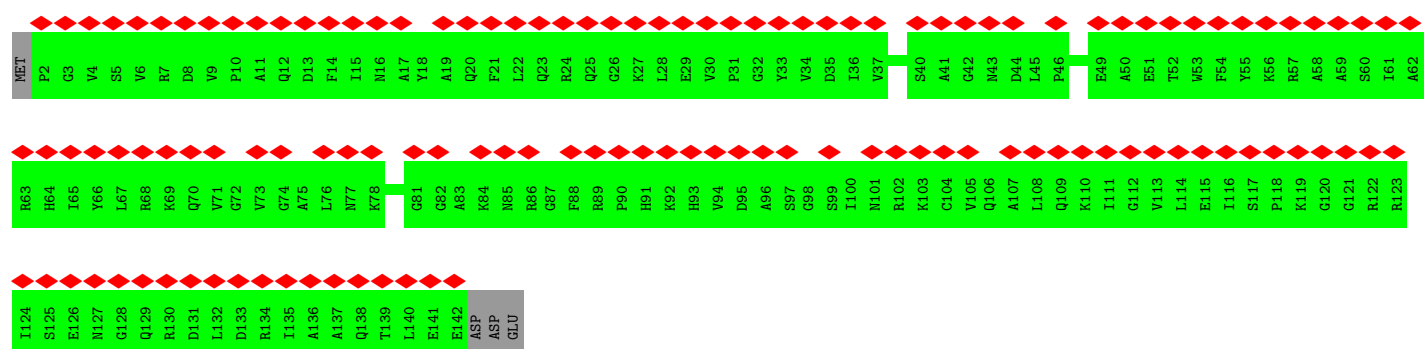
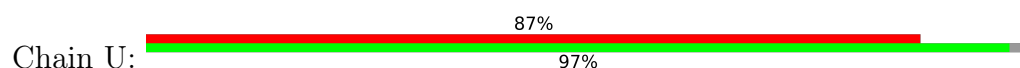
• Molecule 28: Ribosomal 40S subunit protein S17B



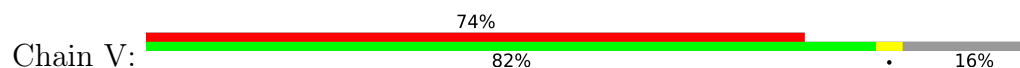
• Molecule 29: Ribosomal 40S subunit protein S18B

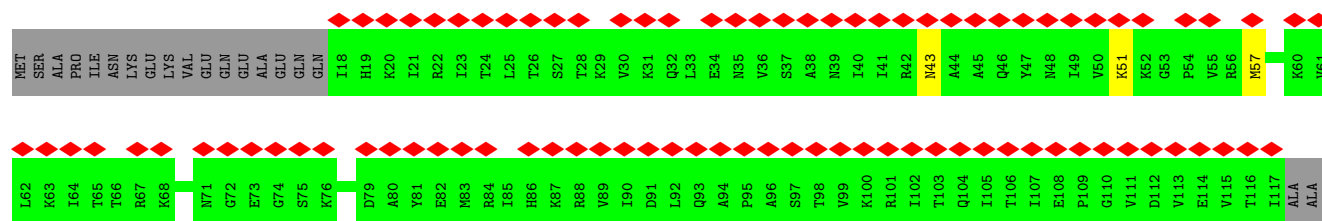


• Molecule 30: Ribosomal 40S subunit protein S19A



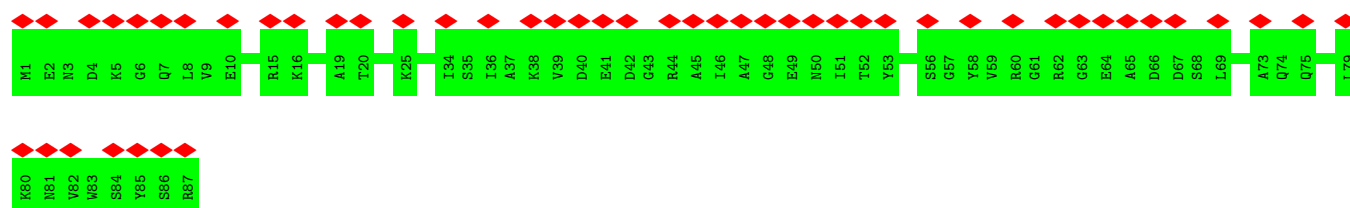
• Molecule 31: Ribosomal 40S subunit protein S20





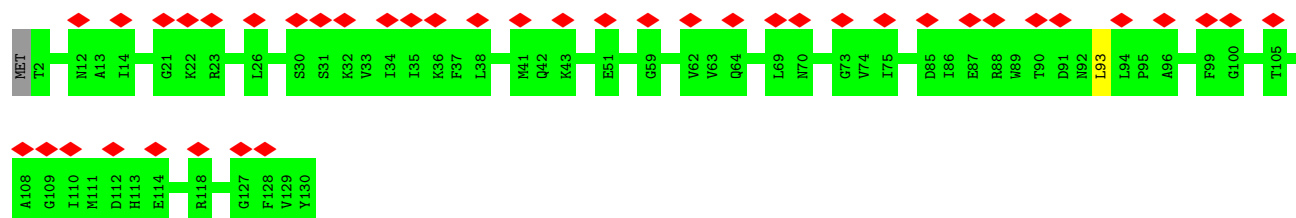
- Molecule 32: 40S ribosomal protein S21

Chain W: 57%  
100%



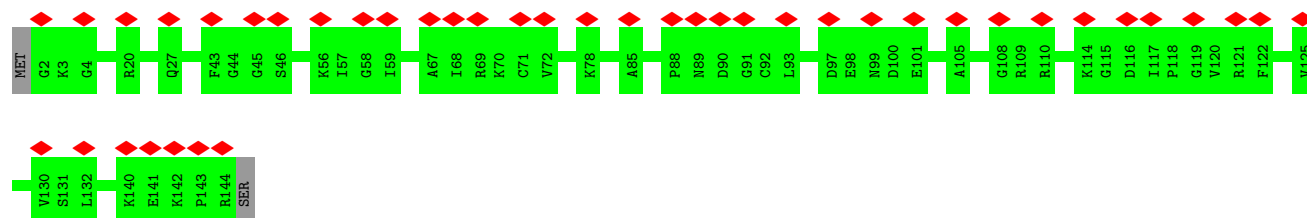
- Molecule 33: 40S ribosomal protein S22-A

Chain X: 32%  
98%



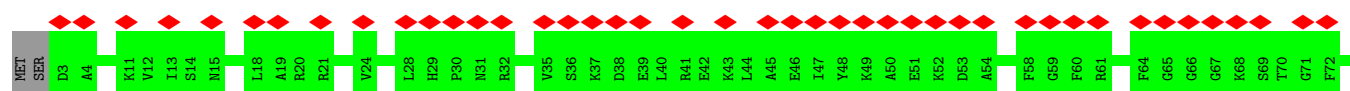
- Molecule 34: Ribosomal 40S subunit protein S23B

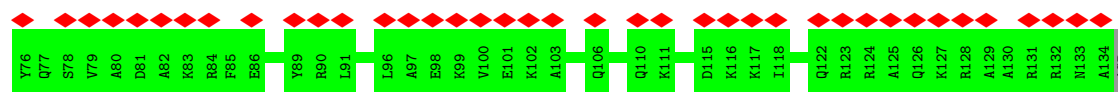
Chain Y: 29%  
99%



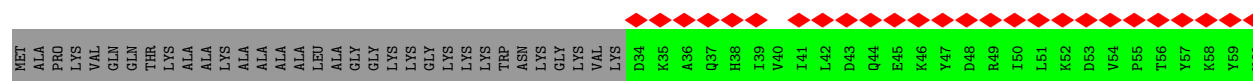
- Molecule 35: 40S ribosomal protein S24

Chain Z: 61%  
98%

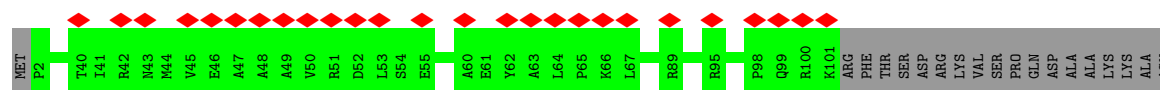
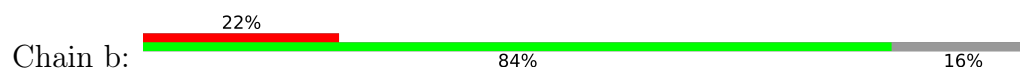




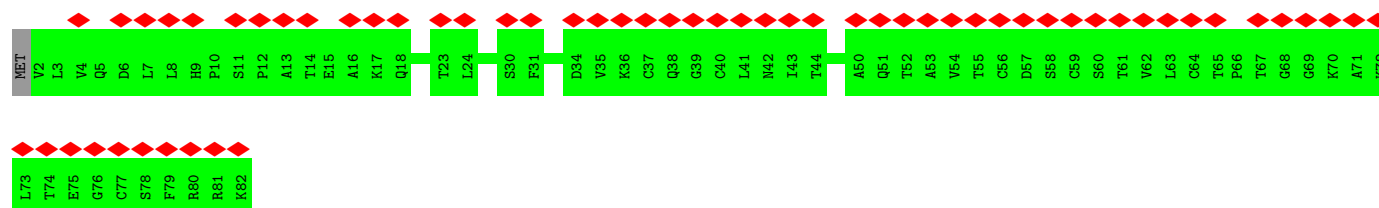
- Molecule 36: 40S ribosomal protein S25



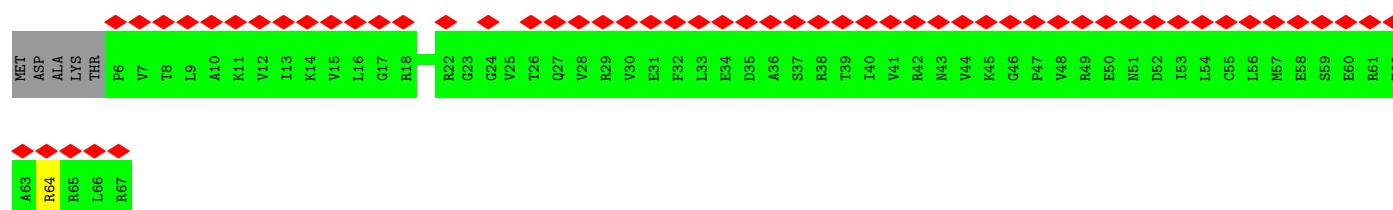
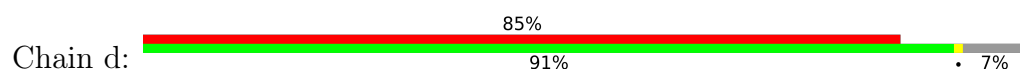
- Molecule 37: 40S ribosomal protein S26



- Molecule 38: 40S ribosomal protein S27



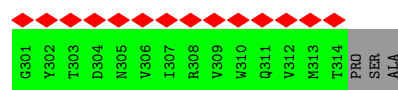
- Molecule 39: Ribosomal 40S subunit protein S28B



- Molecule 40: Ribosomal 40S subunit protein S29A

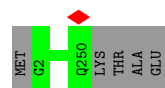






- Molecule 44: Ribosomal 60S subunit protein L2A

Chain j: 98%



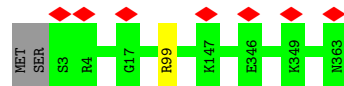
- Molecule 45: 60S ribosomal protein L3

Chain k: 99%



- Molecule 46: Ribosomal 60S subunit protein L4B

Chain l: 99%



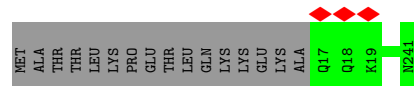
- Molecule 47: Ribosomal 60S subunit protein L5

Chain m: 6% 98%



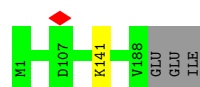
- Molecule 48: Ribosomal 60S subunit protein L7A

Chain o: 93% 7%

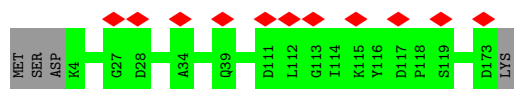


- Molecule 49: Ribosomal 60S subunit protein L9B

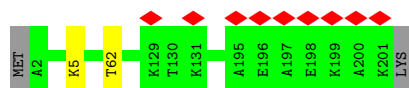
Chain q: 98%



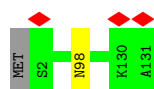
- Molecule 50: Ribosomal 60S subunit protein L11B



- Molecule 51: 60S ribosomal protein L13



- Molecule 52: Ribosomal 60S subunit protein L14B



- Molecule 53: Ribosomal protein L15



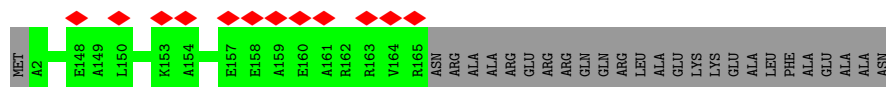
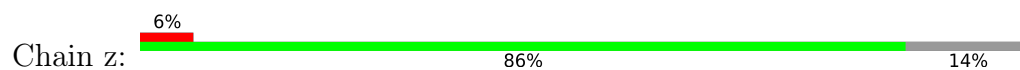
- Molecule 54: Ribosomal 60S subunit protein L16A




- Molecule 55: Ribosomal 60S subunit protein L18A

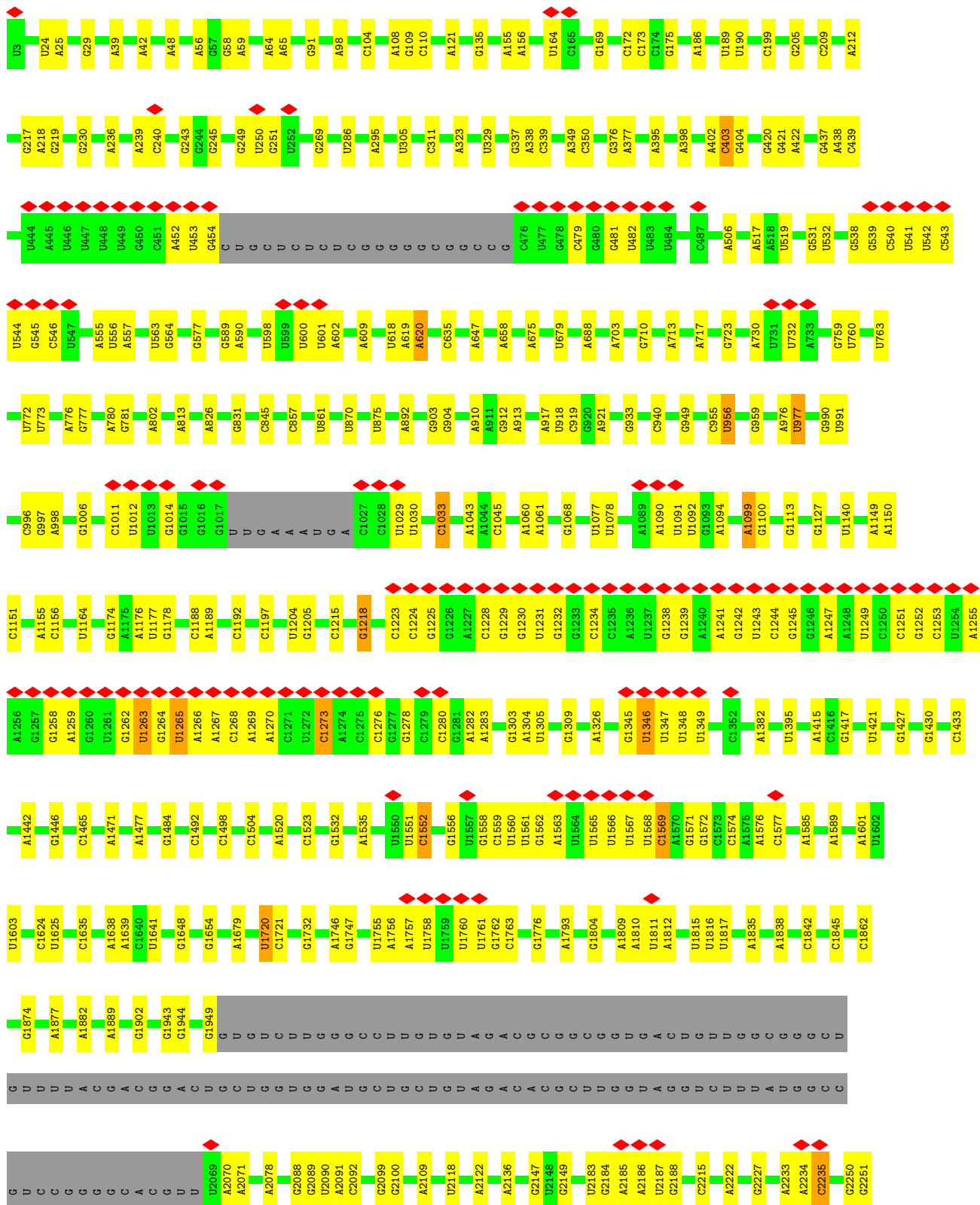


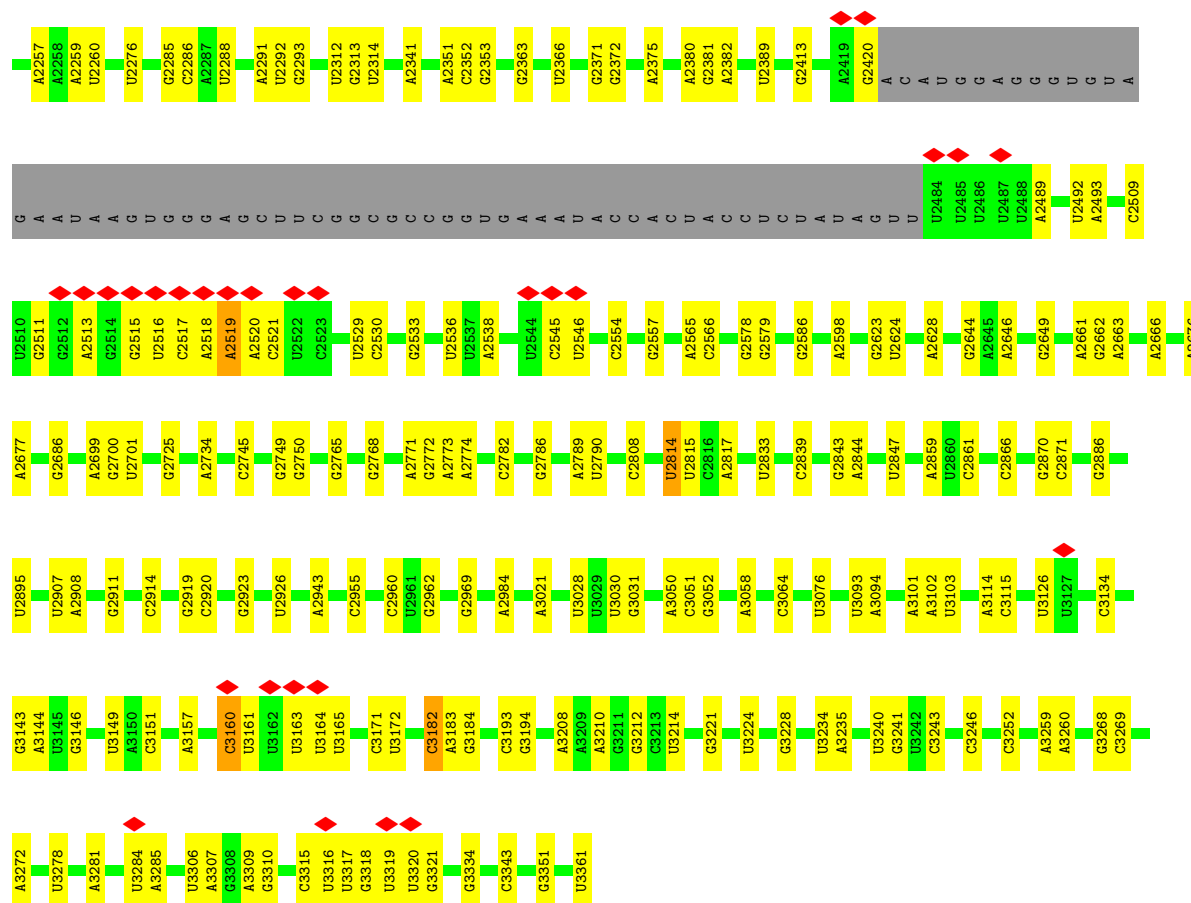
- Molecule 56: Ribosomal protein L19



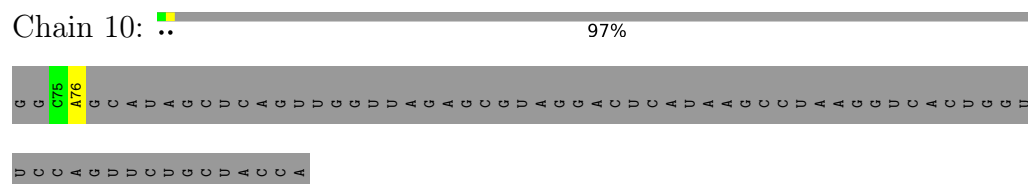
• Molecule 57: 25S rRNA

Chain 1: 

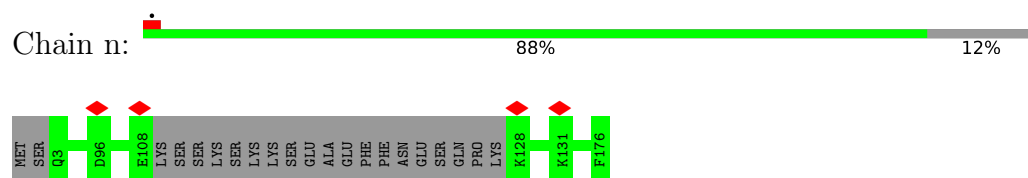




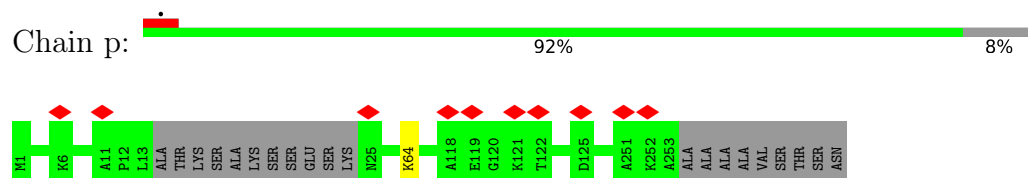
### • Molecule 58: Endogenous tRNA



### • Molecule 59: 60S ribosomal protein L6

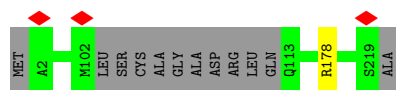


### • Molecule 60: 60S ribosomal protein L8



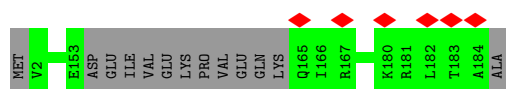
- Molecule 61: Ribosomal 60S subunit protein L10

Chain r:  94% 5%



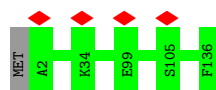
- Molecule 62: Ribosomal 60S subunit protein L17B

Chain x:  93% 7%



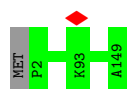
- Molecule 63: 60S ribosomal protein L27

Chain AA:  99%



- Molecule 64: Ribosomal 60S subunit protein L28

Chain AB:  99%



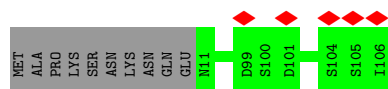
- Molecule 65: 60S ribosomal protein L29

Chain AC:  11% 98%



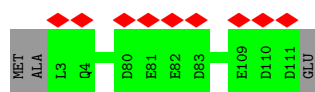
- Molecule 66: Ribosomal 60S subunit protein L30

Chain AD:  5% 91% 9%



- Molecule 67: Ribosomal 60S subunit protein L31B

Chain AE:  8% 97%



- Molecule 68: Ribosomal 60S subunit protein L32



- Molecule 69: Ribosomal 60S subunit protein L33A



- Molecule 70: Large ribosomal subunit protein eL34



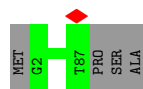
- Molecule 71: Ribosomal 60S subunit protein L35A



- Molecule 72: 60S ribosomal protein L36

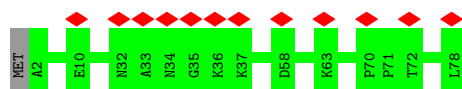


- Molecule 73: Ribosomal protein L37



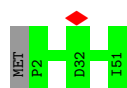
- Molecule 74: Ribosomal 60S subunit protein L38

Chain AL:  15% 99%



- Molecule 75: 60S ribosomal protein L39

Chain AM:  98%



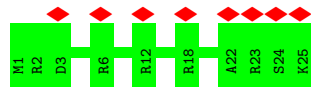
- Molecule 76: Rpl40bp

Chain AN:  100%



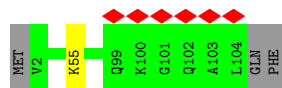
- Molecule 77: 60S ribosomal protein L41

Chain AO:  32% 100%



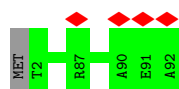
- Molecule 78: Ribosomal 60S subunit protein L42A

Chain AP:  6% 96%



- Molecule 79: Ribosomal 60S subunit protein L43A

Chain AQ:  99%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	51014	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	47.3	Depositor
Minimum defocus (nm)	5000	Depositor
Maximum defocus (nm)	16000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.318	Depositor
Minimum map value	-1.278	Depositor
Average map value	-0.004	Depositor
Map value standard deviation	0.094	Depositor
Recommended contour level	0.25	Depositor
Map size ( $\text{\AA}$ )	429.24, 429.24, 429.24	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.022, 1.022, 1.022	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, YMZ, OMC, MLZ, OMG, SPK

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	0	0.42	0/1483	0.58	0/1997
2	2	0.42	0/1305	0.56	0/1749
3	3	0.59	0/2884	0.78	0/4492
4	4	0.64	0/3702	0.80	1/5764 (0.0%)
5	5	0.32	0/871	0.58	0/1175
6	6	0.38	0/994	0.58	0/1339
7	7	0.41	0/528	0.62	0/701
8	8	0.37	0/990	0.55	0/1337
9	9	0.35	0/999	0.56	0/1334
10	A	0.34	0/39022	0.87	34/60803 (0.1%)
11	B	0.29	0/1666	0.60	1/2273 (0.0%)
12	C	0.29	0/1750	0.59	0/2354
13	D	0.29	0/1648	0.55	1/2237 (0.0%)
14	E	0.29	0/1731	0.63	0/2324
15	F	0.27	0/2096	0.57	0/2822
16	G	0.29	0/1631	0.64	1/2199 (0.0%)
17	H	0.27	0/1845	0.62	1/2464 (0.0%)
18	I	0.26	0/792	0.55	0/1062
19	J	0.27	0/1238	0.59	0/1658
20	K	0.29	0/1478	0.64	0/1978
21	L	0.28	0/801	0.62	0/1081
22	M	0.28	0/1154	0.55	0/1553
23	N	0.29	0/892	0.69	0/1203
24	O	0.29	0/1210	0.60	0/1631
25	P	0.29	0/953	0.69	0/1279
26	Q	0.30	0/954	0.67	1/1282 (0.1%)
27	R	0.26	0/1109	0.61	1/1486 (0.1%)
28	S	0.26	0/494	0.56	0/658
29	T	0.28	0/1186	0.73	2/1590 (0.1%)
30	U	0.29	0/1120	0.60	0/1508
31	V	0.26	0/800	0.61	1/1082 (0.1%)
32	W	0.27	0/683	0.59	0/918

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	X	0.29	0/1049	0.60	1/1412 (0.1%)
34	Y	0.29	0/1128	0.60	0/1505
35	Z	0.27	0/1086	0.61	0/1447
36	a	0.26	0/585	0.55	0/789
37	b	0.29	0/811	0.63	0/1085
38	c	0.27	0/624	0.53	0/843
39	d	0.26	0/489	0.69	0/654
40	e	0.26	0/466	0.57	0/620
41	f	0.30	0/451	0.61	0/601
42	g	0.26	0/585	0.64	1/778 (0.1%)
43	h	0.26	0/2451	0.58	0/3337
44	j	0.39	0/1931	0.60	0/2592
45	k	0.41	0/3156	0.57	0/4246
46	l	0.39	0/2799	0.56	0/3777
47	m	0.36	0/2447	0.56	0/3294
48	o	0.40	0/1855	0.53	0/2492
49	q	0.35	0/1519	0.57	0/2043
50	s	0.31	0/1390	0.60	0/1861
51	t	0.40	0/1637	0.61	0/2195
52	u	0.36	0/1044	0.58	0/1407
53	v	0.45	0/1753	0.61	0/2347
54	w	0.41	0/1620	0.57	0/2167
55	y	0.38	0/1511	0.63	0/2022
56	z	0.35	0/1352	0.64	0/1800
57	1	0.66	0/75238	0.85	44/117289 (0.0%)
58	10	0.49	0/46	0.70	0/69
59	n	0.34	0/1258	0.55	0/1696
60	p	0.34	0/1907	0.52	0/2567
61	r	0.39	0/1724	0.60	0/2314
62	x	0.39	0/1398	0.60	0/1879
63	AA	0.34	0/1112	0.50	0/1488
64	AB	0.40	0/1199	0.55	0/1607
65	AC	0.34	0/522	0.56	0/692
66	AD	0.35	0/738	0.54	0/994
67	AE	0.35	0/902	0.56	0/1212
68	AF	0.41	0/1039	0.59	0/1390
69	AG	0.42	0/895	0.57	0/1201
70	AH	0.38	0/934	0.61	0/1242
71	AI	0.32	0/1004	0.60	0/1337
72	AJ	0.32	0/780	0.59	0/1033
73	AK	0.38	0/690	0.65	0/916
74	AL	0.34	0/632	0.55	0/842
75	AM	0.33	0/458	0.60	0/609

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
76	AN	0.36	0/436	0.61	0/577
77	AO	0.25	0/237	0.80	0/304
78	AP	0.35	0/840	0.56	0/1108
79	AQ	0.37	0/705	0.66	0/940
All	All	0.49	0/208442	0.77	90/305953 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
25	P	0	1
61	r	0	1
All	All	0	2

There are no bond length outliers.

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	T	116	LEU	CA-CB-CG	10.91	140.40	115.30
10	A	451	C	N1-C2-O2	8.18	123.81	118.90
10	A	451	C	C2-N1-C1'	7.45	126.99	118.80
57	1	1218	G	O4'-C1'-N9	7.27	114.02	108.20
57	1	3160	C	C2-N1-C1'	7.21	126.73	118.80
57	1	918	U	C2-N1-C1'	7.21	126.35	117.70
10	A	1375	C	C2-N1-C1'	7.20	126.72	118.80
10	A	824	U	C2-N1-C1'	7.16	126.30	117.70
57	1	2814	U	C2-N1-C1'	7.14	126.27	117.70
57	1	1276	C	N3-C2-O2	-7.02	116.99	121.90
57	1	2215	C	N3-C2-O2	-6.87	117.09	121.90
57	1	3126	U	C2-N1-C1'	6.80	125.86	117.70
57	1	1265	U	N1-C2-O2	6.74	127.52	122.80
10	A	1457	A	C8-N9-C4	-6.72	103.11	105.80
10	A	451	C	N3-C2-O2	-6.71	117.20	121.90
57	1	2814	U	N1-C2-O2	6.66	127.46	122.80
57	1	3182	C	N1-C2-O2	6.59	122.86	118.90
57	1	977	U	C2-N1-C1'	6.58	125.60	117.70
57	1	1720	U	O4'-C1'-N1	6.54	113.43	108.20
10	A	1259	C	N1-C2-O2	6.52	122.81	118.90
57	1	2215	C	N1-C2-O2	6.45	122.77	118.90
10	A	824	U	N1-C2-O2	6.43	127.30	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1259	C	C2-N1-C1'	6.28	125.71	118.80
57	1	3182	C	C2-N1-C1'	6.27	125.70	118.80
57	1	3160	C	C6-N1-C1'	-6.22	113.33	120.80
10	A	579	U	N1-C2-O2	6.17	127.12	122.80
10	A	579	U	C2-N1-C1'	6.13	125.05	117.70
10	A	846	U	C2-N1-C1'	6.11	125.03	117.70
10	A	1242	U	N3-C2-O2	-6.11	117.93	122.20
57	1	1265	U	C2-N1-C1'	6.10	125.02	117.70
10	A	579	U	N3-C2-O2	-6.10	117.93	122.20
57	1	1273	C	N3-C2-O2	-6.07	117.65	121.90
57	1	437	G	N3-C4-N9	-6.05	122.37	126.00
10	A	4	C	C2-N1-C1'	5.97	125.36	118.80
57	1	2519	A	P-O3'-C3'	5.92	126.80	119.70
57	1	2814	U	N3-C2-O2	-5.92	118.06	122.20
57	1	3126	U	N3-C2-O2	-5.89	118.07	122.20
16	G	118	LEU	CA-CB-CG	5.88	128.83	115.30
29	T	113	LEU	CA-CB-CG	5.86	128.77	115.30
57	1	1033	C	C2-N1-C1'	5.83	125.22	118.80
10	A	1242	U	N1-C2-O2	5.81	126.86	122.80
57	1	1265	U	C6-N1-C1'	-5.77	113.13	121.20
57	1	977	U	N1-C2-O2	5.76	126.83	122.80
10	A	1057	C	C2-N1-C1'	5.75	125.12	118.80
42	g	142	LEU	CA-CB-CG	5.74	128.51	115.30
10	A	1462	C	C2-N1-C1'	5.71	125.08	118.80
57	1	3126	U	N1-C2-O2	5.69	126.78	122.80
10	A	1242	U	C2-N1-C1'	5.67	124.50	117.70
26	Q	116	LEU	C-N-CA	-5.67	110.40	122.30
57	1	3182	C	N3-C2-O2	-5.67	117.93	121.90
10	A	1067	C	C2-N1-C1'	5.63	124.99	118.80
10	A	1234	U	C2-N1-C1'	5.61	124.44	117.70
4	4	39	G	O4'-C1'-N9	5.61	112.69	108.20
10	A	804	U	C6-N1-C2	-5.59	117.64	121.00
10	A	824	U	N3-C2-O2	-5.52	118.34	122.20
57	1	977	U	N3-C2-O2	-5.52	118.34	122.20
10	A	1237	C	C2-N1-C1'	5.50	124.85	118.80
57	1	1492	C	C2-N1-C1'	5.47	124.82	118.80
57	1	831	G	O4'-C1'-N9	5.46	112.57	108.20
57	1	2235	C	N1-C2-O2	5.46	122.17	118.90
57	1	620	A	N1-C6-N6	5.44	121.86	118.60
57	1	3030	U	C2-N1-C1'	5.41	124.20	117.70
17	H	144	PHE	C-N-CA	-5.41	108.17	121.70
57	1	1263	U	O4'-C1'-N1	5.38	112.50	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	R	51	LEU	CA-CB-CG	5.38	127.66	115.30
10	A	1327	C	C2-N1-C1'	5.30	124.63	118.80
57	1	1569	C	C2-N1-C1'	5.29	124.62	118.80
57	1	1346	U	P-O3'-C3'	5.28	126.03	119.70
57	1	956	U	C2-N1-C1'	5.27	124.03	117.70
10	A	1259	C	N3-C2-O2	-5.26	118.22	121.90
57	1	1099	A	OP2-P-O3'	5.26	116.78	105.20
10	A	1231	C	N1-C2-O2	5.25	122.05	118.90
57	1	403	C	C6-N1-C2	-5.23	118.21	120.30
57	1	1569	C	C6-N1-C1'	-5.19	114.57	120.80
57	1	2509	C	C2-N1-C1'	5.18	124.50	118.80
10	A	451	C	C6-N1-C2	-5.17	118.23	120.30
10	A	1067	C	N1-C2-O2	5.17	122.00	118.90
10	A	1375	C	C6-N1-C1'	-5.15	114.62	120.80
33	X	93	LEU	C-N-CA	-5.14	108.85	121.70
10	A	561	U	N3-C2-O2	-5.11	118.62	122.20
31	V	57	MET	CA-CB-CG	5.09	121.95	113.30
57	1	3243	C	N1-C2-O2	5.07	121.94	118.90
13	D	129	LEU	CA-CB-CG	5.07	126.96	115.30
57	1	1552	C	N1-C2-O2	5.07	121.94	118.90
10	A	4	C	N1-C2-O2	5.05	121.93	118.90
10	A	451	C	C6-N1-C1'	-5.05	114.74	120.80
57	1	2235	C	C2-N1-C1'	5.05	124.35	118.80
11	B	16	LEU	CA-CB-CG	5.04	126.89	115.30
10	A	1057	C	C6-N1-C1'	-5.02	114.77	120.80
57	1	918	U	C6-N1-C1'	-5.01	114.18	121.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
25	P	118	SER	Peptide
61	r	178	ARG	Mainchain

## 5.2 Too-close contacts ⓘ

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

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	171/172 (99%)	169 (99%)	2 (1%)	0	100	100
2	2	159/160 (99%)	157 (99%)	2 (1%)	0	100	100
5	5	103/124 (83%)	95 (92%)	7 (7%)	1 (1%)	13	42
6	6	129/137 (94%)	126 (98%)	3 (2%)	0	100	100
7	7	60/155 (39%)	60 (100%)	0	0	100	100
8	8	119/142 (84%)	118 (99%)	1 (1%)	0	100	100
9	9	124/127 (98%)	123 (99%)	1 (1%)	0	100	100
11	B	206/261 (79%)	201 (98%)	5 (2%)	0	100	100
12	C	212/256 (83%)	207 (98%)	5 (2%)	0	100	100
13	D	214/249 (86%)	209 (98%)	5 (2%)	0	100	100
14	E	221/251 (88%)	215 (97%)	6 (3%)	0	100	100
15	F	258/262 (98%)	255 (99%)	3 (1%)	0	100	100
16	G	204/225 (91%)	196 (96%)	8 (4%)	0	100	100
17	H	224/236 (95%)	220 (98%)	4 (2%)	0	100	100
18	I	94/186 (50%)	92 (98%)	2 (2%)	0	100	100
19	J	148/206 (72%)	141 (95%)	7 (5%)	0	100	100
20	K	176/189 (93%)	175 (99%)	1 (1%)	0	100	100
21	L	91/118 (77%)	84 (92%)	6 (7%)	1 (1%)	12	39
22	M	139/155 (90%)	136 (98%)	3 (2%)	0	100	100
23	N	114/143 (80%)	98 (86%)	16 (14%)	0	100	100
24	O	148/151 (98%)	145 (98%)	3 (2%)	0	100	100
25	P	125/132 (95%)	122 (98%)	3 (2%)	0	100	100
26	Q	116/142 (82%)	106 (91%)	10 (9%)	0	100	100
27	R	138/142 (97%)	134 (97%)	4 (3%)	0	100	100
28	S	57/137 (42%)	56 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	T	140/145 (97%)	136 (97%)	4 (3%)	0	100	100
30	U	139/145 (96%)	137 (99%)	2 (1%)	0	100	100
31	V	98/119 (82%)	96 (98%)	2 (2%)	0	100	100
32	W	85/87 (98%)	83 (98%)	2 (2%)	0	100	100
33	X	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
34	Y	141/145 (97%)	138 (98%)	3 (2%)	0	100	100
35	Z	130/135 (96%)	130 (100%)	0	0	100	100
36	a	70/105 (67%)	69 (99%)	1 (1%)	0	100	100
37	b	98/119 (82%)	96 (98%)	2 (2%)	0	100	100
38	c	79/82 (96%)	75 (95%)	4 (5%)	0	100	100
39	d	60/67 (90%)	55 (92%)	5 (8%)	0	100	100
40	e	53/56 (95%)	51 (96%)	2 (4%)	0	100	100
41	f	54/63 (86%)	53 (98%)	1 (2%)	0	100	100
42	g	68/193 (35%)	61 (90%)	7 (10%)	0	100	100
43	h	309/317 (98%)	292 (94%)	17 (6%)	0	100	100
44	j	248/254 (98%)	240 (97%)	8 (3%)	0	100	100
45	k	385/389 (99%)	373 (97%)	12 (3%)	0	100	100
46	l	359/363 (99%)	349 (97%)	10 (3%)	0	100	100
47	m	290/298 (97%)	279 (96%)	11 (4%)	0	100	100
48	o	224/241 (93%)	218 (97%)	6 (3%)	0	100	100
49	q	186/191 (97%)	182 (98%)	4 (2%)	0	100	100
50	s	169/174 (97%)	164 (97%)	5 (3%)	0	100	100
51	t	198/202 (98%)	195 (98%)	1 (0%)	2 (1%)	13	42
52	u	128/131 (98%)	125 (98%)	3 (2%)	0	100	100
53	v	201/204 (98%)	198 (98%)	3 (2%)	0	100	100
54	w	197/200 (98%)	195 (99%)	2 (1%)	0	100	100
55	y	186/186 (100%)	183 (98%)	3 (2%)	0	100	100
56	z	163/190 (86%)	161 (99%)	2 (1%)	0	100	100
59	n	152/176 (86%)	150 (99%)	2 (1%)	0	100	100
60	p	238/262 (91%)	229 (96%)	9 (4%)	0	100	100
61	r	204/220 (93%)	201 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
62	x	168/185 (91%)	165 (98%)	3 (2%)	0	100	100
63	AA	133/136 (98%)	132 (99%)	1 (1%)	0	100	100
64	AB	146/149 (98%)	138 (94%)	8 (6%)	0	100	100
65	AC	62/63 (98%)	62 (100%)	0	0	100	100
66	AD	94/106 (89%)	93 (99%)	1 (1%)	0	100	100
67	AE	107/112 (96%)	106 (99%)	1 (1%)	0	100	100
68	AF	124/131 (95%)	123 (99%)	1 (1%)	0	100	100
69	AG	107/107 (100%)	104 (97%)	3 (3%)	0	100	100
70	AH	114/121 (94%)	112 (98%)	2 (2%)	0	100	100
71	AI	118/120 (98%)	114 (97%)	4 (3%)	0	100	100
72	AJ	97/99 (98%)	96 (99%)	1 (1%)	0	100	100
73	AK	84/90 (93%)	81 (96%)	3 (4%)	0	100	100
74	AL	76/78 (97%)	73 (96%)	3 (4%)	0	100	100
75	AM	49/51 (96%)	48 (98%)	1 (2%)	0	100	100
76	AN	51/52 (98%)	51 (100%)	0	0	100	100
77	AO	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
78	AP	101/106 (95%)	100 (99%)	1 (1%)	0	100	100
79	AQ	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
All	All	10672/11870 (90%)	10385 (97%)	283 (3%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
51	t	5	LYS
5	5	20	ALA
21	L	88	PRO
51	t	62	THR

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	158/157 (101%)	158 (100%)	0	100	100
2	2	135/134 (101%)	134 (99%)	1 (1%)	81	90
5	5	95/112 (85%)	94 (99%)	1 (1%)	70	84
6	6	101/103 (98%)	101 (100%)	0	100	100
7	7	56/127 (44%)	56 (100%)	0	100	100
8	8	108/121 (89%)	108 (100%)	0	100	100
9	9	111/112 (99%)	110 (99%)	1 (1%)	75	88
11	B	176/215 (82%)	176 (100%)	0	100	100
12	C	194/229 (85%)	194 (100%)	0	100	100
13	D	174/198 (88%)	174 (100%)	0	100	100
14	E	174/196 (89%)	173 (99%)	1 (1%)	84	91
15	F	218/220 (99%)	218 (100%)	0	100	100
16	G	178/197 (90%)	176 (99%)	2 (1%)	70	84
17	H	195/204 (96%)	194 (100%)	1 (0%)	86	92
18	I	86/167 (52%)	86 (100%)	0	100	100
19	J	126/160 (79%)	126 (100%)	0	100	100
20	K	153/160 (96%)	153 (100%)	0	100	100
21	L	87/104 (84%)	87 (100%)	0	100	100
22	M	122/134 (91%)	121 (99%)	1 (1%)	79	89
23	N	98/123 (80%)	98 (100%)	0	100	100
24	O	129/130 (99%)	129 (100%)	0	100	100
25	P	97/102 (95%)	97 (100%)	0	100	100
26	Q	102/121 (84%)	102 (100%)	0	100	100
27	R	114/116 (98%)	114 (100%)	0	100	100
28	S	54/122 (44%)	54 (100%)	0	100	100
29	T	126/129 (98%)	126 (100%)	0	100	100
30	U	113/117 (97%)	113 (100%)	0	100	100
31	V	90/105 (86%)	88 (98%)	2 (2%)	47	71
32	W	71/71 (100%)	71 (100%)	0	100	100
33	X	112/113 (99%)	112 (100%)	0	100	100
34	Y	116/118 (98%)	116 (100%)	0	100	100
35	Z	109/112 (97%)	109 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	a	64/85 (75%)	64 (100%)	0	100	100
37	b	86/102 (84%)	86 (100%)	0	100	100
38	c	72/73 (99%)	72 (100%)	0	100	100
39	d	54/58 (93%)	53 (98%)	1 (2%)	52	75
40	e	47/48 (98%)	47 (100%)	0	100	100
41	f	48/54 (89%)	48 (100%)	0	100	100
42	g	62/175 (35%)	62 (100%)	0	100	100
43	h	259/263 (98%)	259 (100%)	0	100	100
44	j	191/194 (98%)	191 (100%)	0	100	100
45	k	326/328 (99%)	326 (100%)	0	100	100
46	l	290/292 (99%)	289 (100%)	1 (0%)	91	95
47	m	247/252 (98%)	247 (100%)	0	100	100
48	o	191/204 (94%)	191 (100%)	0	100	100
49	q	167/170 (98%)	166 (99%)	1 (1%)	84	91
50	s	146/149 (98%)	146 (100%)	0	100	100
51	t	166/168 (99%)	166 (100%)	0	100	100
52	u	108/109 (99%)	107 (99%)	1 (1%)	75	88
53	v	177/178 (99%)	177 (100%)	0	100	100
54	w	166/167 (99%)	166 (100%)	0	100	100
55	y	156/154 (101%)	156 (100%)	0	100	100
56	z	135/153 (88%)	135 (100%)	0	100	100
59	n	135/154 (88%)	135 (100%)	0	100	100
60	p	202/216 (94%)	201 (100%)	1 (0%)	86	92
61	r	178/186 (96%)	178 (100%)	0	100	100
62	x	142/154 (92%)	142 (100%)	0	100	100
63	AA	117/118 (99%)	117 (100%)	0	100	100
64	AB	120/121 (99%)	120 (100%)	0	100	100
65	AC	50/49 (102%)	49 (98%)	1 (2%)	50	74
66	AD	81/90 (90%)	81 (100%)	0	100	100
67	AE	98/100 (98%)	98 (100%)	0	100	100
68	AF	111/115 (96%)	109 (98%)	2 (2%)	54	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
69	AG	94/92 (102%)	94 (100%)	0	100	100
70	AH	99/101 (98%)	99 (100%)	0	100	100
71	AI	106/106 (100%)	106 (100%)	0	100	100
72	AJ	79/79 (100%)	78 (99%)	1 (1%)	65	82
73	AK	70/73 (96%)	70 (100%)	0	100	100
74	AL	69/69 (100%)	69 (100%)	0	100	100
75	AM	47/47 (100%)	47 (100%)	0	100	100
76	AN	48/47 (102%)	48 (100%)	0	100	100
77	AO	24/24 (100%)	24 (100%)	0	100	100
78	AP	88/89 (99%)	88 (100%)	0	100	100
79	AQ	72/73 (99%)	72 (100%)	0	100	100
All	All	9166/10008 (92%)	9147 (100%)	19 (0%)	91	96

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	2	83	ARG
5	5	30	GLN
9	9	3	LYS
14	E	77	ARG
16	G	65	ARG
16	G	170	GLN
17	H	191	LYS
22	M	67	ARG
31	V	43	ASN
31	V	51	LYS
39	d	64	ARG
46	l	99	ARG
49	q	141	LYS
52	u	98	ASN
60	p	64	LYS
65	AC	33	LYS
68	AF	17[A]	LYS
68	AF	17[B]	LYS
72	AJ	98	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	8	GLN
1	0	62	ASN
11	B	21	ASN
11	B	30	GLN
11	B	33	ASN
15	F	57	ASN
27	R	102	ASN
29	T	89	GLN
43	h	107	HIS
47	m	151	GLN
49	q	157	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	A	1629/1787 (91%)	371 (22%)	42 (2%)
3	3	120/121 (99%)	9 (7%)	0
4	4	155/158 (98%)	22 (14%)	2 (1%)
57	1	3142/3359 (93%)	540 (17%)	31 (0%)
58	10	1/76 (1%)	1 (100%)	0
All	All	5047/5501 (91%)	943 (18%)	75 (1%)

All (943) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	3	7	G
3	3	22	A
3	3	54	U
3	3	55	A
3	3	65	G
3	3	73	C
3	3	76	A
3	3	102	A
3	3	112	G
4	4	23	U
4	4	34	U
4	4	35	C
4	4	59	A
4	4	62	C
4	4	63	G
4	4	81	A
4	4	84	C

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Mol	Chain	Res	Type
4	4	85	G
4	4	86	U
4	4	87	G
4	4	92	A
4	4	95	G
4	4	102	U
4	4	104	A
4	4	106	C
4	4	111	A
4	4	113	U
4	4	125	U
4	4	126	A
4	4	148	G
4	4	152	G
10	A	17	C
10	A	25	C
10	A	26	A
10	A	27	U
10	A	34	G
10	A	47	A
10	A	57	G
10	A	66	U
10	A	74	U
10	A	75	U
10	A	76	A
10	A	78	A
10	A	79	C
10	A	81	G
10	A	84	A
10	A	104	A
10	A	114	C
10	A	115	G
10	A	123	G
10	A	126	A
10	A	127	G
10	A	128	U
10	A	129	A
10	A	138	C
10	A	139	U
10	A	142	G
10	A	143	A
10	A	150	U

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Mol	Chain	Res	Type
10	A	151	G
10	A	152	G
10	A	154	A
10	A	159	U
10	A	166	A
10	A	168	U
10	A	173	G
10	A	176	U
10	A	177	A
10	A	179	A
10	A	190	U
10	A	191	U
10	A	193	G
10	A	199	G
10	A	200	A
10	A	202	G
10	A	206	U
10	A	211	A
10	A	214	U
10	A	215	A
10	A	216	A
10	A	217	A
10	A	218	A
10	A	247	U
10	A	255	A
10	A	259	U
10	A	260	U
10	A	261	C
10	A	262	G
10	A	266	C
10	A	269	A
10	A	270	U
10	A	274	C
10	A	276	U
10	A	277	G
10	A	278	U
10	A	279	G
10	A	283	G
10	A	285	G
10	A	297	A
10	A	312	C
10	A	314	A

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Mol	Chain	Res	Type
10	A	318	U
10	A	319	C
10	A	320	G
10	A	335	G
10	A	336	C
10	A	350	A
10	A	357	A
10	A	358	A
10	A	359	C
10	A	388	G
10	A	398	A
10	A	400	C
10	A	402	G
10	A	414	A
10	A	421	G
10	A	422	C
10	A	423	A
10	A	424	G
10	A	432	G
10	A	437	U
10	A	442	C
10	A	446	C
10	A	452	A
10	A	458	A
10	A	466	A
10	A	475	A
10	A	480	U
10	A	482	C
10	A	483	A
10	A	485	G
10	A	501	G
10	A	502	U
10	A	503	A
10	A	504	A
10	A	505	U
10	A	506	U
10	A	509	A
10	A	512	G
10	A	513	A
10	A	515	U
10	A	518	A
10	A	519	A

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Mol	Chain	Res	Type
10	A	525	A
10	A	530	U
10	A	534	C
10	A	536	A
10	A	537	G
10	A	539	A
10	A	540	A
10	A	547	G
10	A	553	A
10	A	554	A
10	A	555	G
10	A	556	U
10	A	557	C
10	A	563	C
10	A	566	G
10	A	575	G
10	A	576	U
10	A	580	U
10	A	592	A
10	A	593	G
10	A	604	A
10	A	609	U
10	A	617	A
10	A	618	A
10	A	620	A
10	A	621	A
10	A	633	A
10	A	730	U
10	A	739	A
10	A	740	A
10	A	741	A
10	A	750	G
10	A	751	U
10	A	756	A
10	A	759	A
10	A	760	G
10	A	762	C
10	A	764	U
10	A	765	U
10	A	766	U
10	A	767	G
10	A	768	C

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Mol	Chain	Res	Type
10	A	770	C
10	A	771	G
10	A	773	A
10	A	778	U
10	A	779	U
10	A	796	A
10	A	798	A
10	A	799	G
10	A	802	C
10	A	803	G
10	A	804	U
10	A	805	U
10	A	807	U
10	A	808	G
10	A	814	A
10	A	815	U
10	A	816	U
10	A	818	U
10	A	819	G
10	A	820	U
10	A	821	U
10	A	823	G
10	A	824	U
10	A	825	U
10	A	826	U
10	A	828	U
10	A	831	G
10	A	840	A
10	A	842	U
10	A	848	A
10	A	856	G
10	A	857	G
10	A	869	A
10	A	871	U
10	A	875	C
10	A	877	G
10	A	878	U
10	A	879	U
10	A	881	U
10	A	891	A
10	A	898	G
10	A	909	A

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Mol	Chain	Res	Type
10	A	910	G
10	A	911	A
10	A	918	A
10	A	920	U
10	A	945	U
10	A	951	A
10	A	973	A
10	A	975	C
10	A	977	A
10	A	988	A
10	A	989	U
10	A	997	U
10	A	998	A
10	A	1004	A
10	A	1005	A
10	A	1011	A
10	A	1013	C
10	A	1017	G
10	A	1024	A
10	A	1025	G
10	A	1039	U
10	A	1042	U
10	A	1043	U
10	A	1044	U
10	A	1047	U
10	A	1055	A
10	A	1056	U
10	A	1057	C
10	A	1058	G
10	A	1059	G
10	A	1060	C
10	A	1061	A
10	A	1067	C
10	A	1077	A
10	A	1081	C
10	A	1085	G
10	A	1123	A
10	A	1135	G
10	A	1143	C
10	A	1145	A
10	A	1152	G
10	A	1168	A

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Mol	Chain	Res	Type
10	A	1169	A
10	A	1170	U
10	A	1179	A
10	A	1181	A
10	A	1184	G
10	A	1185	G
10	A	1186	G
10	A	1187	A
10	A	1193	A
10	A	1202	A
10	A	1203	G
10	A	1206	A
10	A	1207	C
10	A	1212	A
10	A	1215	A
10	A	1219	A
10	A	1220	C
10	A	1221	A
10	A	1229	A
10	A	1230	G
10	A	1231	C
10	A	1236	U
10	A	1243	U
10	A	1250	G
10	A	1270	U
10	A	1284	G
10	A	1299	U
10	A	1300	U
10	A	1301	G
10	A	1306	A
10	A	1325	U
10	A	1330	A
10	A	1336	G
10	A	1339	G
10	A	1342	A
10	A	1343	G
10	A	1345	A
10	A	1346	U
10	A	1348	U
10	A	1349	G
10	A	1352	G
10	A	1355	A

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Mol	Chain	Res	Type
10	A	1356	U
10	A	1357	A
10	A	1359	U
10	A	1360	C
10	A	1364	U
10	A	1365	C
10	A	1369	G
10	A	1370	A
10	A	1376	U
10	A	1380	G
10	A	1381	A
10	A	1382	U
10	A	1384	U
10	A	1385	C
10	A	1392	A
10	A	1397	A
10	A	1398	G
10	A	1399	U
10	A	1400	U
10	A	1401	U
10	A	1410	A
10	A	1413	A
10	A	1414	G
10	A	1415	G
10	A	1422	A
10	A	1431	G
10	A	1433	C
10	A	1445	C
10	A	1446	A
10	A	1455	A
10	A	1457	A
10	A	1458	C
10	A	1461	A
10	A	1462	C
10	A	1463	G
10	A	1468	C
10	A	1476	A
10	A	1477	U
10	A	1483	U
10	A	1491	G
10	A	1503	A
10	A	1508	G

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Mol	Chain	Res	Type
10	A	1510	G
10	A	1511	A
10	A	1523	G
10	A	1524	C
10	A	1529	G
10	A	1530	A
10	A	1542	A
10	A	1544	U
10	A	1546	G
10	A	1547	U
10	A	1556	A
10	A	1560	A
10	A	1561	G
10	A	1569	U
10	A	1571	G
10	A	1574	A
10	A	1575	G
10	A	1577	G
10	A	1580	A
10	A	1582	U
10	A	1584	A
10	A	1588	G
10	A	1621	C
10	A	1644	U
10	A	1645	G
10	A	1665	C
10	A	1667	G
10	A	1670	U
10	A	1671	G
10	A	1672	G
10	A	1673	U
10	A	1674	U
10	A	1677	G
10	A	1700	G
10	A	1704	C
10	A	1737	A
10	A	1743	A
10	A	1747	G
10	A	1749	A
10	A	1753	A
10	A	1756	U
10	A	1767	G

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Mol	Chain	Res	Type
10	A	1769	A
10	A	1770	C
10	A	1779	G
10	A	1780	G
10	A	1781	A
10	A	1782	U
10	A	1783	C
57	1	24	U
57	1	25	A
57	1	29	G
57	1	39	A
57	1	42	A
57	1	48	A
57	1	56	A
57	1	58	G
57	1	59	A
57	1	64	A
57	1	65	A
57	1	91	G
57	1	98	A
57	1	104	C
57	1	108	A
57	1	109	G
57	1	110	C
57	1	121	A
57	1	135	G
57	1	155	A
57	1	156	A
57	1	164	U
57	1	169	G
57	1	172	C
57	1	173	C
57	1	175	G
57	1	186	A
57	1	189	U
57	1	190	U
57	1	199	C
57	1	205	G
57	1	209	C
57	1	212	A
57	1	217	G
57	1	218	A

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Mol	Chain	Res	Type
57	1	219	G
57	1	230	G
57	1	236	A
57	1	239	A
57	1	240	C
57	1	243	G
57	1	245	G
57	1	249	G
57	1	250	U
57	1	251	G
57	1	269	G
57	1	286	U
57	1	295	A
57	1	305	U
57	1	311	C
57	1	323	A
57	1	329	U
57	1	337	G
57	1	338	A
57	1	339	C
57	1	349	A
57	1	350	C
57	1	376	G
57	1	377	A
57	1	395	A
57	1	398	A
57	1	402	A
57	1	403	C
57	1	404	G
57	1	420	G
57	1	421	G
57	1	422	A
57	1	438	A
57	1	439	C
57	1	452	A
57	1	453	U
57	1	454	G
57	1	479	C
57	1	481	G
57	1	482	U
57	1	506	A
57	1	517	A

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Mol	Chain	Res	Type
57	1	519	U
57	1	531	G
57	1	532	U
57	1	538	G
57	1	539	G
57	1	540	C
57	1	541	U
57	1	542	U
57	1	543	C
57	1	544	U
57	1	545	G
57	1	546	C
57	1	555	A
57	1	556	U
57	1	557	A
57	1	564	G
57	1	577	G
57	1	589	G
57	1	590	A
57	1	598	U
57	1	600	U
57	1	601	U
57	1	602	A
57	1	609	A
57	1	618	U
57	1	619	A
57	1	620	A
57	1	635	C
57	1	647	A
57	1	658	A
57	1	675	A
57	1	679	U
57	1	688	A
57	1	703	A
57	1	710	G
57	1	713	A
57	1	717	A
57	1	723	G
57	1	730	A
57	1	732	U
57	1	760	U
57	1	763	U

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Mol	Chain	Res	Type
57	1	772	U
57	1	773	U
57	1	776	A
57	1	777	G
57	1	780	A
57	1	781	G
57	1	802	A
57	1	813	A
57	1	826	A
57	1	845	C
57	1	857	C
57	1	861	U
57	1	870	U
57	1	875	U
57	1	892	A
57	1	903	G
57	1	904	G
57	1	910	A
57	1	912	G
57	1	913	A
57	1	917	A
57	1	919	C
57	1	921	A
57	1	933	G
57	1	940	C
57	1	949	G
57	1	955	C
57	1	956	U
57	1	959	G
57	1	976	A
57	1	977	U
57	1	990	G
57	1	991	U
57	1	996	C
57	1	997	G
57	1	998	A
57	1	1006	G
57	1	1011	C
57	1	1012	U
57	1	1014	G
57	1	1030	U
57	1	1033	C

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Mol	Chain	Res	Type
57	1	1043	A
57	1	1045	C
57	1	1060	A
57	1	1061	A
57	1	1068	G
57	1	1077	U
57	1	1078	U
57	1	1090	A
57	1	1091	U
57	1	1092	U
57	1	1094	A
57	1	1099	A
57	1	1100	G
57	1	1113	G
57	1	1127	G
57	1	1140	U
57	1	1149	A
57	1	1150	A
57	1	1151	C
57	1	1155	A
57	1	1156	C
57	1	1164	U
57	1	1174	G
57	1	1176	A
57	1	1177	U
57	1	1178	G
57	1	1188	C
57	1	1189	A
57	1	1192	C
57	1	1197	C
57	1	1204	U
57	1	1205	G
57	1	1215	C
57	1	1218	G
57	1	1223	C
57	1	1224	C
57	1	1225	G
57	1	1228	C
57	1	1229	G
57	1	1230	G
57	1	1231	U
57	1	1232	G

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Mol	Chain	Res	Type
57	1	1234	C
57	1	1238	G
57	1	1239	G
57	1	1241	A
57	1	1242	G
57	1	1243	U
57	1	1244	C
57	1	1245	G
57	1	1247	A
57	1	1249	U
57	1	1251	C
57	1	1252	G
57	1	1253	C
57	1	1255	A
57	1	1258	G
57	1	1259	A
57	1	1262	G
57	1	1263	U
57	1	1264	G
57	1	1265	U
57	1	1266	A
57	1	1267	A
57	1	1268	C
57	1	1269	A
57	1	1270	A
57	1	1273	C
57	1	1278	G
57	1	1280	C
57	1	1282	A
57	1	1283	A
57	1	1303	G
57	1	1304	A
57	1	1305	U
57	1	1309	G
57	1	1326	A
57	1	1345	G
57	1	1346	U
57	1	1347	U
57	1	1348	U
57	1	1349	U
57	1	1382	A
57	1	1395	U

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Mol	Chain	Res	Type
57	1	1415	A
57	1	1417	G
57	1	1421	U
57	1	1427	G
57	1	1430	G
57	1	1433	C
57	1	1442	A
57	1	1446	G
57	1	1465	C
57	1	1471	A
57	1	1477	A
57	1	1484	G
57	1	1498	C
57	1	1504	C
57	1	1520	A
57	1	1523	C
57	1	1532	G
57	1	1535	A
57	1	1551	U
57	1	1552	C
57	1	1556	G
57	1	1558	G
57	1	1559	C
57	1	1560	U
57	1	1561	U
57	1	1562	G
57	1	1563	A
57	1	1565	U
57	1	1566	U
57	1	1567	U
57	1	1568	U
57	1	1569	C
57	1	1571	G
57	1	1572	G
57	1	1574	C
57	1	1576	A
57	1	1577	C
57	1	1585	A
57	1	1589	A
57	1	1601	A
57	1	1603	U
57	1	1624	C

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Mol	Chain	Res	Type
57	1	1625	U
57	1	1635	C
57	1	1638	A
57	1	1639	A
57	1	1641	U
57	1	1648	G
57	1	1654	G
57	1	1679	A
57	1	1720	U
57	1	1721	C
57	1	1732	G
57	1	1746	A
57	1	1747	G
57	1	1755	U
57	1	1756	A
57	1	1757	A
57	1	1758	U
57	1	1760	U
57	1	1761	U
57	1	1762	G
57	1	1763	C
57	1	1776	G
57	1	1793	A
57	1	1804	G
57	1	1809	A
57	1	1810	A
57	1	1811	U
57	1	1812	A
57	1	1815	U
57	1	1816	U
57	1	1817	U
57	1	1835	A
57	1	1838	A
57	1	1842	C
57	1	1845	C
57	1	1862	C
57	1	1874	G
57	1	1877	A
57	1	1882	A
57	1	1889	A
57	1	1902	G
57	1	1944	G

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Mol	Chain	Res	Type
57	1	1949	G
57	1	2070	A
57	1	2071	A
57	1	2078	A
57	1	2088	G
57	1	2089	G
57	1	2090	U
57	1	2091	A
57	1	2092	C
57	1	2099	G
57	1	2100	G
57	1	2109	A
57	1	2118	U
57	1	2122	A
57	1	2136	A
57	1	2147	G
57	1	2149	G
57	1	2183	U
57	1	2184	G
57	1	2185	A
57	1	2186	A
57	1	2187	U
57	1	2188	G
57	1	2222	A
57	1	2227	G
57	1	2233	A
57	1	2234	A
57	1	2235	C
57	1	2250	G
57	1	2251	G
57	1	2257	A
57	1	2259	A
57	1	2260	U
57	1	2276	U
57	1	2285	G
57	1	2286	C
57	1	2288	U
57	1	2291	A
57	1	2292	U
57	1	2293	G
57	1	2312	U
57	1	2313	G

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Mol	Chain	Res	Type
57	1	2314	U
57	1	2341	A
57	1	2351	A
57	1	2352	C
57	1	2353	G
57	1	2363	G
57	1	2366	U
57	1	2371	G
57	1	2372	G
57	1	2375	A
57	1	2380	A
57	1	2381	G
57	1	2382	A
57	1	2389	U
57	1	2413	G
57	1	2420	G
57	1	2489	A
57	1	2492	U
57	1	2493	A
57	1	2511	G
57	1	2513	A
57	1	2515	G
57	1	2516	U
57	1	2517	C
57	1	2518	A
57	1	2519	A
57	1	2520	A
57	1	2521	C
57	1	2529	U
57	1	2530	C
57	1	2533	G
57	1	2536	U
57	1	2538	A
57	1	2545	C
57	1	2546	U
57	1	2554	C
57	1	2557	G
57	1	2565	A
57	1	2566	C
57	1	2578	G
57	1	2579	G
57	1	2586	G

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Mol	Chain	Res	Type
57	1	2598	A
57	1	2623	G
57	1	2624	U
57	1	2628	A
57	1	2644	G
57	1	2646	A
57	1	2649	G
57	1	2661	A
57	1	2662	G
57	1	2663	A
57	1	2666	A
57	1	2676	A
57	1	2677	A
57	1	2686	G
57	1	2699	A
57	1	2700	G
57	1	2701	U
57	1	2725	G
57	1	2734	A
57	1	2745	C
57	1	2749	G
57	1	2750	G
57	1	2768	G
57	1	2771	A
57	1	2772	G
57	1	2773	A
57	1	2774	A
57	1	2782	C
57	1	2786	G
57	1	2789	A
57	1	2790	U
57	1	2814	U
57	1	2815	U
57	1	2817	A
57	1	2833	U
57	1	2839	C
57	1	2843	G
57	1	2844	A
57	1	2847	U
57	1	2859	A
57	1	2861	C
57	1	2866	C

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Mol	Chain	Res	Type
57	1	2870	G
57	1	2871	C
57	1	2886	G
57	1	2895	U
57	1	2907	U
57	1	2908	A
57	1	2911	G
57	1	2914	C
57	1	2919	G
57	1	2920	C
57	1	2923	G
57	1	2926	U
57	1	2943	A
57	1	2955	C
57	1	2960	C
57	1	2962	G
57	1	2969	G
57	1	2984	A
57	1	3021	A
57	1	3028	U
57	1	3031	G
57	1	3050	A
57	1	3051	C
57	1	3052	G
57	1	3058	A
57	1	3064	C
57	1	3076	U
57	1	3094	A
57	1	3101	A
57	1	3102	A
57	1	3103	U
57	1	3114	A
57	1	3115	C
57	1	3134	C
57	1	3143	G
57	1	3144	A
57	1	3146	G
57	1	3149	U
57	1	3151	C
57	1	3157	A
57	1	3160	C
57	1	3161	U

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Mol	Chain	Res	Type
57	1	3163	U
57	1	3164	U
57	1	3165	U
57	1	3171	C
57	1	3172	U
57	1	3182	C
57	1	3183	A
57	1	3184	G
57	1	3194	G
57	1	3208	A
57	1	3210	A
57	1	3212	G
57	1	3214	U
57	1	3221	G
57	1	3224	U
57	1	3228	G
57	1	3235	A
57	1	3241	G
57	1	3246	C
57	1	3252	C
57	1	3259	A
57	1	3260	A
57	1	3268	G
57	1	3269	C
57	1	3272	A
57	1	3278	U
57	1	3281	A
57	1	3284	U
57	1	3285	A
57	1	3306	U
57	1	3307	A
57	1	3309	A
57	1	3310	G
57	1	3316	U
57	1	3317	U
57	1	3318	G
57	1	3319	U
57	1	3320	U
57	1	3321	G
57	1	3334	G
57	1	3343	C
57	1	3351	G

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Mol	Chain	Res	Type
57	1	3361	U
58	10	76	A

All (75) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	4	85	G
4	4	125	U
10	A	25	C
10	A	78	A
10	A	137	A
10	A	151	G
10	A	176	U
10	A	214	U
10	A	259	U
10	A	265	U
10	A	278	U
10	A	451	C
10	A	502	U
10	A	504	A
10	A	505	U
10	A	514	G
10	A	518	A
10	A	529	C
10	A	533	A
10	A	553	A
10	A	556	U
10	A	740	A
10	A	763	C
10	A	769	U
10	A	817	U
10	A	820	U
10	A	824	U
10	A	855	C
10	A	874	U
10	A	876	A
10	A	1168	A
10	A	1335	U
10	A	1355	A
10	A	1359	U
10	A	1369	G
10	A	1396	A

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Mol	Chain	Res	Type
10	A	1398	G
10	A	1457	A
10	A	1467	C
10	A	1523	G
10	A	1555	C
10	A	1573	A
10	A	1579	A
10	A	1581	G
57	1	172	C
57	1	403	C
57	1	538	G
57	1	563	U
57	1	601	U
57	1	759	G
57	1	912	G
57	1	1029	U
57	1	1060	A
57	1	1099	A
57	1	1346	U
57	1	1347	U
57	1	1559	C
57	1	1561	U
57	1	1576	A
57	1	1762	G
57	1	1815	U
57	1	1943	G
57	1	2090	U
57	1	2515	G
57	1	2519	A
57	1	2789	A
57	1	2790	U
57	1	3093	U
57	1	3193	C
57	1	3234	U
57	1	3240	U
57	1	3284	U
57	1	3309	A
57	1	3315	C
57	1	3317	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
57	OMC	1	2808	57	19,22,23	2.86	8 (42%)	26,31,34	1.01	2 (7%)
78	MLZ	AP	40	78	8,9,10	0.72	0	4,9,11	0.92	0
78	MLZ	AP	55	78	8,9,10	0.84	0	4,9,11	2.17	1 (25%)
6	MLZ	6	110	6	8,9,10	0.72	0	4,9,11	1.09	0
57	OMG	1	2765	57	18,26,27	2.40	8 (44%)	19,38,41	1.52	4 (21%)

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
57	OMC	1	2808	57	-	3/9/27/28	0/2/2/2
78	MLZ	AP	40	78	-	0/7/8/10	-
78	MLZ	AP	55	78	-	3/7/8/10	-
6	MLZ	6	110	6	-	3/7/8/10	-
57	OMG	1	2765	57	-	0/5/27/28	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	1	2808	OMC	C2-N3	5.97	1.48	1.36
57	1	2808	OMC	C6-C5	5.77	1.48	1.35
57	1	2765	OMG	C2-N3	5.21	1.45	1.33
57	1	2808	OMC	C4-N4	4.83	1.45	1.33
57	1	2765	OMG	C4-N3	4.65	1.48	1.37
57	1	2808	OMC	C4-N3	4.45	1.43	1.34
57	1	2808	OMC	C2-N1	4.08	1.48	1.40
57	1	2765	OMG	C2-N2	3.75	1.43	1.34
57	1	2765	OMG	C6-N1	3.71	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	1	2808	OMC	O2-C2	-3.33	1.17	1.23
57	1	2765	OMG	C5-C4	-2.84	1.35	1.43
57	1	2808	OMC	C6-N1	2.81	1.44	1.38
57	1	2765	OMG	C5-C6	2.53	1.52	1.47
57	1	2765	OMG	O6-C6	-2.53	1.18	1.23
57	1	2808	OMC	C5-C4	2.21	1.48	1.42
57	1	2765	OMG	C2-N1	2.20	1.43	1.37

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
78	AP	55	MLZ	CD-CG-CB	-3.59	100.92	113.62
57	1	2765	OMG	C5-C6-N1	3.51	120.14	113.95
57	1	2765	OMG	C2-N1-C6	-2.95	119.67	125.10
57	1	2808	OMC	O2-C2-N3	-2.64	118.04	122.33
57	1	2765	OMG	C8-N7-C5	2.59	107.93	102.99
57	1	2765	OMG	O6-C6-C5	-2.47	119.55	124.37
57	1	2808	OMC	C1'-N1-C2	2.25	123.44	118.42

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	6	110	MLZ	N-CA-CB-CG
6	6	110	MLZ	C-CA-CB-CG
57	1	2808	OMC	O4'-C1'-N1-C2
57	1	2808	OMC	O4'-C1'-N1-C6
57	1	2808	OMC	C1'-C2'-O2'-CM2
78	AP	55	MLZ	CG-CD-CE-NZ
78	AP	55	MLZ	CA-CB-CG-CD
78	AP	55	MLZ	CE-CD-CG-CB
6	6	110	MLZ	CD-CE-NZ-CM

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 10 ligands modelled in this entry, 7 are monoatomic - leaving 3 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  $|Z| > 2$  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
81	YMZ	j	301	-	28,28,28	0.45	0	41,43,43	0.65	2 (4%)
81	YMZ	1	3401	-	28,28,28	0.44	0	41,43,43	0.57	2 (4%)
82	SPK	1	3402	-	13,13,13	0.33	0	12,12,12	0.91	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
81	YMZ	j	301	-	-	15/20/28/28	0/3/3/3
81	YMZ	1	3401	-	-	8/20/28/28	0/3/3/3
82	SPK	1	3402	-	-	3/11/11/11	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	j	301	YMZ	CAN-NAQ-CAX	3.21	113.62	111.62
81	1	3401	YMZ	CAN-NAQ-CAX	2.67	113.29	111.62
81	1	3401	YMZ	CAO-CAX-NAQ	-2.10	108.82	111.90
81	j	301	YMZ	CAO-CAX-NAQ	-2.02	108.93	111.90

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
81	j	301	YMZ	CAV-CAT-CAZ-FAE
81	j	301	YMZ	CAV-CAT-CAZ-FAF

*Continued on next page...*

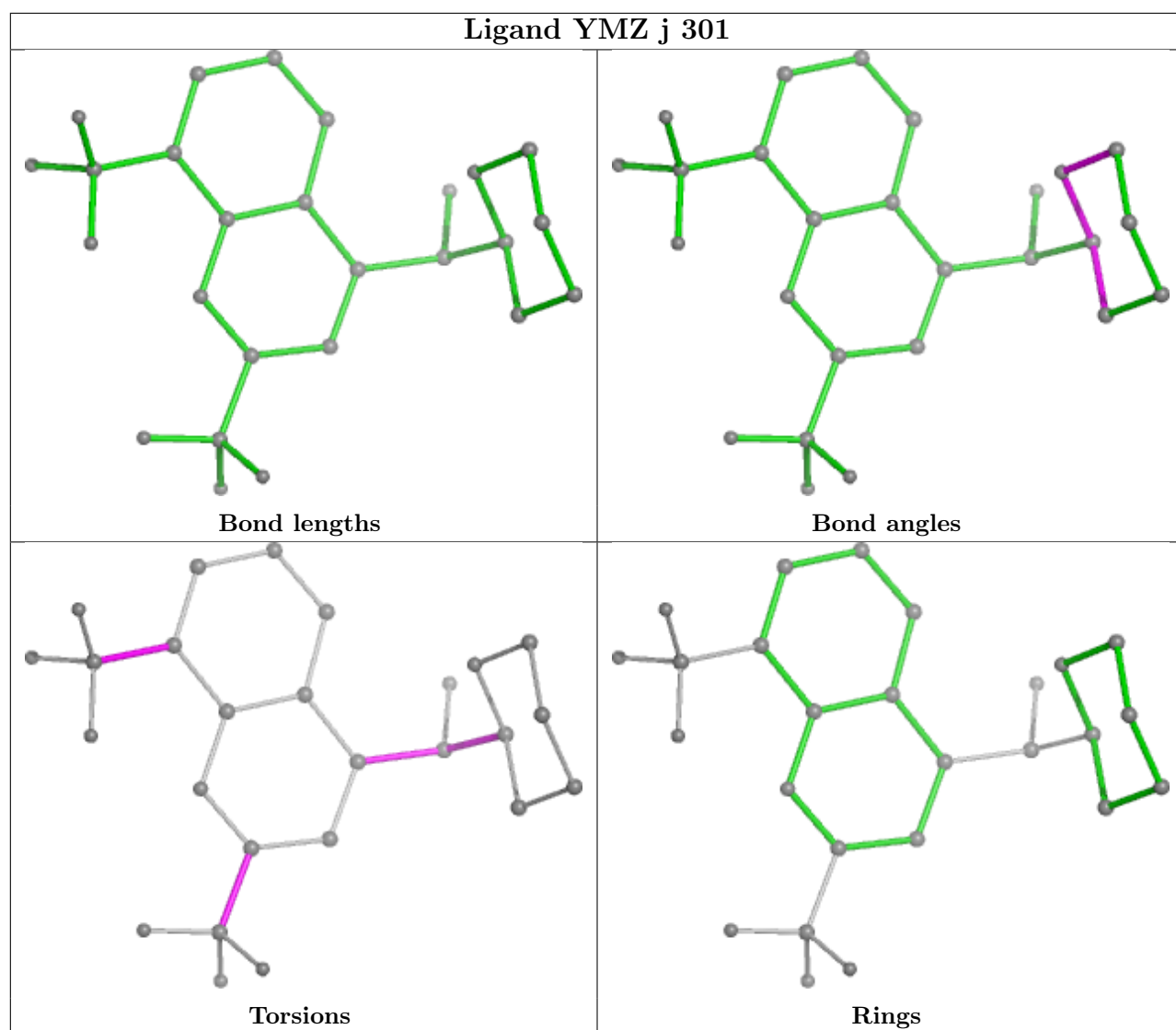
*Continued from previous page...*

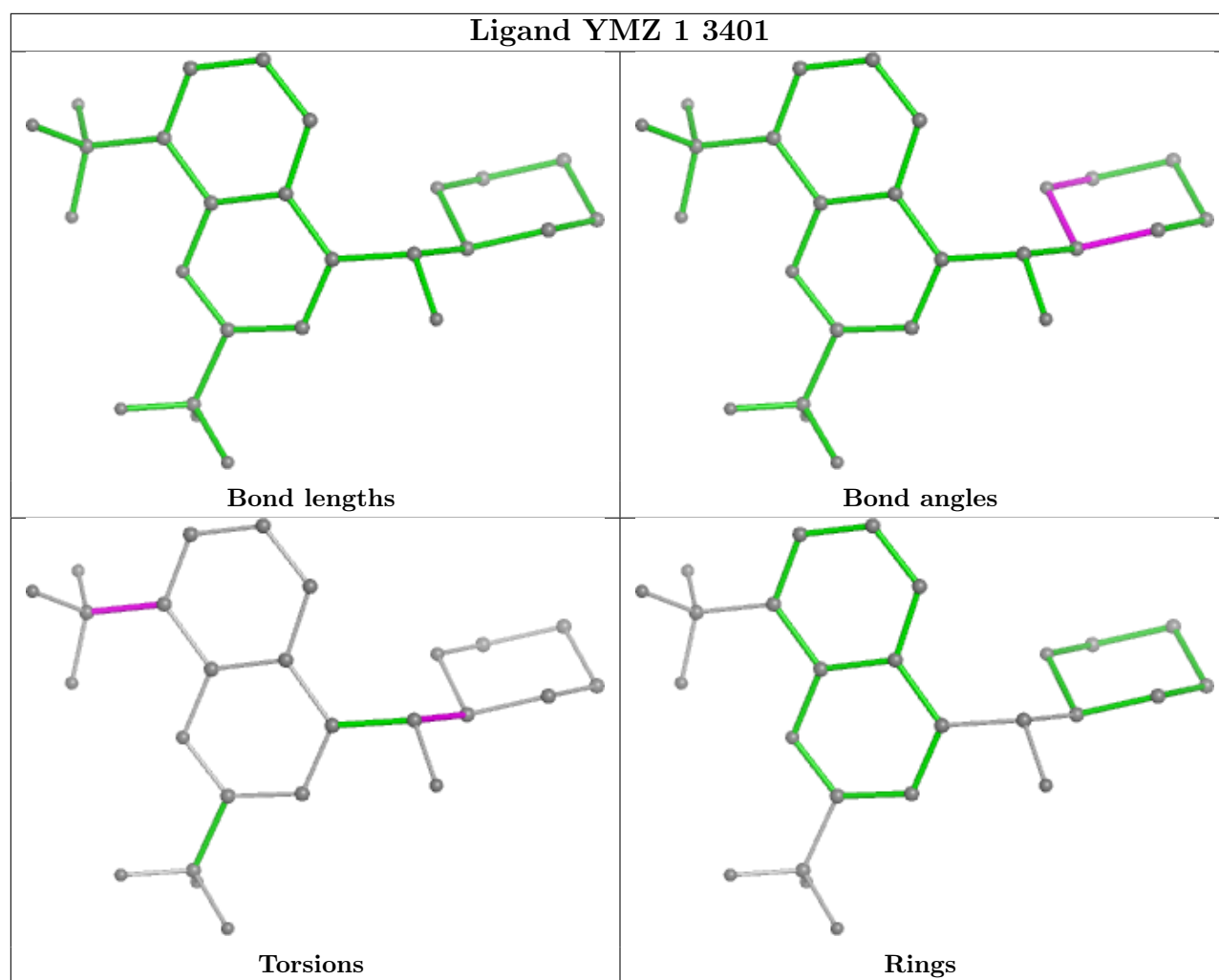
Mol	Chain	Res	Type	Atoms
81	j	301	YMZ	CAV-CAT-CAZ-FAG
81	1	3401	YMZ	CAV-CAT-CAZ-FAE
81	1	3401	YMZ	CAV-CAT-CAZ-FAF
81	1	3401	YMZ	CAV-CAT-CAZ-FAG
82	1	3402	SPK	C2-C3-C4-N5
81	1	3401	YMZ	CAI-CAT-CAZ-FAF
81	1	3401	YMZ	CAI-CAT-CAZ-FAG
81	1	3401	YMZ	CAI-CAT-CAZ-FAE
81	j	301	YMZ	CAK-CAS-CAW-OAA
81	j	301	YMZ	CAU-CAS-CAW-OAA
81	1	3401	YMZ	CAS-CAW-CAX-CAO
81	j	301	YMZ	CAI-CAT-CAZ-FAE
81	j	301	YMZ	CAI-CAT-CAZ-FAF
81	j	301	YMZ	CAI-CAT-CAZ-FAG
82	1	3402	SPK	C12-C11-N10-C9
81	j	301	YMZ	NAP-CAR-CAY-FAB
81	j	301	YMZ	CAK-CAR-CAY-FAB
82	1	3402	SPK	N10-C11-C12-C13
81	j	301	YMZ	NAP-CAR-CAY-FAC
81	j	301	YMZ	CAK-CAR-CAY-FAD
81	j	301	YMZ	NAP-CAR-CAY-FAD
81	j	301	YMZ	CAK-CAR-CAY-FAC
81	j	301	YMZ	OAA-CAW-CAX-CAO
81	1	3401	YMZ	CAS-CAW-CAX-NAQ

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 than 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.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

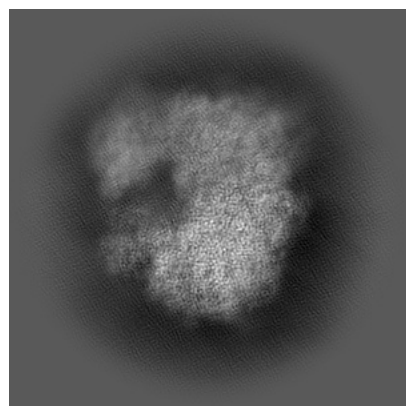
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50957. These allow visual inspection of the internal detail of the map and identification of artifacts.

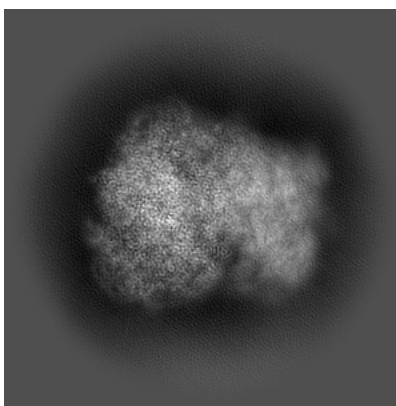
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

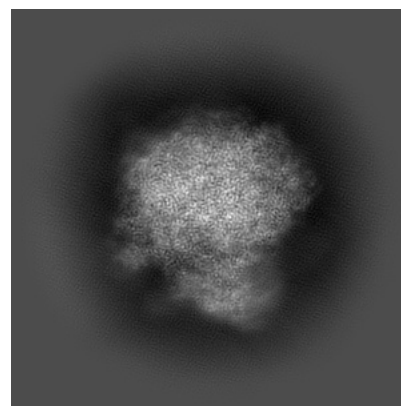
#### 6.1.1 Primary map



X

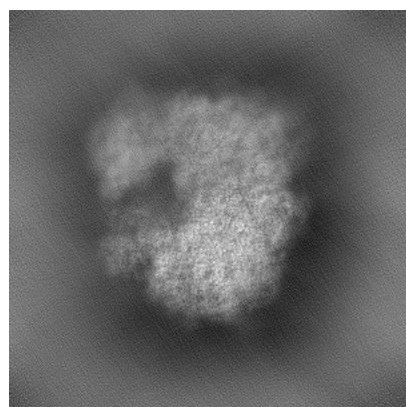


Y

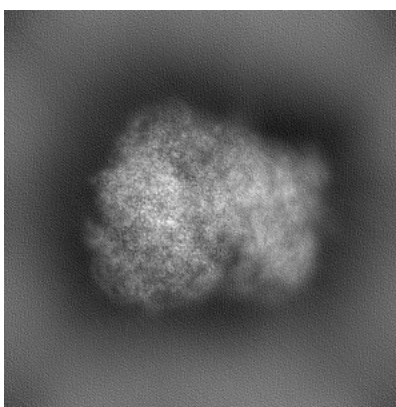


Z

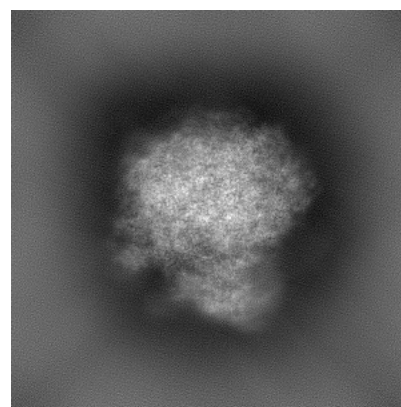
#### 6.1.2 Raw map



X



Y

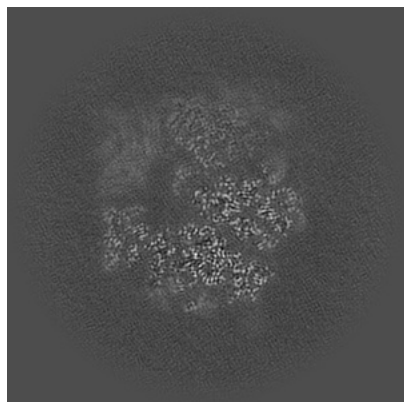


Z

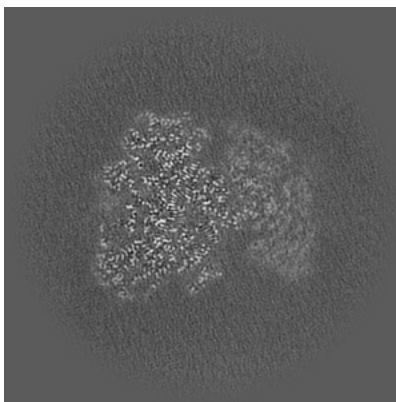
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

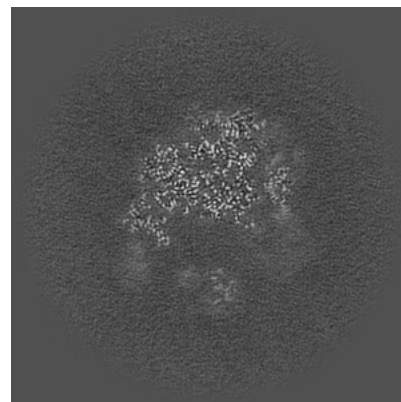
### 6.2.1 Primary map



X Index: 210

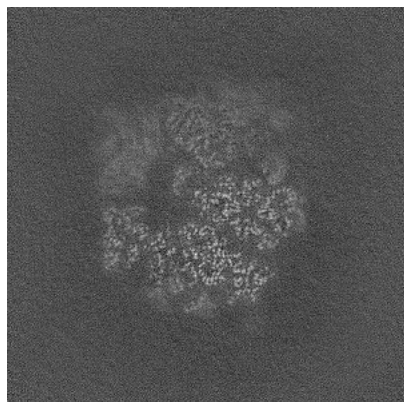


Y Index: 210

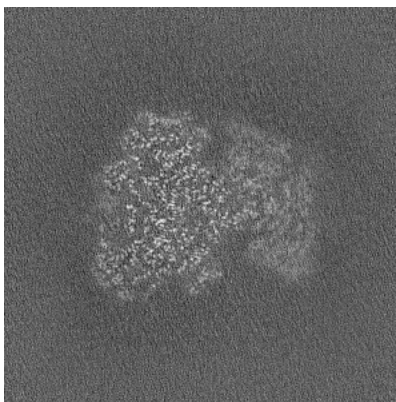


Z Index: 210

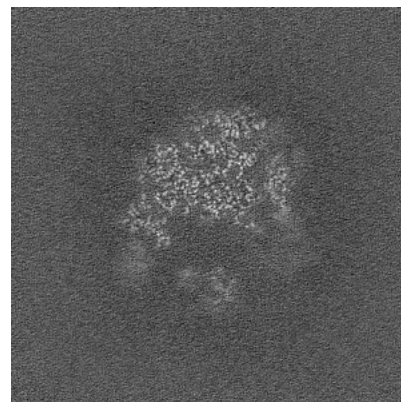
### 6.2.2 Raw map



X Index: 210



Y Index: 210

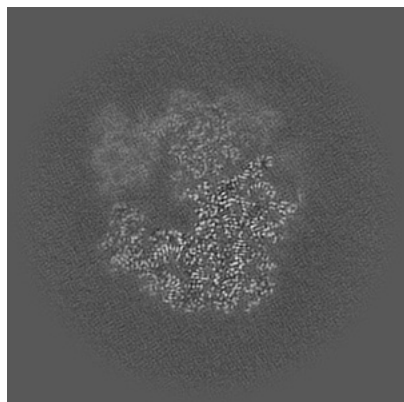


Z Index: 210

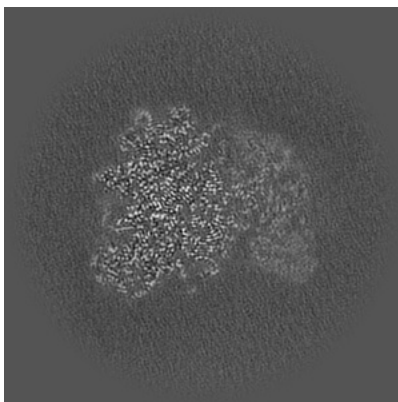
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

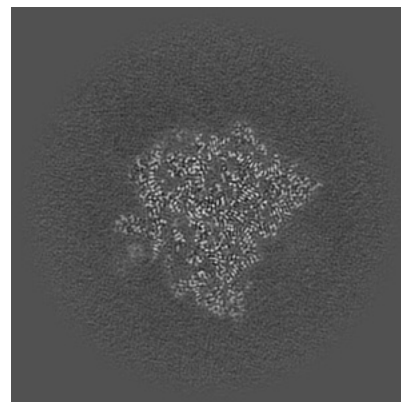
### 6.3.1 Primary map



X Index: 227

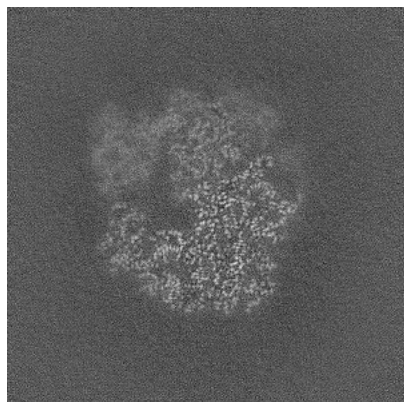


Y Index: 216

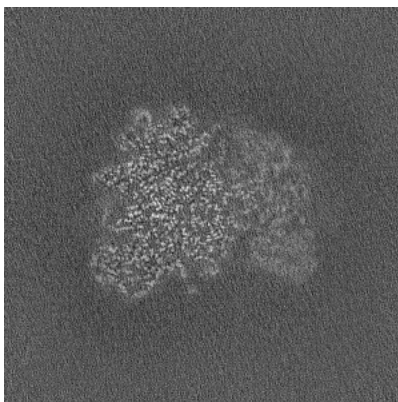


Z Index: 173

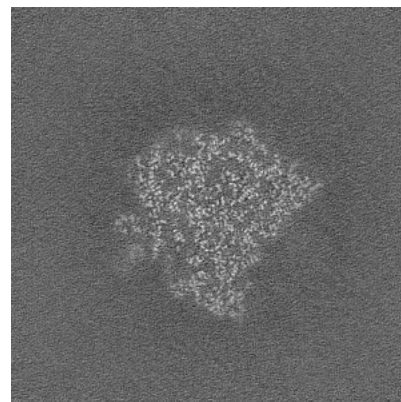
### 6.3.2 Raw map



X Index: 227



Y Index: 216

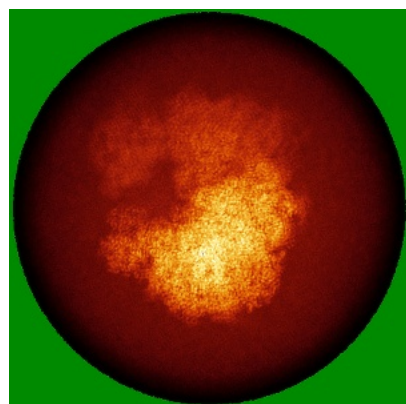


Z Index: 173

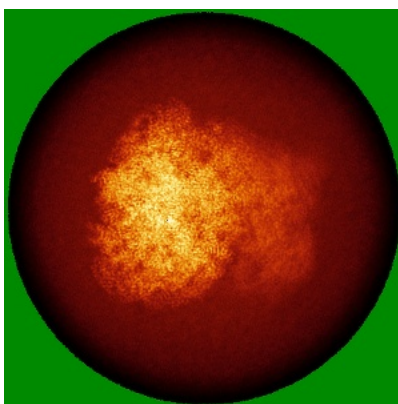
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

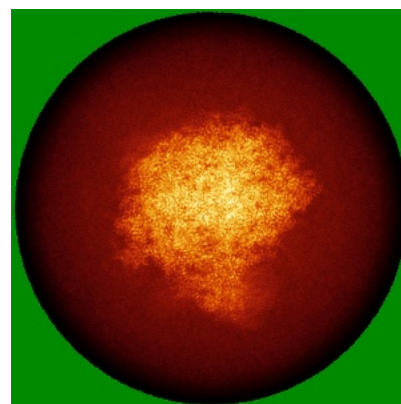
### 6.4.1 Primary map



X

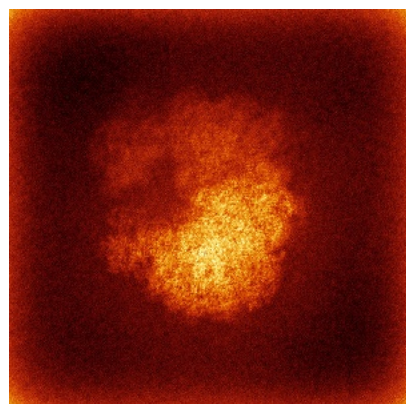


Y

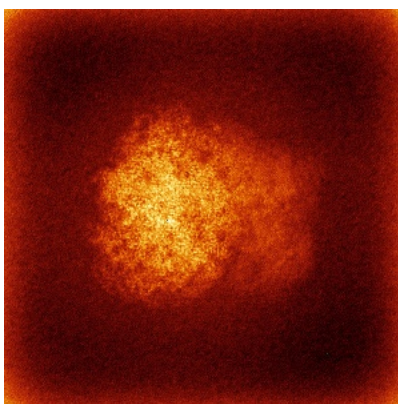


Z

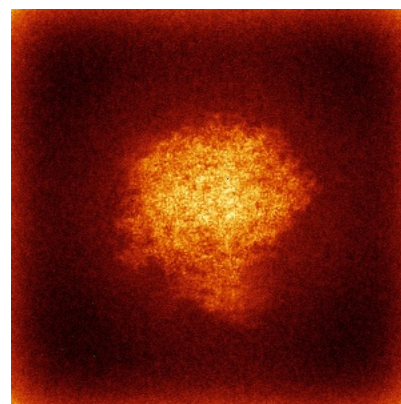
### 6.4.2 Raw map



X



Y

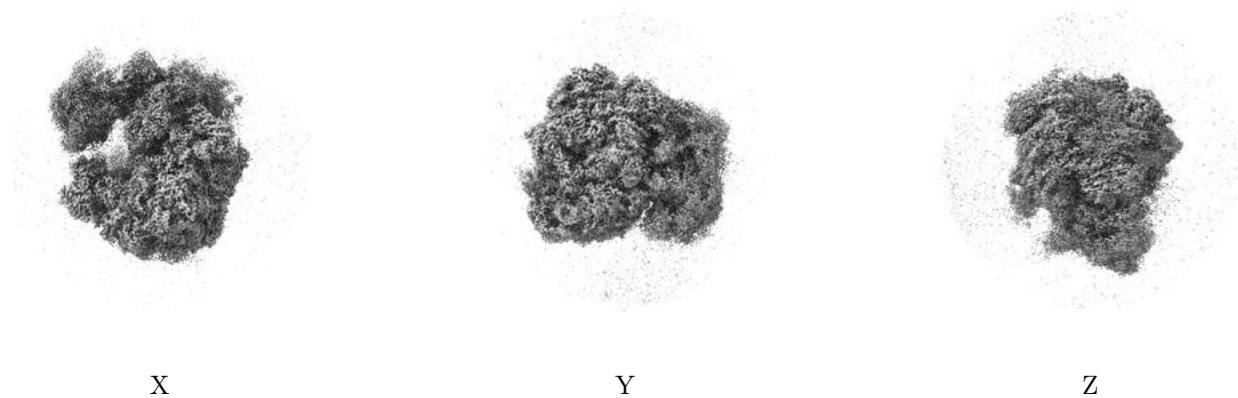


Z

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

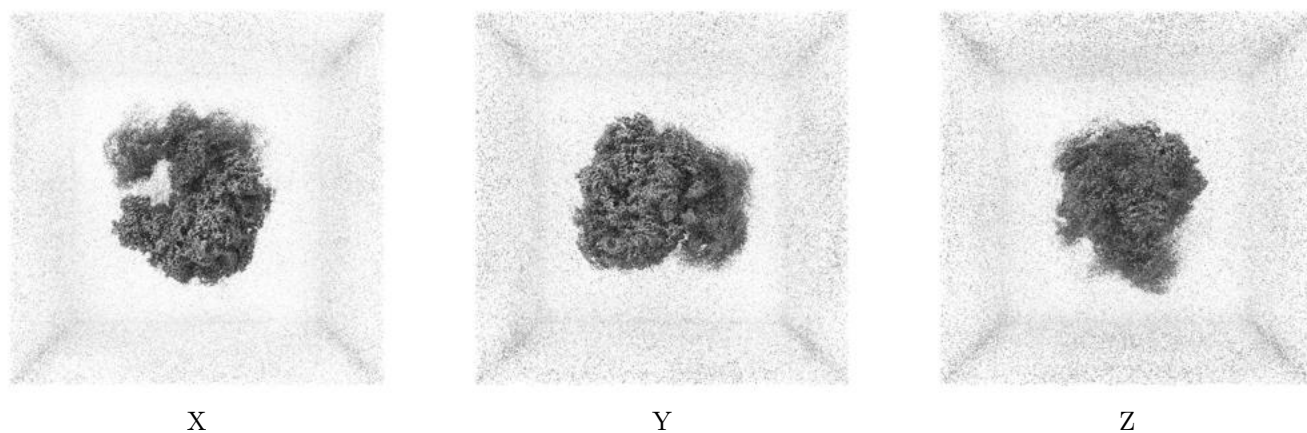
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. 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



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

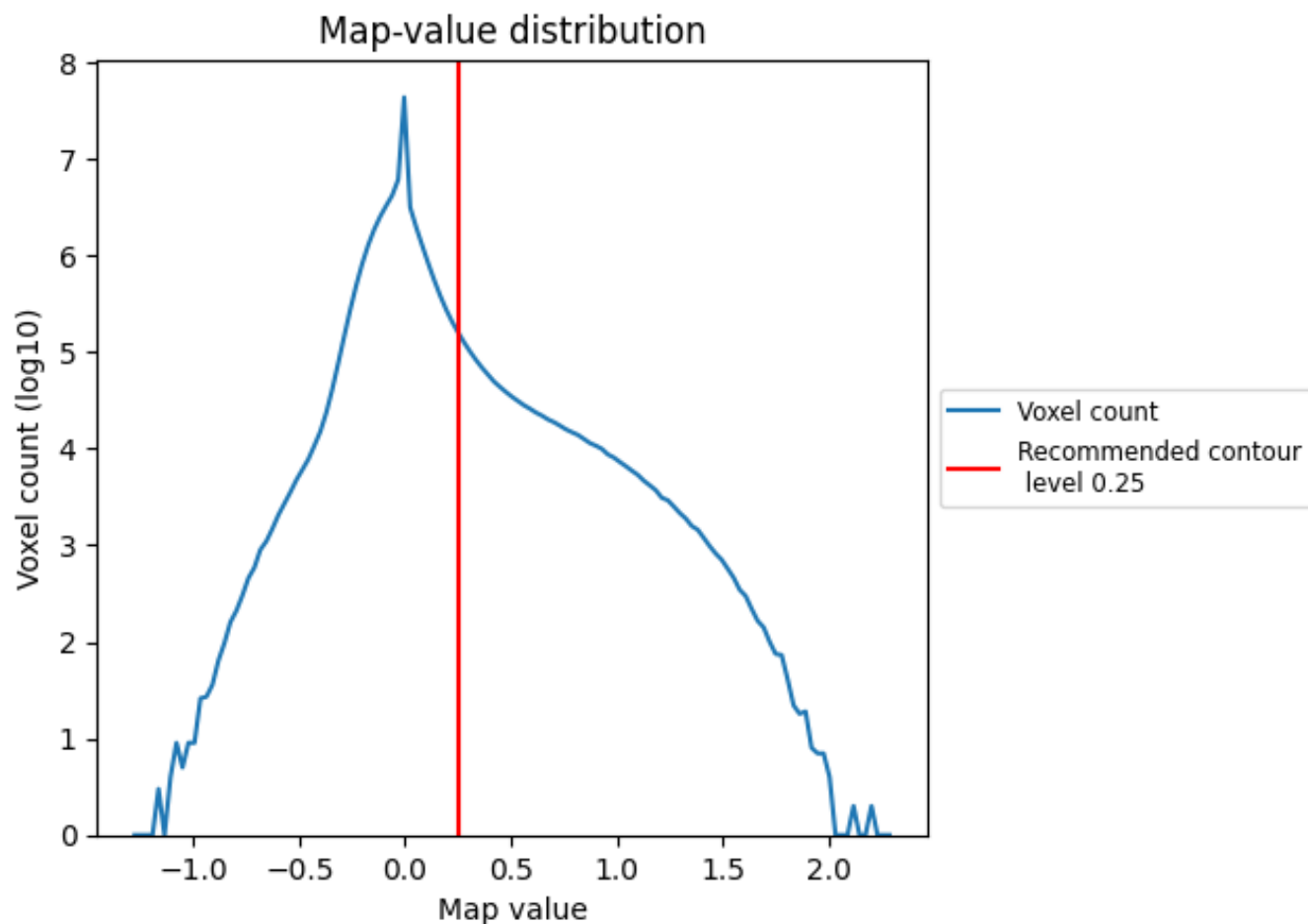
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

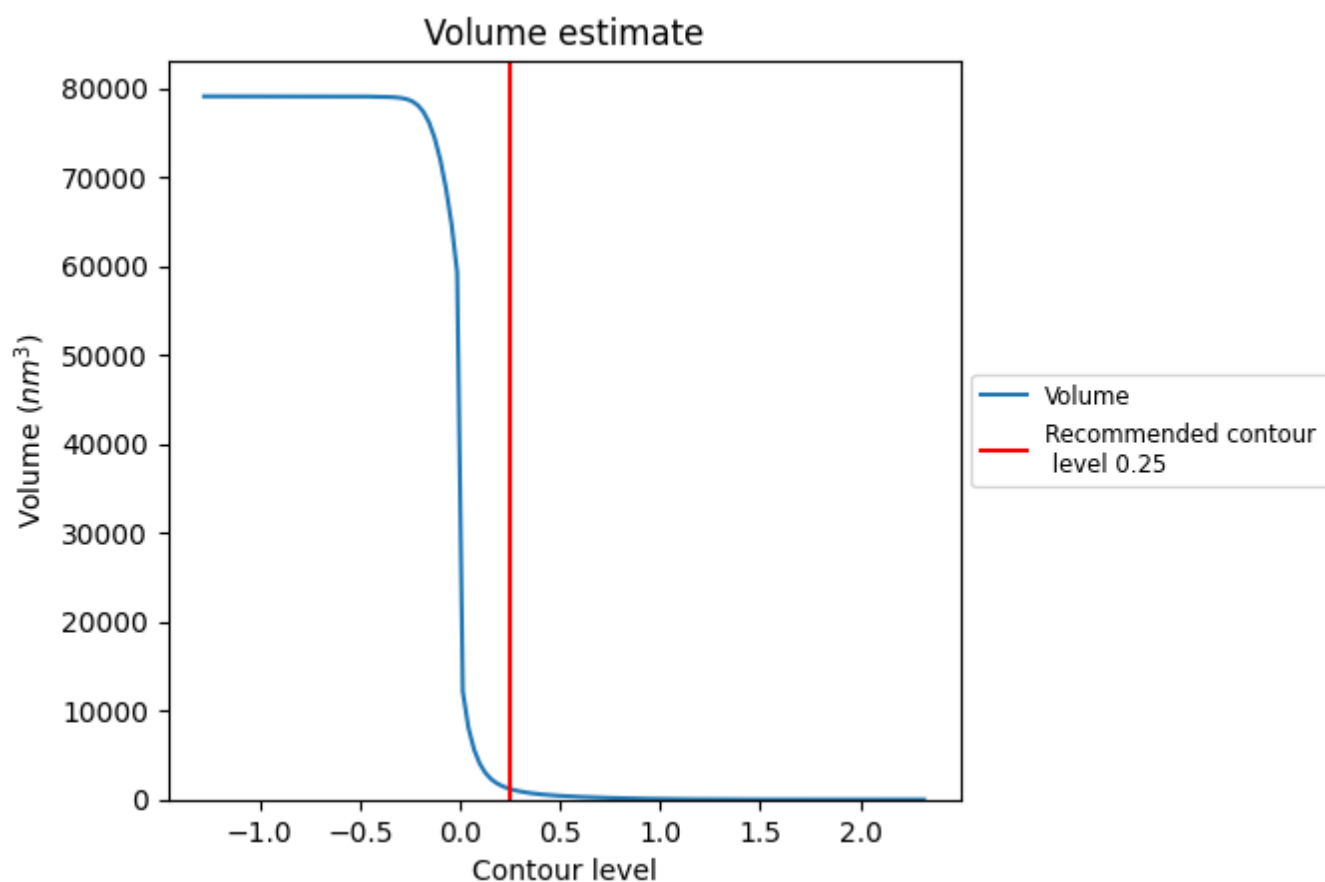
This section contains the results of statistical analysis of the map.

### 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.

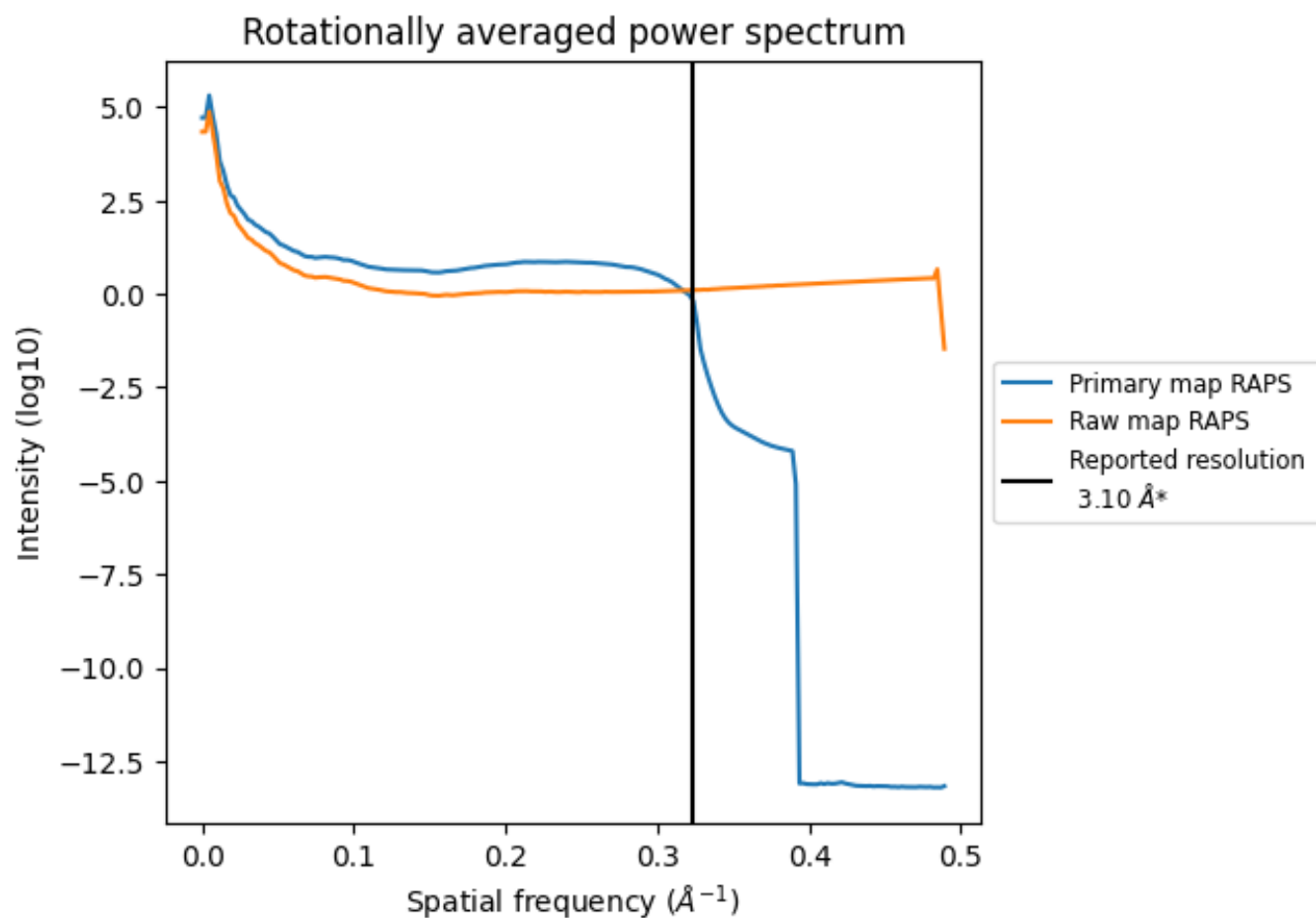
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1201  $\text{nm}^3$ ; this corresponds to an approximate mass of 1085 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 ⓘ

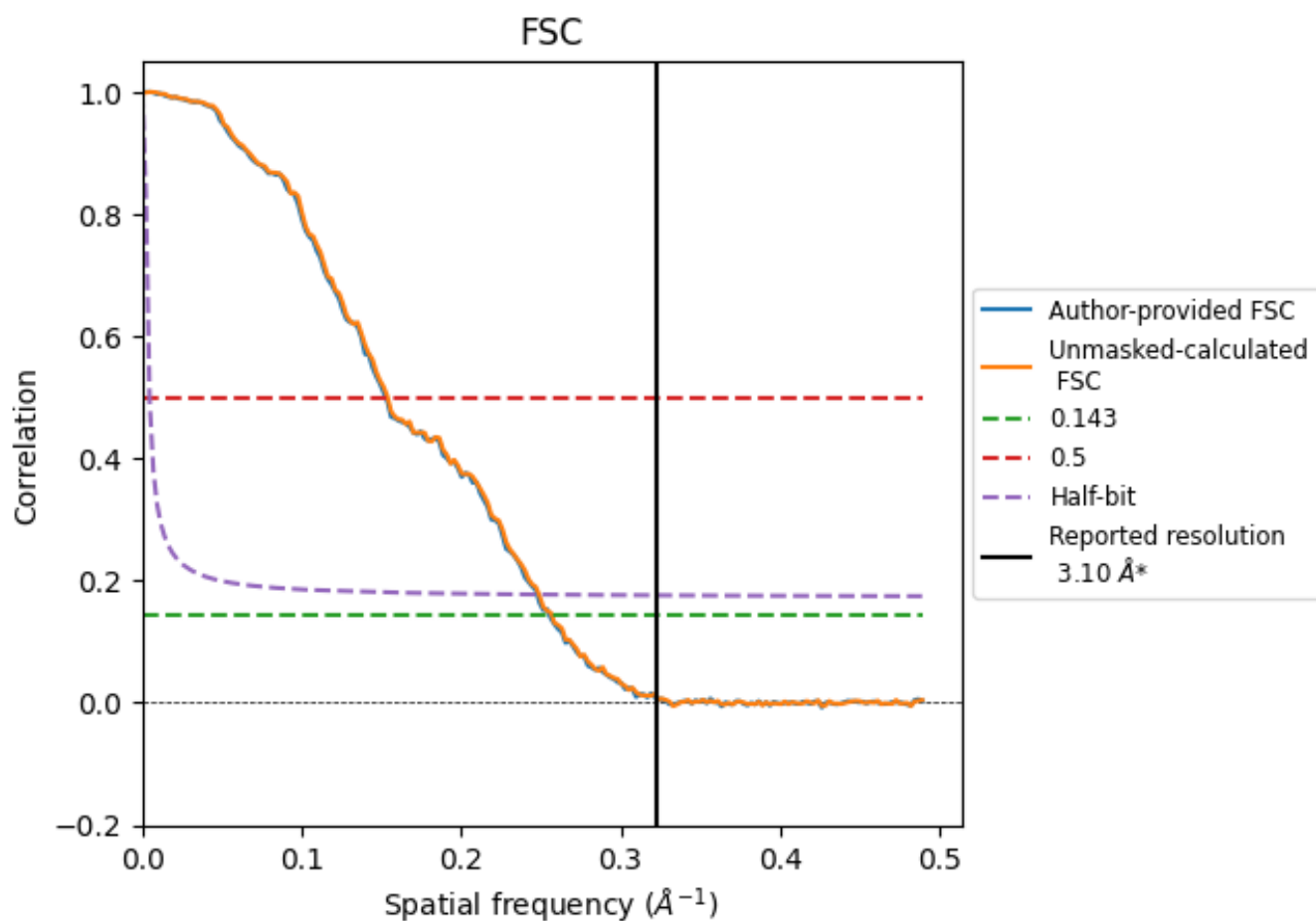


\*Reported resolution corresponds to spatial frequency of 0.323  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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 [i](#)



\*Reported resolution corresponds to spatial frequency of 0.323 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.91	6.55	4.04
Unmasked-calculated*	3.89	6.50	4.02

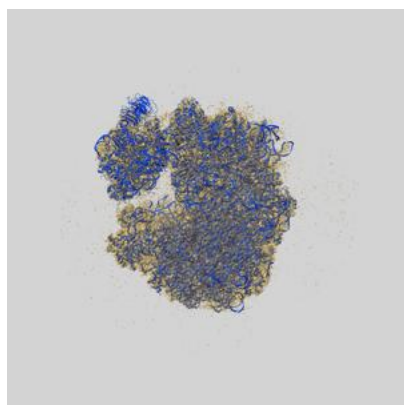
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.91 differs from the reported value 3.1 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.89 differs from the reported value 3.1 by more than 10 %

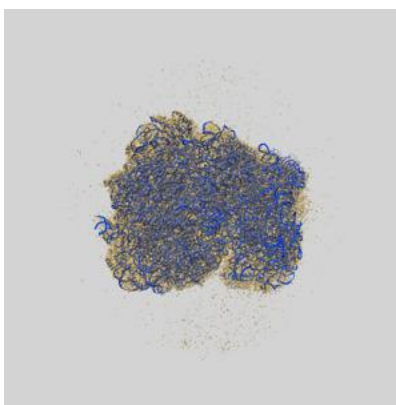
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-50957 and PDB model 9G1Z. Per-residue inclusion information can be found in section [3](#) on page [19](#).

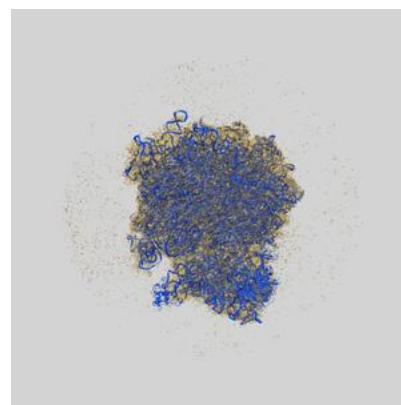
### 9.1 Map-model overlay [i](#)



X



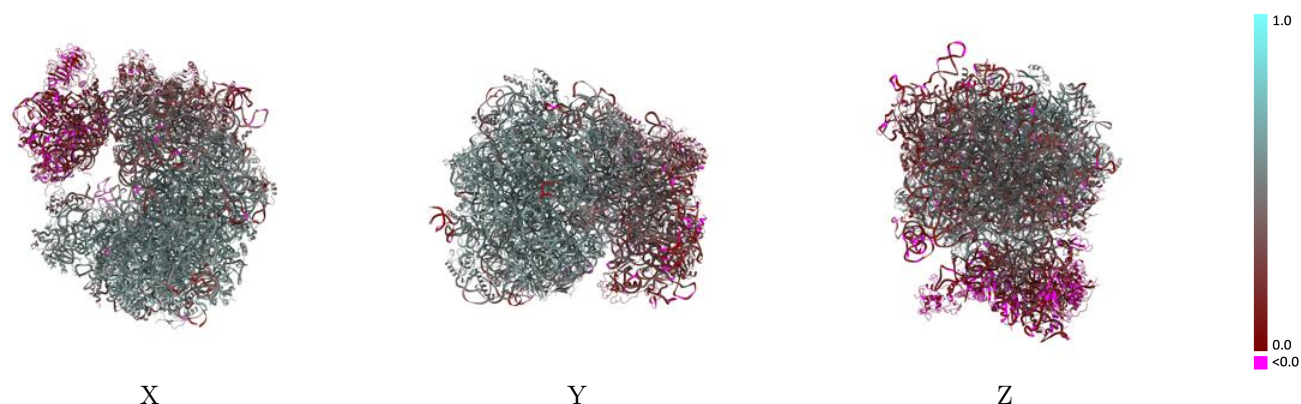
Y



Z

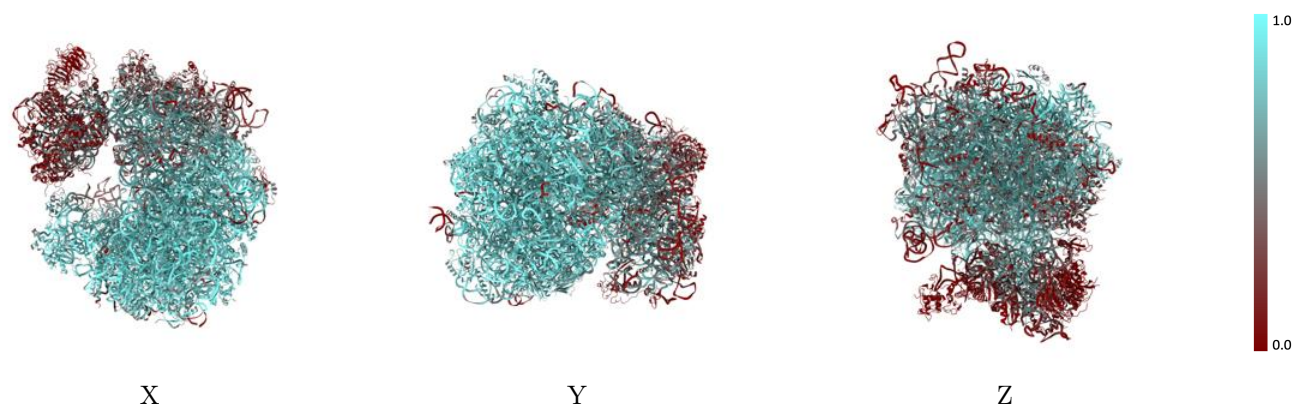
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



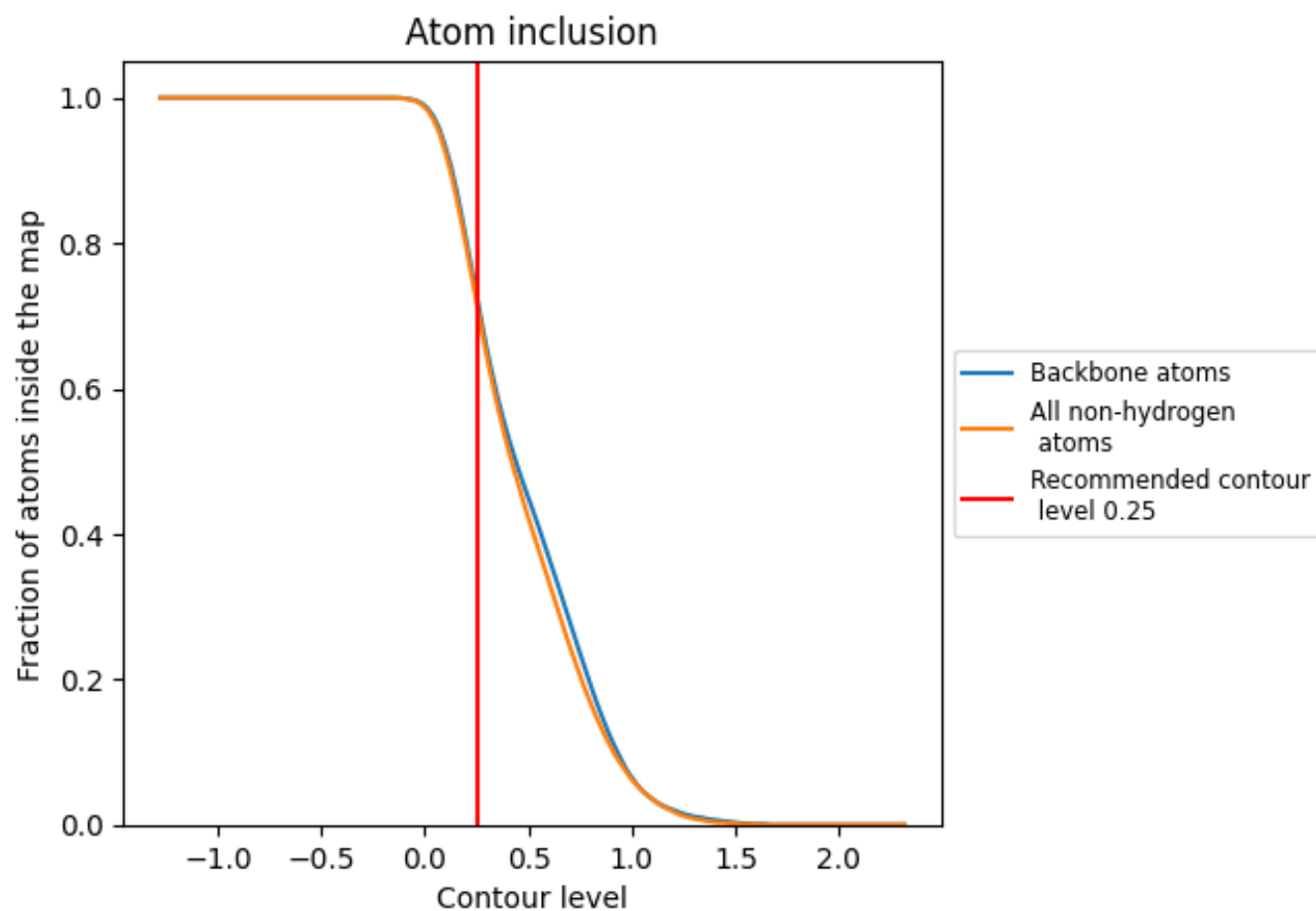
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 [i](#)



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 (0.25).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 72% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7180	 0.4380
0	 0.8650	 0.5590
1	 0.9000	 0.5270
10	 0.5710	 0.4990
2	 0.8370	 0.5390
3	 0.9500	 0.5450
4	 0.9520	 0.5560
5	 0.2950	 0.3590
6	 0.8780	 0.5590
7	 0.8590	 0.5360
8	 0.8590	 0.5440
9	 0.8460	 0.5520
A	 0.5970	 0.3130
AA	 0.7740	 0.5090
AB	 0.9030	 0.5760
AC	 0.8030	 0.5090
AD	 0.7640	 0.4990
AE	 0.7970	 0.5320
AF	 0.9000	 0.5630
AG	 0.9010	 0.5740
AH	 0.8080	 0.5310
AI	 0.8550	 0.5440
AJ	 0.8280	 0.5290
AK	 0.9280	 0.5770
AL	 0.6430	 0.4880
AM	 0.9090	 0.5690
AN	 0.8350	 0.5480
AO	 0.5440	 0.4280
AP	 0.8230	 0.5470
AQ	 0.8360	 0.5310
B	 0.3380	 0.2680
C	 0.4590	 0.3470
D	 0.5170	 0.3570
E	 0.2000	 0.1490
F	 0.3790	 0.2860









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Chain	Atom inclusion	Q-score
G	 0.1170	 0.1170
H	 0.3490	 0.2410
I	 0.2160	 0.2690
J	 0.5220	 0.4090
K	 0.3840	 0.2730
L	 0.1090	 0.0910
M	 0.4290	 0.3730
N	 0.0130	 0.0890
O	 0.4840	 0.3640
P	 0.5020	 0.3960
Q	 0.0970	 0.0980
R	 0.2380	 0.1400
S	 0.2740	 0.2310
T	 0.1340	 0.1380
U	 0.1680	 0.1390
V	 0.1590	 0.1110
W	 0.3740	 0.2770
X	 0.5170	 0.3720
Y	 0.5370	 0.3650
Z	 0.3530	 0.2410
a	 0.0780	 0.0880
b	 0.5780	 0.4140
c	 0.2980	 0.2970
d	 0.0840	 0.1310
e	 0.3360	 0.1890
f	 0.3280	 0.2130
g	 0.0230	 0.0690
h	 0.0470	 0.1020
j	 0.8780	 0.5690
k	 0.8790	 0.5580
l	 0.8720	 0.5530
m	 0.7860	 0.5030
n	 0.8020	 0.5130
o	 0.8560	 0.5510
p	 0.7760	 0.5170
q	 0.8160	 0.5320
r	 0.8260	 0.5470
s	 0.7100	 0.4680
t	 0.8390	 0.5330
u	 0.8030	 0.5220
v	 0.9260	 0.5780
w	 0.8600	 0.5510

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*Continued from previous page...*

Chain	Atom inclusion	Q-score
x	 0.8700	 0.5490
y	 0.8820	 0.5660
z	 0.8150	 0.5160