



wwPDB EM Validation Summary Report ⓘ

Apr 21, 2026 – 02:30 pm BST

PDB ID : 9QWT / pdb_00009qwt
EMDB ID : EMD-53427
Title : Mouse Ribosome RPS15 (uS19) P131S rotated-2 PRE state
Authors : Santo, P.E.; Astier, A.; Plisson-Chastang, C.
Deposited on : 2025-04-15
Resolution : 3.10 Å(reported)
Based on initial model : 7LS1

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

We welcome your comments at 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>.

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

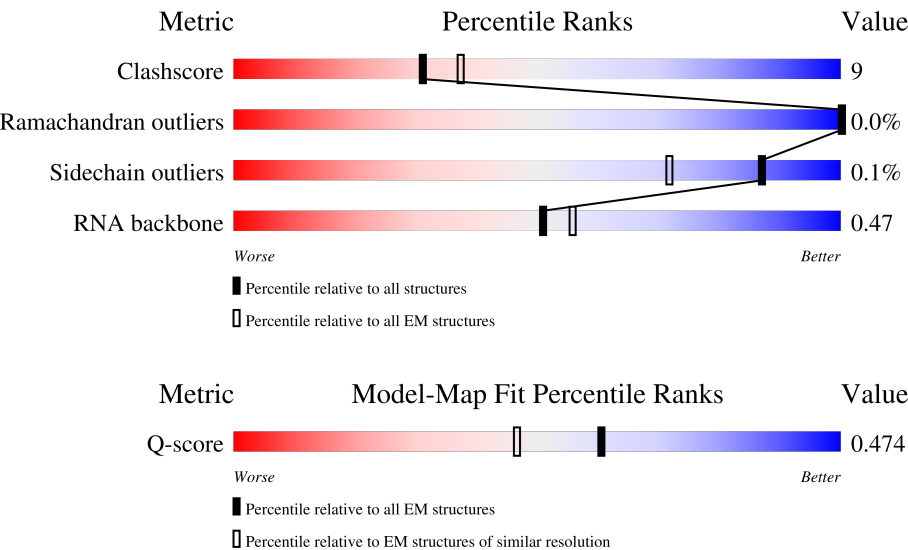
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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.





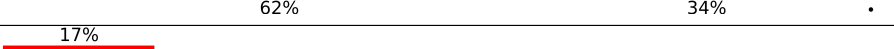




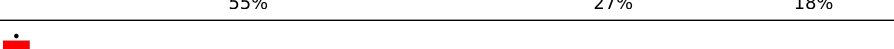



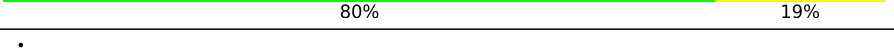

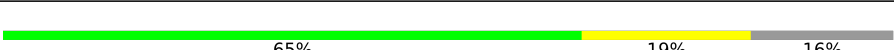


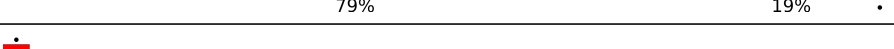







Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14724 (2.60 - 3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	A1	270	<div><div></div><div>59%23%18%</div></div>
2	A2	3615	<div><div>7%</div><div>55%36%6%</div><div></div></div>
3	A3	152	<div><div>5%</div><div>57%34%9%</div><div></div></div>

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Mol	Chain	Length	Quality of chain
4	B1	266	
5	B2	121	
6	B3	145	
7	Bv	76	
8	Bx	10	
9	By	22	
10	C1	192	
11	C2	156	
12	C3	119	
13	D1	214	
14	D2	257	
15	D3	83	
16	E1	178	
17	E2	403	
18	E3	142	
19	F1	211	
20	F2	419	
21	F3	114	
22	G1	217	
23	G2	297	
24	G3	69	
25	H1	204	
26	H2	296	
27	H3	56	
28	I2	203	



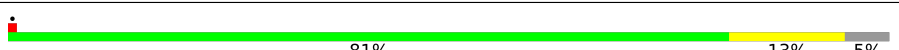
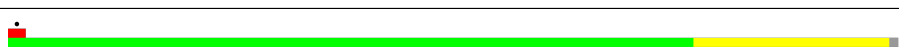

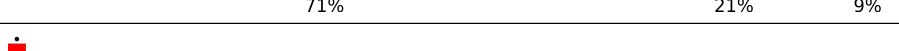
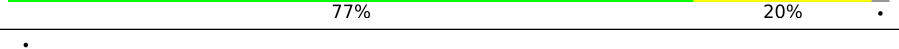





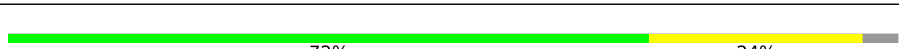


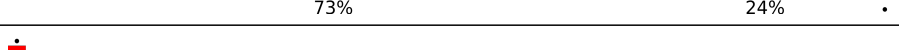

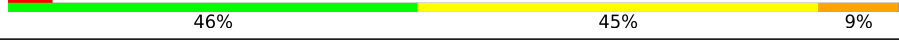






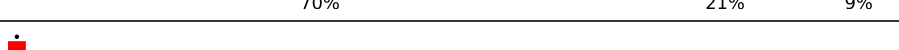
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Mol	Chain	Length	Quality of chain
29	I3	317	
30	J2	184	
31	J3	293	
32	K2	188	
33	K3	249	
34	L2	196	
35	L3	194	
36	M2	176	
37	M3	132	
38	N2	160	
39	N3	151	
40	O2	128	
41	O3	151	
42	P2	140	
43	P3	130	
44	Q2	157	
45	Q3	133	
46	R2	156	
47	R3	125	
48	S2	145	
49	S3	84	
50	T2	136	
51	T3	133	
52	U2	148	
53	V2	160	

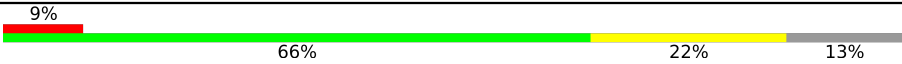
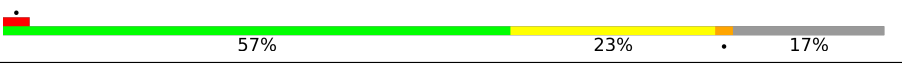
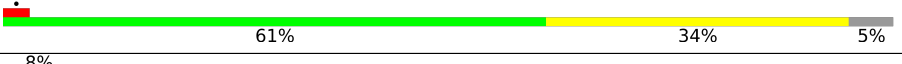

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Mol	Chain	Length	Quality of chain
54	W2	115	
55	X2	125	
56	Y2	135	
57	Z2	110	
58	a2	117	
59	b2	123	
60	c2	105	
61	d2	97	
62	e2	70	
63	f2	51	
64	g2	128	
65	h2	25	
66	i2	105	
67	j2	92	
68	k2	137	
69	m2	1633	
70	n2	73	
71	o2	295	
72	p2	264	
73	q2	242	
74	r2	257	
75	s2	204	
76	t2	194	
77	u2	208	
78	v2	165	

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Mol	Chain	Length	Quality of chain
79	w2	158	
80	x2	145	
81	y2	146	
82	z2	135	

2 Entry composition

There are 87 unique types of molecules in this entry. The entry contains 206855 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 Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A1	222	Total	C	N	O	S	0	0
			1843	1185	353	297	8		

- Molecule 2 is a RNA chain called 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A2	3512	Total	C	N	O	P	0	0
			75341	33588	13744	24498	3511		

- Molecule 3 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A3	139	Total	C	N	O	S	0	0
			1154	725	233	195	1		

- Molecule 4 is a protein called Large ribosomal subunit protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B1	217	Total	C	N	O	S	1	0
			1764	1127	340	293	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B2	119	Total	C	N	O	P	0	0
			2538	1132	454	834	118		

- Molecule 6 is a protein called Small ribosomal subunit protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B3	140	Total	C	N	O	S	0	0
			1091	686	210	192	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B3	88	MET	ARG	conflict	UNP Q9CZX8

- Molecule 7 is a RNA chain called transfer RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Bv	66	Total	C	N	O	P	0	0
			1412	629	255	462	66		

- Molecule 8 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Bx	10	Total	C	N	O	P	0	0
			200	90	20	80	10		

- Molecule 9 is a protein called Nascent protein chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	By	22	Total	C	N	O	0	0
			110	66	22	22		

- Molecule 10 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C1	190	Total	C	N	O	S	0	0
			1519	956	284	273	6		

- Molecule 11 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C2	156	Total	C	N	O	P	0	0
			3315	1481	585	1094	155		

- Molecule 12 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	C3	97	Total	C	N	O	S	0	0
			769	483	144	138	4		

- Molecule 13 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D1	204	Total	C	N	O	S	0	0
			1656	1052	319	272	13		

- Molecule 14 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	D2	245	Total	C	N	O	S	0	0
			1876	1177	383	310	6		

- Molecule 15 is a protein called Small ribosomal subunit protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	D3	83	Total	C	N	O	S	0	0
			589	369	111	104	5		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D3	25	GLY	ALA	conflict	UNP Q9CQR2
D3	41	LYS	ARG	conflict	UNP Q9CQR2
D3	42	VAL	THR	conflict	UNP Q9CQR2
D3	54	ALA	GLY	conflict	UNP Q9CQR2

- Molecule 16 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	E1	174	Total	C	N	O	S	0	0
			1397	880	260	251	6		

- Molecule 17 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	E2	402	Total	C	N	O	S	0	0
			3238	2060	609	555	14		

- Molecule 18 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	E3	139	Total	C	N	O	S	0	0
			1080	682	214	181	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E3	?	-	PRO	deletion	UNP P62267

- Molecule 19 is a protein called Large ribosomal subunit protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	F1	203	Total	C	N	O	S	0	0
			1643	1029	339	271	4		

- Molecule 20 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	F2	352	Total	C	N	O	S	0	0
			2823	1776	566	466	15		

- Molecule 21 is a protein called Small ribosomal subunit protein eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	F3	97	Total	C	N	O	S	0	0
			774	481	160	128	5		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F3	?	-	PRO	deletion	UNP P62855
F3	101	PRO	ARG	conflict	UNP P62855

- Molecule 22 is a protein called Large ribosomal subunit protein eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	G1	139	Total	C	N	O	S	0	0
			1143	732	221	183	7		

- Molecule 23 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	G2	293	Total	C	N	O	S	0	0
			2389	1509	441	425	14		

- Molecule 24 is a protein called Small ribosomal subunit protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	G3	56	Total	C	N	O	S	0	0
			435	267	85	81	2		

- Molecule 25 is a protein called Large ribosomal subunit protein eL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	H1	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 26 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	H2	218	Total	C	N	O	S	0	0
			1766	1130	337	295	4		

- Molecule 27 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	H3	51	Total	C	N	O	S	0	0
			427	269	87	66	5		

- Molecule 28 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	I2	198	Total	C	N	O	S	0	0
			1618	1043	316	253	6		

- Molecule 29 is a protein called Small ribosomal subunit protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	I3	234	Total	C	N	O	S	0	0
			1800	1135	318	337	10		

- Molecule 30 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	J2	153	Total	C	N	O	S	0	0
			1242	777	241	215	9		

- Molecule 31 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	J3	217	Total	C	N	O	S	0	0
			1590	1039	276	266	9		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J3	61	MET	ILE	conflict	UNP P25444

- Molecule 32 is a protein called Large ribosomal subunit protein eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	K2	186	Total	C	N	O	S	0	0
			1511	946	313	248	4		

- Molecule 33 is a protein called Small ribosomal subunit protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	K3	211	Total	C	N	O	S	0	0
			1708	1073	342	286	7		

- Molecule 34 is a protein called Large ribosomal subunit protein eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	L2	169	Total	C	N	O	S	0	0
			1408	873	304	222	9		

- Molecule 35 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	L3	179	Total	C	N	O	S	0	0
			1495	953	299	241	2		

- Molecule 36 is a protein called Large ribosomal subunit protein eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	M2	175	Total	C	N	O	S	0	0
			1450	924	283	233	10		

- Molecule 37 is a protein called Small ribosomal subunit protein eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	M3	84	Total	C	N	O	S	0	0
			525	332	97	91	5		

- Molecule 38 is a protein called Large ribosomal subunit protein eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	N2	159	Total	C	N	O	S	0	0
			1299	824	252	217	6		

- Molecule 39 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	N3	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 40 is a protein called Large ribosomal subunit protein eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	O2	101	Total	C	N	O	S	0	0
			825	529	144	150	2		

- Molecule 41 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	O3	135	Total	C	N	O	S	0	0
			1003	615	198	184	6		

- Molecule 42 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	P2	129	Total	C	N	O	S	0	0
			969	613	182	169	5		

- Molecule 43 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	P3	129	Total	C	N	O	S	0	0
			1027	655	192	174	6		

- Molecule 44 is a protein called Large ribosomal subunit protein eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Q2	62	Total	C	N	O	S	0	0
			519	332	101	83	3		

- Molecule 45 is a protein called Small ribosomal subunit protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Q3	121	Total	C	N	O	S	0	0
			981	620	192	164	5		

- Molecule 46 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	R2	118	Total	C	N	O	S	0	0
			967	618	181	167	1		

- Molecule 47 is a protein called Small ribosomal subunit protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	R3	73	Total	C	N	O	S	0	0
			585	374	108	102	1		

- Molecule 48 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	S2	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 49 is a protein called Small ribosomal subunit protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	S3	79	Total	C	N	O	S	0	0
			618	386	115	110	7		

- Molecule 50 is a protein called Large ribosomal subunit protein eL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	T2	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 51 is a protein called Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	T3	44	Total	C	N	O	S	0	0
			355	218	81	55	1		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T3	55	PRO	ASN	conflict	UNP P62862
T3	56	ASN	VAL	conflict	UNP P62862
T3	57	ALA	VAL	conflict	UNP P62862

- Molecule 52 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	U2	147	Total	C	N	O	S	0	0
			1164	736	239	185	4		

- Molecule 53 is a protein called Large ribosomal subunit protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	V2	117	Total	C	N	O	S	0	0
			945	596	198	146	5		

- Molecule 54 is a protein called Large ribosomal subunit protein eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	W2	94	Total	C	N	O	S	0	0
			732	465	130	131	6		

- Molecule 55 is a protein called Large ribosomal subunit protein eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	X2	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 56 is a protein called Large ribosomal subunit protein eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	Y2	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 57 is a protein called Large ribosomal subunit protein eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Z2	109	Total	C	N	O	S	0	0
			876	555	174	143	4		

- Molecule 58 is a protein called Large ribosomal subunit protein eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	a2	107	Total	C	N	O	S	0	0
			854	535	176	137	6		

- Molecule 59 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	b2	120	Total	C	N	O	S	0	0
			1001	634	201	165	1		

- Molecule 60 is a protein called Large ribosomal subunit protein eL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	c2	102	Total	C	N	O	S	0	0
			832	521	177	129	5		

- Molecule 61 is a protein called Large ribosomal subunit protein eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	d2	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 62 is a protein called Large ribosomal subunit protein eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	e2	69	Total	C	N	O	S	0	0
			568	365	103	99	1		

- Molecule 63 is a protein called Large ribosomal subunit protein eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	f2	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

- Molecule 64 is a protein called Ubiquitin-ribosomal protein eL40 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	g2	52	Total	C	N	O	S	0	0
			429	266	90	67	6		

- Molecule 65 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	h2	24	Total	C	N	O	S	0	0
			230	139	62	26	3		

- Molecule 66 is a protein called Large ribosomal subunit protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	i2	103	Total	C	N	O	S	0	0
			842	528	172	136	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
i2	?	-	GLN	deletion	UNP P83882

- Molecule 67 is a protein called Large ribosomal subunit protein eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	j2	89	Total	C	N	O	S	0	0
			694	436	133	118	7		

- Molecule 68 is a protein called Large ribosomal subunit protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	k2	125	Total	C	N	O	S	0	0
			1001	621	207	168	5		

- Molecule 69 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	m2	1623	Total	C	N	O	P	0	0
			34685	15498	6234	11330	1623		

- Molecule 70 is a RNA chain called transfer RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	n2	73	Total	C	N	O	P	0	0
			1562	698	291	501	72		

- Molecule 71 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	o2	215	Total	C	N	O	S	0	0
			1704	1083	298	315	8		

- Molecule 72 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	p2	212	Total	C	N	O	S	0	0
			1722	1093	308	307	14		

- Molecule 73 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	q2	213	Total	C	N	O	S	0	0
			1655	1056	301	291	7		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
q2	195	THR	SER	conflict	UNP P62908
q2	?	-	ASP	deletion	UNP P62908

- Molecule 74 is a protein called Small ribosomal subunit protein eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	r2	257	Total	C	N	O	S	0	0
			2031	1298	381	344	8		

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
r2	46	VAL	ILE	conflict	UNP P62702
r2	78	VAL	THR	conflict	UNP P62702
r2	80	VAL	ILE	conflict	UNP P62702
r2	93	GLU	ASP	conflict	UNP P62702
r2	98	HIS	ASN	conflict	UNP P62702
r2	102	VAL	ILE	conflict	UNP P62702

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Chain	Residue	Modelled	Actual	Comment	Reference
r2	116	VAL	PRO	conflict	UNP P62702
r2	130	THR	PHE	conflict	UNP P62702
r2	133	VAL	THR	conflict	UNP P62702
r2	153	VAL	LEU	conflict	UNP P62702
r2	160	VAL	ILE	conflict	UNP P62702
r2	165	GLY	GLU	conflict	UNP P62702
r2	170	ILE	THR	conflict	UNP P62702
r2	171	ASN	ASP	conflict	UNP P62702
r2	184	ILE	THR	conflict	UNP P62702
r2	192	VAL	ILE	conflict	UNP P62702
r2	230	ASN	LYS	conflict	UNP P62702
r2	248	VAL	ILE	conflict	UNP P62702
r2	258	THR	ALA	conflict	UNP P62702

- Molecule 75 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	s2	185	Total	C	N	O	S	0	0
			1468	919	277	265	7		

- Molecule 76 is a protein called Small ribosomal subunit protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	t2	174	Total	C	N	O	S	0	0
			1322	857	246	218	1		

- Molecule 77 is a protein called Small ribosomal subunit protein eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	u2	179	Total	C	N	O	S	0	0
			1397	879	274	239	5		

- Molecule 78 is a protein called Small ribosomal subunit protein eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	v2	83	Total	C	N	O	S	0	0
			705	462	122	115	6		

- Molecule 79 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	w2	138	Total	C	N	O	S	0	0
			1134	722	214	192	6		

- Molecule 80 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	x2	120	Total	C	N	O	S	0	0
			999	635	188	169	7		

- Molecule 81 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	y2	139	Total	C	N	O	S	0	0
			1109	704	210	192	3		

- Molecule 82 is a protein called Small ribosomal subunit protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	z2	125	Total	C	N	O	S	0	0
			1011	634	187	186	4		

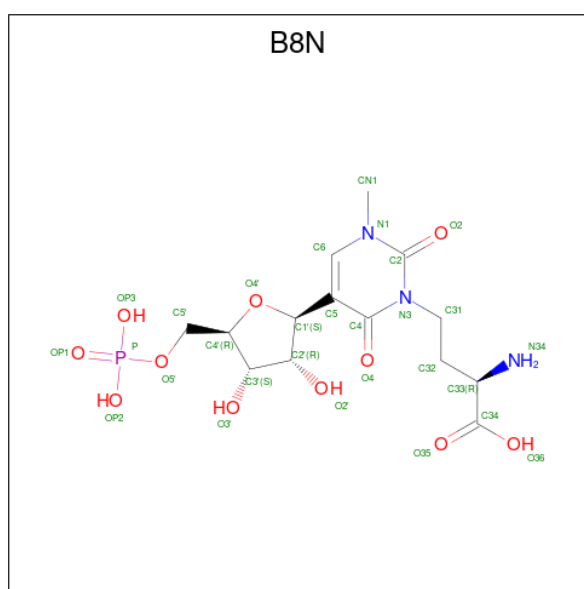
- Molecule 83 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
83	A2	84	Total	Mg	0
			84	84	
83	E3	1	Total	Mg	0
			1	1	
83	H1	1	Total	Mg	0
			1	1	
83	P2	1	Total	Mg	0
			1	1	
83	d2	1	Total	Mg	0
			1	1	
83	m2	35	Total	Mg	0
			35	35	

- Molecule 84 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

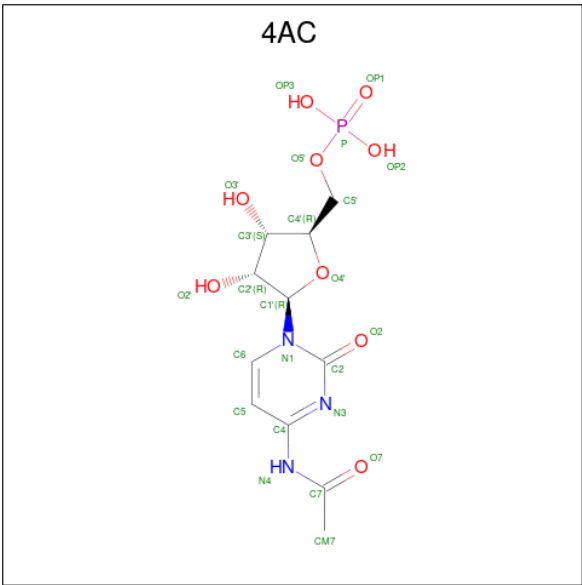
Mol	Chain	Residues	Atoms		AltConf
84	F3	1	Total	Zn	0
			1	1	
84	H3	1	Total	Zn	0
			1	1	
84	d2	1	Total	Zn	0
			1	1	
84	g2	1	Total	Zn	0
			1	1	
84	i2	1	Total	Zn	0
			1	1	
84	j2	1	Total	Zn	0
			1	1	

- Molecule 85 is (2 {R})-2-azanyl-4-[5-[(2 {S},3 {R},4 {S},5 {R})-3,4-bis(oxidanyl)-5-(phosphonoxymethyl)oxolan-2-yl]-3-methyl-2,6-bis(oxidanylidene)pyrimidin-1-yl]butanoic acid (CCD ID: B8N) (formula: C₁₄H₂₂N₃O₁₁P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
85	m2	1	Total	C	N	O	P	0
			28	14	3	10	1	

- Molecule 86 is N(4)-ACETYLCYTIDINE-5'-MONOPHOSPHATE (CCD ID: 4AC) (formula: C₁₁H₁₆N₃O₉P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
86	m2	1	Total	C	N	O	P	0
			23	11	3	8	1	

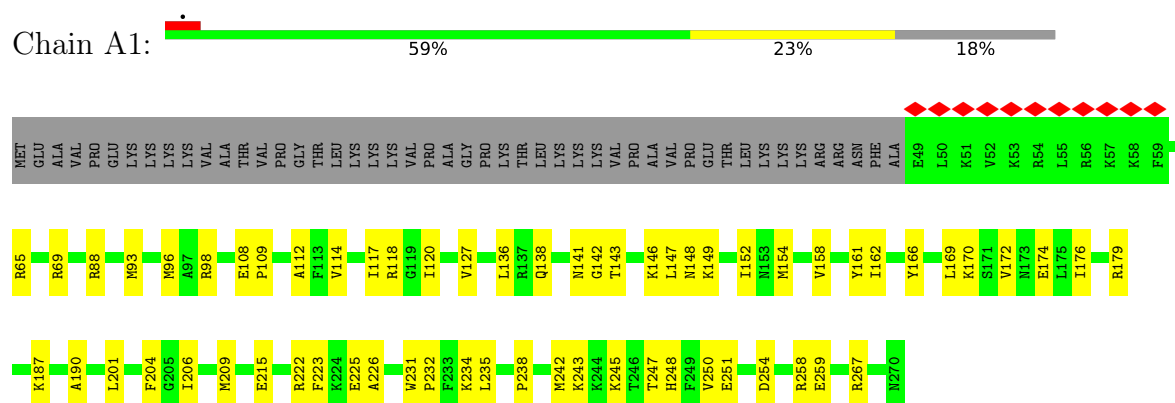
- Molecule 87 is water.

Mol	Chain	Residues	Atoms		AltConf
87	B1	1	Total	O	0
			1	1	

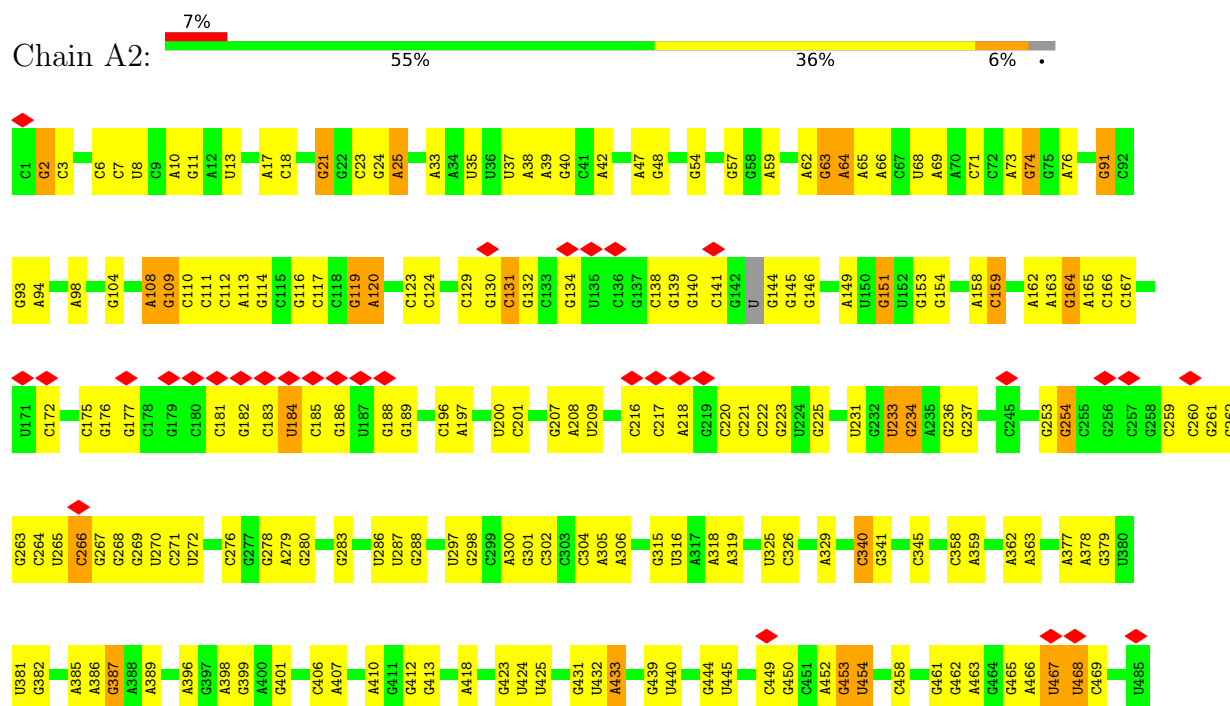
3 Residue-property plots

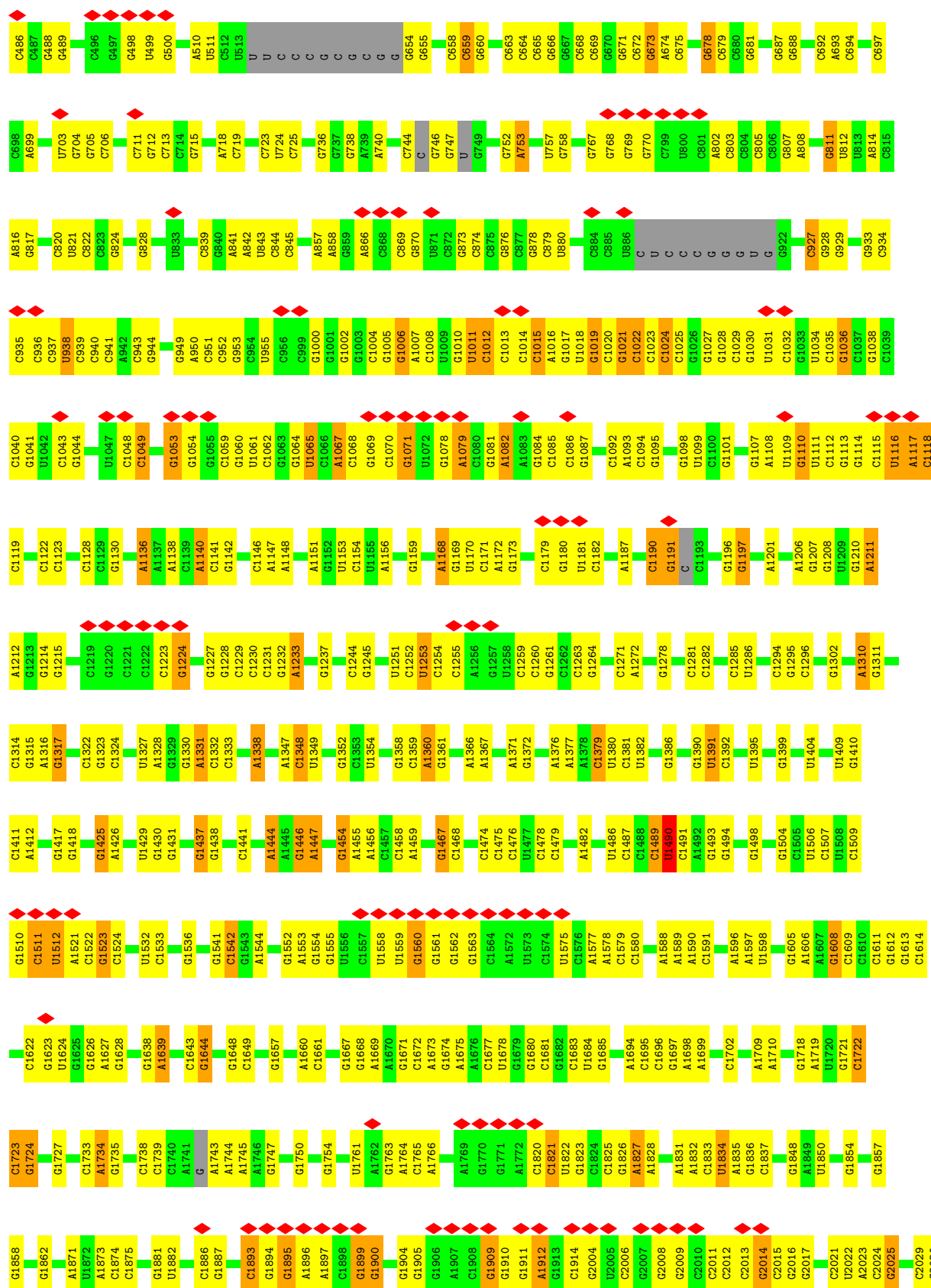
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Large ribosomal subunit protein uL30

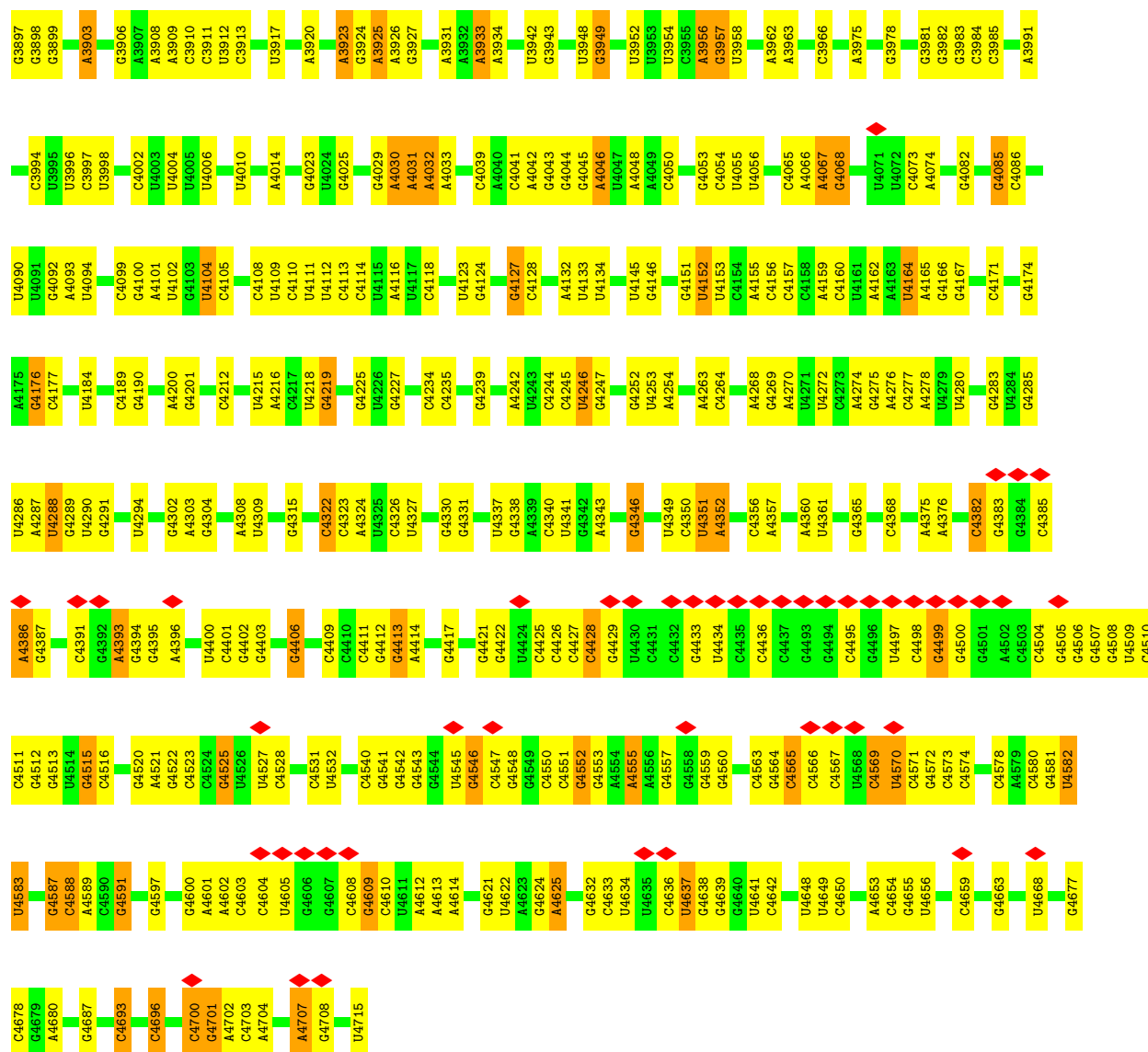


- Molecule 2: 28S ribosomal RNA

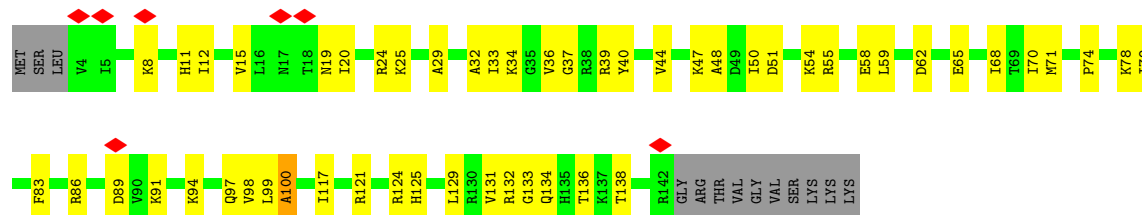






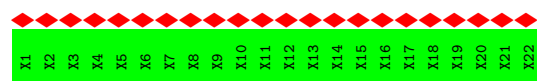


- Molecule 3: Small ribosomal subunit protein uS13

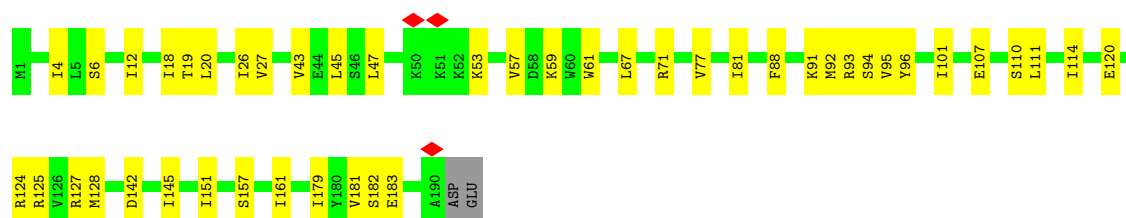
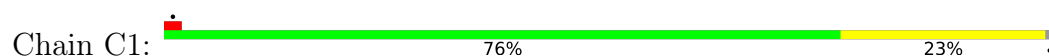


- Molecule 4: Large ribosomal subunit protein eL8

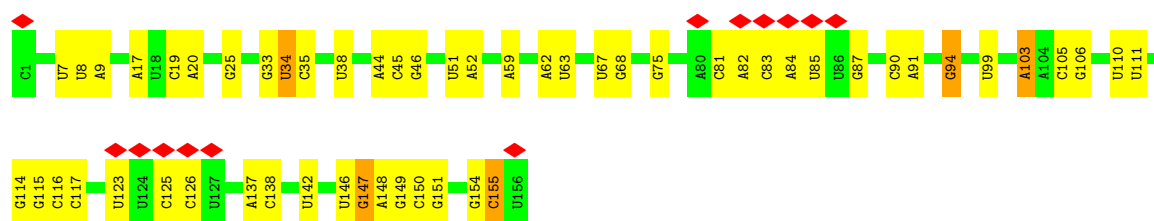




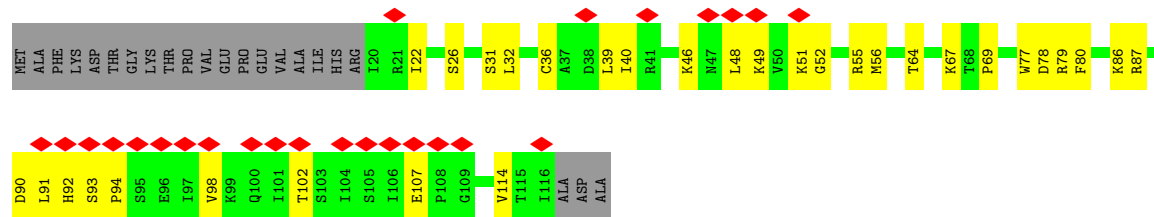
- Molecule 10: Large ribosomal subunit protein uL6



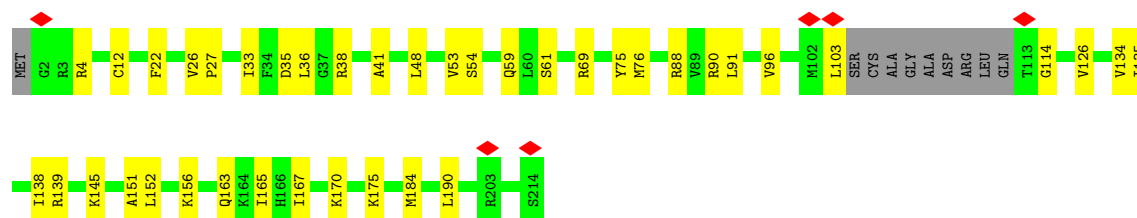
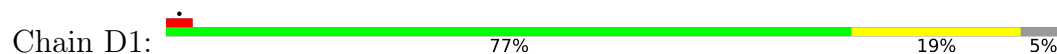
- Molecule 11: 5.8S ribosomal RNA




- Molecule 12: Small ribosomal subunit protein uS10

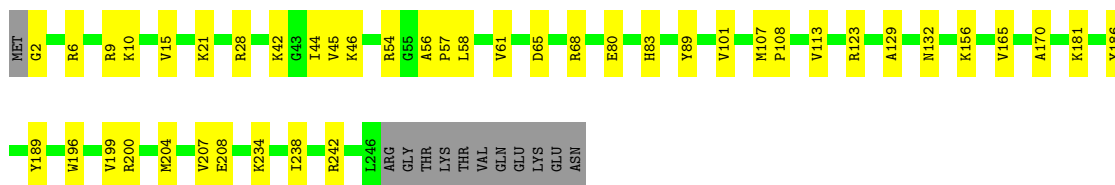


- Molecule 13: Large ribosomal subunit protein uL16




- Molecule 14: Large ribosomal subunit protein uL2

Chain D2:  79% 17% 5%




- Molecule 15: Small ribosomal subunit protein eS21

Chain D3:  78% 22%



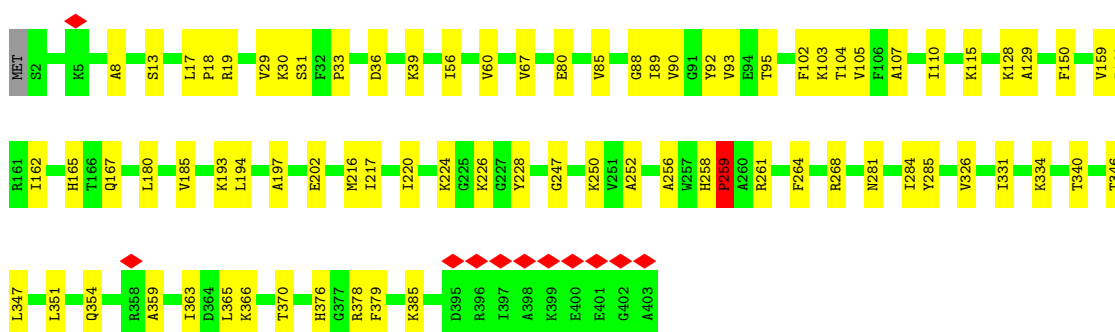
- Molecule 16: Large ribosomal subunit protein uL5

Chain E1:  5% 72% 25% .




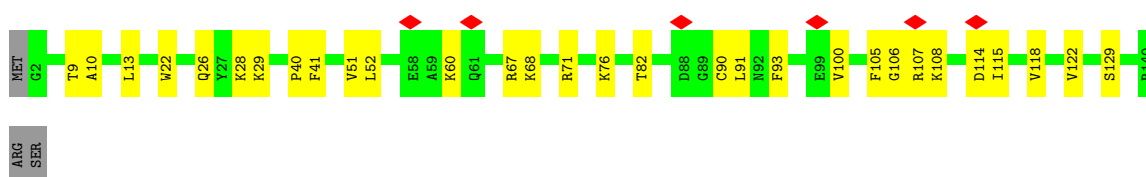
- Molecule 17: Large ribosomal subunit protein uL3

Chain E2:  80% 19%

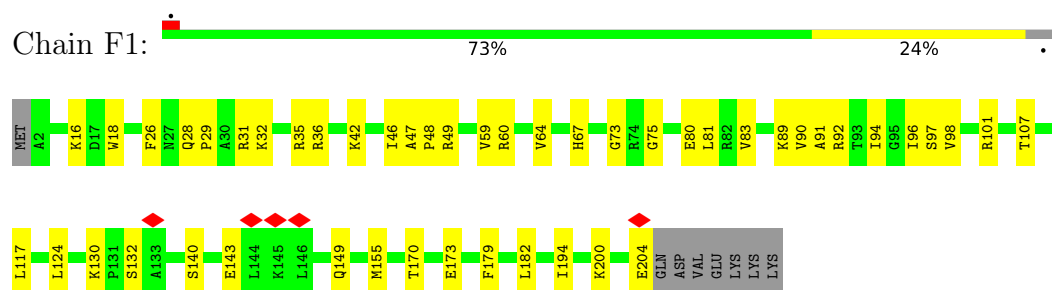


- Molecule 18: Small ribosomal subunit protein uS12

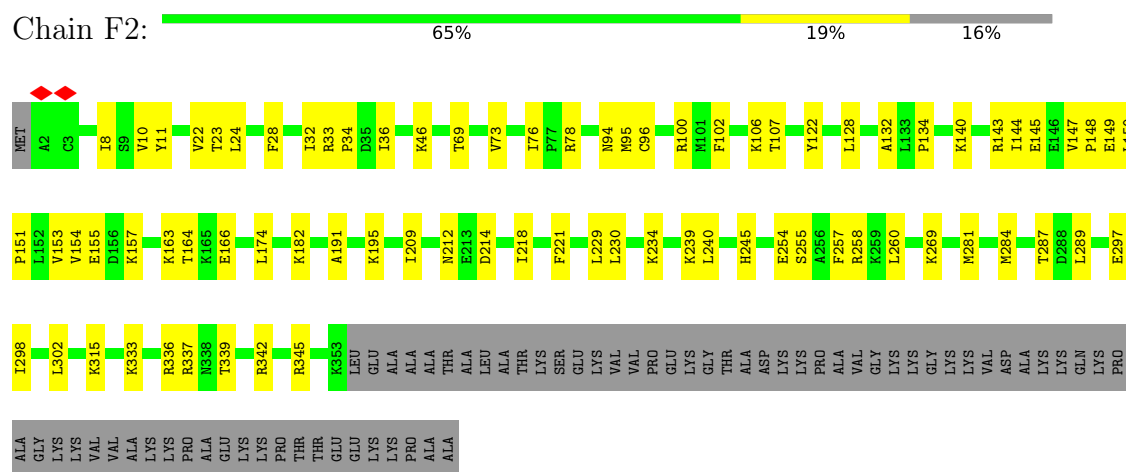
Chain E3:  77% 21%



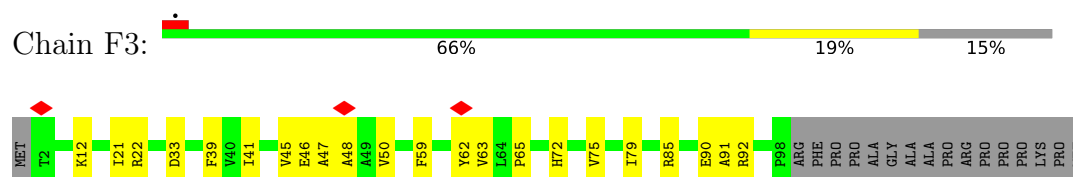
- Molecule 19: Large ribosomal subunit protein eL13



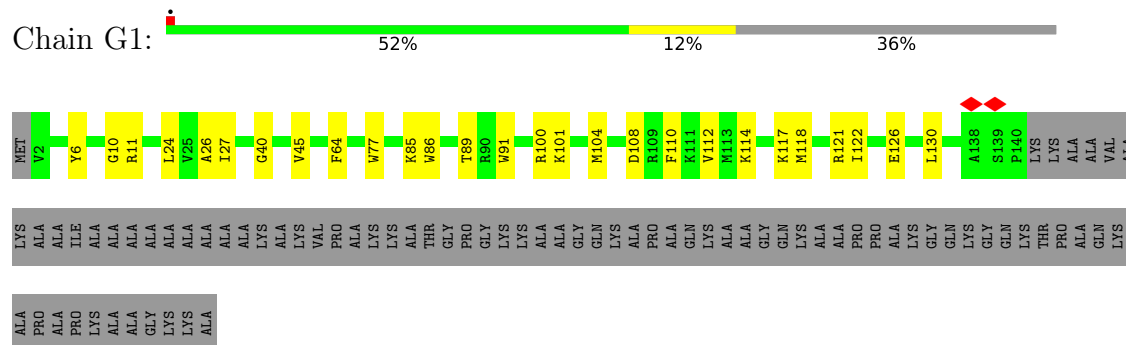
- Molecule 20: Large ribosomal subunit protein uL4



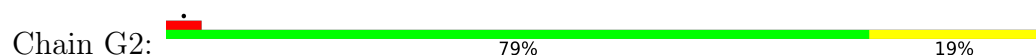
- Molecule 21: Small ribosomal subunit protein eS26

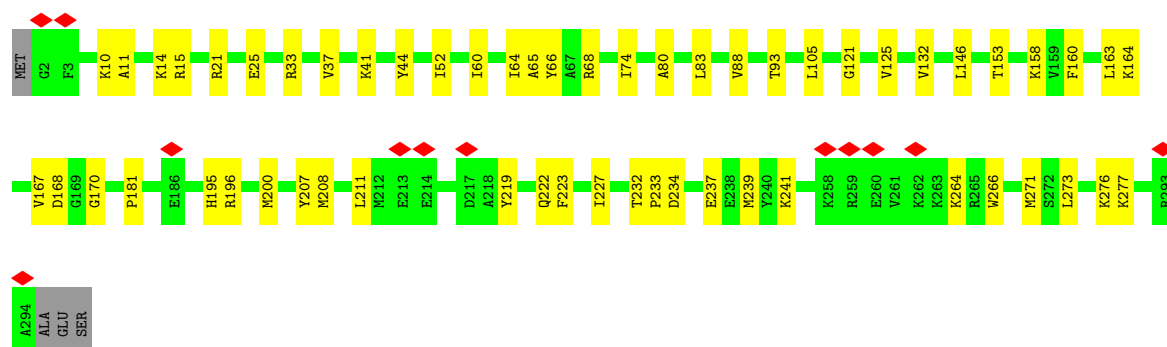


- Molecule 22: Large ribosomal subunit protein eL14

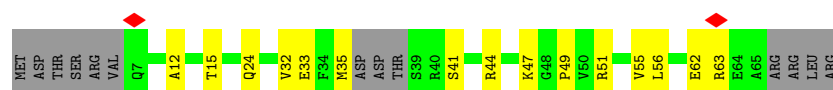


- Molecule 23: Large ribosomal subunit protein uL18

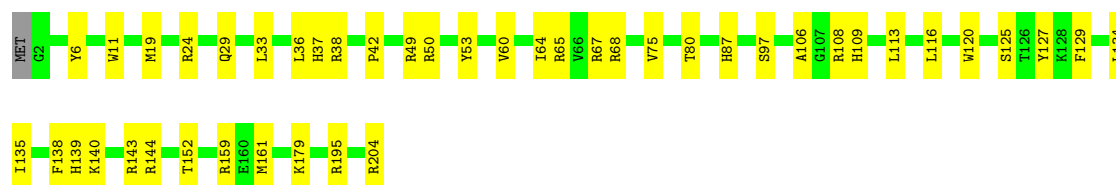
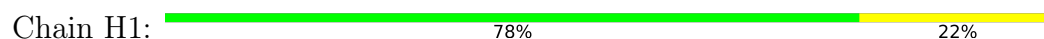




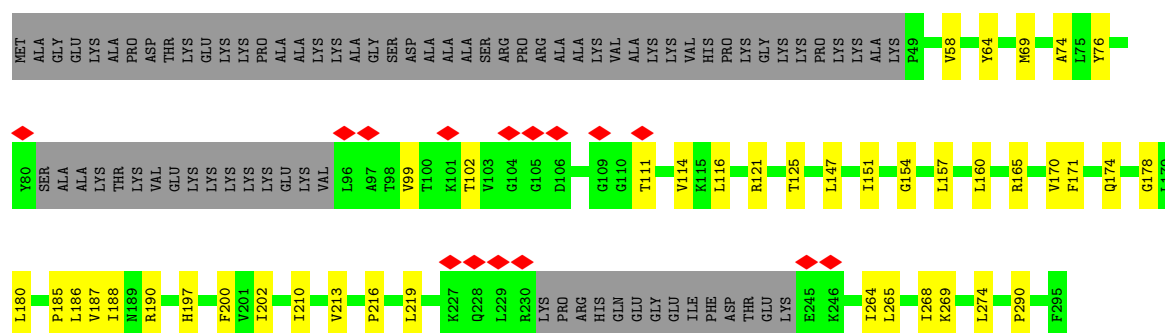
- Molecule 24: Small ribosomal subunit protein eS28



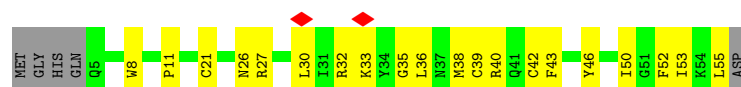
- Molecule 25: Large ribosomal subunit protein eL15



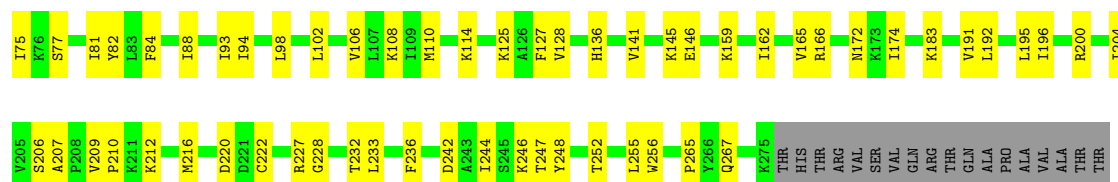
- Molecule 26: Large ribosomal subunit protein eL6



- Molecule 27: Small ribosomal subunit protein uS14

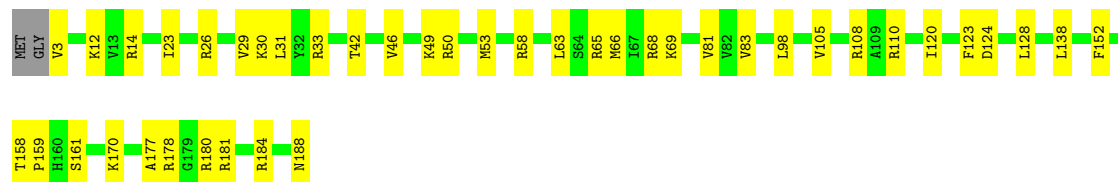


- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | ASP | ASP | ALA | GLY | ALA | ALA | GLY | PRO | PRO | GLY | LEU | GLY | GLY | ARG | ARG | PHE | GLY | SER | GLY | LEU | ARG | GLY | ARG | ARG | GLY | ARG | GLY | ALA | ALA | GLU | ASP | LYS | PHE |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|



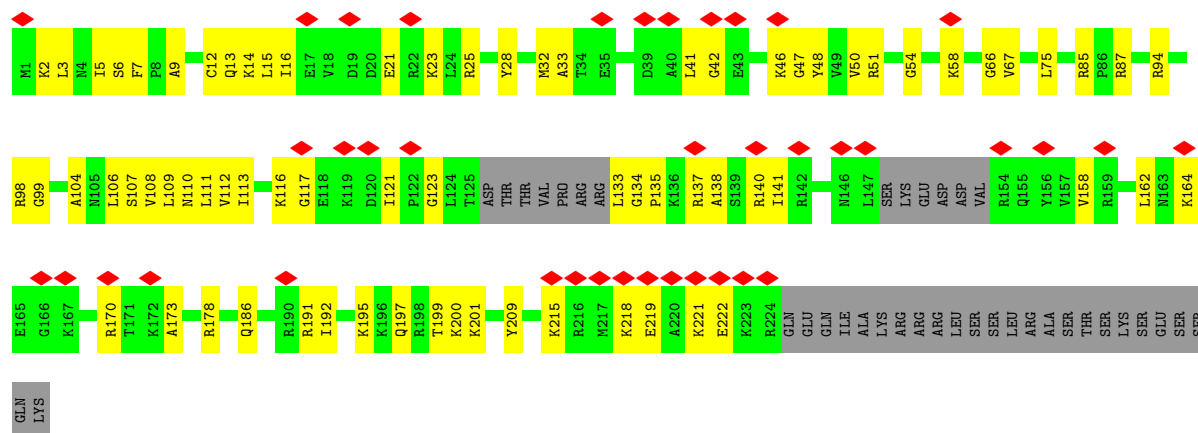
• Molecule 32: Large ribosomal subunit protein eL18

Chain K2: 77% 22%



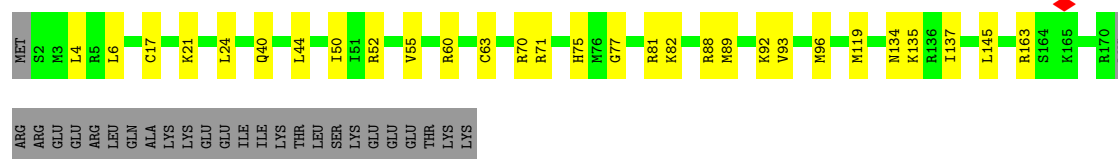
• Molecule 33: Small ribosomal subunit protein eS6

Chain K3: 16% 55% 30% 15%



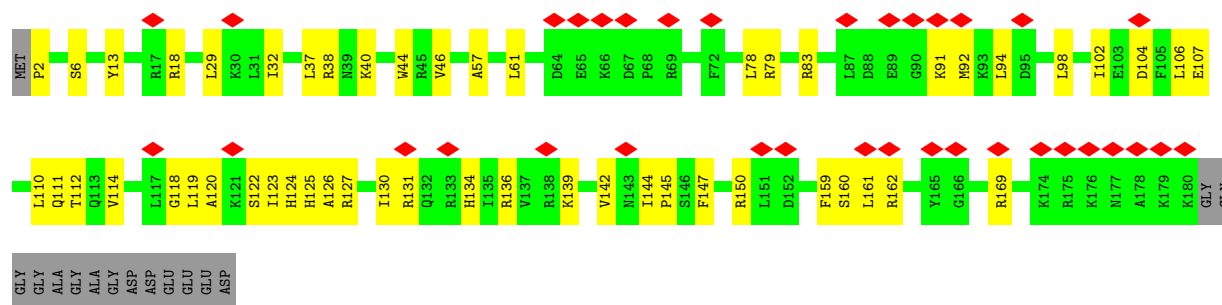
• Molecule 34: Large ribosomal subunit protein eL19

Chain L2: 71% 15% 14%



• Molecule 35: Small ribosomal subunit protein uS4

Chain L3: 18% 65% 27% 8%



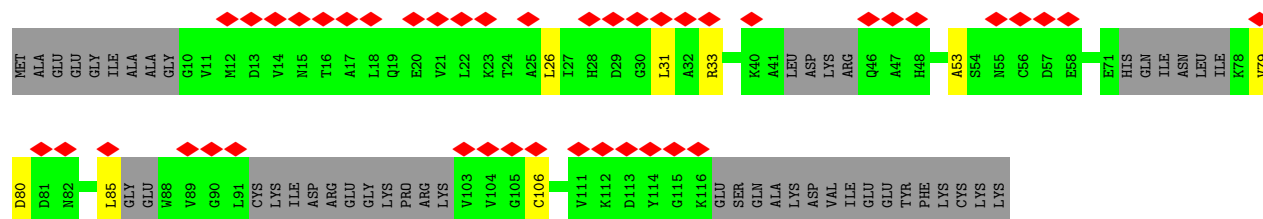
- Molecule 36: Large ribosomal subunit protein eL20

Chain M2: 79% 20%



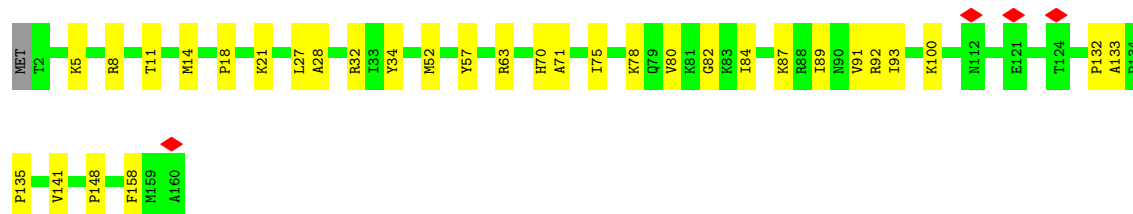
- Molecule 37: Small ribosomal subunit protein eS12

Chain M3: 33% 58% 6% 36%



- Molecule 38: Large ribosomal subunit protein eL21

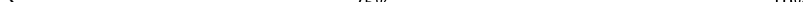
Chain N2: 79% 20%



- Molecule 39: Small ribosomal subunit protein uS15

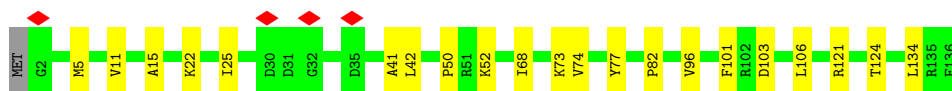
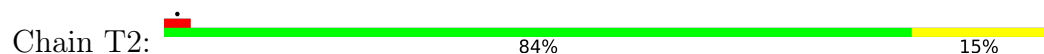
Chain N3: 72% 26%



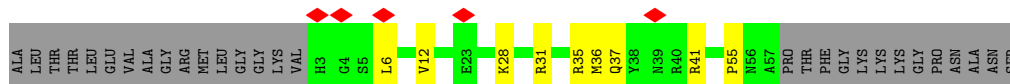
Chain S3: 



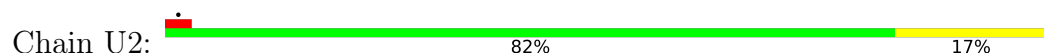
- Molecule 50: Large ribosomal subunit protein eL27



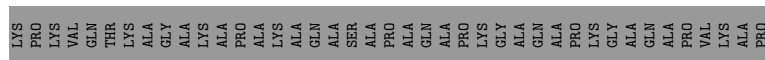
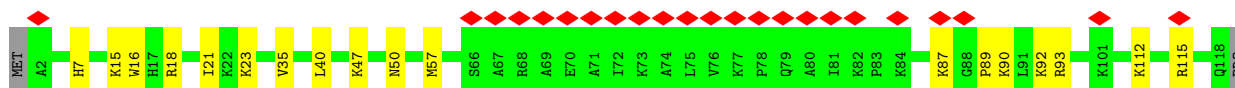
- Molecule 51: Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein



- Molecule 52: Large ribosomal subunit protein uL15



- Molecule 53: Large ribosomal subunit protein eL29

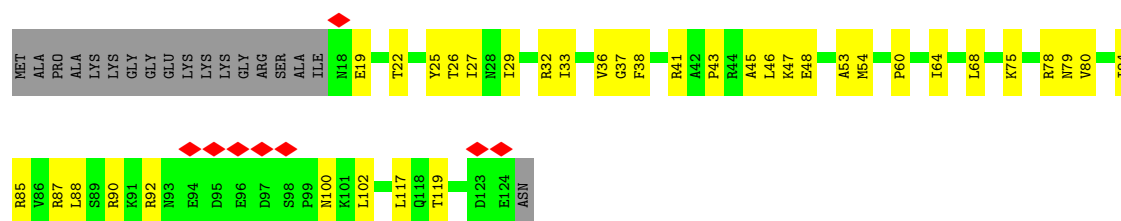


- Molecule 54: Large ribosomal subunit protein eL30

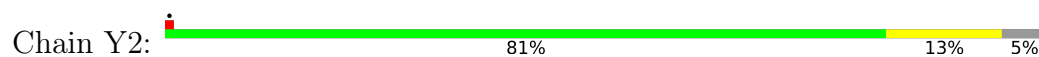


- Molecule 55: Large ribosomal subunit protein eL31

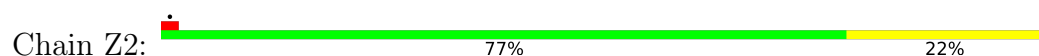




- Molecule 56: Large ribosomal subunit protein eL32



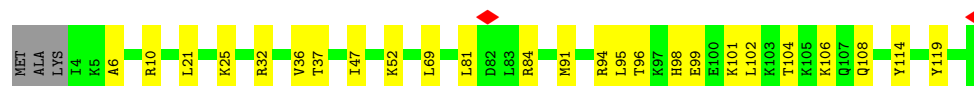
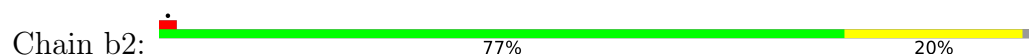
- Molecule 57: Large ribosomal subunit protein eL33



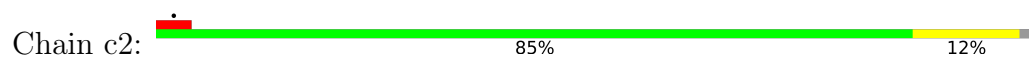
- Molecule 58: Large ribosomal subunit protein eL34



- Molecule 59: Large ribosomal subunit protein uL29

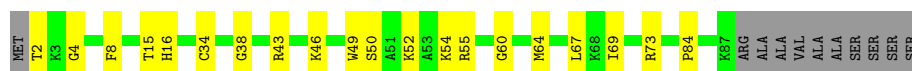


- Molecule 60: Large ribosomal subunit protein eL36

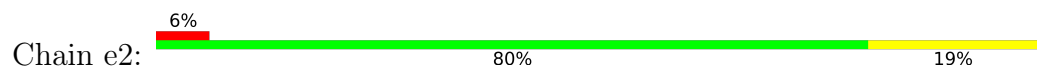


- Molecule 61: Large ribosomal subunit protein eL37

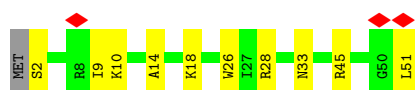
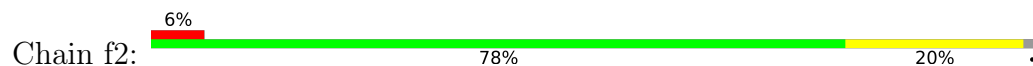




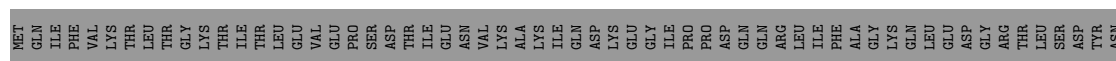
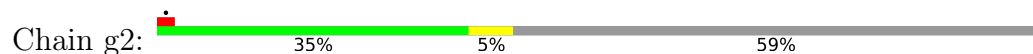
- Molecule 62: Large ribosomal subunit protein eL38



- Molecule 63: Large ribosomal subunit protein eL39



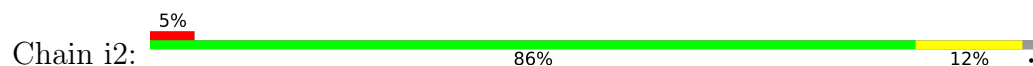
- Molecule 64: Ubiquitin-ribosomal protein eL40 fusion protein



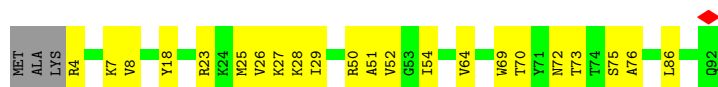
- Molecule 65: 60S ribosomal protein L41



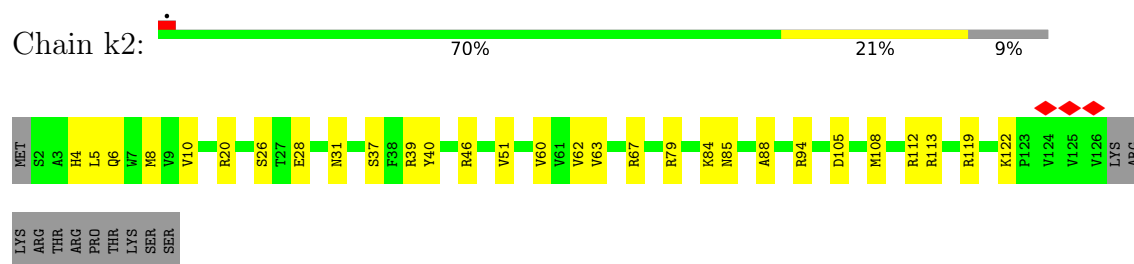
- Molecule 66: Large ribosomal subunit protein eL42



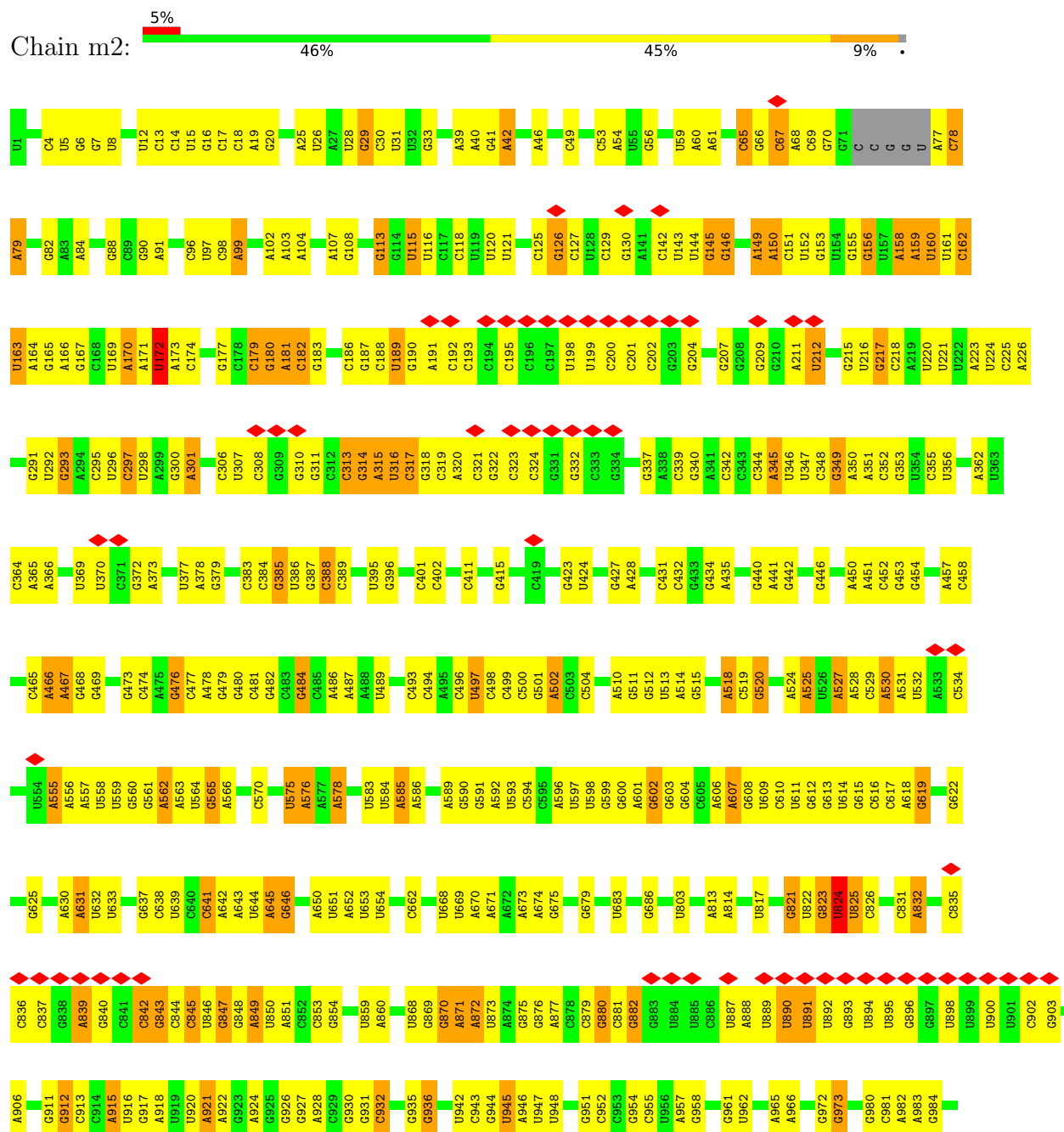
- Molecule 67: Large ribosomal subunit protein eL43

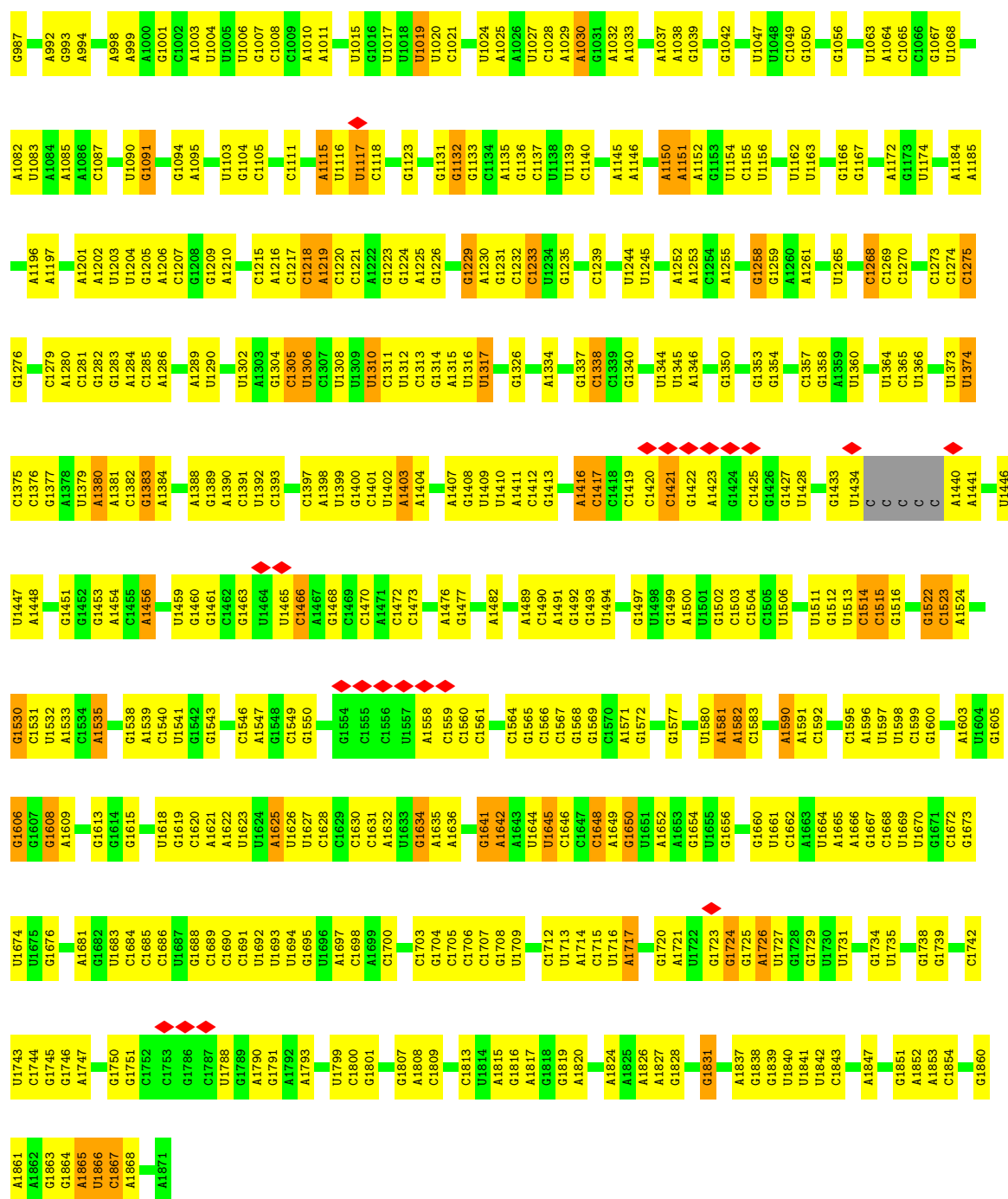


- Molecule 68: Large ribosomal subunit protein eL28



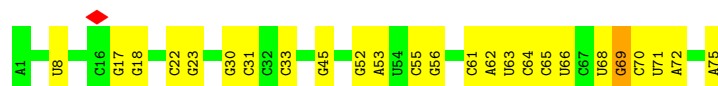
- Molecule 69: 18S ribosomal RNA





- Molecule 70: transfer RNA

Chain n2: 66% 33%

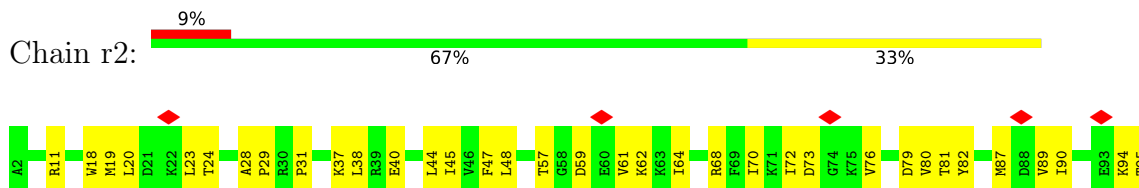


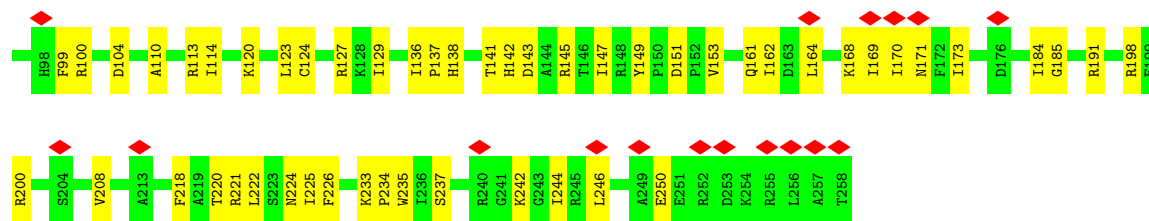
- Molecule 71: Small ribosomal subunit protein uS2

- Molecule 72: 40S ribosomal protein S3a

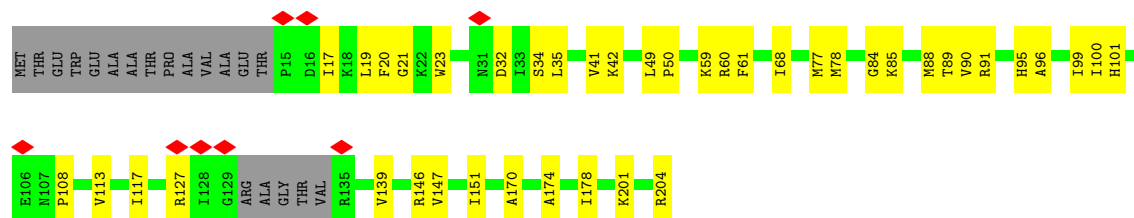
- Molecule 73: Small ribosomal subunit protein uS3

- Molecule 74: Small ribosomal subunit protein eS4

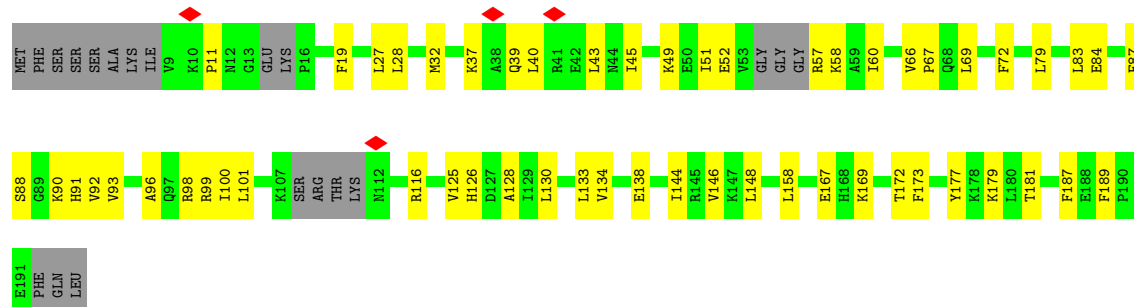




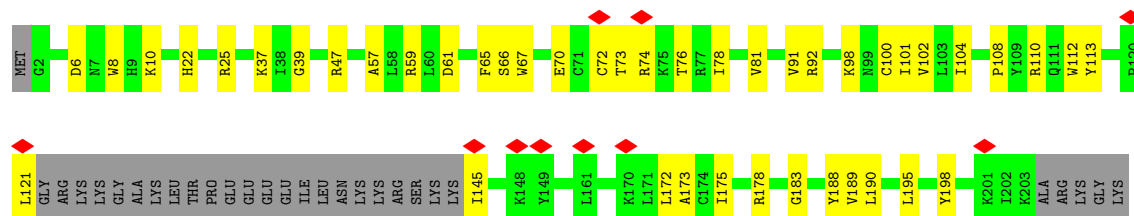
• Molecule 75: Small ribosomal subunit protein uS7



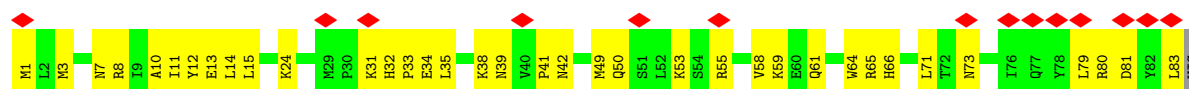
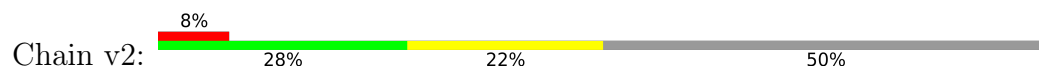
• Molecule 76: Small ribosomal subunit protein eS7



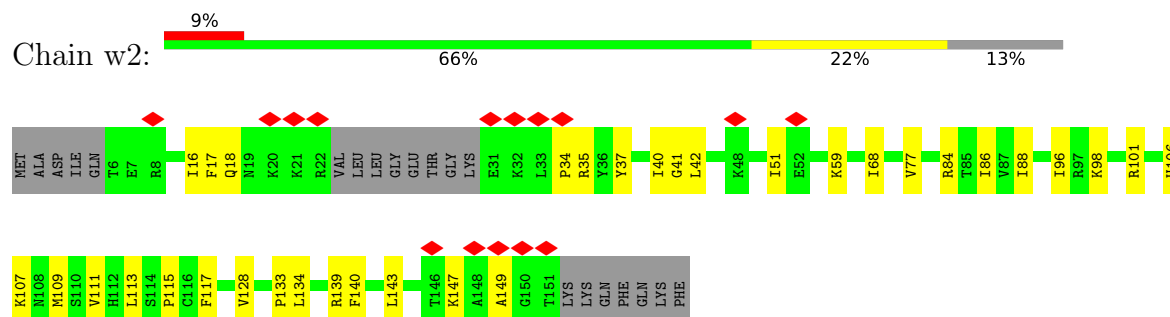
• Molecule 77: Small ribosomal subunit protein eS8



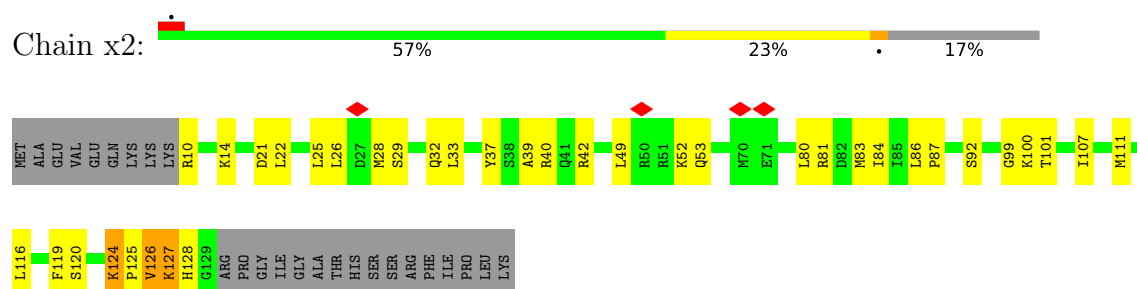
• Molecule 78: Small ribosomal subunit protein eS10



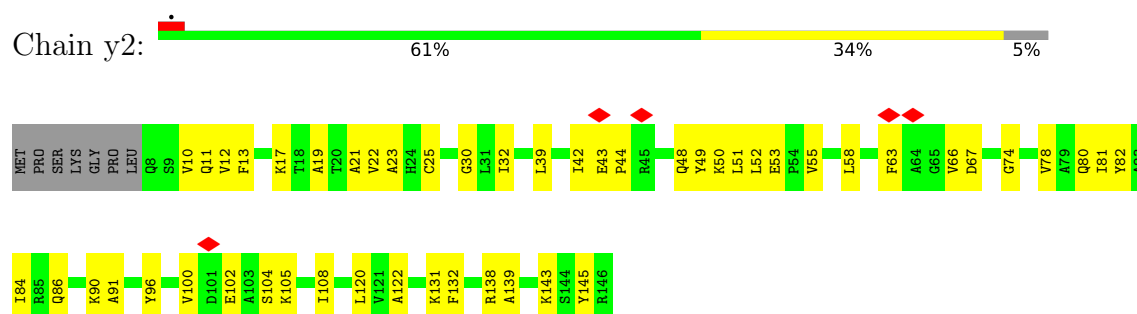
- Molecule 79: Small ribosomal subunit protein uS17



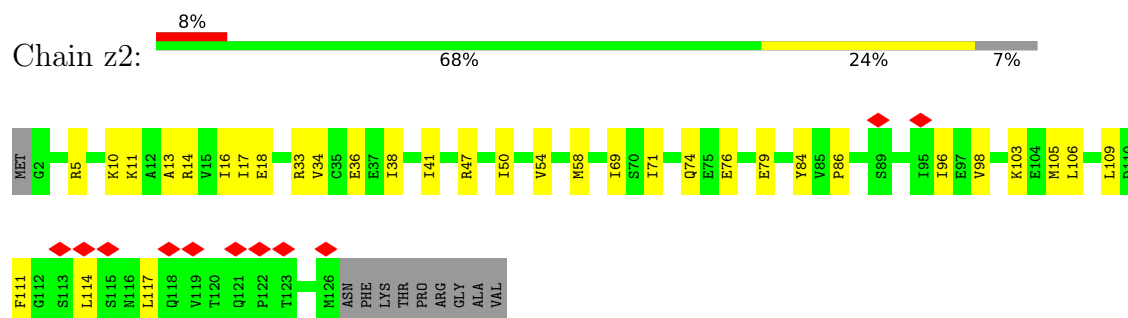
- Molecule 80: Small ribosomal subunit protein uS19



- Molecule 81: Small ribosomal subunit protein uS9



- Molecule 82: Small ribosomal subunit protein eS17



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	134861	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 ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2900	Depositor
Magnification	100000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	2.353	Depositor
Minimum map value	-0.049	Depositor
Average map value	0.014	Depositor
Map value standard deviation	0.085	Depositor
Recommended contour level	0.0823	Depositor
Map size (Å)	315.12, 315.12, 315.12	wwPDB
Map dimensions	312, 312, 312	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.01, 1.01, 1.01	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 4AC, ZN, 5MC, B8N, OMC, B8T, PSU, MG, OMG, UR3, OMU, 2MG, 1MA, A2M

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	A1	0.37	0/1877	0.38	0/2502
2	A2	0.44	0/82439	0.34	0/128559
3	A3	0.30	0/1172	0.45	1/1570 (0.1%)
4	B1	0.32	0/1799	0.44	0/2424
5	B2	0.45	0/2836	0.32	0/4421
6	B3	0.27	0/1109	0.46	0/1484
7	Bv	0.20	0/1576	0.29	0/2451
8	Bx	0.36	0/219	0.40	0/336
10	C1	0.32	0/1537	0.39	0/2065
11	C2	0.45	0/3675	0.32	0/5725
12	C3	0.23	0/778	0.35	0/1045
13	D1	0.34	0/1694	0.36	0/2261
14	D2	0.39	0/1914	0.39	0/2567
15	D3	0.30	0/596	0.38	0/800
16	E1	0.29	0/1420	0.43	0/1899
17	E2	0.36	0/3305	0.43	1/4422 (0.0%)
18	E3	0.29	0/1097	0.40	0/1464
19	F1	0.34	0/1674	0.39	0/2241
20	F2	0.37	0/2877	0.42	0/3860
21	F3	0.37	0/786	0.45	0/1053
22	G1	0.32	0/1165	0.40	0/1558
23	G2	0.32	0/2435	0.38	0/3260
24	G3	0.25	0/436	0.33	0/582
25	H1	0.45	0/1746	0.39	0/2338
26	H2	0.28	0/1799	0.37	0/2413
27	H3	0.35	0/437	0.47	0/580
28	I2	0.39	0/1648	0.40	0/2203
29	I3	0.21	0/1827	0.43	0/2467
30	J2	0.37	0/1268	0.41	0/1700
31	J3	0.31	0/1626	0.46	0/2211
32	K2	0.40	0/1535	0.41	0/2048
33	K3	0.20	0/1728	0.39	0/2295

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
34	L2	0.33	0/1424	0.33	0/1884
35	L3	0.22	0/1520	0.40	0/2030
36	M2	0.38	0/1490	0.43	0/2000
37	M3	0.12	0/527	0.34	0/718
38	N2	0.35	0/1327	0.35	0/1771
39	N3	0.30	0/1226	0.40	0/1649
40	O2	0.21	0/839	0.32	0/1126
41	O3	0.31	0/1016	0.43	0/1363
42	P2	0.36	0/983	0.40	0/1319
43	P3	0.33	0/1044	0.42	0/1398
44	Q2	0.36	0/532	0.34	0/708
45	Q3	0.16	0/997	0.42	0/1325
46	R2	0.34	0/984	0.38	0/1323
47	R3	0.23	0/591	0.38	0/794
48	S2	0.32	0/1132	0.37	0/1504
49	S3	0.24	0/629	0.36	0/841
50	T2	0.31	0/1130	0.33	0/1507
51	T3	0.18	0/358	0.31	0/467
52	U2	0.38	0/1193	0.39	0/1593
53	V2	0.31	0/963	0.36	0/1275
54	W2	0.31	0/742	0.34	0/996
55	X2	0.35	0/903	0.37	0/1216
56	Y2	0.39	0/1071	0.36	0/1429
57	Z2	0.39	0/895	0.42	0/1198
58	a2	0.39	0/864	0.44	0/1152
59	b2	0.30	0/1009	0.37	0/1332
60	c2	0.28	0/843	0.33	0/1115
61	d2	0.41	0/720	0.44	0/952
62	e2	0.26	0/574	0.30	0/760
63	f2	0.36	0/454	0.29	0/599
64	g2	0.32	0/435	0.32	0/575
65	h2	0.39	0/231	0.52	0/294
66	i2	0.34	0/855	0.39	0/1128
67	j2	0.39	0/704	0.37	0/935
68	k2	0.38	0/1016	0.40	0/1363
69	m2	0.41	0/38048	0.33	0/59291
70	n2	0.26	0/1746	0.23	0/2717
71	o2	0.31	0/1741	0.46	0/2366
72	p2	0.30	0/1749	0.40	0/2340
73	q2	0.24	0/1681	0.40	0/2261
74	r2	0.24	0/2072	0.42	0/2793
75	s2	0.27	0/1489	0.44	0/1999
76	t2	0.27	0/1341	0.48	0/1803

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
77	u2	0.25	0/1424	0.38	0/1918
78	v2	0.24	0/725	0.55	0/974
79	w2	0.29	0/1154	0.36	0/1543
80	x2	0.34	0/1018	0.48	0/1359
81	y2	0.29	0/1126	0.46	0/1506
82	z2	0.24	0/1023	0.39	0/1373
All	All	0.39	0/219588	0.36	2/322686 (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
17	E2	0	2
60	c2	0	1
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A3	100	ALA	CB-CA-C	-5.38	109.91	117.23
17	E2	259	PRO	N-CA-C	-5.07	102.03	112.47

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	E2	258	HIS	Peptide
17	E2	259	PRO	Peptide
60	c2	63	VAL	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A1	1843	0	1975	52	0
2	A2	75341	0	38147	864	0
3	A3	1154	0	1210	43	0
4	B1	1764	0	1892	46	0
5	B2	2538	0	1286	20	0
6	B3	1091	0	1130	42	0
7	Bv	1412	0	716	22	0
8	Bx	200	0	101	3	0
9	By	110	0	31	0	0
10	C1	1519	0	1603	30	0
11	C2	3315	0	1685	23	0
12	C3	769	0	837	21	0
13	D1	1656	0	1706	29	0
14	D2	1876	0	1970	33	0
15	D3	589	0	566	16	0
16	E1	1397	0	1425	30	0
17	E2	3238	0	3380	61	0
18	E3	1080	0	1147	23	0
19	F1	1643	0	1750	36	0
20	F2	2823	0	2996	56	0
21	F3	774	0	821	16	0
22	G1	1143	0	1219	20	0
23	G2	2389	0	2420	48	0
24	G3	435	0	461	12	0
25	H1	1701	0	1749	41	0
26	H2	1766	0	1902	30	0
27	H3	427	0	426	22	0
28	I2	1618	0	1775	31	0
29	I3	1800	0	1770	64	0
30	J2	1242	0	1274	27	0
31	J3	1590	0	1606	43	0
32	K2	1511	0	1636	35	0
33	K3	1708	0	1864	63	0
34	L2	1408	0	1550	22	0
35	L3	1495	0	1615	57	0
36	M2	1450	0	1488	29	0
37	M3	525	0	439	8	0
38	N2	1299	0	1368	30	0
39	N3	1202	0	1289	31	0
40	O2	825	0	850	8	0
41	O3	1003	0	1028	31	0
42	P2	969	0	1031	22	0
43	P3	1027	0	1067	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	Q2	519	0	533	8	0
45	Q3	981	0	1039	42	0
46	R2	967	0	1040	21	0
47	R3	585	0	640	19	0
48	S2	1115	0	1205	25	0
49	S3	618	0	634	9	0
50	T2	1107	0	1182	16	0
51	T3	355	0	391	10	0
52	U2	1164	0	1213	23	0
53	V2	945	0	1037	14	0
54	W2	732	0	769	14	0
55	X2	888	0	930	26	0
56	Y2	1053	0	1147	14	0
57	Z2	876	0	912	14	0
58	a2	854	0	945	23	0
59	b2	1001	0	1138	19	0
60	c2	832	0	917	10	0
61	d2	705	0	737	13	0
62	e2	568	0	635	10	0
63	f2	444	0	483	10	0
64	g2	429	0	465	6	0
65	h2	230	0	276	5	0
66	i2	842	0	912	12	0
67	j2	694	0	738	18	0
68	k2	1001	0	1066	21	0
69	m2	34685	0	17531	556	0
70	n2	1562	0	797	15	0
71	o2	1704	0	1702	60	0
72	p2	1722	0	1794	41	0
73	q2	1655	0	1750	42	0
74	r2	2031	0	2138	60	0
75	s2	1468	0	1519	35	0
76	t2	1322	0	1365	39	0
77	u2	1397	0	1378	35	0
78	v2	705	0	722	31	0
79	w2	1134	0	1197	27	0
80	x2	999	0	1046	37	0
81	y2	1109	0	1174	39	0
82	z2	1011	0	1063	25	0
83	A2	84	0	0	0	0
83	E3	1	0	0	0	0
83	H1	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
83	P2	1	0	0	0	0
83	d2	1	0	0	0	0
83	m2	35	0	0	0	0
84	F3	1	0	0	0	0
84	H3	1	0	0	0	0
84	d2	1	0	0	0	0
84	g2	1	0	0	0	0
84	i2	1	0	0	0	0
84	j2	1	0	0	0	0
85	m2	28	0	0	1	0
86	m2	23	0	13	2	0
87	B1	1	0	0	0	0
All	All	206855	0	152374	3151	0

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

The worst 5 of 3151 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A2:3348:A:H62	2:A2:3479:G:N2	1.34	1.24
2:A2:3348:A:N6	2:A2:3479:G:H21	1.35	1.23
2:A2:444:G:H1	2:A2:1117:A:N6	1.59	1.00
69:m2:153:G:H1	69:m2:165:G:H22	1.08	0.99
69:m2:1731:U:H3	69:m2:1807:G:H1	1.11	0.95

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A1	220/270 (82%)	213 (97%)	7 (3%)	0	100	100
3	A3	137/152 (90%)	120 (88%)	16 (12%)	1 (1%)	18	49
4	B1	214/266 (80%)	207 (97%)	7 (3%)	0	100	100
6	B3	136/145 (94%)	127 (93%)	9 (7%)	0	100	100
10	C1	188/192 (98%)	182 (97%)	6 (3%)	0	100	100
12	C3	95/119 (80%)	91 (96%)	4 (4%)	0	100	100
13	D1	200/214 (94%)	194 (97%)	6 (3%)	0	100	100
14	D2	243/257 (95%)	229 (94%)	14 (6%)	0	100	100
15	D3	81/83 (98%)	75 (93%)	6 (7%)	0	100	100
16	E1	172/178 (97%)	165 (96%)	7 (4%)	0	100	100
17	E2	400/403 (99%)	383 (96%)	17 (4%)	0	100	100
18	E3	137/142 (96%)	124 (90%)	13 (10%)	0	100	100
19	F1	201/211 (95%)	189 (94%)	12 (6%)	0	100	100
20	F2	350/419 (84%)	334 (95%)	16 (5%)	0	100	100
21	F3	95/114 (83%)	89 (94%)	6 (6%)	0	100	100
22	G1	137/217 (63%)	134 (98%)	3 (2%)	0	100	100
23	G2	291/297 (98%)	283 (97%)	8 (3%)	0	100	100
24	G3	52/69 (75%)	52 (100%)	0	0	100	100
25	H1	201/204 (98%)	195 (97%)	6 (3%)	0	100	100
26	H2	212/296 (72%)	207 (98%)	5 (2%)	0	100	100
27	H3	49/56 (88%)	44 (90%)	5 (10%)	0	100	100
28	I2	196/203 (97%)	190 (97%)	6 (3%)	0	100	100
29	I3	208/317 (66%)	183 (88%)	24 (12%)	1 (0%)	24	57
30	J2	151/184 (82%)	145 (96%)	6 (4%)	0	100	100
31	J3	215/293 (73%)	192 (89%)	22 (10%)	1 (0%)	24	57
32	K2	184/188 (98%)	172 (94%)	12 (6%)	0	100	100
33	K3	205/249 (82%)	200 (98%)	5 (2%)	0	100	100
34	L2	167/196 (85%)	164 (98%)	3 (2%)	0	100	100
35	L3	177/194 (91%)	158 (89%)	18 (10%)	1 (1%)	21	52
36	M2	173/176 (98%)	163 (94%)	10 (6%)	0	100	100
37	M3	74/132 (56%)	66 (89%)	8 (11%)	0	100	100
38	N2	157/160 (98%)	154 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	N3	147/151 (97%)	131 (89%)	16 (11%)	0	100	100
40	O2	99/128 (77%)	98 (99%)	1 (1%)	0	100	100
41	O3	133/151 (88%)	124 (93%)	9 (7%)	0	100	100
42	P2	127/140 (91%)	122 (96%)	5 (4%)	0	100	100
43	P3	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
44	Q2	60/157 (38%)	56 (93%)	4 (7%)	0	100	100
45	Q3	117/133 (88%)	108 (92%)	9 (8%)	0	100	100
46	R2	116/156 (74%)	113 (97%)	3 (3%)	0	100	100
47	R3	71/125 (57%)	67 (94%)	4 (6%)	0	100	100
48	S2	132/145 (91%)	128 (97%)	4 (3%)	0	100	100
49	S3	75/84 (89%)	70 (93%)	5 (7%)	0	100	100
50	T2	133/136 (98%)	131 (98%)	2 (2%)	0	100	100
51	T3	40/133 (30%)	39 (98%)	1 (2%)	0	100	100
52	U2	145/148 (98%)	137 (94%)	8 (6%)	0	100	100
53	V2	115/160 (72%)	112 (97%)	3 (3%)	0	100	100
54	W2	92/115 (80%)	89 (97%)	3 (3%)	0	100	100
55	X2	105/125 (84%)	100 (95%)	5 (5%)	0	100	100
56	Y2	126/135 (93%)	123 (98%)	3 (2%)	0	100	100
57	Z2	107/110 (97%)	105 (98%)	2 (2%)	0	100	100
58	a2	105/117 (90%)	102 (97%)	3 (3%)	0	100	100
59	b2	118/123 (96%)	117 (99%)	1 (1%)	0	100	100
60	c2	100/105 (95%)	97 (97%)	3 (3%)	0	100	100
61	d2	84/97 (87%)	80 (95%)	4 (5%)	0	100	100
62	e2	67/70 (96%)	67 (100%)	0	0	100	100
63	f2	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
64	g2	50/128 (39%)	49 (98%)	1 (2%)	0	100	100
65	h2	22/25 (88%)	22 (100%)	0	0	100	100
66	i2	101/105 (96%)	96 (95%)	5 (5%)	0	100	100
67	j2	87/92 (95%)	84 (97%)	3 (3%)	0	100	100
68	k2	123/137 (90%)	118 (96%)	5 (4%)	0	100	100
71	o2	213/295 (72%)	197 (92%)	16 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
72	p2	210/264 (80%)	190 (90%)	20 (10%)	0	100	100
73	q2	211/242 (87%)	206 (98%)	5 (2%)	0	100	100
74	r2	255/257 (99%)	234 (92%)	21 (8%)	0	100	100
75	s2	181/204 (89%)	169 (93%)	12 (7%)	0	100	100
76	t2	166/194 (86%)	149 (90%)	17 (10%)	0	100	100
77	u2	175/208 (84%)	166 (95%)	9 (5%)	0	100	100
78	v2	81/165 (49%)	64 (79%)	16 (20%)	1 (1%)	10	37
79	w2	134/158 (85%)	124 (92%)	10 (8%)	0	100	100
80	x2	118/145 (81%)	109 (92%)	9 (8%)	0	100	100
81	y2	137/146 (94%)	121 (88%)	16 (12%)	0	100	100
82	z2	123/135 (91%)	115 (94%)	8 (6%)	0	100	100
All	All	10694/12621 (85%)	10120 (95%)	569 (5%)	5 (0%)	100	100

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A3	91	LYS
29	I3	52	TYR
31	J3	77	SER
78	v2	42	ASN
35	L3	122	SER

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	A1	193/234 (82%)	193 (100%)	0	100	100
3	A3	121/132 (92%)	121 (100%)	0	100	100
4	B1	189/223 (85%)	187 (99%)	2 (1%)	65	78
6	B3	111/115 (96%)	111 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	C1	169/171 (99%)	169 (100%)	0	100	100
12	C3	90/107 (84%)	90 (100%)	0	100	100
13	D1	174/181 (96%)	174 (100%)	0	100	100
14	D2	188/199 (94%)	188 (100%)	0	100	100
15	D3	53/67 (79%)	53 (100%)	0	100	100
16	E1	147/149 (99%)	147 (100%)	0	100	100
17	E2	347/348 (100%)	347 (100%)	0	100	100
18	E3	111/114 (97%)	111 (100%)	0	100	100
19	F1	170/178 (96%)	170 (100%)	0	100	100
20	F2	298/348 (86%)	298 (100%)	0	100	100
21	F3	84/97 (87%)	84 (100%)	0	100	100
22	G1	118/157 (75%)	118 (100%)	0	100	100
23	G2	246/249 (99%)	246 (100%)	0	100	100
24	G3	49/62 (79%)	49 (100%)	0	100	100
25	H1	171/172 (99%)	171 (100%)	0	100	100
26	H2	196/256 (77%)	196 (100%)	0	100	100
27	H3	45/49 (92%)	45 (100%)	0	100	100
28	I2	170/173 (98%)	170 (100%)	0	100	100
29	I3	197/275 (72%)	197 (100%)	0	100	100
30	J2	134/163 (82%)	134 (100%)	0	100	100
31	J3	155/224 (69%)	155 (100%)	0	100	100
32	K2	164/165 (99%)	164 (100%)	0	100	100
33	K3	182/218 (84%)	182 (100%)	0	100	100
34	L2	149/175 (85%)	149 (100%)	0	100	100
35	L3	160/168 (95%)	160 (100%)	0	100	100
36	M2	155/156 (99%)	155 (100%)	0	100	100
37	M3	35/108 (32%)	35 (100%)	0	100	100
38	N2	139/140 (99%)	139 (100%)	0	100	100
39	N3	130/131 (99%)	130 (100%)	0	100	100
40	O2	91/114 (80%)	91 (100%)	0	100	100
41	O3	103/119 (87%)	103 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	P2	100/107 (94%)	100 (100%)	0	100	100
43	P3	110/113 (97%)	110 (100%)	0	100	100
44	Q2	54/126 (43%)	54 (100%)	0	100	100
45	Q3	103/115 (90%)	103 (100%)	0	100	100
46	R2	106/133 (80%)	106 (100%)	0	100	100
47	R3	65/103 (63%)	65 (100%)	0	100	100
48	S2	124/135 (92%)	124 (100%)	0	100	100
49	S3	71/76 (93%)	71 (100%)	0	100	100
50	T2	117/118 (99%)	117 (100%)	0	100	100
51	T3	35/105 (33%)	35 (100%)	0	100	100
52	U2	120/121 (99%)	120 (100%)	0	100	100
53	V2	98/124 (79%)	98 (100%)	0	100	100
54	W2	79/97 (81%)	79 (100%)	0	100	100
55	X2	98/110 (89%)	98 (100%)	0	100	100
56	Y2	114/121 (94%)	114 (100%)	0	100	100
57	Z2	88/89 (99%)	88 (100%)	0	100	100
58	a2	93/100 (93%)	93 (100%)	0	100	100
59	b2	108/110 (98%)	108 (100%)	0	100	100
60	c2	86/89 (97%)	86 (100%)	0	100	100
61	d2	73/80 (91%)	73 (100%)	0	100	100
62	e2	64/65 (98%)	64 (100%)	0	100	100
63	f2	47/48 (98%)	47 (100%)	0	100	100
64	g2	48/116 (41%)	48 (100%)	0	100	100
65	h2	23/24 (96%)	23 (100%)	0	100	100
66	i2	91/93 (98%)	91 (100%)	0	100	100
67	j2	73/75 (97%)	73 (100%)	0	100	100
68	k2	109/121 (90%)	109 (100%)	0	100	100
71	o2	180/242 (74%)	180 (100%)	0	100	100
72	p2	193/229 (84%)	193 (100%)	0	100	100
73	q2	176/201 (88%)	176 (100%)	0	100	100
74	r2	220/220 (100%)	220 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
75	s2	157/170 (92%)	157 (100%)	0	100	100
76	t2	132/174 (76%)	132 (100%)	0	100	100
77	u2	137/180 (76%)	137 (100%)	0	100	100
78	v2	75/136 (55%)	75 (100%)	0	100	100
79	w2	125/142 (88%)	125 (100%)	0	100	100
80	x2	109/130 (84%)	105 (96%)	4 (4%)	30	61
81	y2	115/121 (95%)	115 (100%)	0	100	100
82	z2	113/121 (93%)	113 (100%)	0	100	100
All	All	9263/10717 (86%)	9257 (100%)	6 (0%)	87	90

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
80	x2	125	PRO
80	x2	126	VAL
80	x2	127	LYS
4	B1	137[B]	ARG
4	B1	137[A]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 107 such sidechains are listed below:

Mol	Chain	Res	Type
35	L3	134	HIS
53	V2	6	ASN
77	u2	181	GLN
36	M2	50	GLN
45	Q3	94	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	C2	155/156 (99%)	28 (18%)	0
2	A2	3484/3615 (96%)	679 (19%)	13 (0%)
5	B2	118/121 (97%)	11 (9%)	0
69	m2	1612/1633 (98%)	391 (24%)	0
7	Bv	63/76 (82%)	28 (44%)	0
70	n2	70/73 (95%)	8 (11%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	Bx	9/10 (90%)	4 (44%)	0
All	All	5511/5684 (96%)	1149 (20%)	13 (0%)

5 of 1149 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	A2	2	G
2	A2	13	U
2	A2	17	A
2	A2	21	G
2	A2	25	A

5 of 13 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	A2	3253	G
2	A2	3532	A
2	A2	4582	U
2	A2	4277	C
2	A2	4351	U

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

105 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	$\# Z > 2$
2	5MC	A2	4099	2	18,22,23	0.47	0	26,32,35	0.61	0
2	OMC	A2	2559	2	19,22,23	0.42	0	26,31,34	0.38	0
69	A2M	m2	578	69	22,25,26	0.10	0	31,36,39	0.27	0
2	PSU	A2	3371	2	18,21,22	0.61	0	22,30,33	0.57	0
2	OMC	A2	2106	2	19,22,23	0.36	0	26,31,34	0.40	0
2	1MA	A2	4067	2	21,25,26	0.41	0	31,37,40	0.45	0
2	OMC	A2	3525	2	19,22,23	0.38	0	26,31,34	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
69	PSU	m2	824	69	18,21,22	0.58	0	22,30,33	0.64	1 (4%)
2	PSU	A2	3945	2	18,21,22	0.61	0	22,30,33	0.60	0
69	OMU	m2	172	69	19,22,23	0.29	0	26,31,34	0.58	1 (3%)
2	OMU	A2	4272	2	19,22,23	0.48	0	26,31,34	0.68	0
2	PSU	A2	4094	2	18,21,22	0.67	1 (5%)	22,30,33	0.58	0
69	A2M	m2	1680	69	22,25,26	0.16	0	31,36,39	0.23	0
2	A2M	A2	398	2	22,25,26	0.14	0	31,36,39	0.36	0
2	OMG	A2	3400	2	23,26,27	0.40	0	33,38,41	0.37	0
69	OMG	m2	646	69	23,26,27	0.49	0	33,38,41	0.39	0
2	OMG	A2	1438	2	23,26,27	0.34	0	33,38,41	0.39	0
69	OMG	m2	603	69	23,26,27	0.43	0	33,38,41	0.32	0
69	PSU	m2	614	69	18,21,22	0.60	1 (5%)	22,30,33	0.63	1 (4%)
69	B8T	m2	1339	69	19,22,23	0.48	0	26,31,34	0.42	0
69	PSU	m2	825	69	18,21,22	0.57	0	22,30,33	0.61	1 (4%)
2	OMC	A2	2579	2	19,22,23	0.39	0	26,31,34	0.42	0
2	OMC	A2	3543	2	19,22,23	0.38	0	26,31,34	0.46	0
2	PSU	A2	1395	2	18,21,22	0.73	1 (5%)	22,30,33	0.53	0
2	OMG	A2	3555	2,83	23,26,27	0.49	0	33,38,41	0.51	0
2	A2M	A2	3481	2	22,25,26	0.15	0	31,36,39	0.27	0
2	A2M	A2	1337	2	22,25,26	0.21	0	31,36,39	0.52	0
2	PSU	A2	1490	2	18,21,22	0.75	1 (5%)	22,30,33	0.42	0
69	OMG	m2	685	69	23,26,27	0.49	0	33,38,41	0.44	0
69	OMG	m2	511	69,83	23,26,27	0.35	0	33,38,41	0.43	0
2	A2M	A2	1347	2,83	22,25,26	0.13	0	31,36,39	0.53	0
2	OMC	A2	3357	2	19,22,23	0.34	0	26,31,34	0.49	0
2	OMC	A2	3464	2	19,22,23	0.37	0	26,31,34	0.40	0
2	A2M	A2	3374	2	22,25,26	0.15	0	31,36,39	0.37	0
2	OMU	A2	4150	2	19,22,23	0.34	0	26,31,34	0.50	0
2	OMG	A2	4044	2	23,26,27	0.45	0	33,38,41	0.35	0
69	OMU	m2	116	69	19,22,23	0.33	0	26,31,34	0.43	0
2	OMG	A2	2119	2	23,26,27	0.47	0	33,38,41	0.44	0
2	OMU	A2	3581	2	19,22,23	0.41	0	26,31,34	0.62	0
2	PSU	A2	4152	2	18,21,22	0.58	0	22,30,33	0.63	0
2	OMU	A2	2592	2	19,22,23	0.39	0	26,31,34	0.63	0
2	PSU	A2	2263	2	18,21,22	0.66	0	22,30,33	0.56	0
2	OMG	A2	1130	2	23,26,27	0.52	0	33,38,41	0.60	1 (3%)
2	OMC	A2	2120	2	19,22,23	0.40	0	26,31,34	0.48	0
69	OMC	m2	355	69	19,22,23	0.37	0	26,31,34	0.41	0
2	A2M	A2	4223	2	22,25,26	0.14	0	31,36,39	0.18	0
69	A2M	m2	27	69	22,25,26	0.20	0	31,36,39	0.30	0
69	A2M	m2	486	69	22,25,26	0.12	0	31,36,39	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	A2M	A2	1140	2	22,25,26	0.15	0	31,36,39	0.25	0
2	A2M	A2	3441	2	22,25,26	0.16	0	31,36,39	0.35	0
2	OMU	A2	3474	2	19,22,23	0.38	0	26,31,34	0.38	0
2	PSU	A2	4280	2	18,21,22	0.63	1 (5%)	22,30,33	0.57	0
2	PSU	A2	3385	2	18,21,22	0.63	0	22,30,33	0.56	0
69	OMC	m2	519	69	19,22,23	0.35	0	26,31,34	0.49	0
2	A2M	A2	2542	2	22,25,26	0.19	0	31,36,39	0.30	0
69	OMU	m2	121	69	19,22,23	0.37	0	26,31,34	0.48	0
2	OMG	A2	4275	2	23,26,27	0.46	0	33,38,41	0.52	0
2	PSU	A2	4183	2	18,21,22	0.63	0	22,30,33	0.42	0
2	5MC	A2	3438	2,83	18,22,23	0.39	0	26,32,35	0.45	0
2	OMG	A2	4289	2	23,26,27	0.47	0	33,38,41	0.40	0
2	OMC	A2	4188	2	19,22,23	0.42	0	26,31,34	0.53	0
2	OMC	A2	1683	2,83	19,22,23	0.42	0	26,31,34	0.63	0
2	OMC	A2	3497	2	19,22,23	0.40	0	26,31,34	0.36	0
69	OMU	m2	430	69	19,22,23	0.32	0	26,31,34	0.47	0
2	OMG	A2	3283	2	23,26,27	0.43	0	33,38,41	0.53	0
2	PSU	A2	4288	2	18,21,22	0.61	0	22,30,33	0.60	0
2	A2M	A2	4175	2,83	22,25,26	0.19	0	31,36,39	0.44	0
69	PSU	m2	1083	69	18,21,22	0.65	1 (5%)	22,30,33	0.67	0
2	A2M	A2	2156	2	22,25,26	0.18	0	31,36,39	0.21	0
2	OMC	A2	1154	2	19,22,23	0.40	0	26,31,34	0.57	0
2	A2M	A2	1137	2	22,25,26	0.13	0	31,36,39	0.26	0
69	A2M	m2	1033	69	22,25,26	0.18	0	31,36,39	0.29	0
69	OMG	m2	438	69	23,26,27	0.43	0	33,38,41	0.39	0
69	OMC	m2	1705	69	19,22,23	0.34	0	26,31,34	0.47	0
2	OMG	A2	3880	2	23,26,27	0.38	0	33,38,41	0.49	0
69	A2M	m2	670	69,83	22,25,26	0.21	0	31,36,39	0.29	0
2	A2M	A2	2118	2,83	22,25,26	0.16	0	31,36,39	0.24	0
2	PSU	A2	4055	2	18,21,22	0.69	1 (5%)	22,30,33	0.59	1 (4%)
2	OMG	A2	2179	2	23,26,27	0.42	0	33,38,41	0.40	0
2	A2M	A2	3380	2	22,25,26	0.13	0	31,36,39	0.31	0
2	OMG	A2	4022	2	23,26,27	0.46	0	33,38,41	0.39	0
2	OMG	A2	1335	2	23,26,27	0.45	0	33,38,41	0.40	0
2	A2M	A2	3486	2	22,25,26	0.17	0	31,36,39	0.44	0
2	OMC	A2	4108	2	19,22,23	0.40	0	26,31,34	0.39	0
2	OMC	A2	2177	2,83	19,22,23	0.39	0	26,31,34	0.38	0
2	OMG	A2	4151	2	23,26,27	0.40	0	33,38,41	0.46	0
69	PSU	m2	1245	69	18,21,22	0.65	0	22,30,33	0.58	0
2	A2M	A2	2570	2	22,25,26	0.19	0	31,36,39	0.26	0
2	OMC	A2	2616	2	19,22,23	0.35	0	26,31,34	0.42	0
2	OMU	A2	3958	2	19,22,23	0.40	0	26,31,34	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PSU	A2	4102	2,83	18,21,22	0.68	1 (5%)	22,30,33	0.38	0
69	OMG	m2	869	69	23,26,27	0.35	0	33,38,41	0.34	0
2	OMG	A2	3448	2	23,26,27	0.42	0	33,38,41	0.32	0
69	A2M	m2	99	69,83	22,25,26	0.15	0	31,36,39	0.40	0
2	OMG	A2	4146	2	23,26,27	0.44	0	33,38,41	0.40	0
69	OMC	m2	174	69	19,22,23	0.38	0	26,31,34	0.52	0
69	UR3	m2	1832	69,83	19,22,23	0.41	0	26,32,35	0.37	0
2	A2M	A2	4270	2	22,25,26	0.20	0	31,36,39	0.50	1 (3%)
11	OMG	C2	75	11	23,26,27	0.44	0	33,38,41	0.37	0
2	A2M	A2	1673	2	22,25,26	0.18	0	31,36,39	0.41	0
2	OMG	A2	3848	2	23,26,27	0.43	0	33,38,41	0.43	0
69	OMG	m2	1330	69	23,26,27	0.39	0	33,38,41	0.39	0
69	A2M	m2	514	69	22,25,26	0.16	0	31,36,39	0.26	0
2	2MG	A2	1330	2	23,26,27	0.46	0	32,38,41	0.41	0
2	PSU	A2	1496	2	18,21,22	0.66	0	22,30,33	0.67	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
2	5MC	A2	4099	2	-	3/7/25/26	0/2/2/2
2	OMC	A2	2559	2	-	0/9/27/28	0/2/2/2
69	A2M	m2	578	69	-	2/9/27/28	0/3/3/3
2	PSU	A2	3371	2	-	0/7/25/26	0/2/2/2
2	OMC	A2	2106	2	-	2/9/27/28	0/2/2/2
2	1MA	A2	4067	2	-	2/7/25/26	0/3/3/3
2	OMC	A2	3525	2	-	0/9/27/28	0/2/2/2
69	PSU	m2	824	69	-	0/7/25/26	0/2/2/2
2	PSU	A2	3945	2	-	0/7/25/26	0/2/2/2
69	OMU	m2	172	69	-	3/9/27/28	0/2/2/2
2	OMU	A2	4272	2	-	3/9/27/28	0/2/2/2
2	PSU	A2	4094	2	-	0/7/25/26	0/2/2/2
69	A2M	m2	1680	69	-	1/9/27/28	0/3/3/3
2	A2M	A2	398	2	-	2/9/27/28	0/3/3/3
2	OMG	A2	3400	2	-	0/9/27/28	0/3/3/3
69	OMG	m2	646	69	-	3/9/27/28	0/3/3/3
2	OMG	A2	1438	2	-	1/9/27/28	0/3/3/3
69	OMG	m2	603	69	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
69	PSU	m2	614	69	-	0/7/25/26	0/2/2/2
69	B8T	m2	1339	69	-	2/7/27/28	0/2/2/2
69	PSU	m2	825	69	-	0/7/25/26	0/2/2/2
2	OMC	A2	2579	2	-	1/9/27/28	0/2/2/2
2	OMC	A2	3543	2	-	1/9/27/28	0/2/2/2
2	PSU	A2	1395	2	-	0/7/25/26	0/2/2/2
2	OMG	A2	3555	2,83	-	0/9/27/28	0/3/3/3
2	A2M	A2	3481	2	-	0/9/27/28	0/3/3/3
2	A2M	A2	1337	2	-	1/9/27/28	0/3/3/3
2	PSU	A2	1490	2	-	4/7/25/26	0/2/2/2
69	OMG	m2	685	69	-	0/9/27/28	0/3/3/3
69	OMG	m2	511	69,83	-	0/9/27/28	0/3/3/3
2	A2M	A2	1347	2,83	-	3/9/27/28	0/3/3/3
2	OMC	A2	3357	2	-	4/9/27/28	0/2/2/2
2	OMC	A2	3464	2	-	0/9/27/28	0/2/2/2
2	A2M	A2	3374	2	-	0/9/27/28	0/3/3/3
2	OMU	A2	4150	2	-	0/9/27/28	0/2/2/2
2	OMG	A2	4044	2	-	0/9/27/28	0/3/3/3
69	OMU	m2	116	69	-	0/9/27/28	0/2/2/2
2	OMG	A2	2119	2	-	2/9/27/28	0/3/3/3
2	OMU	A2	3581	2	-	0/9/27/28	0/2/2/2
2	PSU	A2	4152	2	-	1/7/25/26	0/2/2/2
2	OMU	A2	2592	2	-	0/9/27/28	0/2/2/2
2	PSU	A2	2263	2	-	0/7/25/26	0/2/2/2
2	OMG	A2	1130	2	-	0/9/27/28	0/3/3/3
2	OMC	A2	2120	2	-	1/9/27/28	0/2/2/2
69	OMC	m2	355	69	-	1/9/27/28	0/2/2/2
2	A2M	A2	4223	2	-	0/9/27/28	0/3/3/3
69	A2M	m2	27	69	-	3/9/27/28	0/3/3/3
69	A2M	m2	486	69	-	0/9/27/28	0/3/3/3
2	A2M	A2	1140	2	-	3/9/27/28	0/3/3/3
2	A2M	A2	3441	2	-	5/9/27/28	0/3/3/3
2	OMU	A2	3474	2	-	2/9/27/28	0/2/2/2
2	PSU	A2	4280	2	-	2/7/25/26	0/2/2/2
2	PSU	A2	3385	2	-	0/7/25/26	0/2/2/2
69	OMC	m2	519	69	-	2/9/27/28	0/2/2/2
2	A2M	A2	2542	2	-	3/9/27/28	0/3/3/3
69	OMU	m2	121	69	-	0/9/27/28	0/2/2/2
2	OMG	A2	4275	2	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	A2	4183	2	-	2/7/25/26	0/2/2/2
2	5MC	A2	3438	2,83	-	0/7/25/26	0/2/2/2
2	OMG	A2	4289	2	-	3/9/27/28	0/3/3/3
2	OMC	A2	4188	2	-	0/9/27/28	0/2/2/2
2	OMC	A2	1683	2,83	-	0/9/27/28	0/2/2/2
2	OMC	A2	3497	2	-	1/9/27/28	0/2/2/2
69	OMU	m2	430	69	-	4/9/27/28	0/2/2/2
2	OMG	A2	3283	2	-	0/9/27/28	0/3/3/3
2	PSU	A2	4288	2	-	5/7/25/26	0/2/2/2
2	A2M	A2	4175	2,83	-	1/9/27/28	0/3/3/3
69	PSU	m2	1083	69	-	1/7/25/26	0/2/2/2
2	A2M	A2	2156	2	-	0/9/27/28	0/3/3/3
2	OMC	A2	1154	2	-	0/9/27/28	0/2/2/2
2	A2M	A2	1137	2	-	2/9/27/28	0/3/3/3
69	A2M	m2	1033	69	-	0/9/27/28	0/3/3/3
69	OMG	m2	438	69	-	0/9/27/28	0/3/3/3
69	OMC	m2	1705	69	-	0/9/27/28	0/2/2/2
2	OMG	A2	3880	2	-	1/9/27/28	0/3/3/3
69	A2M	m2	670	69,83	-	1/9/27/28	0/3/3/3
2	A2M	A2	2118	2,83	-	0/9/27/28	0/3/3/3
2	PSU	A2	4055	2	-	0/7/25/26	0/2/2/2
2	OMG	A2	2179	2	-	1/9/27/28	0/3/3/3
2	A2M	A2	3380	2	-	2/9/27/28	0/3/3/3
2	OMG	A2	4022	2	-	0/9/27/28	0/3/3/3
2	OMG	A2	1335	2	-	0/9/27/28	0/3/3/3
2	A2M	A2	3486	2	-	0/9/27/28	0/3/3/3
2	OMC	A2	4108	2	-	0/9/27/28	0/2/2/2
2	OMC	A2	2177	2,83	-	2/9/27/28	0/2/2/2
2	OMG	A2	4151	2	-	0/9/27/28	0/3/3/3
69	PSU	m2	1245	69	-	2/7/25/26	0/2/2/2
2	A2M	A2	2570	2	-	0/9/27/28	0/3/3/3
2	OMC	A2	2616	2	-	0/9/27/28	0/2/2/2
2	OMU	A2	3958	2	-	1/9/27/28	0/2/2/2
2	PSU	A2	4102	2,83	-	1/7/25/26	0/2/2/2
69	OMG	m2	869	69	-	0/9/27/28	0/3/3/3
2	OMG	A2	3448	2	-	0/9/27/28	0/3/3/3
69	A2M	m2	99	69,83	-	3/9/27/28	0/3/3/3
2	OMG	A2	4146	2	-	0/9/27/28	0/3/3/3
69	OMC	m2	174	69	-	2/9/27/28	0/2/2/2
69	UR3	m2	1832	69,83	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A2M	A2	4270	2	-	0/9/27/28	0/3/3/3
11	OMG	C2	75	11	-	2/9/27/28	0/3/3/3
2	A2M	A2	1673	2	-	0/9/27/28	0/3/3/3
2	OMG	A2	3848	2	-	0/9/27/28	0/3/3/3
69	OMG	m2	1330	69	-	0/9/27/28	0/3/3/3
69	A2M	m2	514	69	-	0/9/27/28	0/3/3/3
2	2MG	A2	1330	2	-	0/9/27/28	0/3/3/3
2	PSU	A2	1496	2	-	0/7/25/26	0/2/2/2

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A2	1490	PSU	O4'-C1'	-2.27	1.40	1.43
69	m2	1083	PSU	O4'-C1'	-2.27	1.40	1.43
2	A2	1395	PSU	O4'-C1'	-2.15	1.40	1.43
2	A2	4094	PSU	O4'-C1'	-2.15	1.40	1.43
2	A2	4102	PSU	O4'-C1'	-2.13	1.40	1.43

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
69	m2	614	PSU	O4'-C1'-C2'	2.21	108.26	105.14
69	m2	172	OMU	O2'-C2'-C1'	2.18	113.33	109.08
2	A2	4270	A2M	C2'-C3'-C4'	-2.17	97.28	101.99
69	m2	824	PSU	O4'-C1'-C2'	2.09	108.10	105.14
69	m2	825	PSU	O4'-C1'-C2'	2.05	108.04	105.14

There are no chirality outliers.

5 of 100 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	C2	75	OMG	O4'-C4'-C5'-O5'
11	C2	75	OMG	C3'-C4'-C5'-O5'
2	A2	398	A2M	C1'-C2'-O2'-CM'
2	A2	1140	A2M	O4'-C4'-C5'-O5'
2	A2	1140	A2M	C3'-C4'-C5'-O5'

There are no ring outliers.

46 monomers are involved in 64 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A2	4099	5MC	2	0
69	m2	578	A2M	2	0
2	A2	2106	OMC	1	0
2	A2	4067	1MA	1	0
69	m2	824	PSU	1	0
69	m2	172	OMU	1	0
2	A2	398	A2M	2	0
69	m2	646	OMG	1	0
69	m2	603	OMG	3	0
69	m2	825	PSU	2	0
2	A2	2579	OMC	1	0
2	A2	3543	OMC	1	0
2	A2	1490	PSU	1	0
69	m2	511	OMG	3	0
2	A2	3374	A2M	1	0
2	A2	4044	OMG	2	0
69	m2	116	OMU	3	0
2	A2	2119	OMG	1	0
2	A2	4152	PSU	1	0
69	m2	355	OMC	1	0
69	m2	486	A2M	2	0
2	A2	1140	A2M	1	0
2	A2	3441	A2M	1	0
69	m2	519	OMC	1	0
69	m2	121	OMU	3	0
2	A2	4275	OMG	1	0
2	A2	1683	OMC	1	0
2	A2	4288	PSU	1	0
2	A2	1154	OMC	2	0
69	m2	1033	A2M	1	0
69	m2	1705	OMC	2	0
2	A2	2118	A2M	1	0
2	A2	2179	OMG	2	0
2	A2	3380	A2M	1	0
2	A2	4108	OMC	1	0
2	A2	2177	OMC	1	0
2	A2	2570	A2M	2	0
2	A2	3958	OMU	1	0
69	m2	869	OMG	2	0
69	m2	99	A2M	1	0
2	A2	4146	OMG	1	0
69	m2	174	OMC	1	0
2	A2	1673	A2M	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A2	3848	OMG	1	0
69	m2	514	A2M	3	0
2	A2	1330	2MG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 131 ligands modelled in this entry, 129 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ 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	$\# Z > 2$
85	B8N	m2	1935	69	24,29,30	0.69	1 (4%)	29,42,45	0.66	1 (3%)
86	4AC	m2	1936	69	21,24,25	0.39	0	29,34,37	0.36	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
85	B8N	m2	1935	69	-	4/16/34/35	0/2/2/2
86	4AC	m2	1936	69	-	0/11/29/30	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	m2	1935	B8N	O4'-C1'	-2.09	1.40	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	m2	1935	B8N	O4'-C1'-C2'	2.03	108.01	105.14

There are no chirality outliers.

All (4) torsion outliers are listed below:

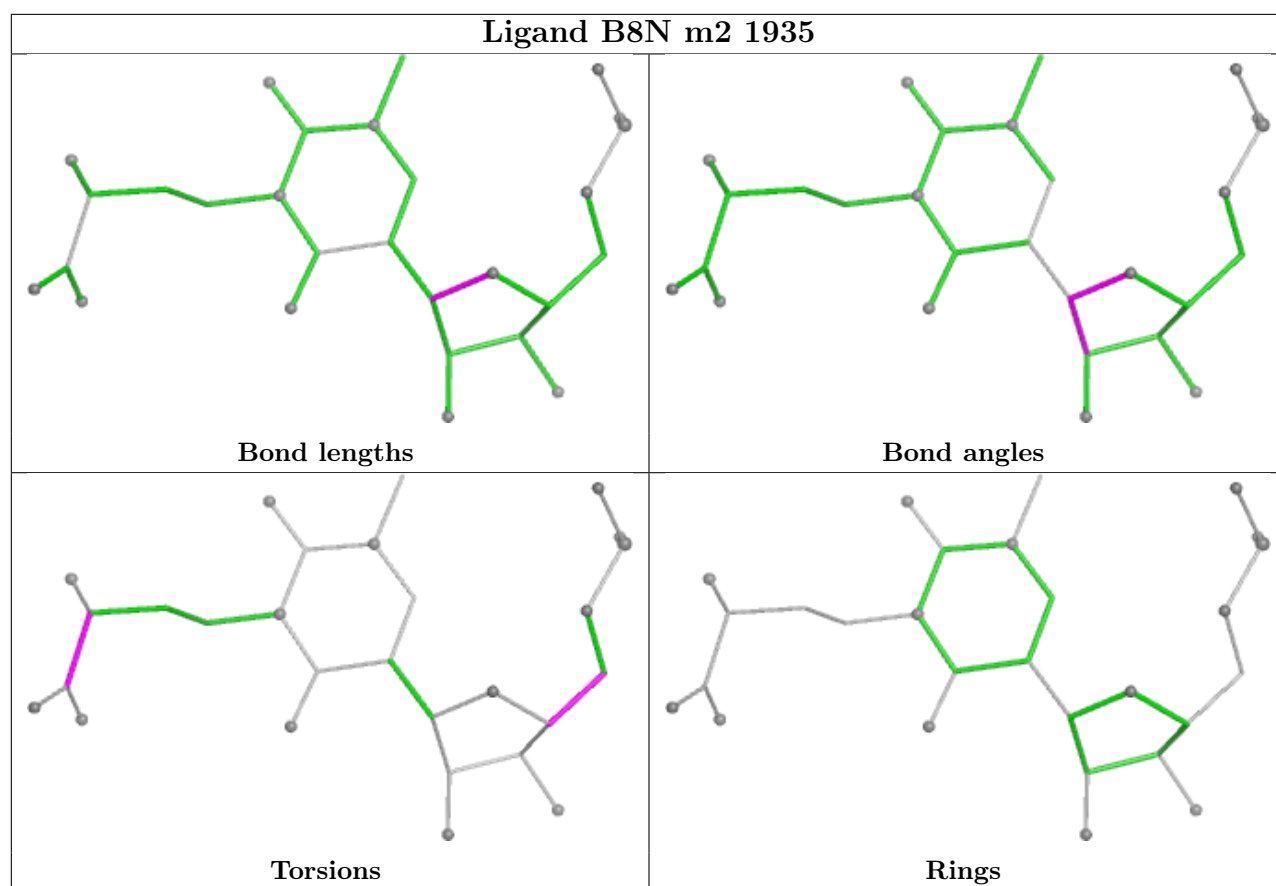
Mol	Chain	Res	Type	Atoms
85	m2	1935	B8N	O4'-C4'-C5'-O5'
85	m2	1935	B8N	C3'-C4'-C5'-O5'
85	m2	1935	B8N	N34-C33-C34-O36
85	m2	1935	B8N	N34-C33-C34-O35

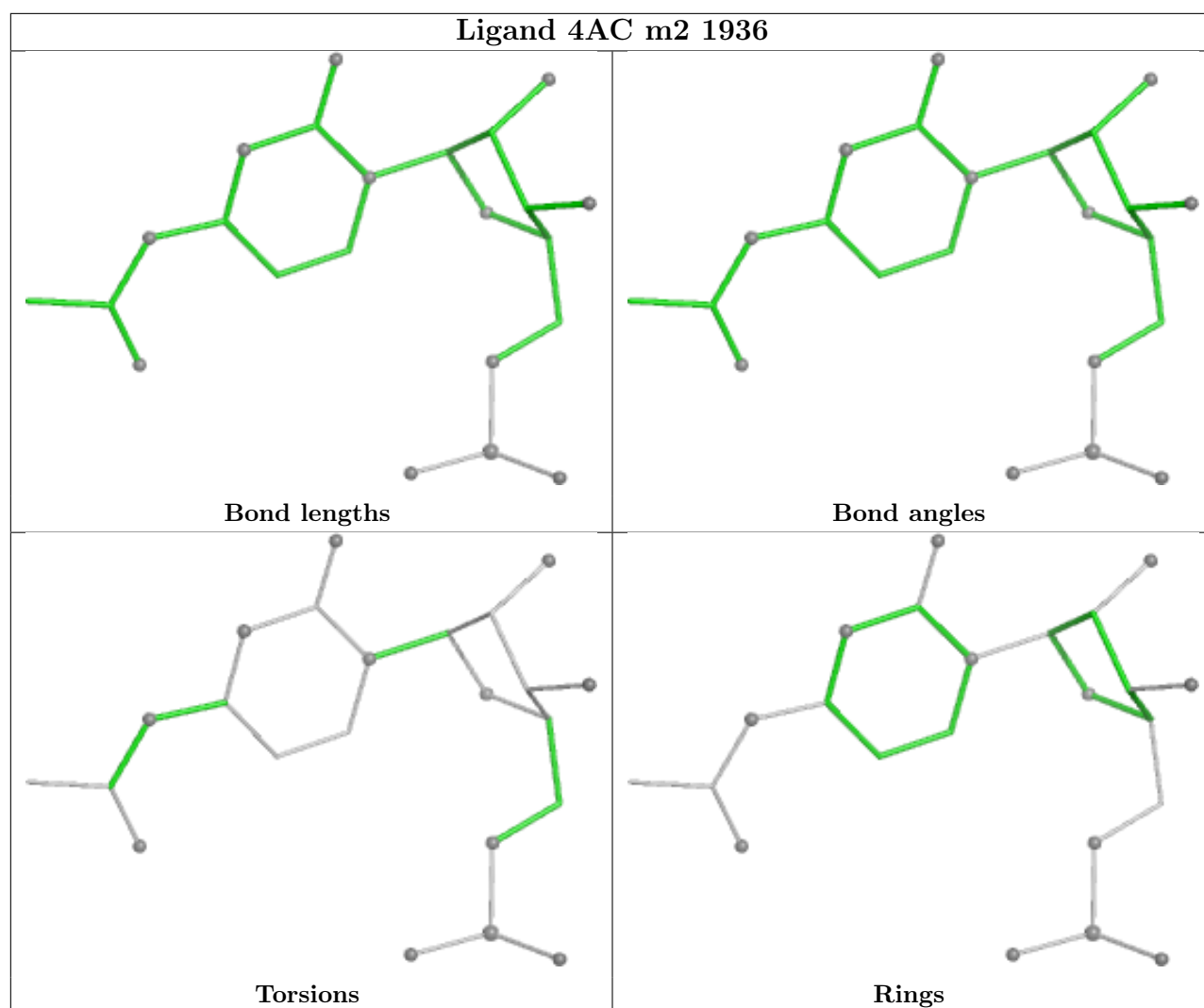
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
85	m2	1935	B8N	1	0
86	m2	1936	4AC	2	0

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	A2	15
69	m2	8
70	n2	2
51	T3	1
32	K2	1

The worst 5 of 27 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	m2	130:G	O3'	141:A	P	26.12
1	A2	1512:U	O3'	1521:A	P	25.45
1	m2	690:U	O3'	801:U	P	17.62
1	A2	4437:C	O3'	4493:G	P	17.51
1	m2	536:G	O3'	554:U	P	16.80

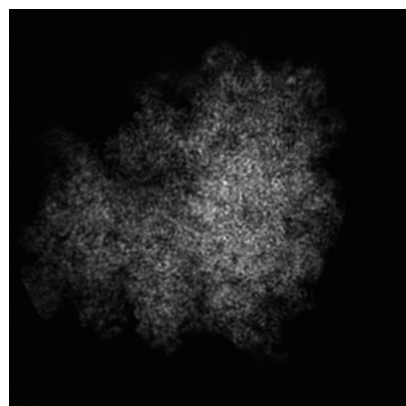
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53427. These allow visual inspection of the internal detail of the map and identification of artifacts.

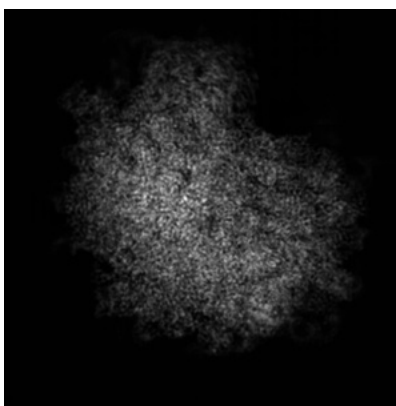
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

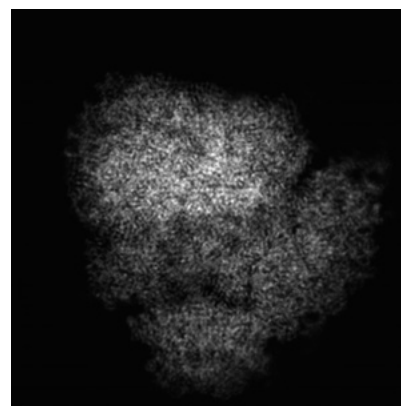
6.1.1 Primary map



X

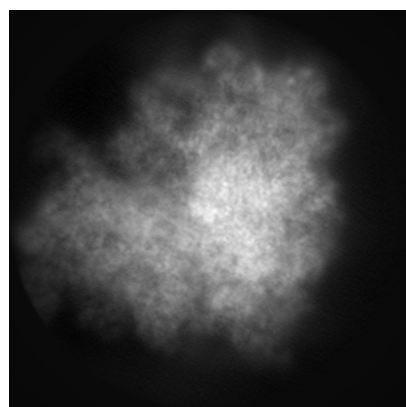


Y

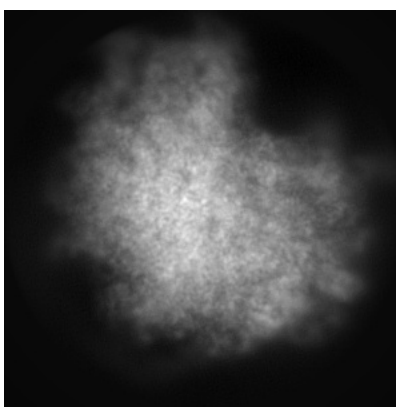


Z

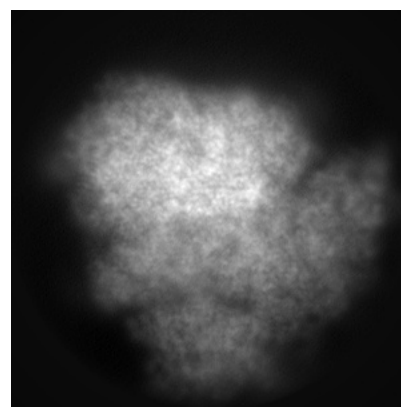
6.1.2 Raw map



X



Y

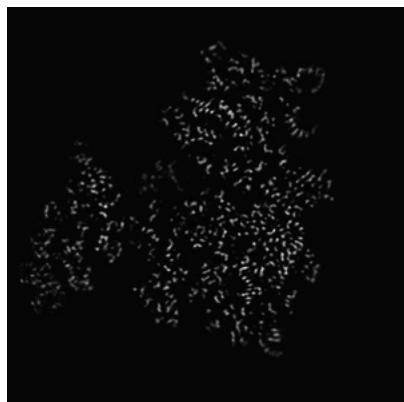


Z

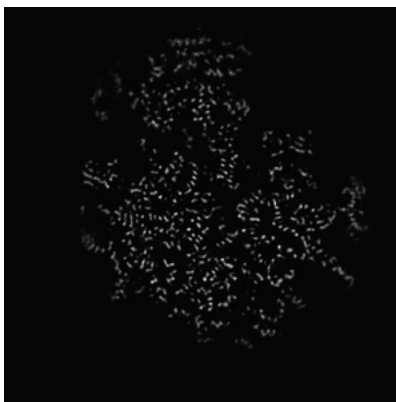
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

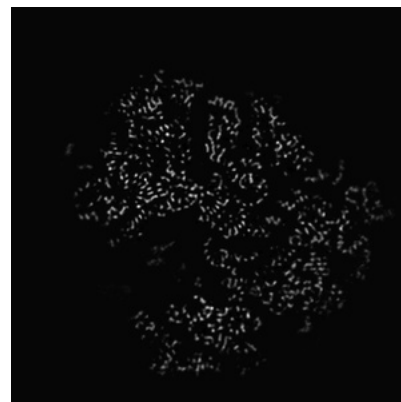
6.2.1 Primary map



X Index: 156

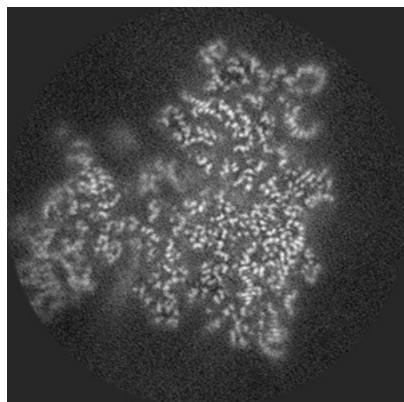


Y Index: 156

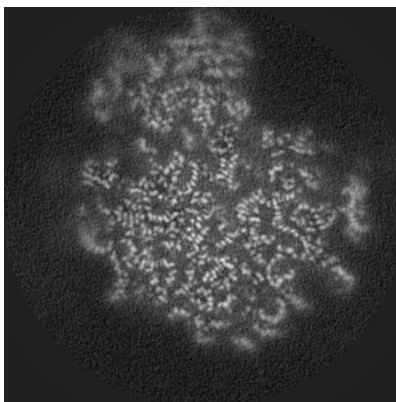


Z Index: 156

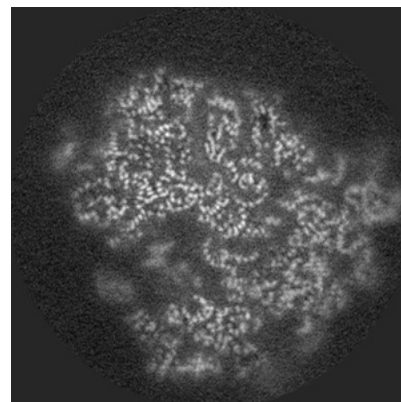
6.2.2 Raw map



X Index: 156



Y Index: 156

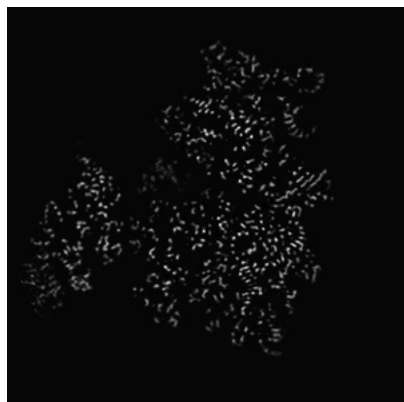


Z Index: 156

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

6.3 Largest variance slices [i](#)

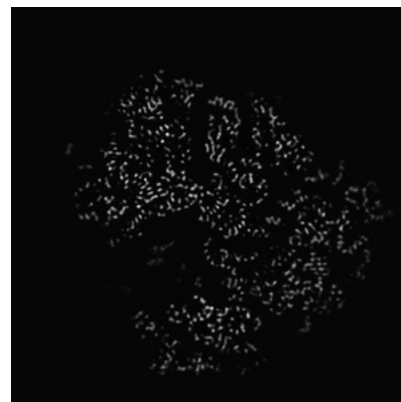
6.3.1 Primary map



X Index: 155

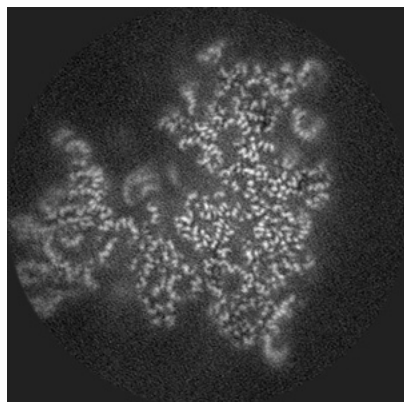


Y Index: 170

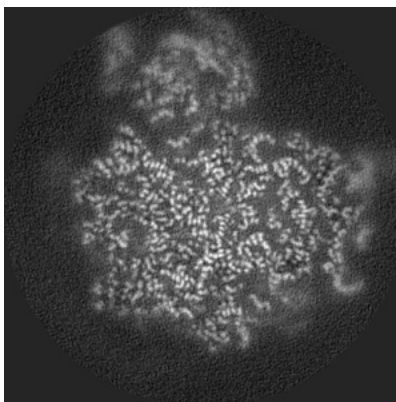


Z Index: 156

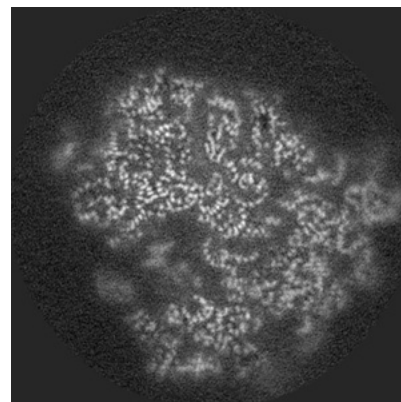
6.3.2 Raw map



X Index: 161



Y Index: 170

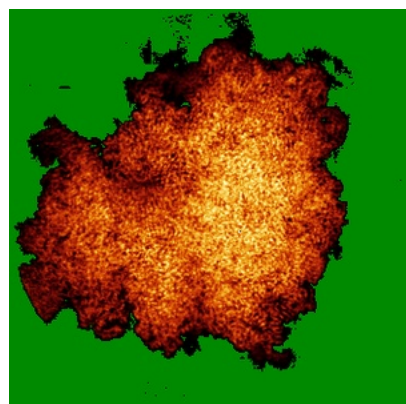


Z Index: 156

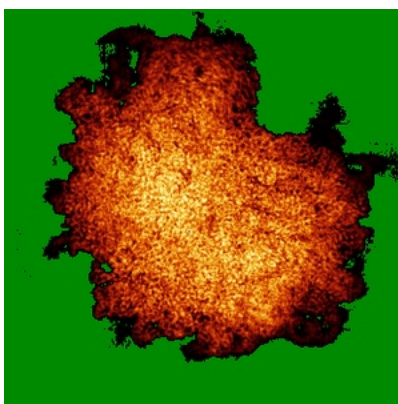
The images above show the largest variance slices of the map in three orthogonal directions.

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

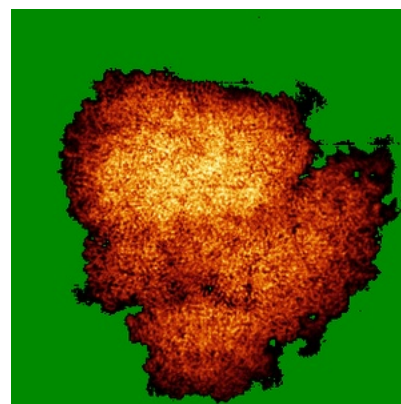
6.4.1 Primary map



X

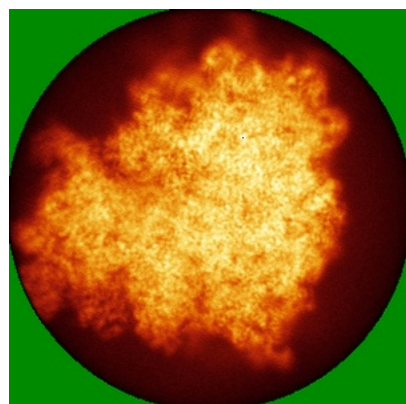


Y

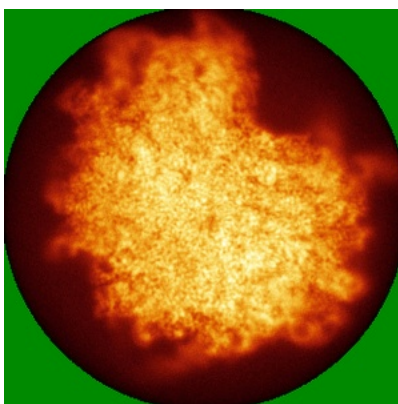


Z

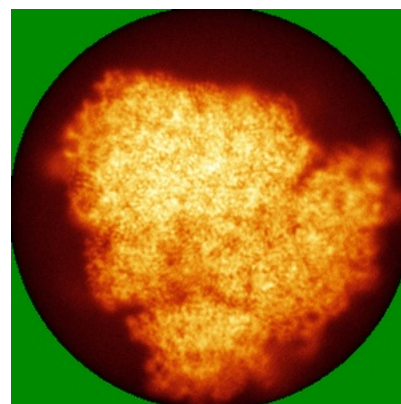
6.4.2 Raw map



X



Y

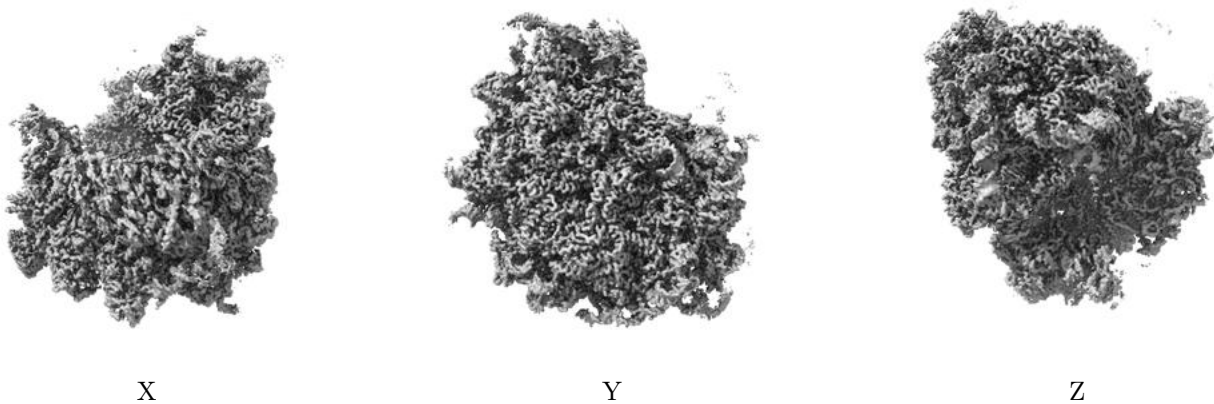


Z

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.

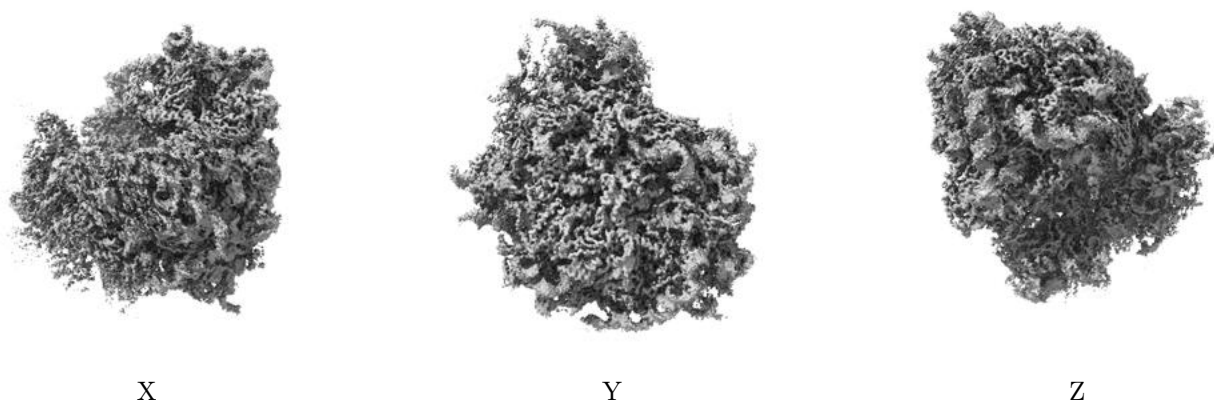
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0823. 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.

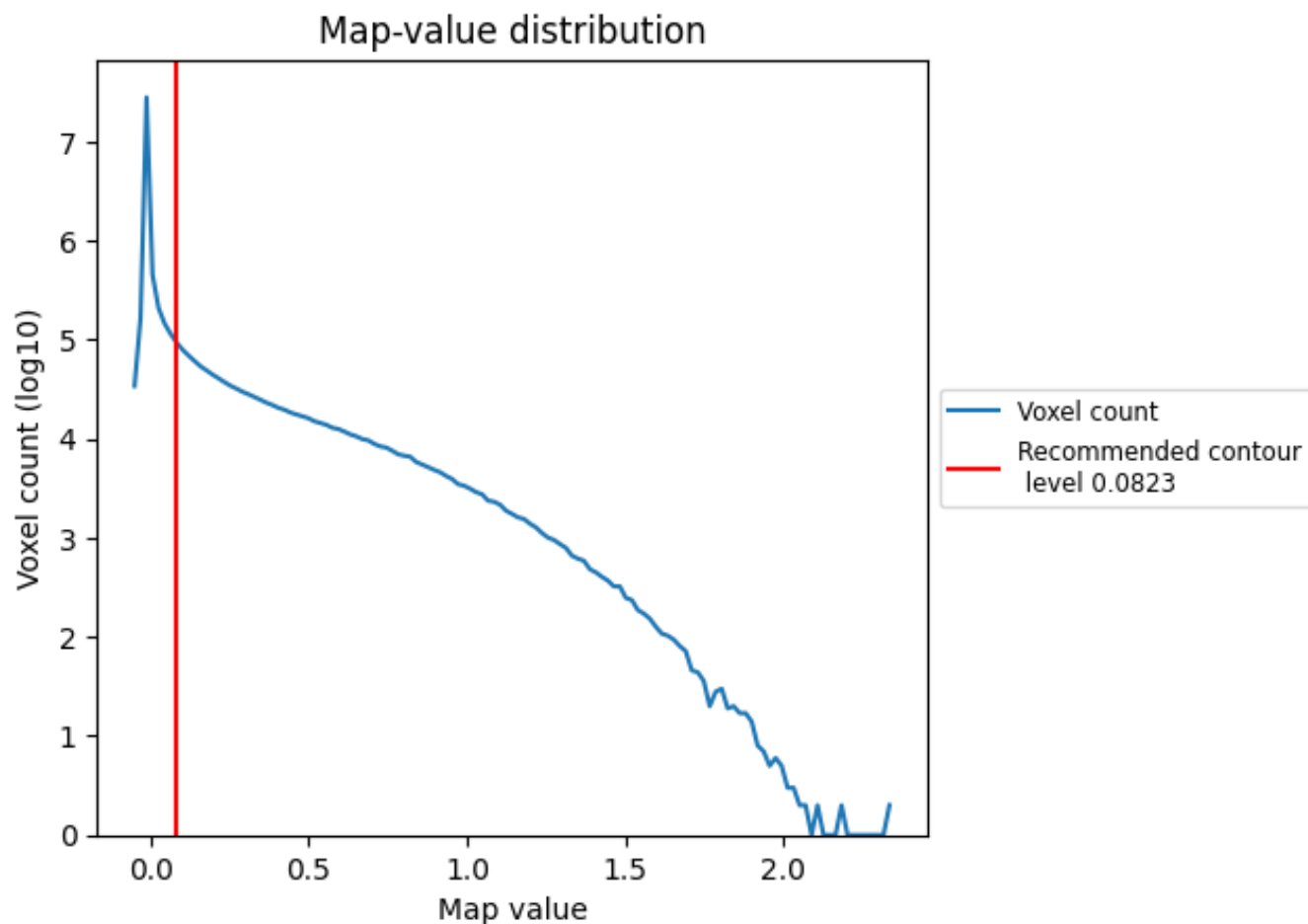
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

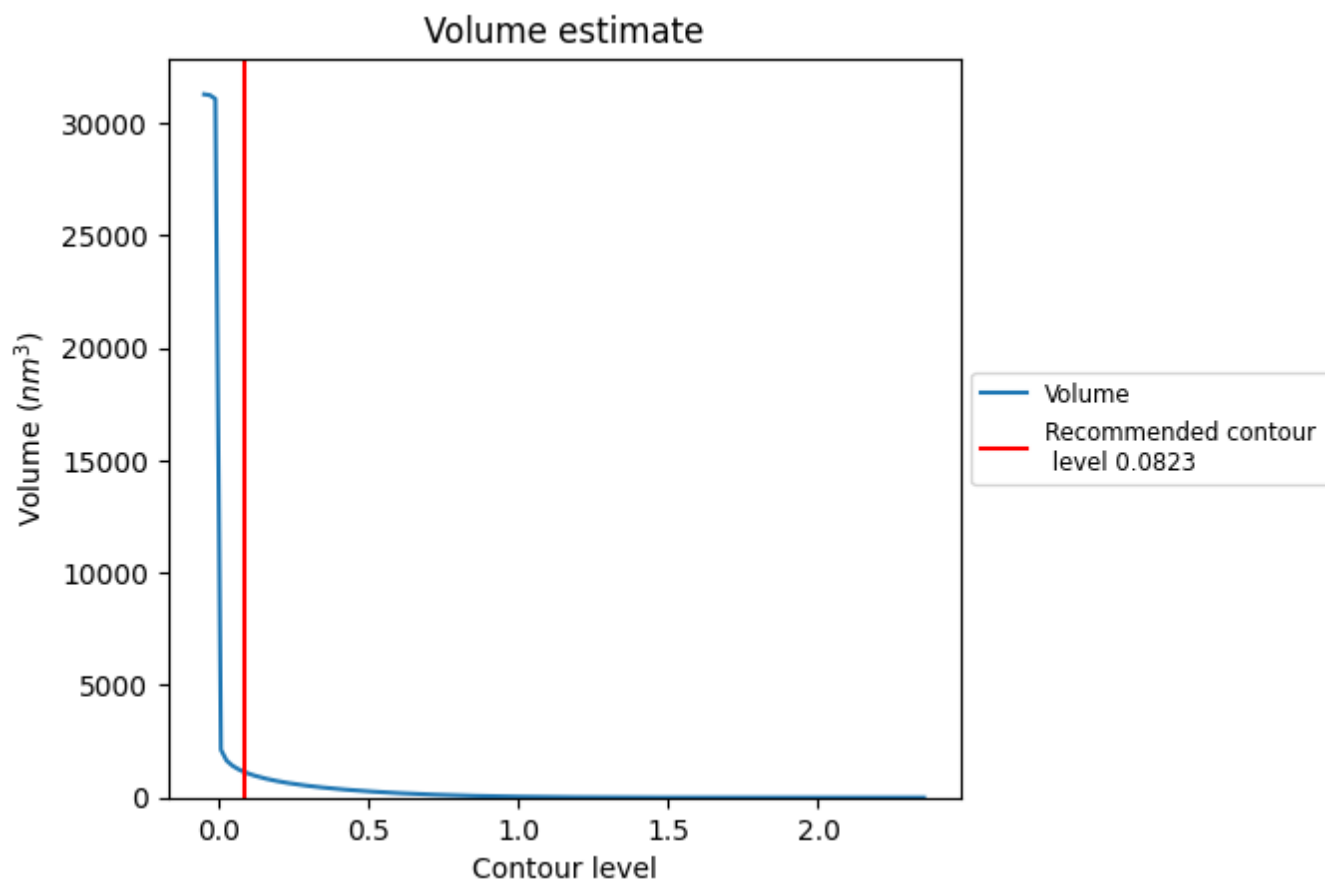
This section contains the results of statistical analysis of the map.

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.

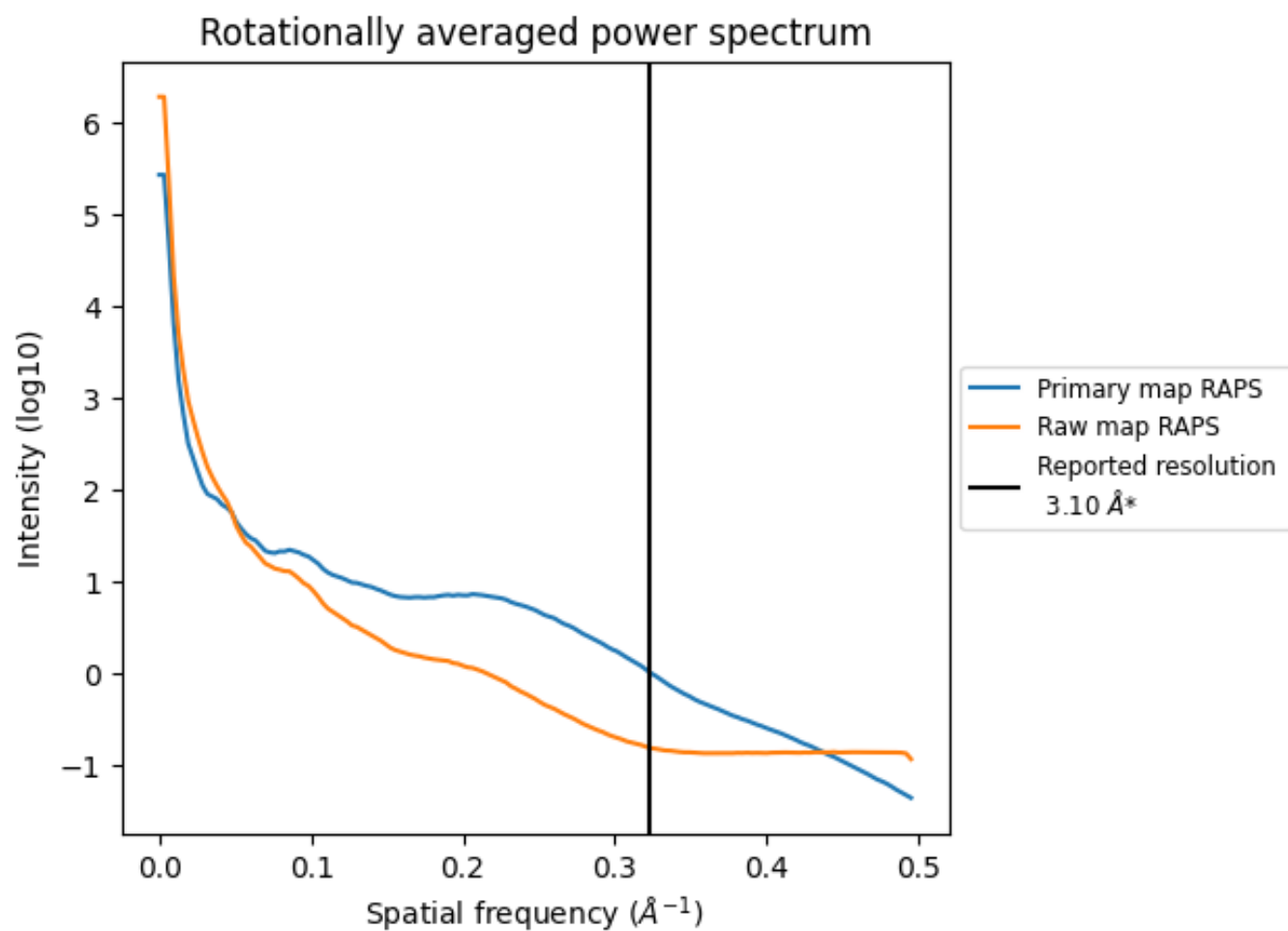
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1154 nm^3 ; this corresponds to an approximate mass of 1043 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 ⓘ

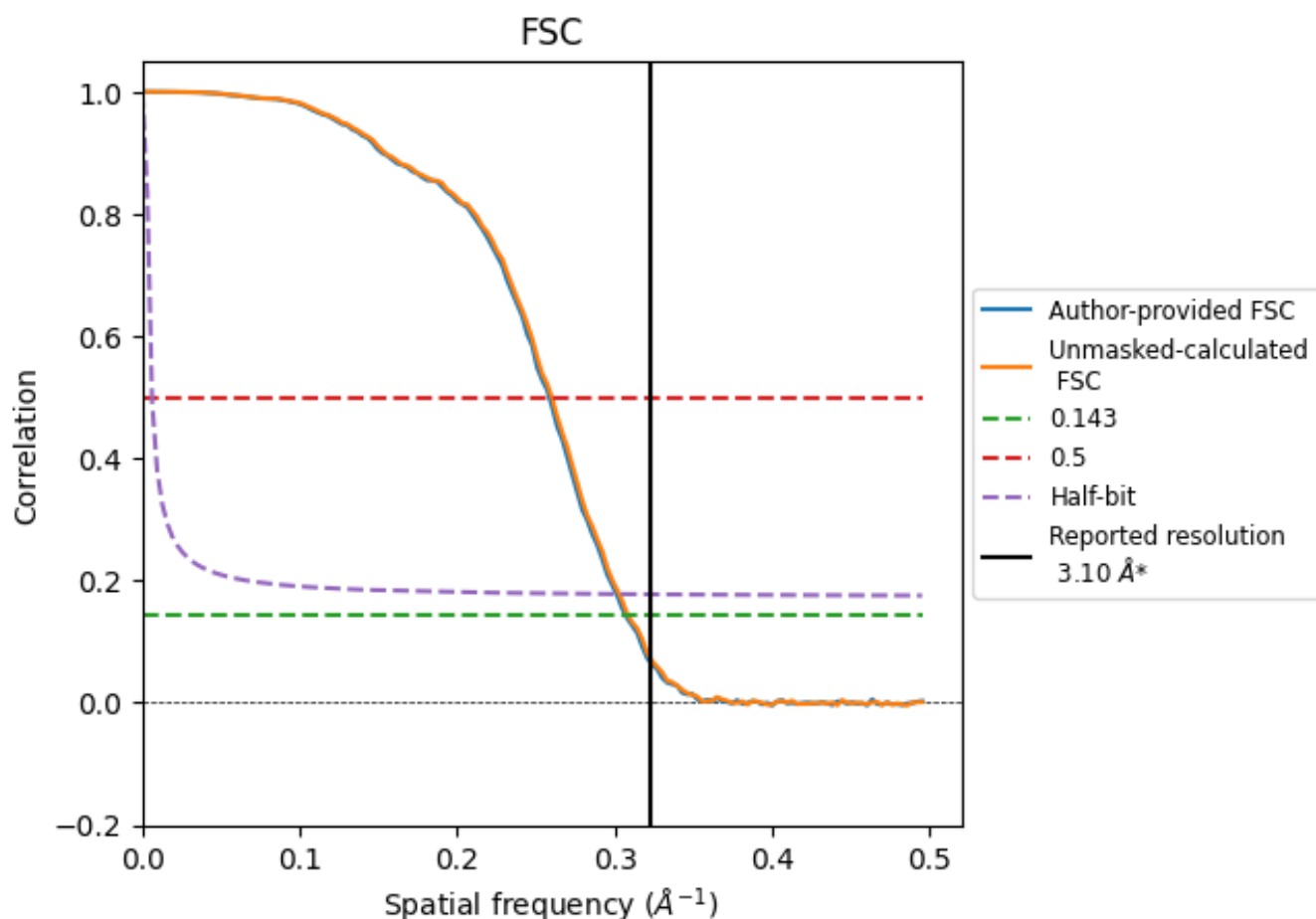


*Reported resolution corresponds to spatial frequency of 0.323 \AA^{-1}

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 \AA^{-1}

8.2 Resolution estimates [i](#)

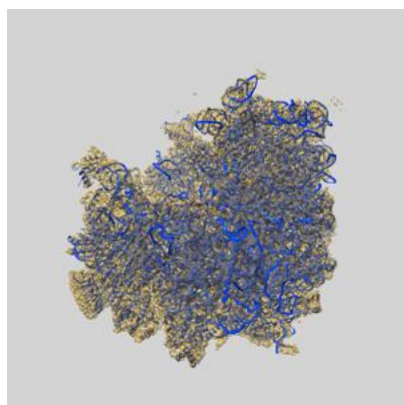
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.26	3.87	3.32
Unmasked-calculated*	3.24	3.85	3.30

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

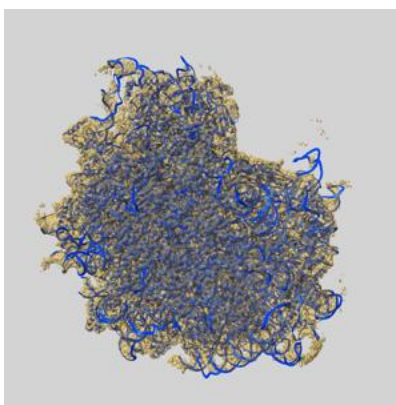
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-53427 and PDB model 9QWT. Per-residue inclusion information can be found in section [3](#) on page [23](#).

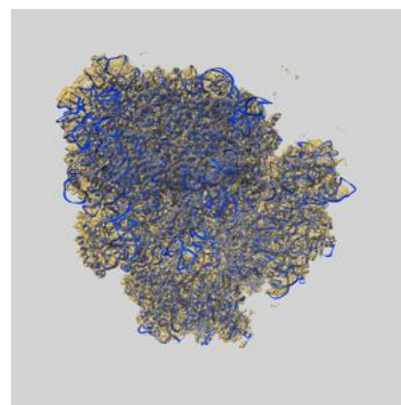
9.1 Map-model overlay [i](#)



X



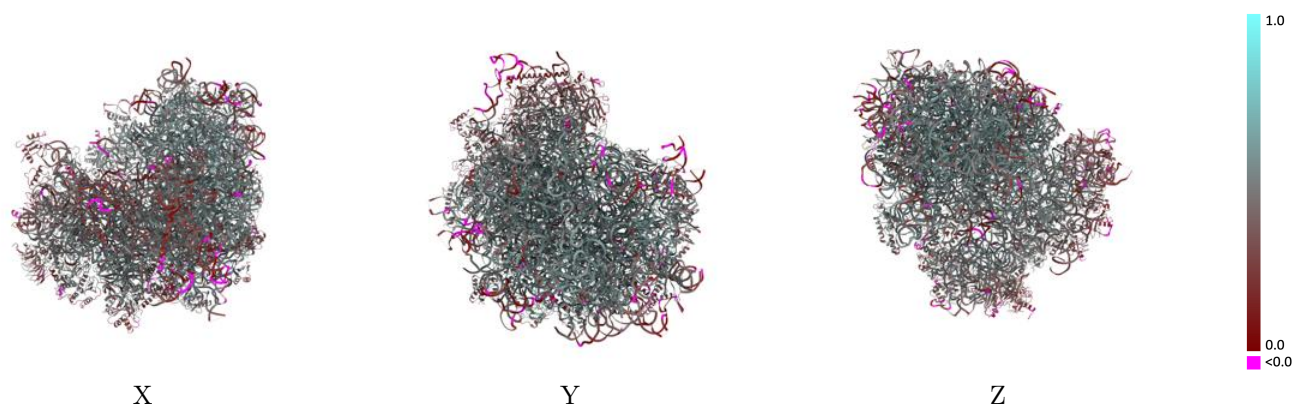
Y



Z

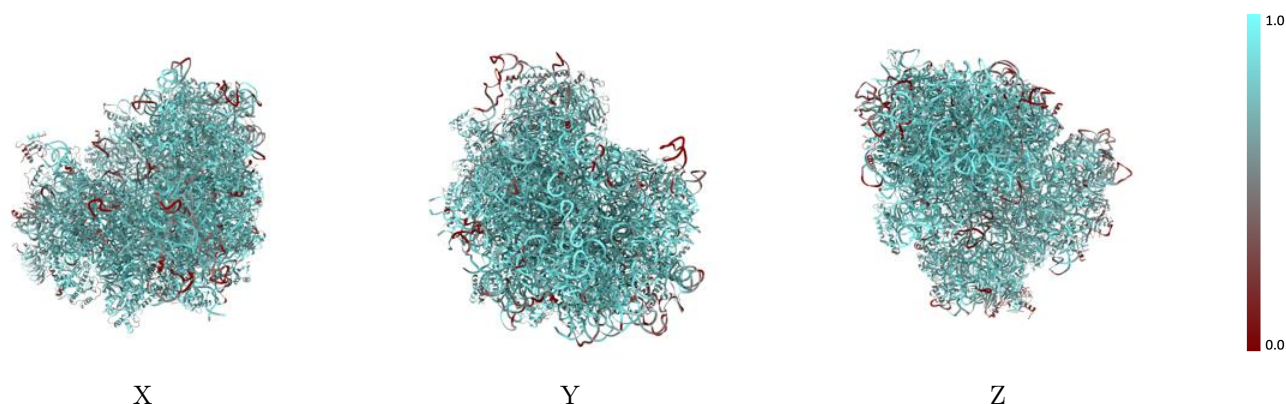
The images above show the 3D surface view of the map at the recommended contour level 0.0823 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



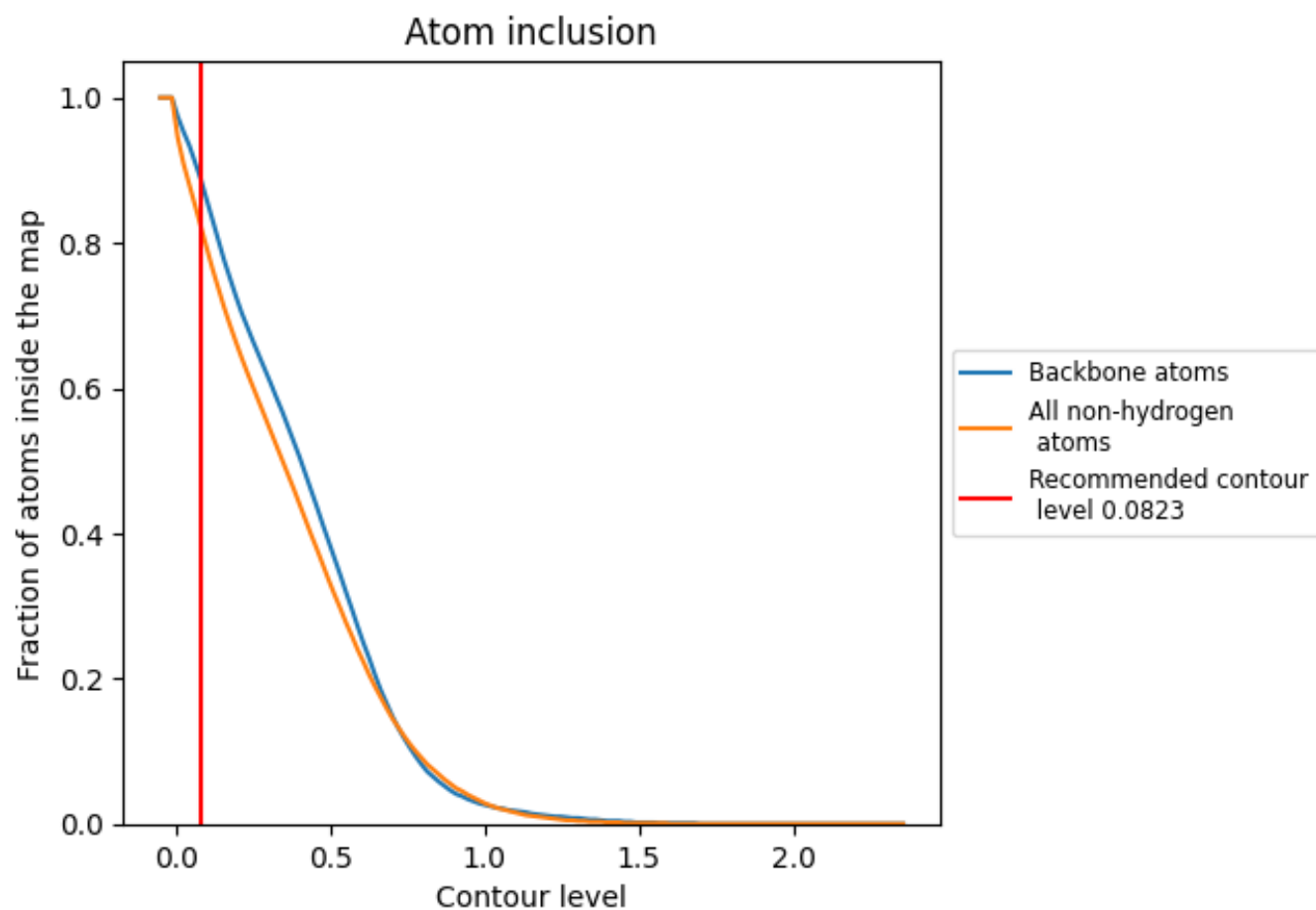
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0823).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 82% 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 (0.0823) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8210	 0.4740
A1	 0.8390	 0.5160
A2	 0.8610	 0.4970
A3	 0.7650	 0.4220
B1	 0.7990	 0.4630
B2	 0.9370	 0.5460
B3	 0.6940	 0.3830
Bv	 0.5950	 0.3020
Bx	 0.8450	 0.4850
By	 0.0000	 0.0310
C1	 0.8080	 0.5000
C2	 0.8580	 0.5040
C3	 0.5720	 0.3270
D1	 0.8290	 0.5070
D2	 0.9090	 0.5630
D3	 0.8130	 0.4670
E1	 0.7540	 0.4390
E2	 0.8310	 0.5170
E3	 0.7700	 0.4400
F1	 0.8250	 0.4950
F2	 0.8710	 0.5350
F3	 0.8310	 0.4950
G1	 0.8500	 0.5040
G2	 0.7850	 0.4740
G3	 0.7150	 0.4290
H1	 0.9130	 0.5720
H2	 0.7770	 0.4820
H3	 0.8150	 0.4350
I2	 0.8760	 0.5370
I3	 0.6500	 0.3200
J2	 0.8670	 0.5380
J3	 0.8300	 0.4860
K2	 0.8880	 0.5460
K3	 0.5880	 0.2800
L2	 0.8110	 0.4850















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Chain	Atom inclusion	Q-score
L3	 0.6050	 0.3090
M2	 0.9020	 0.5490
M3	 0.3770	 0.1880
N2	 0.8240	 0.5040
N3	 0.7960	 0.4510
O2	 0.6980	 0.3980
O3	 0.7660	 0.4530
P2	 0.8750	 0.5430
P3	 0.8350	 0.4930
Q2	 0.8620	 0.5320
Q3	 0.4840	 0.2230
R2	 0.8170	 0.4990
R3	 0.6490	 0.3610
S2	 0.7800	 0.4950
S3	 0.7480	 0.4060
T2	 0.8220	 0.4860
T3	 0.6150	 0.3460
U2	 0.8870	 0.5540
V2	 0.6460	 0.3990
W2	 0.8320	 0.4850
X2	 0.7860	 0.4930
Y2	 0.8630	 0.5440
Z2	 0.9010	 0.5630
a2	 0.8540	 0.5190
b2	 0.8000	 0.4800
c2	 0.7670	 0.4610
d2	 0.8800	 0.5560
e2	 0.7190	 0.4100
f2	 0.8460	 0.5240
g2	 0.8150	 0.5190
h2	 0.8180	 0.4840
i2	 0.8190	 0.5090
j2	 0.8620	 0.5270
k2	 0.8640	 0.5300
m2	 0.8570	 0.4620
n2	 0.7190	 0.3850
o2	 0.7560	 0.4120
p2	 0.7970	 0.4600
q2	 0.6680	 0.3820
r2	 0.6620	 0.3470
s2	 0.7380	 0.4180
t2	 0.7390	 0.3830

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Chain	Atom inclusion	Q-score
u2	 0.7420	 0.3980
v2	 0.6300	 0.3030
w2	 0.7520	 0.4120
x2	 0.7190	 0.4120
y2	 0.7290	 0.4010
z2	 0.6660	 0.3350