



Full wwPDB EM Validation Report ⓘ

Feb 10, 2025 – 09:28 am GMT

PDB ID : 9GFT
EMDB ID : EMD-51318
Title : Structure of the HrpA-bound E. coli disome, Class I
Authors : Esser, H.F.; Berninghausen, O.; Becker, T.; Beckmann, R.
Deposited on : 2024-08-12
Resolution : 3.10 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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:

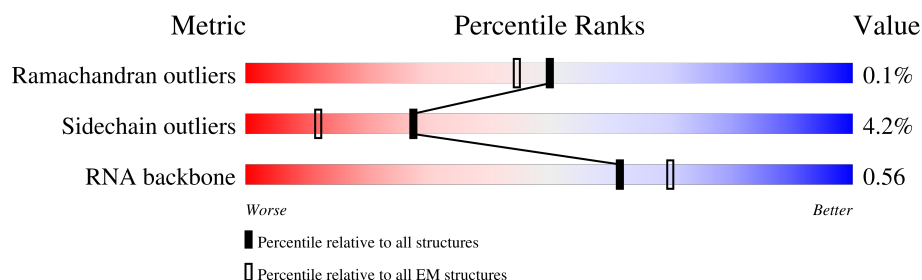
EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

1 Overall quality at a glance

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

The reported resolution of this entry is 3.10 Å.

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









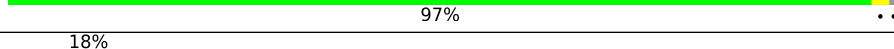
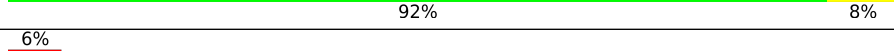
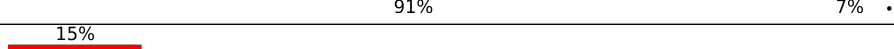
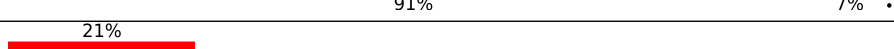
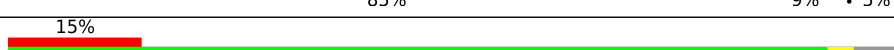
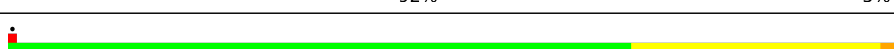
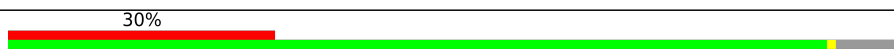
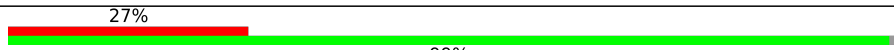
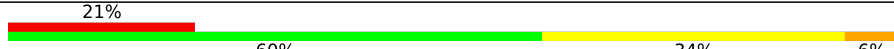


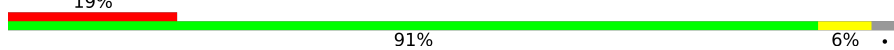
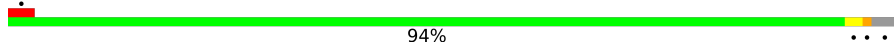
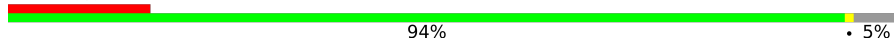
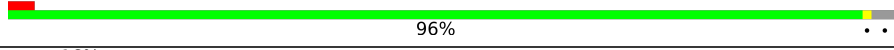
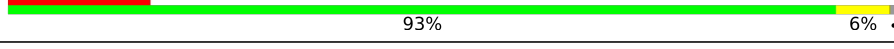
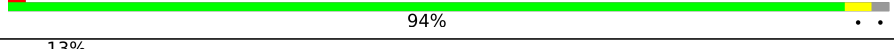
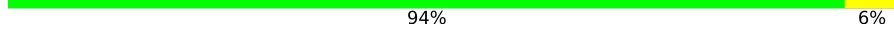

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	0	1542	<div> <div>83%</div> <div>15%</div> <div>..</div> </div>
1	AA	1542	<div> <div>82%</div> <div>16%</div> <div>.</div> </div>
2	1	241	<div> <div>12%</div> <div>87%</div> <div>10%</div> </div>
2	AB	241	<div> <div>27%</div> <div>86%</div> <div>10%</div> </div>
3	2	233	<div> <div>5%</div> <div>87%</div> <div>12%</div> </div>
3	AC	233	<div> <div>17%</div> <div>86%</div> <div>12%</div> </div>
4	3	206	<div> <div>12%</div> <div>97%</div> <div>.</div> </div>
4	AD	206	<div> <div>19%</div> <div>93%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
5	4	167	
5	AE	167	
6	5	135	
6	AF	135	
7	6	179	
7	AG	179	
8	7	130	
8	AH	130	
9	8	130	
9	AI	130	
10	9	103	
10	AJ	103	
11	A	76	
12	A1	71	
12	v	71	
13	A3	77	
14	AK	234	
14	C	234	
15	AL	118	
15	F	118	
16	AM	101	
16	G	101	
17	AN	89	
17	H	89	
18	AO	82	

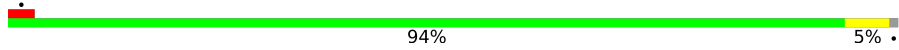
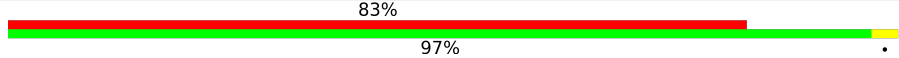
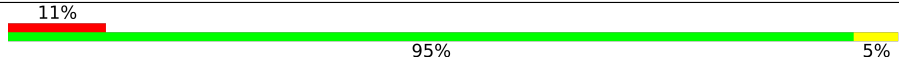
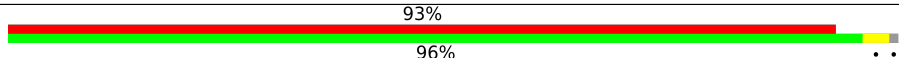

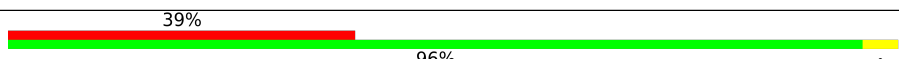
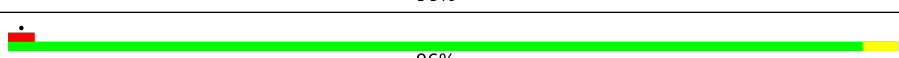
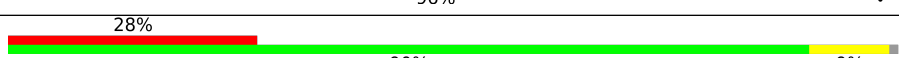
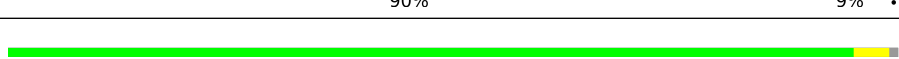
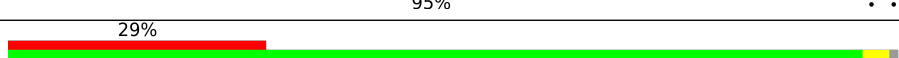
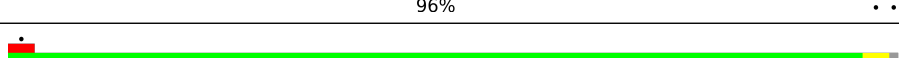
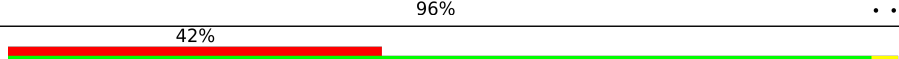
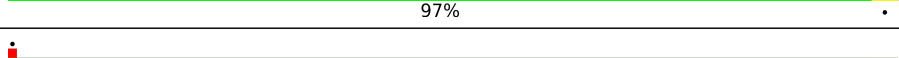
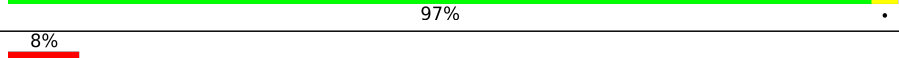
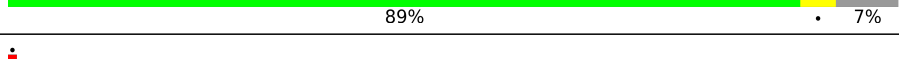
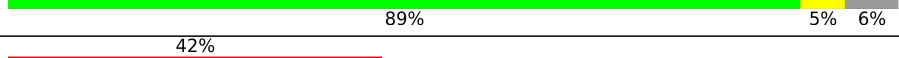
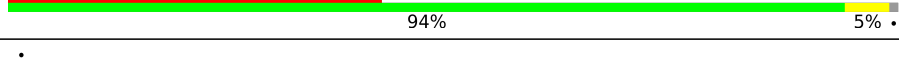
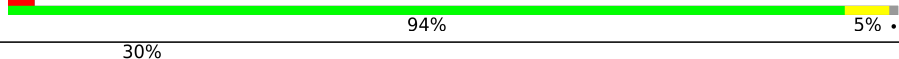
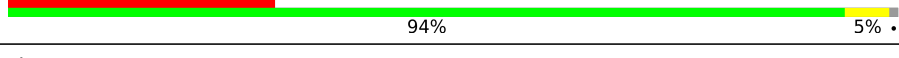
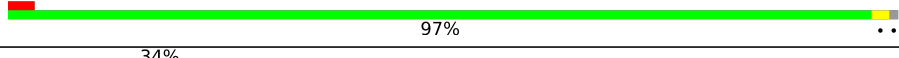
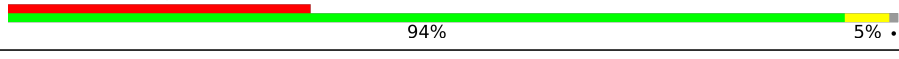
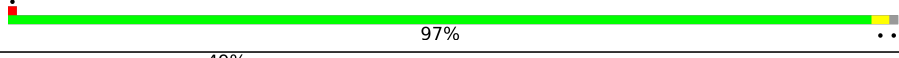
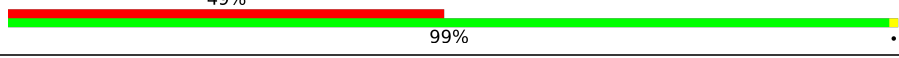
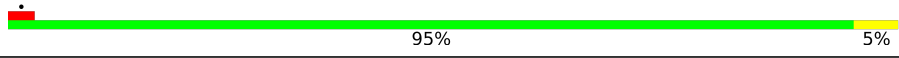
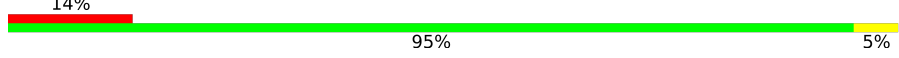
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Mol	Chain	Length	Quality of chain
18	I	82	
19	AP	84	
19	J	84	
20	AQ	75	
20	K	75	
21	AR	92	
21	t	92	
22	AS	87	
22	u	87	
23	AT	70	
23	L	70	
24	AU	76	
25	AV	2903	
25	N	2903	
26	AW	120	
26	O	120	
27	AX	273	
27	P	273	
28	AY	209	
28	Q	209	
29	AZ	201	
29	R	201	
30	Aa	179	
30	S	179	
31	Ab	177	

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Mol	Chain	Length	Quality of chain
31	T	177	
32	Ac	149	
32	U	149	
33	Ad	142	
33	V	142	
34	Ae	142	
34	W	142	
35	Af	123	
35	X	123	
36	Ag	144	
36	Y	144	
37	Ah	136	
37	Z	136	
38	Ai	127	
38	a	127	
39	Aj	117	
39	b	117	
40	Ak	115	
40	c	115	
41	Al	118	
41	d	118	
42	Am	103	
42	e	103	
43	An	110	
43	f	110	

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Mol	Chain	Length	Quality of chain
44	Ao	100	
44	g	100	
45	Ap	104	
45	h	104	
46	Aq	94	
46	i	94	
47	Ar	85	
47	j	85	
48	As	78	
48	k	78	
49	At	63	
49	l	63	
50	Au	59	
50	m	59	
51	Av	57	
52	Aw	55	
52	o	55	
53	Ax	46	
53	p	46	
54	Ay	65	
54	q	65	
55	Az	38	
55	r	38	
56	B	1326	
57	D	129	

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Mol	Chain	Length	Quality of chain
57	y	129	
58	E	124	
58	z	124	
59	M	75	
60	n	56	
61	s	179	
62	w	698	
63	x	165	

2 Entry composition [i](#)

There are 63 unique types of molecules in this entry. The entry contains 307377 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 RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	1533	Total	C	N	O	P	0	0
			32895	14671	6036	10655	1533		
1	AA	1539	Total	C	N	O	P	0	0
			33015	14725	6052	10699	1539		

- Molecule 2 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		
2	AB	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 3 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		
3	AC	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 4 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		
4	AD	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 5 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	150	Total	C	N	O	S	0	0
			1105	687	211	201	6		
5	AE	150	Total	C	N	O	S	0	0
			1105	687	211	201	6		

- Molecule 6 is a protein called Small ribosomal subunit protein bS6, fully modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	100	Total	C	N	O	S	0	0
			817	515	148	148	6		
6	AF	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 7 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		
7	AG	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 8 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	129	Total	C	N	O	S	0	0
			979	616	173	184	6		
8	AH	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 9 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	8	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		
9	AI	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 10 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	9	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	AJ	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 11 is a RNA chain called A-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A	76	Total	C	N	O	P	0	0
			1622	723	290	533	76		

- Molecule 12 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A1	66	Total	C	N	O	S	0	0
			551	340	118	92	1		
12	v	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

- Molecule 13 is a RNA chain called A-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A3	77	Total	C	N	O	P	0	0
			1638	732	291	538	77		

- Molecule 14 is a protein called Large ribosomal subunit protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AK	134	Total	C	N	O	S	0	0
			1026	645	186	193	2		
14	C	134	Total	C	N	O	S	0	0
			1026	645	186	193	2		

- Molecule 15 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AL	114	Total	C	N	O	S	0	0
			883	546	178	156	3		
15	F	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 16 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AM	96	Total	C	N	O	S	0	0
			774	483	160	128	3		
16	G	98	Total	C	N	O	S	0	0
			791	490	161	137	3		

- Molecule 17 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AN	88	Total	C	N	O	S	0	0
			714	439	144	130	1		
17	H	87	Total	C	N	O	S	0	0
			702	433	140	128	1		

- Molecule 18 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AO	82	Total	C	N	O	S	0	0
			649	406	128	114	1		
18	I	82	Total	C	N	O	S	0	0
			648	406	128	113	1		

- Molecule 19 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AP	80	Total	C	N	O	S	0	0
			648	411	121	113	3		
19	J	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 20 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AQ	66	Total	C	N	O	S	0	0
			544	345	102	96	1		
20	K	65	Total	C	N	O	S	0	0
			535	339	100	95	1		

- Molecule 21 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AR	75	Total	C	N	O	S	0	0
			603	387	112	102	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
21	t	77	Total	C	N	O	S	0	0
			620	399	115	104	2		

- Molecule 22 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AS	85	Total	C	N	O	S	0	0
			665	411	137	114	3		
22	u	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 23 is a protein called Large ribosomal subunit protein bL31A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AT	60	Total	C	N	O	S	0	0
			480	299	90	85	6		
23	L	62	Total	C	N	O	S	0	0
			499	309	95	89	6		

- Molecule 24 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AU	76	Total	C	N	O	P	0	0
			1625	724	293	532	76		

- Molecule 25 is a RNA chain called 23S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AV	2897	Total	C	N	O	P	0	0
			62195	27745	11446	20107	2897		
25	N	2897	Total	C	N	O	P	0	0
			62195	27745	11446	20107	2897		

- Molecule 26 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	AW	118	Total	C	N	O	P	0	0
			2529	1126	464	821	118		
26	O	118	Total	C	N	O	P	0	0
			2529	1126	464	821	118		

- Molecule 27 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	AX	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		
27	P	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 28 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	AY	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		
28	Q	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 29 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	AZ	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		
29	R	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 30 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Aa	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		
30	S	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 31 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Ab	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		
31	T	175	Total	C	N	O	S	0	0
			1313	826	241	244	2		

- Molecule 32 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Ac	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
32	U	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 33 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Ad	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		
33	V	134	Total	C	N	O	S	0	0
			979	619	169	185	6		

- Molecule 34 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Ae	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		
34	W	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 35 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Af	122	Total	C	N	O	S	0	0
			938	587	180	165	6		
35	X	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 36 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Ag	142	Total	C	N	O	S	0	0
			1034	643	202	188	1		
36	Y	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 37 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Ah	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		
37	Z	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 38 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Ai	118	Total	C	N	O	S	0	0
			945	585	194	161	5		
38	a	119	Total	C	N	O	S	0	0
			951	588	195	163	5		

- Molecule 39 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Aj	116	Total	C	N	O		0	0
			892	552	178	162			
39	b	116	Total	C	N	O		0	0
			892	552	178	162			

- Molecule 40 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Ak	114	Total	C	N	O	S	0	0
			917	574	179	163	1		
40	c	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 41 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Al	117	Total	C	N	O		0	0
			947	604	192	151			
41	d	117	Total	C	N	O		0	0
			947	604	192	151			

- Molecule 42 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Am	103	Total	C	N	O	S	0	0
			816	516	153	145	2		
42	e	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 43 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	An	110	Total	C	N	O	S	0	0
			857	532	166	156	3		
43	f	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 44 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Ao	93	Total	C	N	O	S	0	0
			738	466	139	131	2		
44	g	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 45 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Ap	102	Total	C	N	O		0	0
			779	492	146	141			
45	h	102	Total	C	N	O		0	0
			779	492	146	141			

- Molecule 46 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Aq	94	Total	C	N	O	S	0	0
			753	479	137	134	3		
46	i	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 47 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Ar	75	Total	C	N	O	S	0	0
			575	356	116	102	1		
47	j	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 48 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	As	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
48	k	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 49 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	At	63	Total	C	N	O	S	0	0
			509	313	99	95	2		
49	l	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 50 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Au	56	Total	C	N	O	S	0	0
			435	272	84	77	2		
50	m	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 51 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Av	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 52 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	Aw	50	Total	C	N	O	0	0
			409	263	75	71		
52	o	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 53 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	Ax	46	Total	C	N	O	S	0	0
			377	228	90	57	2		
53	p	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 54 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Ay	64	Total	C	N	O	S	0	0
			504	323	105	74	2		
54	q	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 55 is a protein called Large ribosomal subunit protein bL36A.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Az	38	Total	C	N	O	S	0	0
			302	185	65	48	4		
55	r	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 56 is a protein called ATP-dependent RNA helicase HrpA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	B	1295	Total	C	N	O	S	0	0
			10462	6619	1887	1924	32		

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-25	MET	-	initiating methionine	UNP P43329
B	-24	GLY	-	expression tag	UNP P43329
B	-23	HIS	-	expression tag	UNP P43329
B	-22	HIS	-	expression tag	UNP P43329
B	-21	HIS	-	expression tag	UNP P43329
B	-20	HIS	-	expression tag	UNP P43329
B	-19	HIS	-	expression tag	UNP P43329
B	-18	HIS	-	expression tag	UNP P43329
B	-17	HIS	-	expression tag	UNP P43329
B	-16	HIS	-	expression tag	UNP P43329
B	-15	ASP	-	expression tag	UNP P43329
B	-14	TYR	-	expression tag	UNP P43329
B	-13	ASP	-	expression tag	UNP P43329
B	-12	ILE	-	expression tag	UNP P43329
B	-11	PRO	-	expression tag	UNP P43329
B	-10	THR	-	expression tag	UNP P43329
B	-9	THR	-	expression tag	UNP P43329
B	-8	LEU	-	expression tag	UNP P43329
B	-7	GLU	-	expression tag	UNP P43329
B	-6	VAL	-	expression tag	UNP P43329
B	-5	LEU	-	expression tag	UNP P43329

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	PHE	-	expression tag	UNP P43329
B	-3	GLN	-	expression tag	UNP P43329
B	-2	GLY	-	expression tag	UNP P43329
B	-1	PRO	-	expression tag	UNP P43329
B	0	GLY	-	expression tag	UNP P43329
B	1	THR	-	expression tag	UNP P43329

- Molecule 57 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	D	117	Total	C	N	O	S	0	0
			877	540	174	160	3		
57	y	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 58 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	E	123	Total	C	N	O	S	0	0
			955	590	196	165	4		
58	z	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 59 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	M	75	Total	C	N	O	P	0	0
			1593	711	281	526	75		

- Molecule 60 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	n	54	Total	C	N	O	S	0	0
			429	260	91	77	1		

- Molecule 61 is a protein called VemP nascent chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	s	37	Total	C	N	O	S	0	0
			316	198	58	58	2		

- Molecule 62 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	w	57	Total	C	N	O	P	0	0
			1175	527	165	426	57		

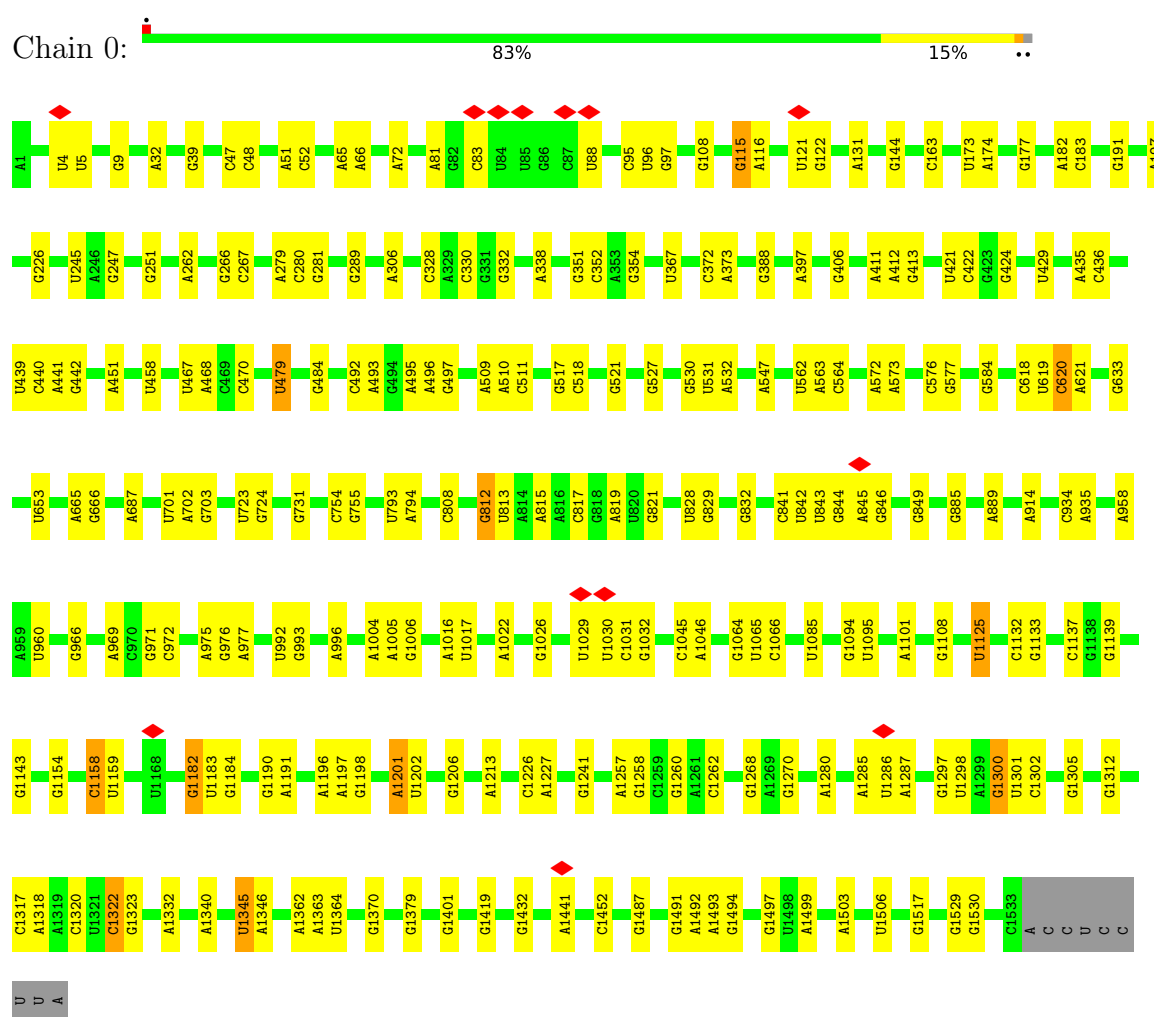
- Molecule 63 is a protein called Large ribosomal subunit protein uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	x	127	Total	C	N	O	S	0	0
			958	605	171	178	4		

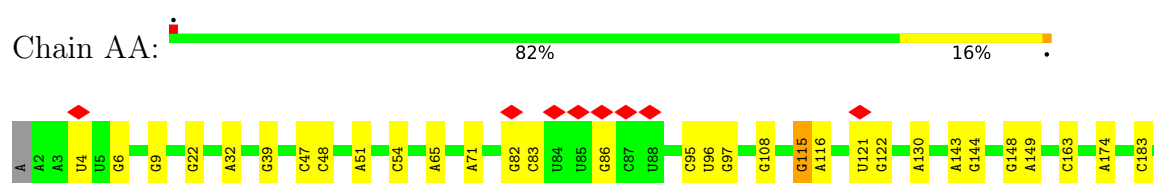
3 Residue-property plots

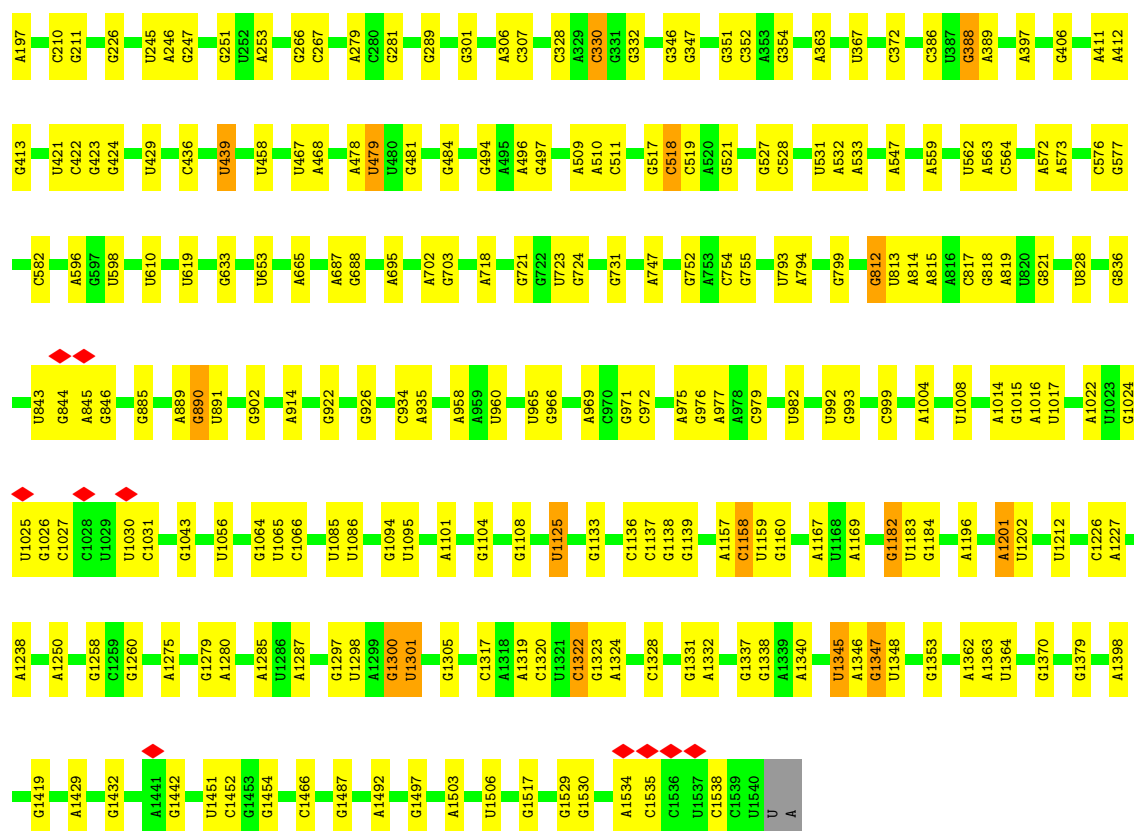
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 16S ribosomal RNA

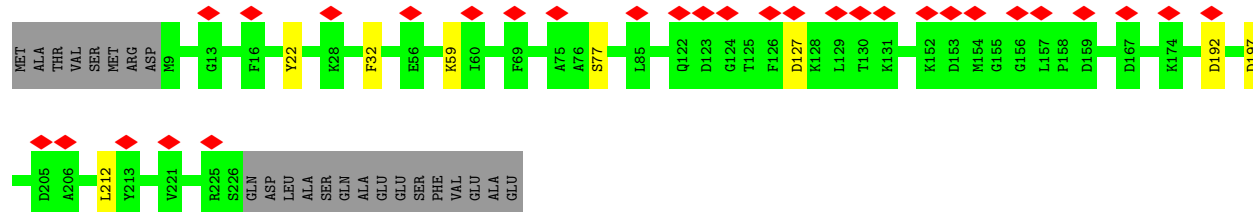
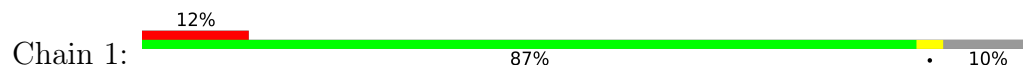


• Molecule 1: 16S ribosomal RNA

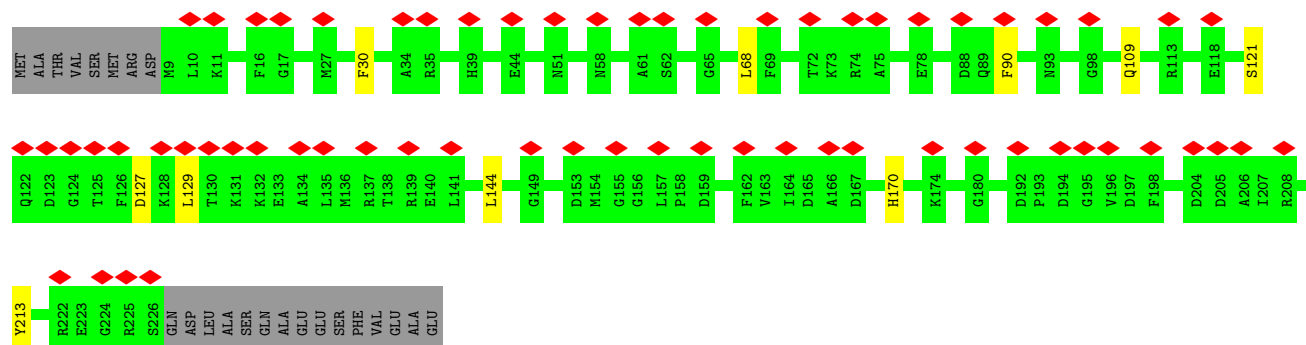
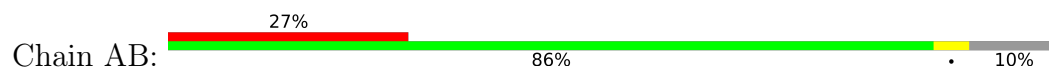




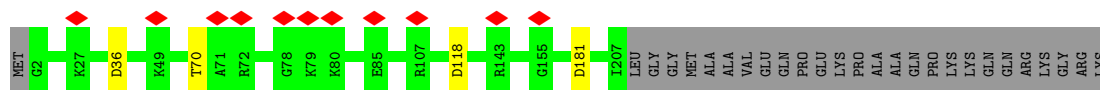
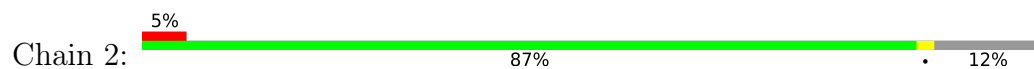
• Molecule 2: Small ribosomal subunit protein uS2



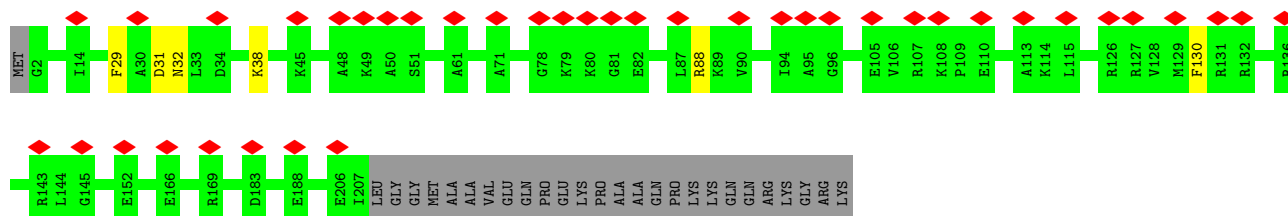
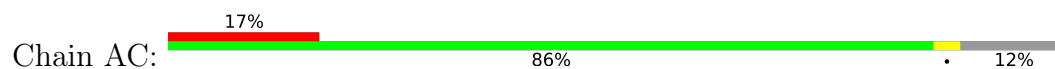
• Molecule 2: Small ribosomal subunit protein uS2



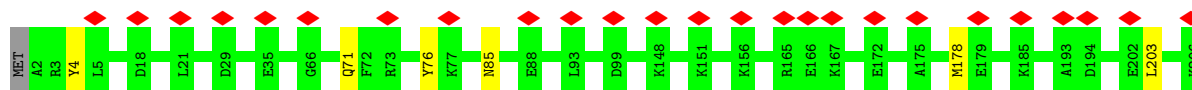
- Molecule 3: Small ribosomal subunit protein uS3



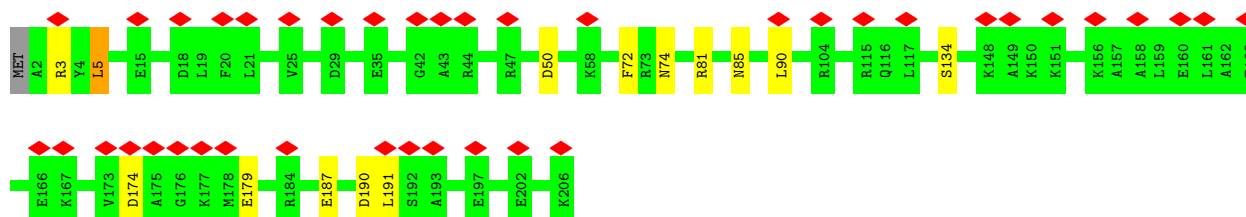
- Molecule 3: Small ribosomal subunit protein uS3



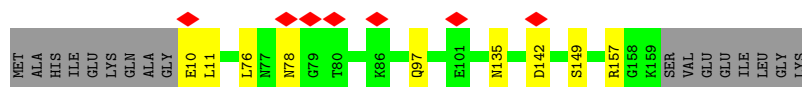
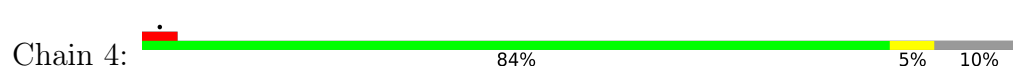
- Molecule 4: Small ribosomal subunit protein uS4



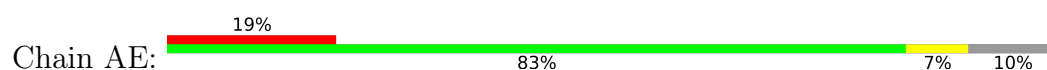
- Molecule 4: Small ribosomal subunit protein uS4

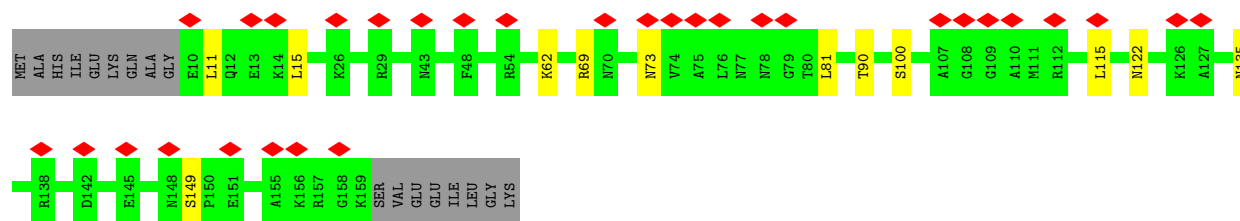


- Molecule 5: Small ribosomal subunit protein uS5

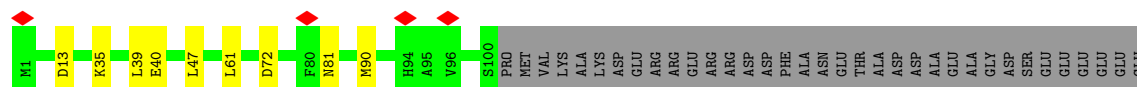


- Molecule 5: Small ribosomal subunit protein uS5

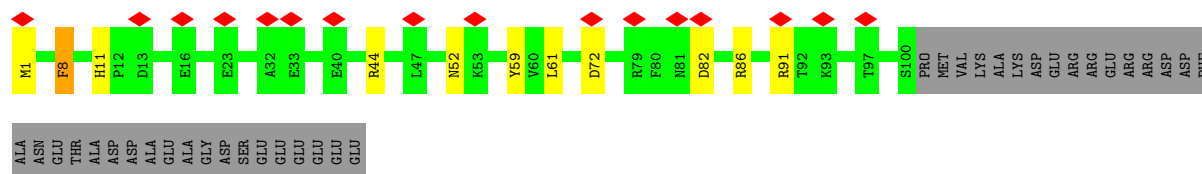




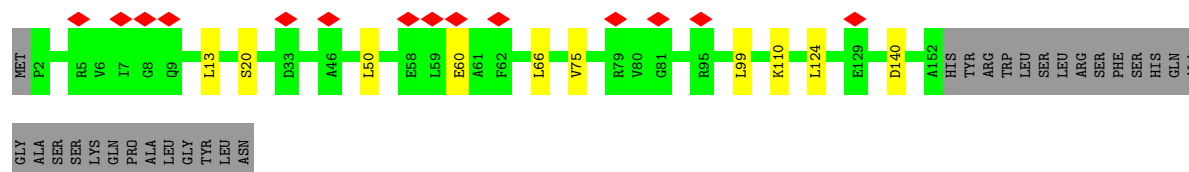
- Molecule 6: Small ribosomal subunit protein bS6, fully modified isoform



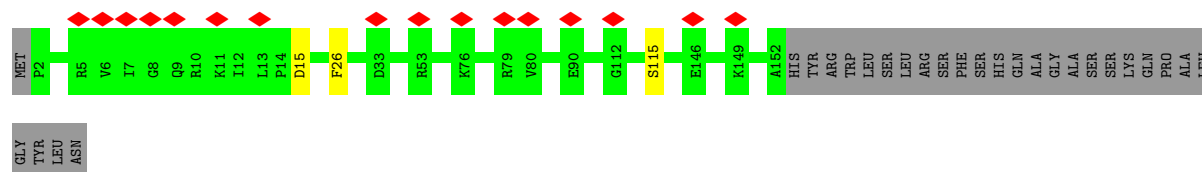
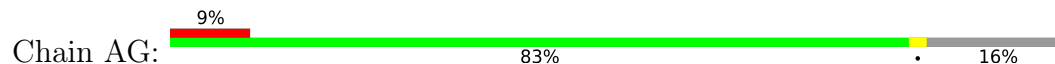
- Molecule 6: Small ribosomal subunit protein bS6, fully modified isoform



- Molecule 7: Small ribosomal subunit protein uS7

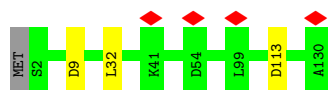


- Molecule 7: Small ribosomal subunit protein uS7

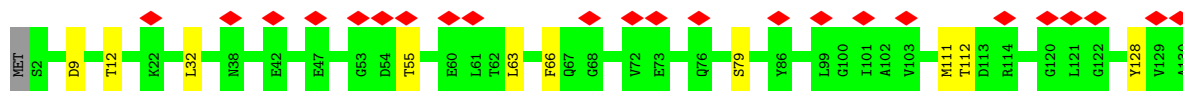
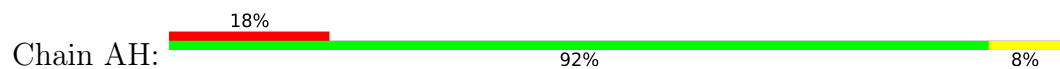


- Molecule 8: Small ribosomal subunit protein uS8

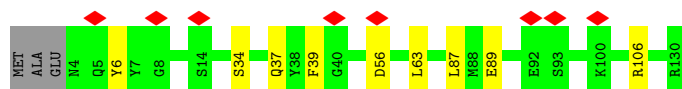




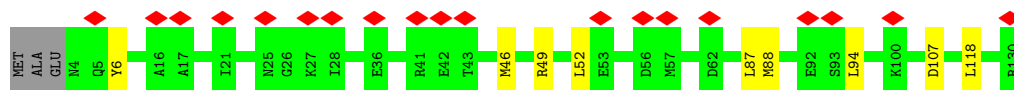
- Molecule 8: Small ribosomal subunit protein uS8



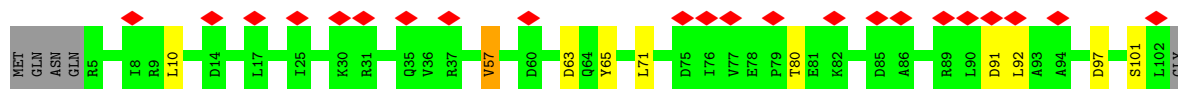
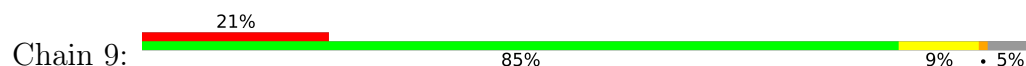
- Molecule 9: Small ribosomal subunit protein uS9



- Molecule 9: Small ribosomal subunit protein uS9



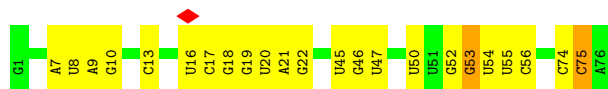
- Molecule 10: Small ribosomal subunit protein uS10



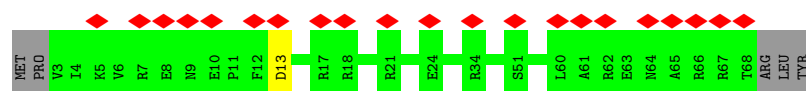
- Molecule 10: Small ribosomal subunit protein uS10



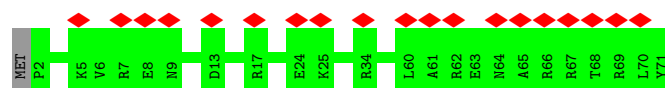
- Molecule 11: A-site tRNA



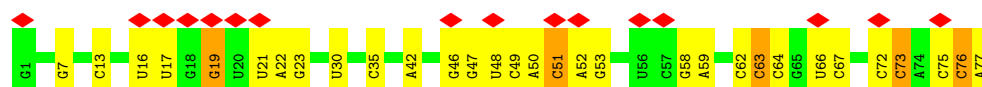
- Molecule 12: Small ribosomal subunit protein bS21



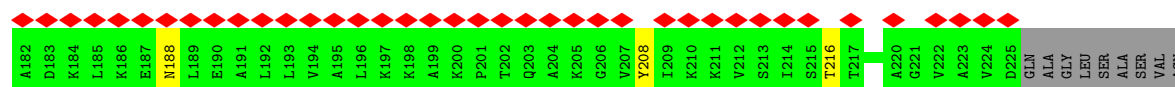
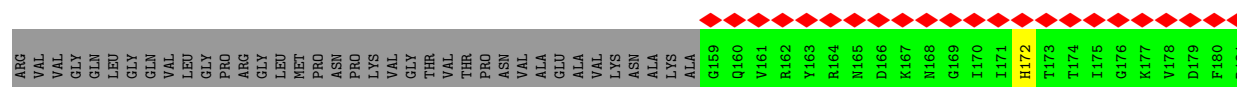
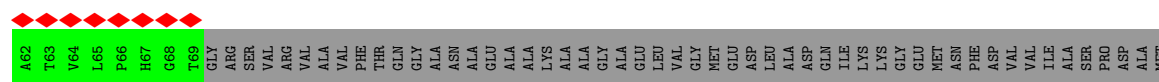
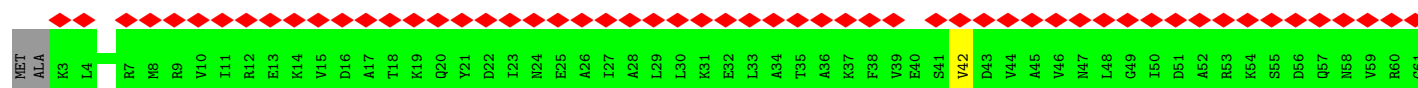
- Molecule 12: Small ribosomal subunit protein bS21



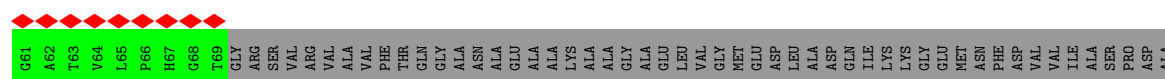
- Molecule 13: A-site tRNA

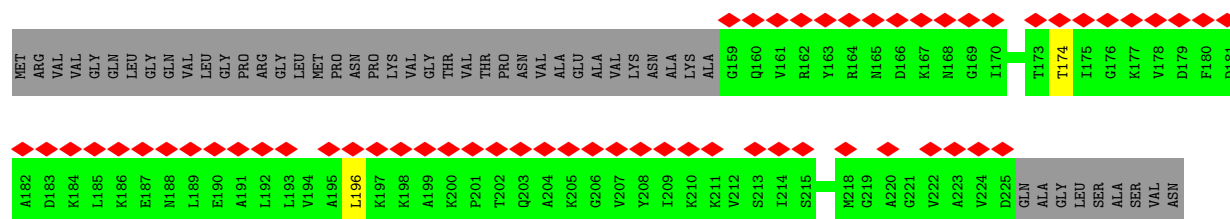


- Molecule 14: Large ribosomal subunit protein uL1

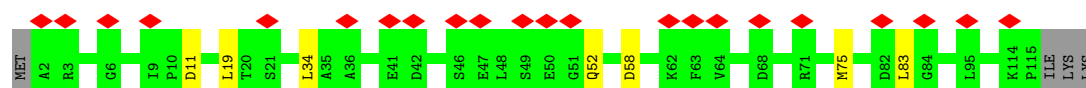
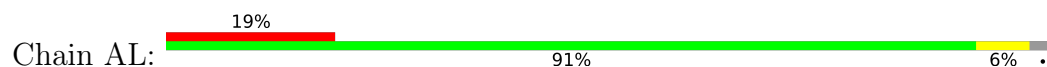


- Molecule 14: Large ribosomal subunit protein uL1

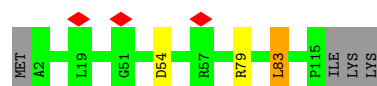




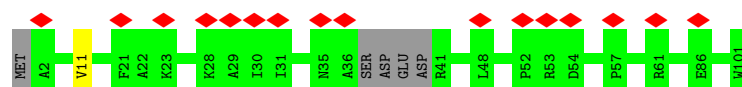
- Molecule 15: Small ribosomal subunit protein uS13



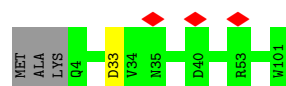
- Molecule 15: Small ribosomal subunit protein uS13



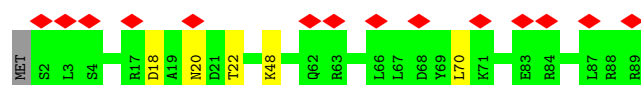
- Molecule 16: Small ribosomal subunit protein uS14



- Molecule 16: Small ribosomal subunit protein uS14



- Molecule 17: Small ribosomal subunit protein uS15

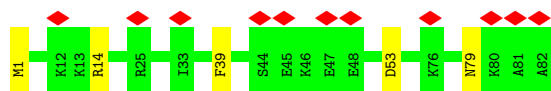


- Molecule 17: Small ribosomal subunit protein uS15

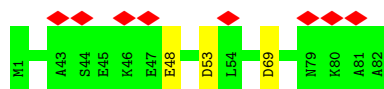




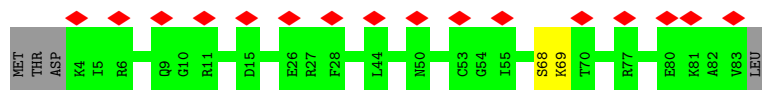
- Molecule 18: Small ribosomal subunit protein bS16



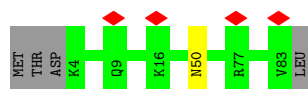
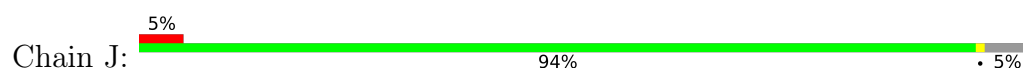
- Molecule 18: Small ribosomal subunit protein bS16



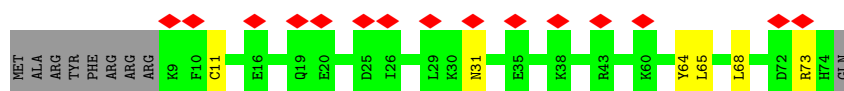
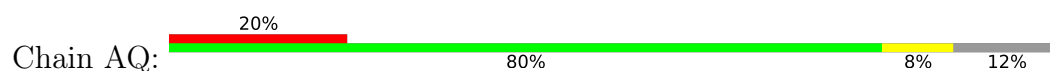
- Molecule 19: Small ribosomal subunit protein uS17



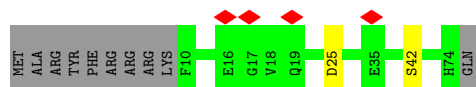
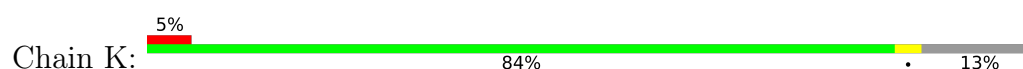
- Molecule 19: Small ribosomal subunit protein uS17



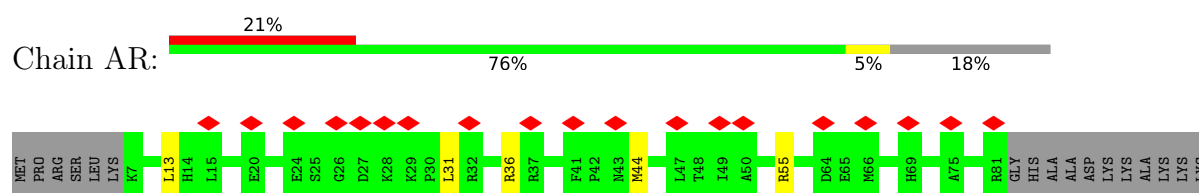
- Molecule 20: Small ribosomal subunit protein bS18



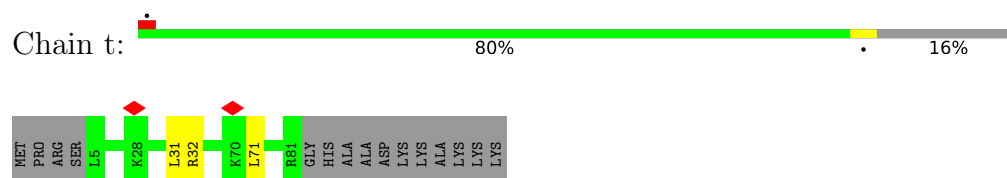
- Molecule 20: Small ribosomal subunit protein bS18



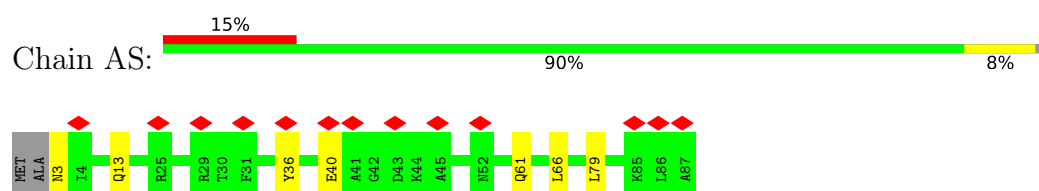
- Molecule 21: Small ribosomal subunit protein uS19



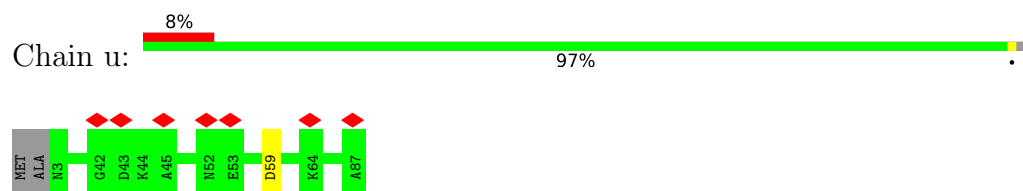
- Molecule 21: Small ribosomal subunit protein uS19



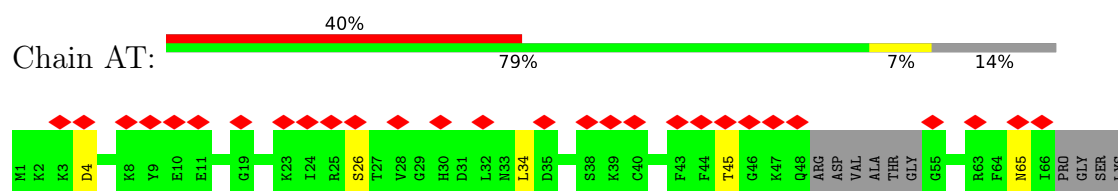
- Molecule 22: Small ribosomal subunit protein bS20



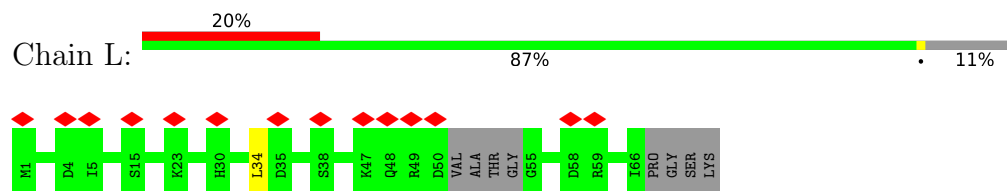
- Molecule 22: Small ribosomal subunit protein bS20



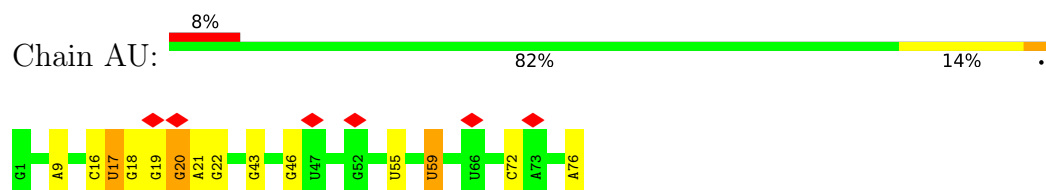
- Molecule 23: Large ribosomal subunit protein bL31A



- Molecule 23: Large ribosomal subunit protein bL31A

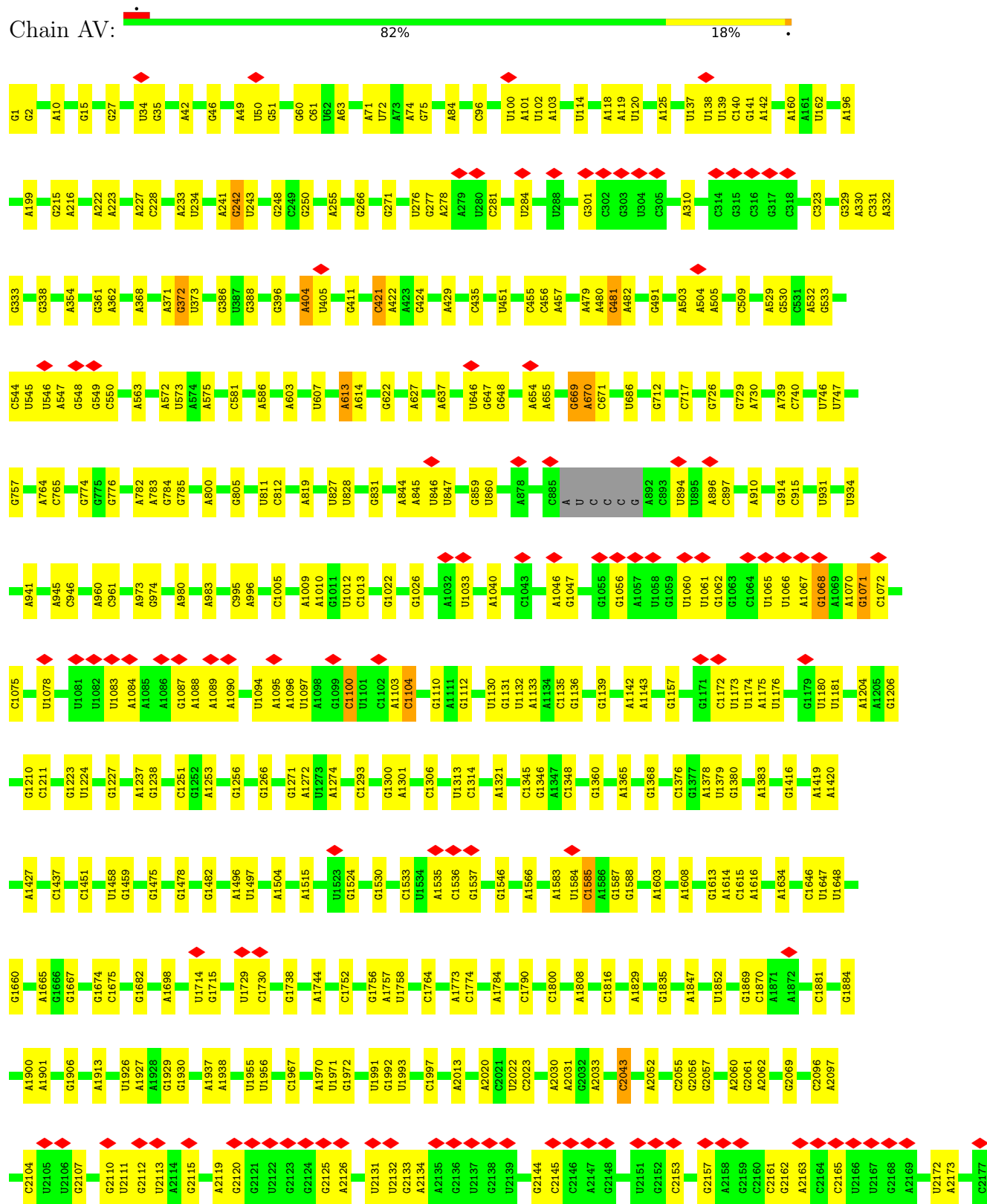


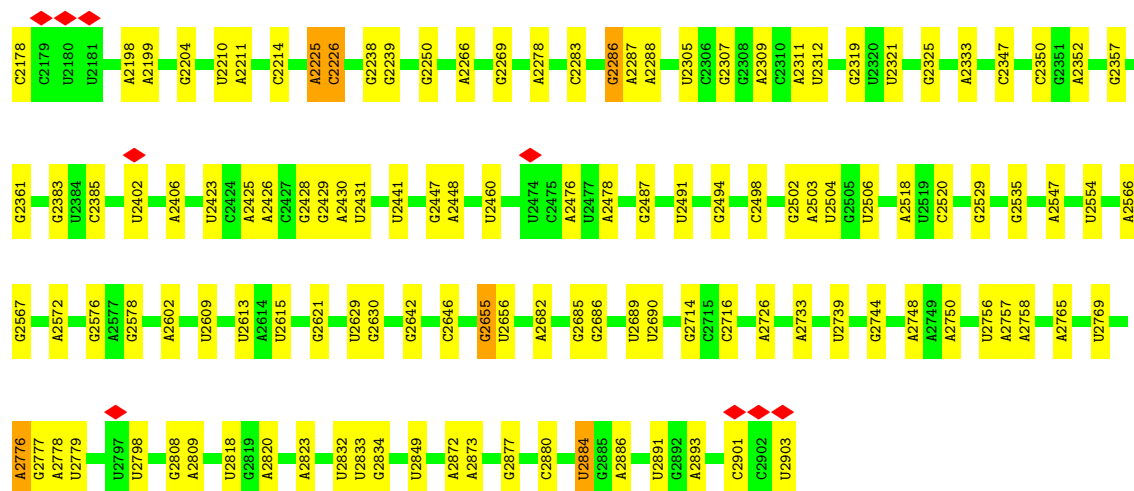
- Molecule 24: P-site tRNA



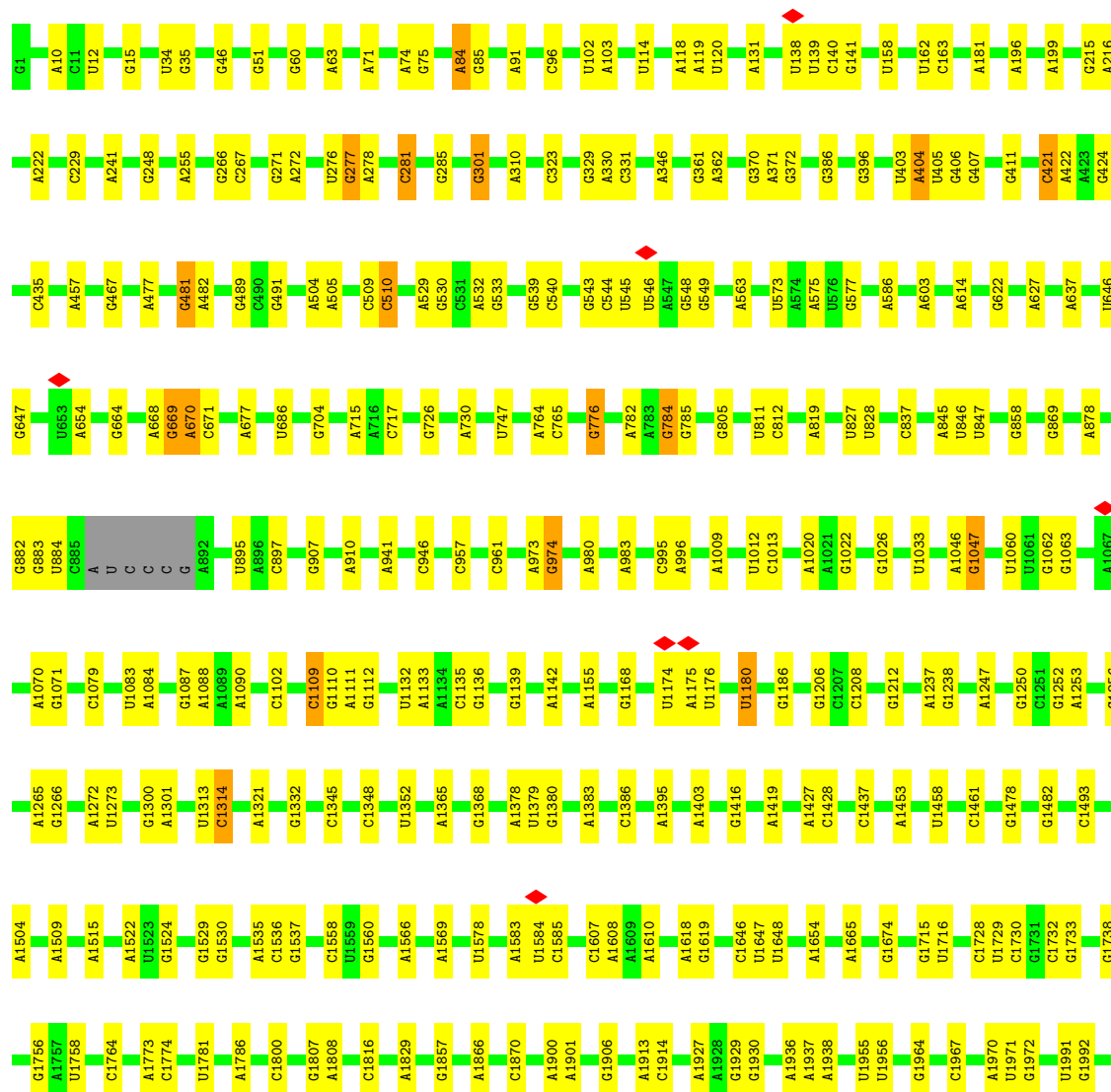
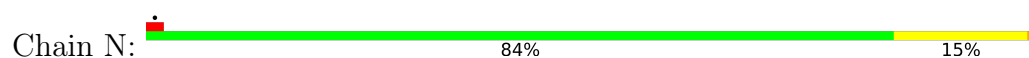
• Molecule 25: 23S RNA

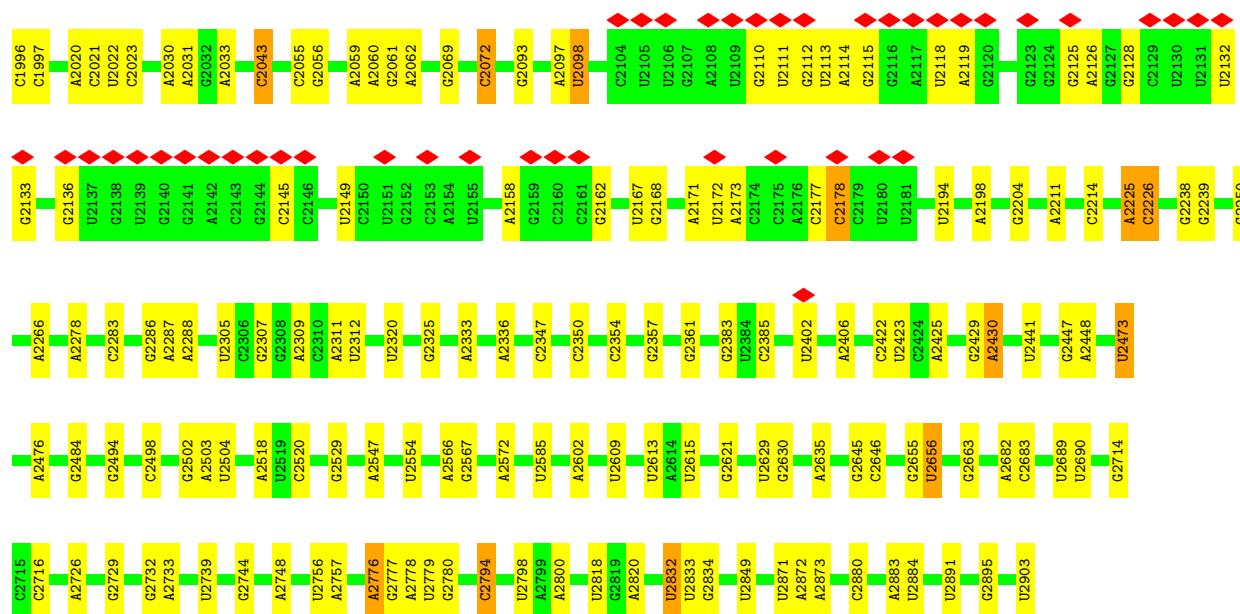
Chain AV:



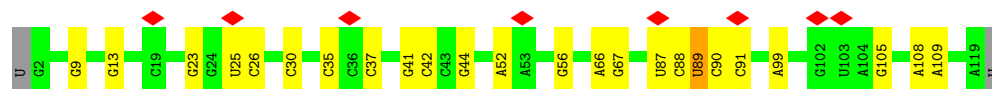
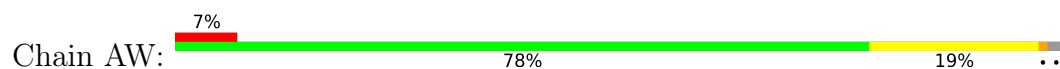


• Molecule 25: 23S RNA

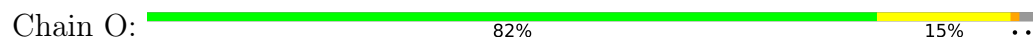




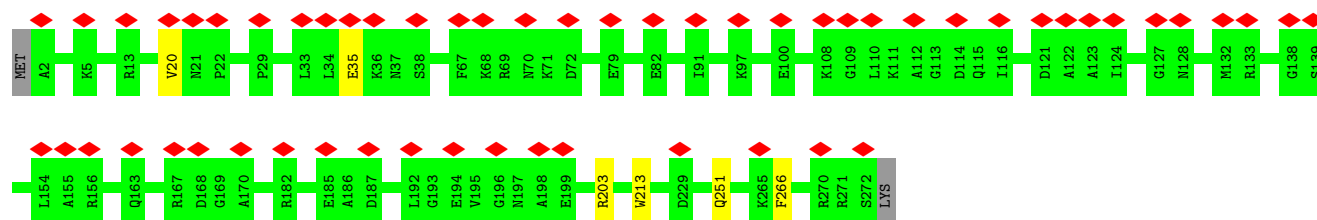
• Molecule 26: 5S ribosomal RNA



• Molecule 26: 5S ribosomal RNA

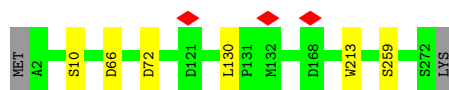


• Molecule 27: Large ribosomal subunit protein uL2



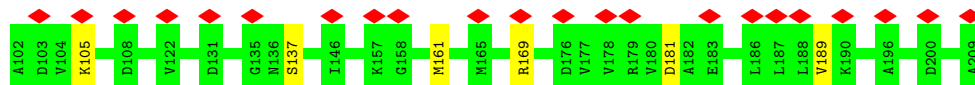
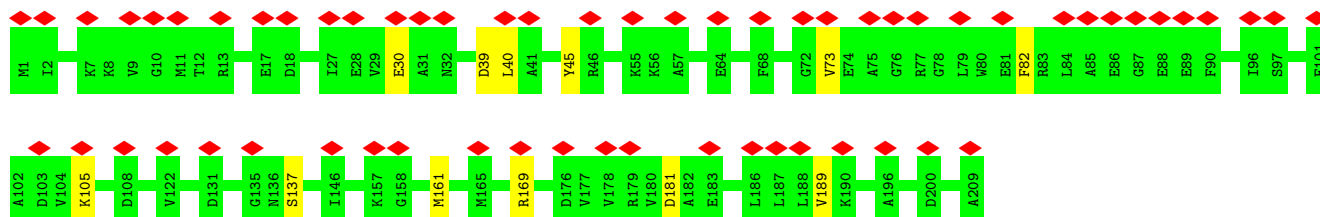
• Molecule 27: Large ribosomal subunit protein uL2





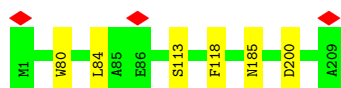
- Molecule 28: 50S ribosomal protein L3

Chain AY: 29% 94% 6%



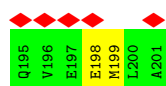
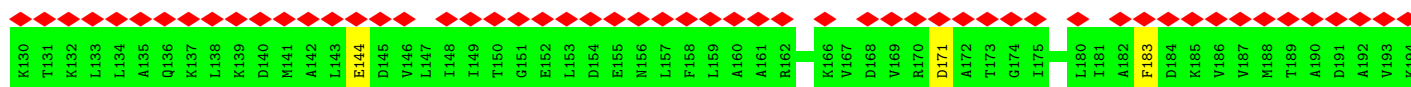
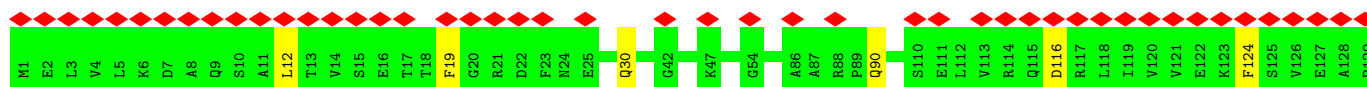
- Molecule 28: 50S ribosomal protein L3

Chain Q: 97%



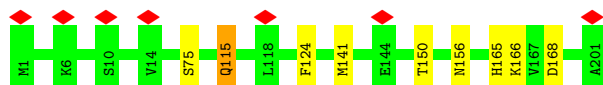
- Molecule 29: Large ribosomal subunit protein uL4

Chain AZ: 53% 95% 5%



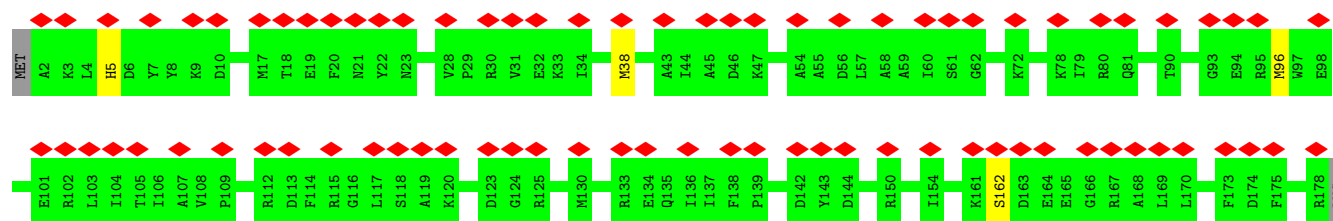
- Molecule 29: Large ribosomal subunit protein uL4

Chain R: 96%

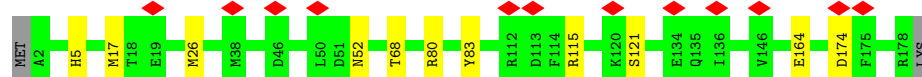


- Molecule 30: Large ribosomal subunit protein uL5

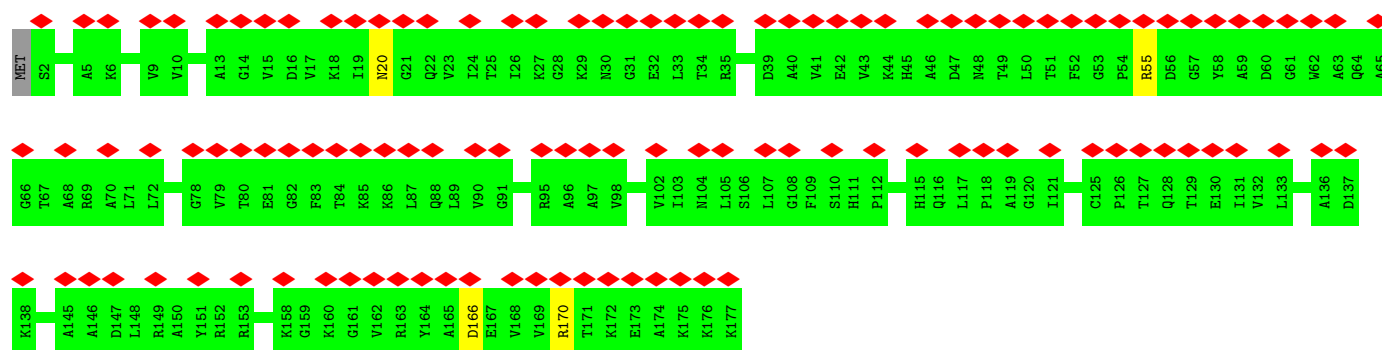
Chain Aa: 44% 97%



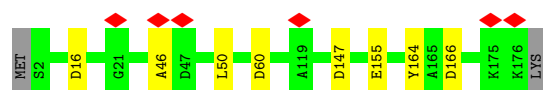
- Molecule 30: Large ribosomal subunit protein uL5



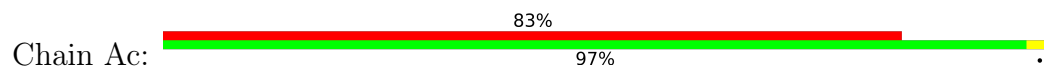
- Molecule 31: Large ribosomal subunit protein uL6

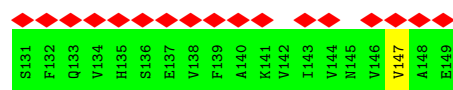


- Molecule 31: Large ribosomal subunit protein uL6

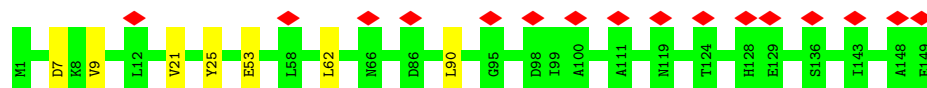


- Molecule 32: Large ribosomal subunit protein bL9

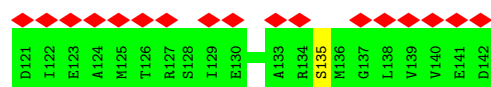
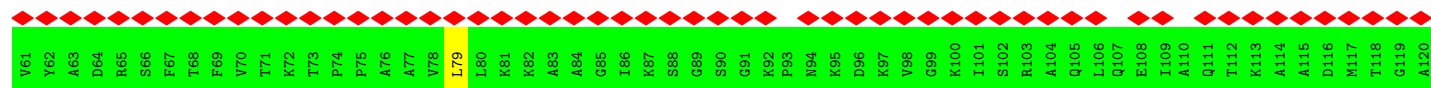
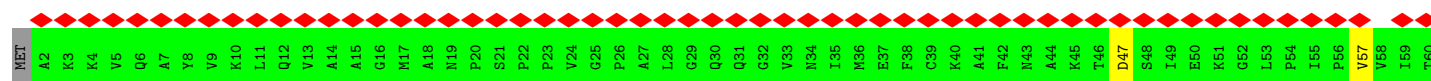




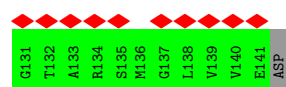
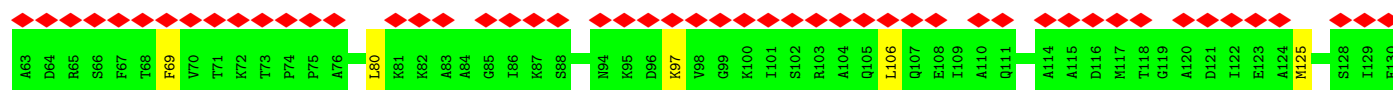
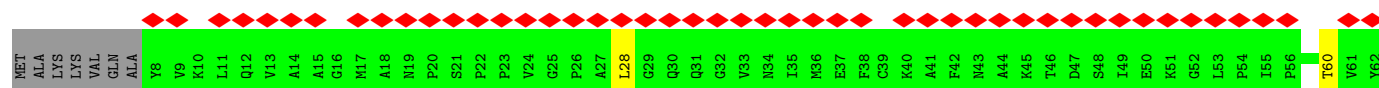
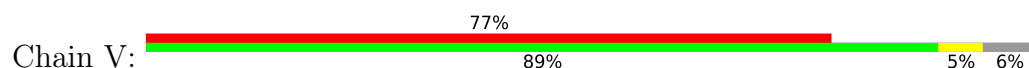
- Molecule 32: Large ribosomal subunit protein bL9



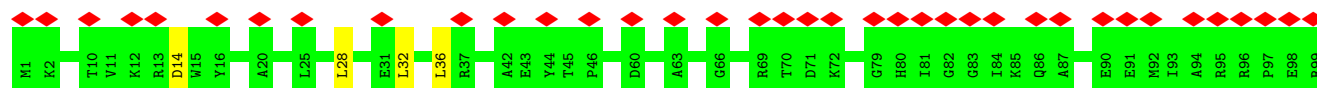
- Molecule 33: 50S ribosomal protein L11

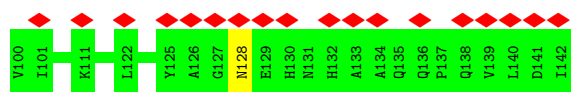


- Molecule 33: 50S ribosomal protein L11



- Molecule 34: Large ribosomal subunit protein uL13





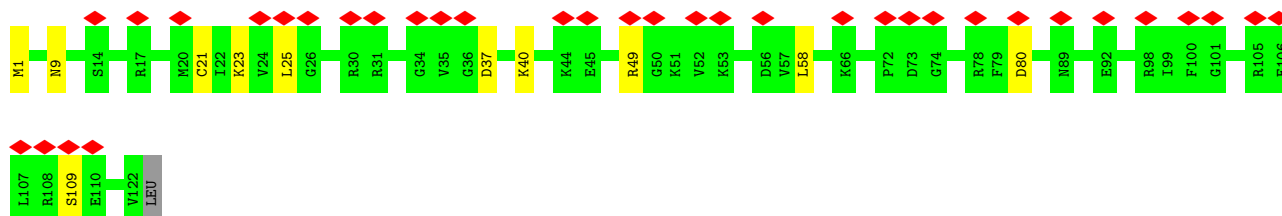
- Molecule 34: Large ribosomal subunit protein uL13

Chain W: 96%



- Molecule 35: Large ribosomal subunit protein uL14

Chain Af: 28% 90% 9%



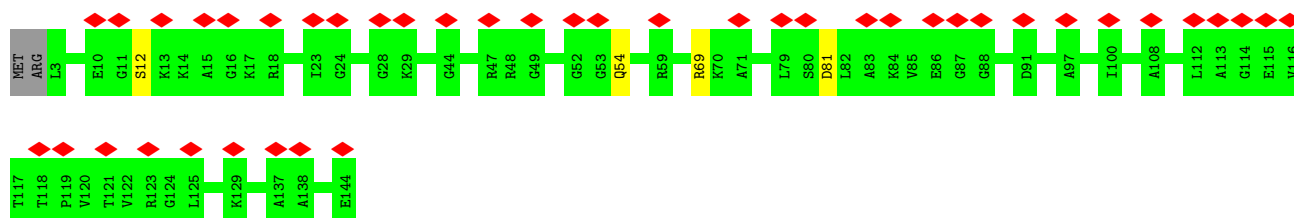
- Molecule 35: Large ribosomal subunit protein uL14

Chain X: 95%



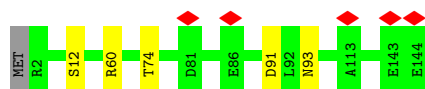
- Molecule 36: Large ribosomal subunit protein uL15

Chain Ag: 29% 96%

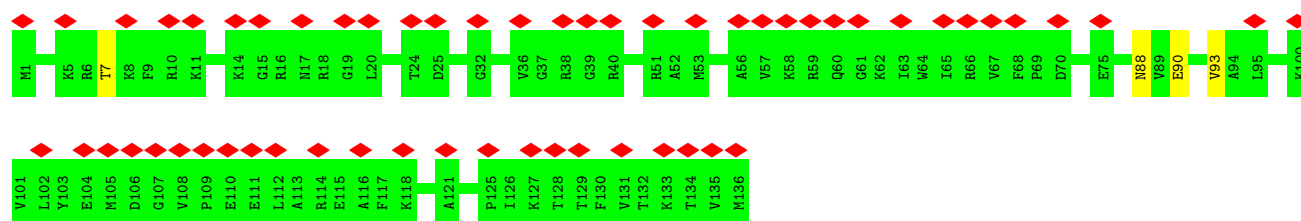
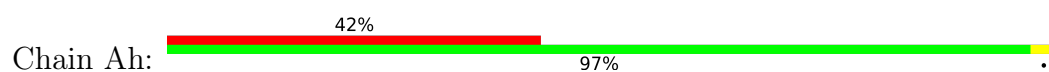


- Molecule 36: Large ribosomal subunit protein uL15

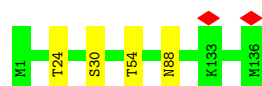
Chain Y: 96%



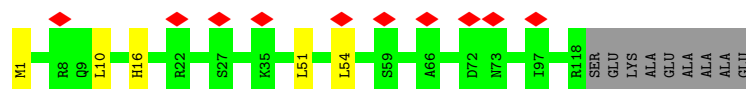
- Molecule 37: 50S ribosomal protein L16



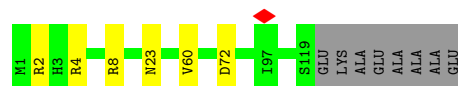
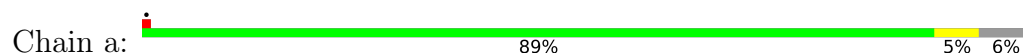
- Molecule 37: 50S ribosomal protein L16



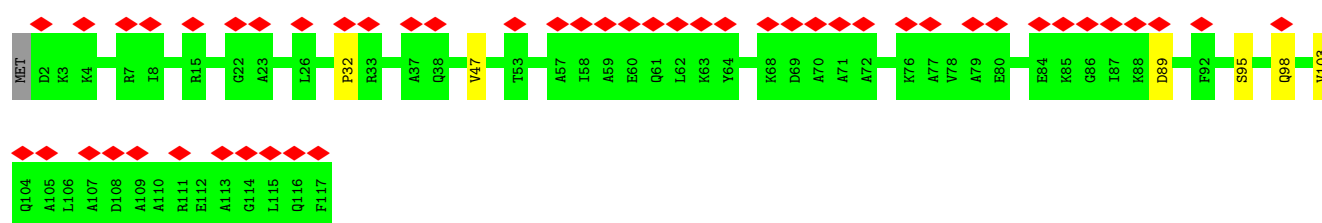
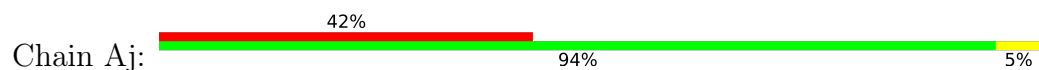
- Molecule 38: Large ribosomal subunit protein bL17



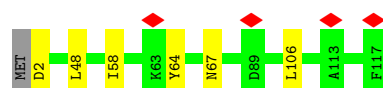
- Molecule 38: Large ribosomal subunit protein bL17



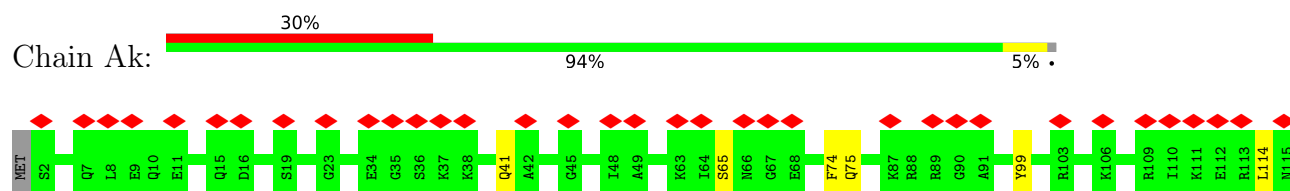
- Molecule 39: Large ribosomal subunit protein uL18



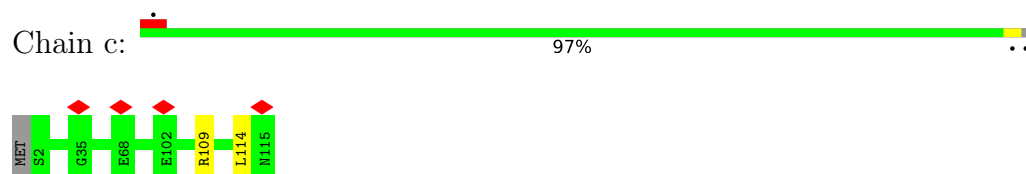
- Molecule 39: Large ribosomal subunit protein uL18



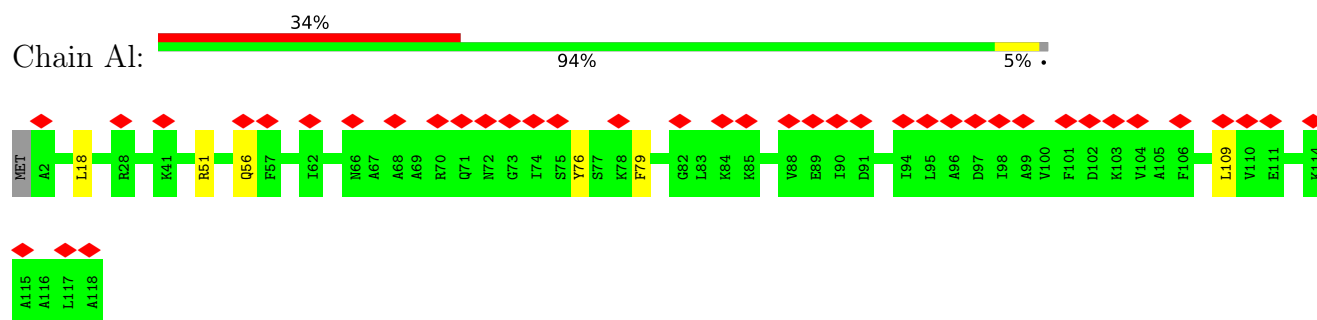
- Molecule 40: Large ribosomal subunit protein bL19



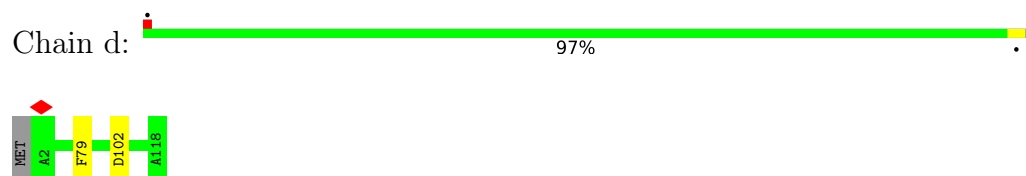
- Molecule 40: Large ribosomal subunit protein bL19



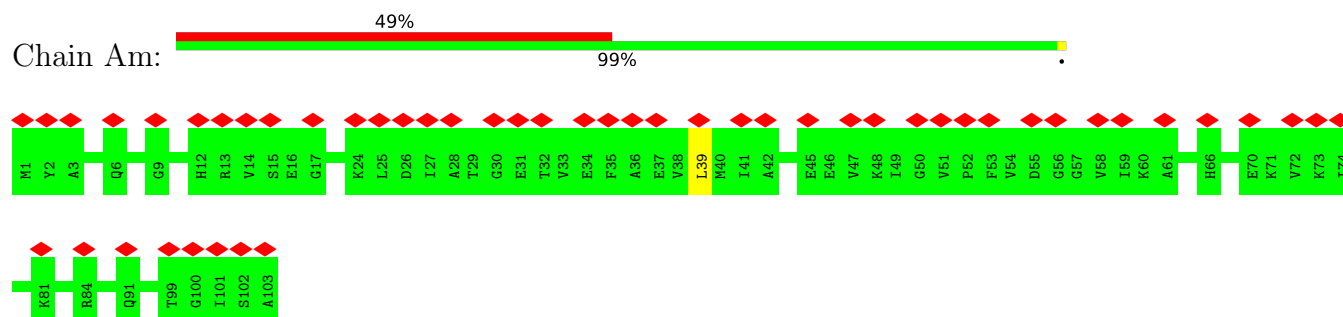
- Molecule 41: Large ribosomal subunit protein bL20



- Molecule 41: Large ribosomal subunit protein bL20

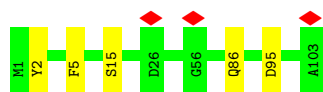


- Molecule 42: Large ribosomal subunit protein bL21

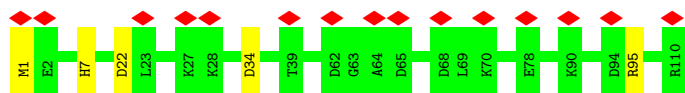


- Molecule 42: Large ribosomal subunit protein bL21





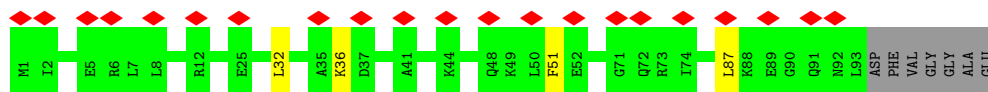
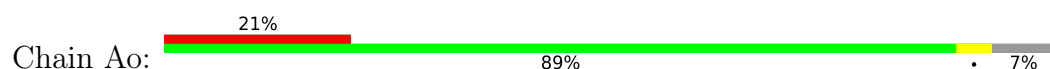
- Molecule 43: Large ribosomal subunit protein uL22



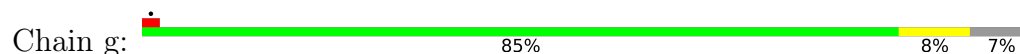
- Molecule 43: Large ribosomal subunit protein uL22



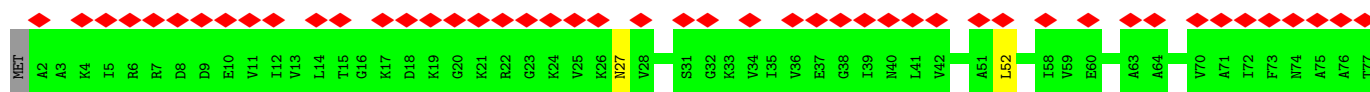
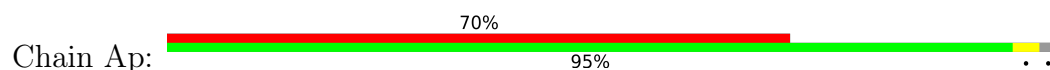
- Molecule 44: Large ribosomal subunit protein uL23



- Molecule 44: Large ribosomal subunit protein uL23

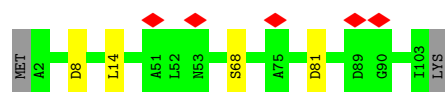


- Molecule 45: Large ribosomal subunit protein uL24

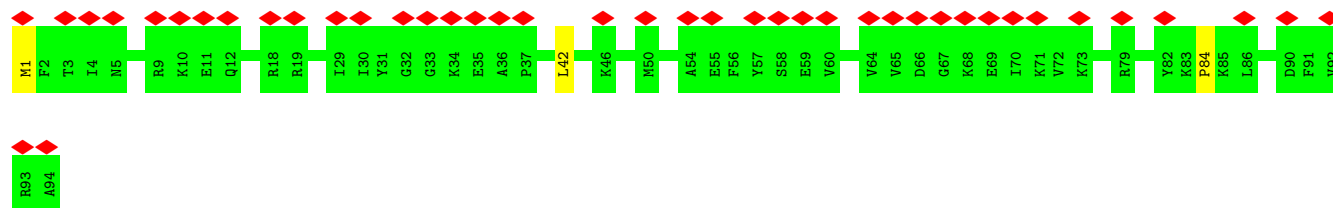


- Molecule 45: Large ribosomal subunit protein uL24

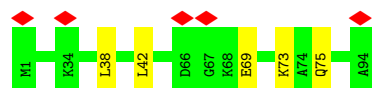




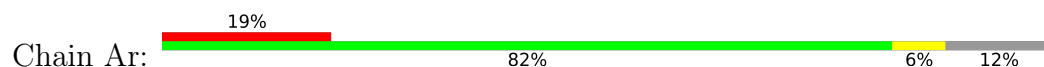
- Molecule 46: Large ribosomal subunit protein bL25



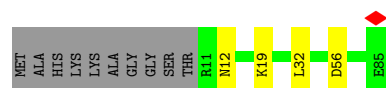
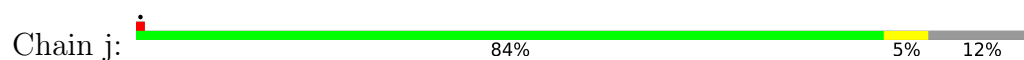
- Molecule 46: Large ribosomal subunit protein bL25



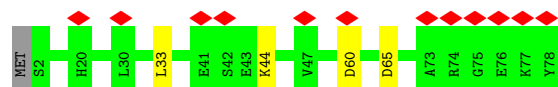
- Molecule 47: Large ribosomal subunit protein bL27



- Molecule 47: Large ribosomal subunit protein bL27

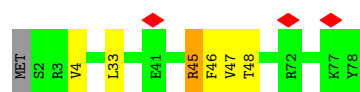


- Molecule 48: Large ribosomal subunit protein bL28

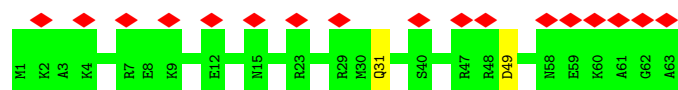


- Molecule 48: Large ribosomal subunit protein bL28

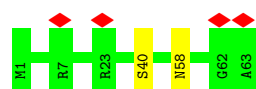




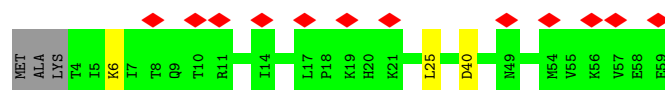
- Molecule 49: Large ribosomal subunit protein uL29



- Molecule 49: Large ribosomal subunit protein uL29



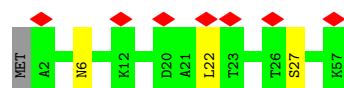
- Molecule 50: Large ribosomal subunit protein uL30



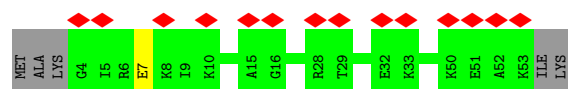
- Molecule 50: Large ribosomal subunit protein uL30



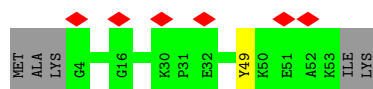
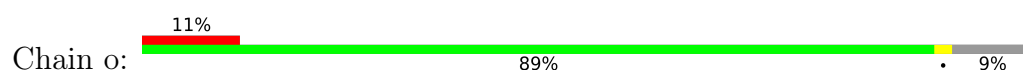
- Molecule 51: Large ribosomal subunit protein bL32



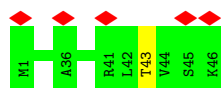
- Molecule 52: Large ribosomal subunit protein bL33



- Molecule 52: Large ribosomal subunit protein bL33



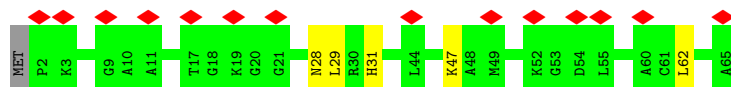
- Molecule 53: Large ribosomal subunit protein bL34



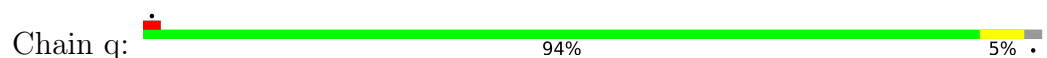
- Molecule 53: Large ribosomal subunit protein bL34



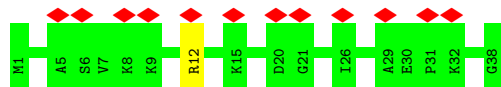
- Molecule 54: Large ribosomal subunit protein bL35



- Molecule 54: Large ribosomal subunit protein bL35

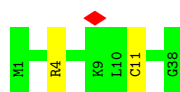


- Molecule 55: Large ribosomal subunit protein bL36A

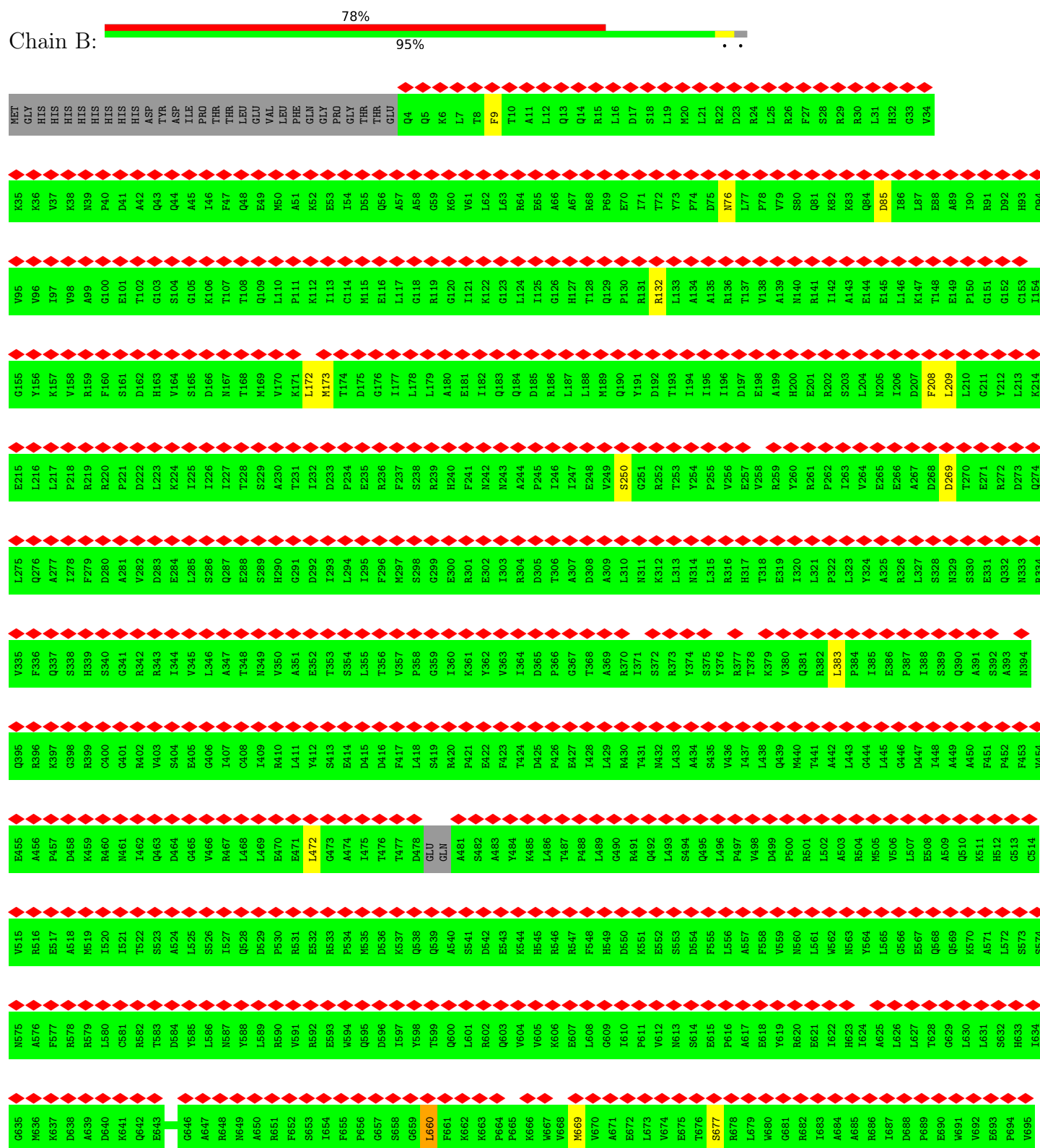


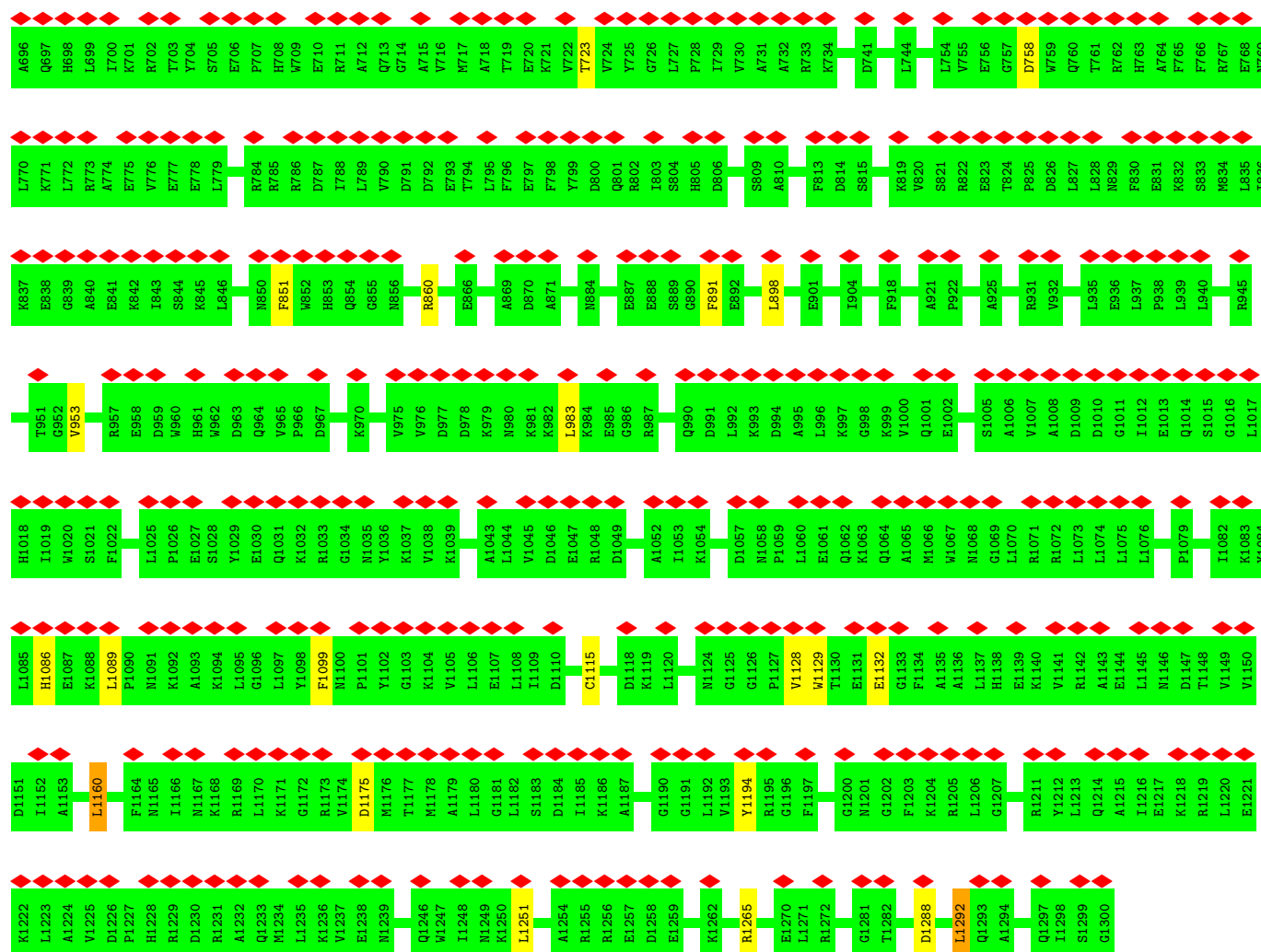
- Molecule 55: Large ribosomal subunit protein bL36A



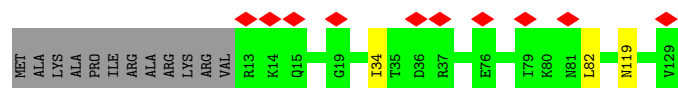
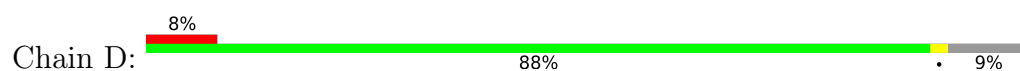


• Molecule 56: ATP-dependent RNA helicase HrpA

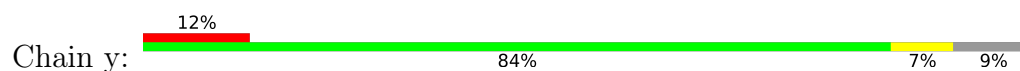




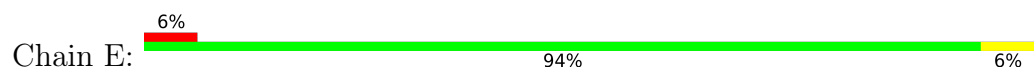
- Molecule 57: Small ribosomal subunit protein uS11



- Molecule 57: Small ribosomal subunit protein uS11



- Molecule 58: Small ribosomal subunit protein uS12



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	17182	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.831	Depositor
Minimum map value	-0.349	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.048	Depositor
Recommended contour level	0.165	Depositor
Map size (Å)	508.9, 508.9, 508.9	wwPDB
Map dimensions	700, 700, 700	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.727, 0.727, 0.727	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	0	0.29	0/36834	0.89	31/57462 (0.1%)
1	AA	0.27	0/36966	0.89	45/57666 (0.1%)
2	1	0.29	0/1735	0.61	1/2338 (0.0%)
2	AB	0.29	0/1735	0.63	2/2338 (0.1%)
3	2	0.29	0/1651	0.66	0/2225
3	AC	0.30	0/1651	0.64	0/2225
4	3	0.29	0/1665	0.65	0/2227
4	AD	0.28	0/1665	0.69	3/2227 (0.1%)
5	4	0.35	0/1118	0.66	0/1504
5	AE	0.34	0/1118	0.73	0/1504
6	5	0.39	0/835	0.87	5/1128 (0.4%)
6	AF	0.42	0/835	0.90	5/1128 (0.4%)
7	6	0.29	0/1195	0.74	6/1602 (0.4%)
7	AG	0.33	0/1195	0.64	0/1602
8	7	0.30	0/989	0.65	1/1326 (0.1%)
8	AH	0.32	0/989	0.72	2/1326 (0.2%)
9	8	0.37	0/1034	0.80	1/1375 (0.1%)
9	AI	0.31	0/1034	0.82	4/1375 (0.3%)
10	9	0.33	0/796	0.75	1/1077 (0.1%)
10	AJ	0.28	0/796	0.74	0/1077
11	A	0.29	0/1812	1.00	9/2823 (0.3%)
12	A1	0.34	0/557	0.71	1/738 (0.1%)
12	v	0.28	0/597	0.66	0/792
13	A3	0.31	0/1830	1.11	16/2849 (0.6%)
14	AK	0.24	0/1033	0.53	0/1387
14	C	0.23	0/1033	0.55	1/1387 (0.1%)
15	AL	0.26	0/892	0.74	1/1193 (0.1%)
15	F	0.31	0/892	0.73	2/1193 (0.2%)
16	AM	0.28	0/785	0.72	0/1043
16	G	0.45	0/803	0.69	0/1070
17	AN	0.32	0/722	0.73	2/964 (0.2%)
17	H	0.32	0/710	0.65	0/950
18	AO	0.37	0/659	0.83	0/884
18	I	0.28	0/658	0.72	1/884 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	AP	0.29	0/657	0.68	0/881
19	J	0.30	0/657	0.65	0/881
20	AQ	0.31	0/553	0.81	2/742 (0.3%)
20	K	0.28	0/544	0.69	0/731
21	AR	0.30	0/618	0.71	2/833 (0.2%)
21	t	0.32	0/635	0.64	1/855 (0.1%)
22	AS	0.30	0/671	0.68	1/888 (0.1%)
22	u	0.28	0/671	0.62	0/888
23	AT	0.26	0/488	0.67	1/649 (0.2%)
23	L	0.31	0/507	0.67	0/674
24	AU	0.29	0/1816	1.02	9/2830 (0.3%)
25	AV	0.27	0/69659	0.90	72/108672 (0.1%)
25	N	0.30	0/69659	0.88	76/108672 (0.1%)
26	AW	0.26	0/2828	0.96	6/4410 (0.1%)
26	O	0.26	0/2828	0.91	5/4410 (0.1%)
27	AX	0.27	0/2121	0.62	0/2852
27	P	0.30	0/2121	0.63	1/2852 (0.0%)
28	AY	0.30	0/1586	0.66	3/2134 (0.1%)
28	Q	0.29	0/1586	0.58	0/2134
29	AZ	0.27	0/1571	0.58	0/2113
29	R	0.30	0/1571	0.62	2/2113 (0.1%)
30	Aa	0.27	0/1434	0.62	0/1926
30	S	0.34	0/1434	0.64	2/1926 (0.1%)
31	Ab	0.29	0/1343	0.61	1/1816 (0.1%)
31	T	0.29	0/1333	0.66	3/1805 (0.2%)
32	Ac	0.28	0/1122	0.65	1/1515 (0.1%)
32	U	0.41	0/1122	0.70	1/1515 (0.1%)
33	Ad	0.33	0/1046	0.58	0/1410
33	V	0.27	0/993	0.61	2/1341 (0.1%)
34	Ae	0.30	0/1152	0.69	2/1551 (0.1%)
34	W	0.33	0/1152	0.67	2/1551 (0.1%)
35	Af	0.29	0/947	0.66	0/1268
35	X	0.30	0/947	0.71	1/1268 (0.1%)
36	Ag	0.25	0/1043	0.60	0/1389
36	Y	0.30	0/1054	0.76	1/1403 (0.1%)
37	Ah	0.26	0/1093	0.61	0/1460
37	Z	0.32	0/1093	0.64	0/1460
38	Ai	0.31	0/958	0.75	2/1281 (0.2%)
38	a	0.30	0/964	0.70	1/1289 (0.1%)
39	Aj	0.28	0/902	0.59	0/1209
39	b	0.28	0/902	0.69	1/1209 (0.1%)
40	Ak	0.39	1/929 (0.1%)	0.73	1/1242 (0.1%)
40	c	0.31	0/929	0.73	1/1242 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
41	Al	0.28	0/960	0.66	1/1278 (0.1%)
41	d	0.27	0/960	0.59	0/1278
42	Am	0.30	0/829	0.72	0/1107
42	e	0.32	0/829	0.72	1/1107 (0.1%)
43	An	0.33	0/864	0.70	2/1156 (0.2%)
43	f	0.27	0/864	0.63	0/1156
44	Ao	0.28	0/744	0.60	0/994
44	g	0.39	0/744	0.71	1/994 (0.1%)
45	Ap	0.29	0/787	0.67	1/1051 (0.1%)
45	h	0.27	0/787	0.58	0/1051
46	Aq	0.32	0/766	0.63	0/1025
46	i	0.33	0/766	0.75	1/1025 (0.1%)
47	Ar	0.30	0/582	0.77	3/769 (0.4%)
47	j	0.33	0/582	0.74	1/769 (0.1%)
48	As	0.26	0/635	0.71	1/848 (0.1%)
48	k	0.43	1/635 (0.2%)	0.72	1/848 (0.1%)
49	At	0.29	0/510	0.68	0/677
49	l	0.41	0/510	0.67	0/677
50	Au	0.29	0/439	0.72	0/587
50	m	0.27	0/453	0.72	1/605 (0.2%)
51	Av	0.33	0/450	0.67	0/599
52	Aw	0.31	0/416	0.68	0/554
52	o	0.37	0/416	0.70	0/554
53	Ax	0.27	0/380	0.73	0/498
53	p	0.25	0/380	0.74	0/498
54	Ay	0.26	0/513	0.71	1/676 (0.1%)
54	q	0.26	0/513	0.62	0/676
55	Az	0.25	0/303	0.61	0/397
55	r	0.29	0/303	0.64	0/397
56	B	0.27	0/10668	0.57	7/14419 (0.0%)
57	D	0.31	0/893	0.68	0/1205
57	y	0.33	0/893	0.70	0/1205
58	E	0.31	0/969	0.75	2/1300 (0.2%)
58	z	0.37	0/969	0.73	0/1300
59	M	0.27	0/1778	0.90	1/2768 (0.0%)
60	n	0.25	0/435	0.66	0/581
61	s	0.37	0/326	0.66	1/441 (0.2%)
62	w	0.32	0/1302	1.07	13/2018 (0.6%)
63	x	0.27	0/970	0.61	2/1307 (0.2%)
All	All	0.29	2/333181 (0.0%)	0.84	384/496574 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	k	45	ARG	C-N	5.68	1.47	1.34
40	Ak	75	GLN	C-N	5.41	1.46	1.34

All (384) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	AV	613	A	O4'-C1'-N9	10.79	116.84	108.20
1	0	1125	U	C2-N1-C1'	9.96	129.65	117.70
25	N	1313	U	C2-N1-C1'	9.95	129.64	117.70
13	A3	76	C	N1-C2-O2	9.94	124.86	118.90
13	A3	76	C	C2-N1-C1'	9.82	129.60	118.80
25	N	1313	U	N1-C2-O2	8.86	129.00	122.80
25	N	1313	U	N3-C2-O2	-8.85	116.01	122.20
26	O	89	U	C2-N1-C1'	8.74	128.19	117.70
25	AV	2506	U	C2-N1-C1'	8.74	128.19	117.70
1	AA	386	C	N3-C2-O2	-8.67	115.83	121.90
1	0	1125	U	N3-C4-O4	8.66	125.46	119.40
25	N	510	C	N1-C2-O2	8.65	124.09	118.90
25	AV	2013	A	N1-C6-N6	-8.56	113.46	118.60
1	0	1125	U	C5-C4-O4	-8.43	120.84	125.90
58	E	109	ASP	CB-CG-OD1	8.39	125.85	118.30
20	AQ	65	LEU	CA-CB-CG	8.24	134.26	115.30
25	AV	1313	U	C2-N1-C1'	8.20	127.55	117.70
40	c	114	LEU	CA-CB-CG	8.17	134.10	115.30
25	AV	2506	U	N1-C2-O2	8.13	128.49	122.80
26	O	89	U	N1-C2-O2	8.08	128.46	122.80
1	0	1322	C	N1-C2-O2	8.06	123.73	118.90
26	AW	89	U	C2-N1-C1'	8.04	127.35	117.70
25	N	2473	U	N1-C2-O2	8.03	128.42	122.80
25	N	2656	U	C2-N1-C1'	8.02	127.33	117.70
13	A3	76	C	N3-C2-O2	-7.98	116.32	121.90
25	N	2794	C	C2-N1-C1'	7.83	127.42	118.80
25	AV	1774	C	N3-C2-O2	-7.71	116.51	121.90
1	AA	1125	U	C2-N1-C1'	7.63	126.86	117.70
25	N	2656	U	N1-C2-O2	7.59	128.11	122.80
26	AW	89	U	N1-C2-O2	7.59	128.11	122.80
25	N	1774	C	N3-C2-O2	-7.57	116.60	121.90
45	Ap	52	LEU	CA-CB-CG	7.57	132.70	115.30
11	A	75	C	C2-N1-C1'	7.48	127.03	118.80
25	N	510	C	C2-N1-C1'	7.42	126.96	118.80
25	N	1348	C	N1-C2-O2	7.39	123.34	118.90
4	AD	174	ASP	CB-CG-OD1	7.34	124.91	118.30
25	AV	2506	U	N3-C2-O2	-7.34	117.06	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	N	2473	U	C2-N1-C1'	7.30	126.46	117.70
1	0	1322	C	C2-N1-C1'	7.26	126.78	118.80
25	AV	1071	G	C4-N9-C1'	7.25	135.93	126.50
32	Ac	122	LEU	CA-CB-CG	7.25	131.97	115.30
62	w	534	G	C4-N9-C1'	7.23	135.90	126.50
6	5	72	ASP	CB-CG-OD1	7.22	124.79	118.30
25	N	837	C	N3-C2-O2	-7.21	116.86	121.90
1	0	754	C	C2-N1-C1'	7.16	126.67	118.80
1	AA	528	C	N1-C2-O2	7.15	123.19	118.90
56	B	1292	LEU	CA-CB-CG	7.15	131.74	115.30
6	AF	91	ARG	NE-CZ-NH2	7.15	123.87	120.30
32	U	7	ASP	CB-CG-OD1	7.14	124.73	118.30
9	8	56	ASP	CB-CG-OD1	7.12	124.71	118.30
26	AW	89	U	N3-C2-O2	-7.11	117.22	122.20
26	O	89	U	N3-C2-O2	-7.08	117.25	122.20
13	A3	30	U	C2-N1-C1'	7.04	126.15	117.70
25	N	2473	U	N3-C2-O2	-7.03	117.28	122.20
25	AV	1313	U	N1-C2-O2	6.99	127.69	122.80
11	A	75	C	N1-C2-O2	6.98	123.09	118.90
25	AV	1068	G	N3-C4-C5	-6.94	125.13	128.60
25	AV	1313	U	N3-C2-O2	-6.94	117.34	122.20
36	Y	91	ASP	CB-CG-OD1	6.93	124.54	118.30
31	T	147	ASP	CB-CG-OD1	6.92	124.52	118.30
8	AH	9	ASP	CB-CG-OD1	6.88	124.50	118.30
6	5	90	MET	CA-C-N	-6.87	102.09	117.20
9	AI	107	ASP	CB-CG-OD1	6.87	124.48	118.30
34	W	141	ASP	CB-CG-OD1	6.87	124.48	118.30
25	N	837	C	N1-C2-O2	6.86	123.02	118.90
50	m	25	LEU	CA-CB-CG	6.84	131.02	115.30
25	AV	1068	G	N3-C4-N9	6.83	130.10	126.00
25	N	2656	U	C5-C6-N1	6.81	126.11	122.70
6	5	90	MET	C-N-CA	-6.78	104.76	121.70
13	A3	76	C	C6-N1-C1'	-6.77	112.68	120.80
25	N	2682	A	C5-C6-N1	6.77	121.08	117.70
25	AV	1068	G	C4-N9-C1'	6.76	135.29	126.50
25	N	2098	U	C2-N1-C1'	6.75	125.79	117.70
25	AV	2013	A	C5-C6-N1	6.69	121.05	117.70
1	AA	979	C	N1-C2-O2	6.69	122.91	118.90
25	AV	1061	U	C2-N1-C1'	6.68	125.71	117.70
18	I	53	ASP	CB-CG-OD1	6.64	124.28	118.30
62	w	555	G	P-O3'-C3'	6.63	127.65	119.70
43	An	22	ASP	CB-CG-OD1	6.60	124.24	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	53	G	C4-N9-C1'	6.59	135.07	126.50
62	w	555	G	C4-N9-C1'	6.59	135.06	126.50
56	B	1160	LEU	CA-CB-CG	6.58	130.43	115.30
44	g	52	GLU	CA-CB-CG	6.56	127.83	113.40
28	AY	181	ASP	CB-CG-OD1	6.56	124.20	118.30
34	Ae	28	LEU	CA-CB-CG	6.55	130.37	115.30
47	Ar	56	ASP	CB-CG-OD1	6.54	124.19	118.30
1	0	1125	U	C6-N1-C1'	-6.54	112.05	121.20
56	B	383	LEU	CA-CB-CG	6.53	130.31	115.30
15	AL	75	MET	CA-CB-CG	6.52	124.39	113.30
15	F	83	LEU	CA-CB-CG	6.51	130.28	115.30
26	AW	26	C	N1-C2-O2	6.50	122.80	118.90
13	A3	30	U	N3-C2-O2	-6.48	117.66	122.20
62	w	543	A	P-O3'-C3'	6.48	127.48	119.70
20	AQ	68	LEU	CA-CB-CG	6.48	130.20	115.30
25	AV	1774	C	N1-C2-O2	6.47	122.78	118.90
42	e	95	ASP	CB-CG-OD1	6.47	124.12	118.30
13	A3	30	U	N1-C2-O2	6.46	127.32	122.80
13	A3	76	C	C6-N1-C2	-6.46	117.72	120.30
62	w	534	G	N3-C4-N9	6.45	129.87	126.00
1	AA	582	C	N1-C2-O2	6.44	122.76	118.90
25	AV	1072	C	N1-C2-O2	6.44	122.76	118.90
28	AY	39	ASP	CB-CG-OD1	6.42	124.07	118.30
62	w	534	G	N3-C4-C5	-6.41	125.39	128.60
25	N	1774	C	N1-C2-O2	6.41	122.74	118.90
25	N	404	A	P-O3'-C3'	6.38	127.36	119.70
25	N	1313	U	C6-N1-C1'	-6.38	112.27	121.20
9	AI	87	LEU	CA-CB-CG	6.38	129.96	115.30
25	N	510	C	N3-C2-O2	-6.37	117.44	121.90
25	AV	421	C	P-O3'-C3'	6.37	127.34	119.70
39	b	106	LEU	CA-CB-CG	6.29	129.77	115.30
25	N	1079	C	C2-N1-C1'	6.28	125.71	118.80
25	AV	1061	U	N1-C2-O2	6.27	127.19	122.80
58	E	21	VAL	CG1-CB-CG2	-6.26	100.88	110.90
25	N	2682	A	N1-C6-N6	-6.25	114.85	118.60
54	Ay	29	LEU	CA-CB-CG	6.25	129.68	115.30
24	AU	72	C	C2-N1-C1'	6.25	125.67	118.80
31	T	16	ASP	CB-CG-OD1	6.25	123.92	118.30
25	AV	2225	A	P-O3'-C3'	6.24	127.19	119.70
11	A	53	G	C8-N9-C1'	-6.23	118.90	127.00
13	A3	51	C	P-O3'-C3'	6.23	127.18	119.70
62	w	555	G	N3-C4-C5	-6.23	125.49	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1322	C	N3-C2-O2	-6.23	117.54	121.90
25	AV	242	G	P-O3'-C3'	6.23	127.17	119.70
13	A3	63	C	O4'-C1'-N1	6.21	113.17	108.20
1	AA	1201	A	P-O3'-C3'	6.18	127.11	119.70
47	Ar	15	ASP	CB-CG-OD1	6.17	123.86	118.30
6	AF	86	ARG	NE-CZ-NH2	6.17	123.38	120.30
1	0	1201	A	P-O3'-C3'	6.17	127.10	119.70
63	x	59	LEU	CA-CB-CG	6.16	129.47	115.30
23	AT	4	ASP	CB-CG-OD1	6.16	123.84	118.30
25	N	2225	A	P-O3'-C3'	6.15	127.08	119.70
10	9	97	ASP	CB-CG-OD1	6.15	123.84	118.30
25	AV	404	A	P-O3'-C3'	6.15	127.08	119.70
25	AV	1071	G	C8-N9-C1'	-6.15	119.01	127.00
25	N	84	A	P-O3'-C3'	6.14	127.07	119.70
1	0	1320	C	C2-N1-C1'	6.13	125.54	118.80
25	N	1109	C	P-O3'-C3'	6.13	127.05	119.70
1	0	1320	C	N1-C2-O2	6.12	122.57	118.90
1	0	479	U	N1-C2-O2	6.12	127.08	122.80
25	N	421	C	P-O3'-C3'	6.12	127.04	119.70
25	N	1314	C	C2-N1-C1'	6.12	125.53	118.80
25	N	271	G	O4'-C1'-N9	6.11	113.08	108.20
62	w	534	G	C8-N9-C1'	-6.10	119.06	127.00
13	A3	63	C	C2-N1-C1'	-6.10	112.09	118.80
1	0	1132	C	C2-N1-C1'	6.09	125.50	118.80
1	AA	979	C	C2-N1-C1'	6.09	125.49	118.80
1	AA	1086	U	N1-C2-O2	6.08	127.06	122.80
13	A3	73	C	O4'-C1'-N1	6.08	113.06	108.20
1	AA	979	C	N3-C2-O2	-6.06	117.66	121.90
1	0	812	G	P-O3'-C3'	6.05	126.97	119.70
40	Ak	114	LEU	CA-CB-CG	6.05	129.22	115.30
25	AV	2013	A	C4-C5-C6	-6.05	113.98	117.00
1	AA	386	C	C6-N1-C2	-6.04	117.89	120.30
6	5	90	MET	O-C-N	6.02	132.34	122.70
31	Ab	55	ARG	NE-CZ-NH2	6.02	123.31	120.30
1	AA	979	C	C6-N1-C2	-6.01	117.90	120.30
25	AV	1071	G	N3-C4-N9	5.99	129.59	126.00
25	AV	1348	C	N1-C2-O2	5.98	122.49	118.90
25	AV	1614	A	C5-C6-N1	5.98	120.69	117.70
1	0	115	G	P-O3'-C3'	5.97	126.87	119.70
62	w	553	C	C2-N1-C1'	5.97	125.37	118.80
62	w	555	G	N3-C4-N9	5.96	129.58	126.00
25	N	670	A	P-O3'-C3'	5.96	126.85	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	N	2098	U	N1-C2-O2	5.95	126.97	122.80
25	AV	670	A	P-O3'-C3'	5.93	126.82	119.70
1	AA	1322	C	N1-C2-O2	5.93	122.46	118.90
11	A	53	G	N3-C4-N9	5.93	129.56	126.00
13	A3	63	C	C6-N1-C1'	5.92	127.90	120.80
1	AA	1158	C	C2-N1-C1'	5.91	125.30	118.80
25	N	974	G	C4-N9-C1'	5.91	134.18	126.50
25	AV	1956	U	N3-C2-O2	-5.90	118.07	122.20
26	O	89	U	C6-N1-C1'	-5.90	112.94	121.20
25	AV	61	C	N1-C2-O2	5.88	122.43	118.90
25	AV	2776	A	P-O3'-C3'	5.88	126.75	119.70
25	N	2178	C	N3-C2-O2	-5.88	117.79	121.90
25	N	2656	U	N3-C2-O2	-5.88	118.09	122.20
47	j	56	ASP	CB-CG-OD1	5.88	123.59	118.30
25	AV	1071	G	N3-C4-C5	-5.87	125.67	128.60
15	F	79	ARG	NE-CZ-NH2	5.86	123.23	120.30
25	N	323	C	C2-N1-C1'	5.86	125.24	118.80
25	N	2776	A	P-O3'-C3'	5.85	126.72	119.70
25	N	1956	U	N3-C2-O2	-5.84	118.11	122.20
25	N	1348	C	N3-C2-O2	-5.84	117.81	121.90
38	Ai	54	LEU	CA-CB-CG	5.84	128.73	115.30
25	AV	1585	C	N1-C2-O2	5.82	122.39	118.90
34	Ae	36	LEU	CA-CB-CG	5.82	128.67	115.30
25	AV	607	U	N1-C2-O2	5.81	126.87	122.80
25	N	2682	A	C4-C5-C6	-5.80	114.10	117.00
25	AV	2901	C	N1-C2-O2	5.80	122.38	118.90
1	AA	54	C	N3-C2-O2	-5.79	117.85	121.90
25	AV	2153	C	N3-C2-O2	-5.79	117.85	121.90
35	X	87	LEU	CA-CB-CG	5.79	128.60	115.30
1	AA	115	G	P-O3'-C3'	5.78	126.64	119.70
11	A	75	C	N3-C2-O2	-5.75	117.87	121.90
38	a	72	ASP	CB-CG-OD1	5.74	123.47	118.30
25	AV	1314	C	C2-N1-C1'	5.73	125.10	118.80
25	N	1348	C	C2-N1-C1'	5.73	125.10	118.80
25	N	669	G	C4-N9-C1'	5.72	133.94	126.50
25	AV	1	G	C4-N9-C1'	5.72	133.94	126.50
30	S	26	MET	CA-CB-CG	5.72	123.02	113.30
25	AV	1956	U	N1-C2-O2	5.71	126.80	122.80
25	N	1180	U	C2-N1-C1'	5.71	124.55	117.70
8	7	9	ASP	CB-CG-OD1	5.68	123.42	118.30
25	N	1956	U	N1-C2-O2	5.68	126.78	122.80
25	AV	1615	C	O4'-C1'-N1	5.68	112.74	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	W	96	ARG	NE-CZ-NH2	5.67	123.14	120.30
6	AF	8	PHE	CB-CG-CD1	5.67	124.77	120.80
1	AA	528	C	N3-C2-O2	-5.66	117.94	121.90
25	AV	669	G	C4-N9-C1'	5.65	133.85	126.50
25	AV	2506	U	C6-N1-C1'	-5.64	113.30	121.20
48	As	33	LEU	CA-CB-CG	5.62	128.23	115.30
25	N	2043	C	C2-N1-C1'	5.62	124.98	118.80
25	AV	2506	U	C5-C6-N1	5.61	125.50	122.70
1	AA	1301	U	C2-N1-C1'	5.61	124.43	117.70
25	AV	137	U	N3-C2-O2	-5.61	118.28	122.20
21	AR	13	LEU	CA-CB-CG	5.60	128.18	115.30
28	AY	40	LEU	CA-CB-CG	5.60	128.17	115.30
25	N	2716	C	C2-N1-C1'	5.57	124.93	118.80
22	AS	79	LEU	CA-CB-CG	5.57	128.11	115.30
1	AA	1086	U	N3-C2-O2	-5.57	118.30	122.20
25	AV	607	U	N3-C2-O2	-5.57	118.31	122.20
25	AV	1068	G	C8-N9-C1'	-5.57	119.77	127.00
25	AV	581	C	C5-C6-N1	5.56	123.78	121.00
7	6	124	LEU	CA-CB-CG	5.56	128.09	115.30
1	AA	386	C	N1-C2-N3	5.56	123.09	119.20
25	AV	234	U	N3-C2-O2	-5.55	118.31	122.20
25	N	2794	C	C6-N1-C1'	-5.55	114.14	120.80
13	A3	19	G	O4'-C1'-N9	-5.55	103.76	108.20
25	N	2430	A	C2-N3-C4	5.55	113.37	110.60
1	AA	479	U	N1-C2-O2	5.53	126.67	122.80
25	N	281	C	C2-N1-C1'	5.52	124.88	118.80
25	AV	372	G	P-O3'-C3'	5.52	126.32	119.70
25	AV	2739	U	N3-C2-O2	-5.52	118.34	122.20
56	B	983	LEU	CA-CB-CG	5.51	127.97	115.30
25	AV	2901	C	N3-C2-O2	-5.51	118.05	121.90
2	AB	129	LEU	CA-CB-CG	5.51	127.97	115.30
61	s	153	LEU	CA-CB-CG	5.51	127.96	115.30
1	AA	436	C	C2-N1-C1'	5.50	124.85	118.80
25	AV	669	G	N3-C4-N9	5.49	129.30	126.00
9	AI	118	LEU	CA-CB-CG	5.48	127.90	115.30
17	AN	70	LEU	CA-CB-CG	5.48	127.90	115.30
56	B	1251	LEU	CA-CB-CG	5.48	127.90	115.30
25	N	2177	C	N3-C2-O2	-5.47	118.07	121.90
25	N	2683	C	N3-C2-O2	-5.47	118.07	121.90
25	AV	1614	A	C4-C5-C6	-5.47	114.27	117.00
41	Al	18	LEU	CA-CB-CG	5.47	127.88	115.30
27	P	66	ASP	CB-CG-OD1	5.47	123.22	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	6	66	LEU	CA-CB-CG	5.46	127.85	115.30
4	AD	5	LEU	CA-CB-CG	5.46	127.85	115.30
25	N	545	U	C2-N1-C1'	5.45	124.24	117.70
25	N	2098	U	N3-C2-O2	-5.45	118.38	122.20
1	0	479	U	N3-C2-O2	-5.44	118.39	122.20
25	AV	2884	U	C2-N1-C1'	5.44	124.23	117.70
1	AA	890	G	P-O3'-C3'	5.43	126.22	119.70
25	AV	545	U	C2-N1-C1'	5.43	124.22	117.70
33	V	106	LEU	CA-CB-CG	5.43	127.80	115.30
25	N	1047	G	O4'-C1'-N9	5.43	112.54	108.20
1	AA	1279	G	C4-N9-C1'	5.42	133.55	126.50
11	A	50	U	C5-C4-O4	-5.42	122.65	125.90
24	AU	20	G	C4-N9-C1'	5.42	133.54	126.50
25	N	1313	U	C5-C6-N1	5.42	125.41	122.70
1	0	1262	C	N1-C2-O2	5.42	122.15	118.90
24	AU	17	U	N1-C2-O2	5.41	126.58	122.80
25	AV	61	C	N3-C2-O2	-5.41	118.12	121.90
25	AV	2226	C	N1-C2-O2	5.41	122.14	118.90
1	AA	54	C	N1-C2-O2	5.40	122.14	118.90
1	0	530	G	C4-N9-C1'	5.39	133.51	126.50
25	AV	669	G	N3-C4-C5	-5.39	125.90	128.60
26	AW	26	C	N3-C2-O2	-5.39	118.13	121.90
56	B	660	LEU	CA-CB-CG	5.39	127.69	115.30
30	S	174	ASP	CB-CG-OD1	5.37	123.13	118.30
25	AV	717	C	N1-C2-O2	5.36	122.12	118.90
1	0	1158	C	C2-N1-C1'	5.36	124.69	118.80
17	AN	18	ASP	CB-CG-OD1	5.36	123.12	118.30
25	N	2072	C	C2-N1-C1'	5.35	124.69	118.80
25	N	1102	C	N1-C2-O2	5.35	122.11	118.90
62	w	555	G	C8-N9-C1'	-5.35	120.05	127.00
9	AI	52	LEU	CA-CB-CG	5.34	127.59	115.30
1	0	442	G	N3-C4-N9	5.33	129.20	126.00
1	AA	1182	G	P-O3'-C3'	5.33	126.10	119.70
14	C	48	LEU	CA-CB-CG	5.33	127.56	115.30
1	AA	518	C	P-O3'-C3'	5.32	126.08	119.70
24	AU	17	U	N3-C2-O2	-5.32	118.48	122.20
6	AF	1	MET	CB-CG-SD	5.30	128.31	112.40
13	A3	76	C	C5-C6-N1	5.30	123.65	121.00
25	AV	2655	G	P-O3'-C3'	5.30	126.06	119.70
7	6	99	LEU	CA-CB-CG	5.29	127.47	115.30
25	AV	1313	U	C6-N1-C1'	-5.28	113.80	121.20
8	AH	32	LEU	CA-CB-CG	5.28	127.45	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	610	U	N1-C2-O2	5.27	126.49	122.80
24	AU	20	G	N3-C4-C5	-5.27	125.96	128.60
24	AU	17	U	C2-N1-C1'	5.27	124.02	117.70
7	6	50	LEU	CA-CB-CG	5.26	127.41	115.30
25	AV	2043	C	C2-N1-C1'	5.26	124.59	118.80
11	A	75	C	C6-N1-C1'	-5.26	114.49	120.80
2	AB	68	LEU	CA-CB-CG	5.25	127.39	115.30
25	N	12	U	C2-N1-C1'	5.25	124.00	117.70
21	t	71	LEU	CA-CB-CG	5.25	127.38	115.30
1	0	563	A	C4-N9-C1'	5.25	135.75	126.30
38	Ai	10	LEU	CA-CB-CG	5.25	127.38	115.30
25	N	301	G	C4-N9-C1'	-5.25	119.68	126.50
1	0	1125	U	C5-C6-N1	5.24	125.32	122.70
6	5	61	LEU	CA-CB-CG	5.24	127.36	115.30
33	V	125	MET	CA-CB-CG	5.24	122.21	113.30
24	AU	59	U	N1-C2-O2	5.24	126.47	122.80
25	AV	2286	G	P-O3'-C3'	5.24	125.99	119.70
1	AA	598	U	N3-C2-O2	-5.23	118.54	122.20
1	AA	388	G	P-O3'-C3'	5.22	125.97	119.70
1	AA	812	G	P-O3'-C3'	5.22	125.97	119.70
1	AA	1466	C	N3-C2-O2	-5.22	118.24	121.90
1	0	1322	C	C6-N1-C1'	-5.22	114.53	120.80
1	AA	1345	U	P-O3'-C3'	5.22	125.96	119.70
25	AV	1061	U	N3-C2-O2	-5.22	118.55	122.20
12	A1	13	ASP	CB-CG-OD1	5.21	122.99	118.30
1	0	1182	G	P-O3'-C3'	5.21	125.95	119.70
1	0	754	C	C6-N1-C1'	-5.20	114.56	120.80
46	i	38	LEU	CA-CB-CG	5.20	127.25	115.30
1	AA	563	A	C4-N9-C1'	5.20	135.65	126.30
25	AV	114	U	C2-N1-C1'	5.20	123.94	117.70
1	0	1345	U	P-O3'-C3'	5.19	125.93	119.70
25	AV	1615	C	N3-C2-O2	-5.19	118.27	121.90
6	AF	61	LEU	CA-CB-CG	5.18	127.21	115.30
25	N	1180	U	N1-C2-O2	5.18	126.42	122.80
25	N	1728	C	C2-N1-C1'	5.18	124.50	118.80
7	6	110	LYS	CA-CB-CG	5.17	124.78	113.40
1	0	1300	G	P-O3'-C3'	5.17	125.91	119.70
25	N	776	G	C4-N9-C1'	5.17	133.22	126.50
25	N	2226	C	N1-C2-O2	5.17	122.00	118.90
1	AA	1347	G	P-O3'-C3'	5.17	125.90	119.70
59	M	18	G	O4'-C1'-N9	-5.16	104.07	108.20
62	w	553	C	N1-C2-O2	5.16	122.00	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	AV	1100	C	C2-N1-C1'	5.16	124.47	118.80
43	An	95	ARG	NE-CZ-NH2	5.15	122.88	120.30
63	x	38	MET	CA-CB-CG	5.15	122.06	113.30
47	Ar	19	LYS	CA-CB-CG	5.15	124.73	113.40
1	0	479	U	C2-N1-C1'	5.15	123.88	117.70
1	0	620	C	P-O3'-C3'	5.14	125.87	119.70
1	AA	1300	G	P-O3'-C3'	5.14	125.86	119.70
26	AW	89	U	C6-N1-C1'	-5.14	114.01	121.20
13	A3	73	C	C6-N1-C1'	5.13	126.96	120.80
1	AA	582	C	N3-C2-O2	-5.13	118.31	121.90
29	R	168	ASP	CB-CG-OD1	5.13	122.92	118.30
31	T	46	ALA	C-N-CA	5.13	134.53	121.70
21	AR	31	LEU	CA-CB-CG	5.12	127.09	115.30
1	AA	1158	C	N3-C2-O2	-5.12	118.32	121.90
1	AA	307	C	N1-C2-O2	5.12	121.97	118.90
25	N	158	U	C2-N1-C1'	5.11	123.83	117.70
25	N	481	G	P-O3'-C3'	5.11	125.83	119.70
1	AA	1158	C	N1-C2-O2	5.11	121.96	118.90
11	A	53	G	OP1-P-O3'	5.10	116.43	105.20
1	AA	479	U	N3-C2-O2	-5.10	118.63	122.20
25	N	1716	U	C2-N1-C1'	5.10	123.82	117.70
26	O	17	C	C2-N1-C1'	5.10	124.41	118.80
25	N	277	G	P-O3'-C3'	5.09	125.81	119.70
62	w	544	G	N3-C4-C5	-5.09	126.05	128.60
1	AA	754	C	C2-N1-C1'	5.09	124.40	118.80
25	N	12	U	N1-C2-O2	5.09	126.36	122.80
25	N	2656	U	C6-N1-C1'	-5.09	114.07	121.20
48	k	33	LEU	CA-CB-CG	5.09	127.01	115.30
1	AA	1125	U	N1-C2-O2	5.09	126.36	122.80
2	1	212	LEU	CA-CB-CG	5.09	127.00	115.30
25	AV	1104	C	C6-N1-C2	-5.09	118.27	120.30
25	N	510	C	C6-N1-C1'	-5.08	114.70	120.80
25	N	12	U	N3-C2-O2	-5.08	118.65	122.20
25	AV	1	G	N3-C4-C5	-5.07	126.07	128.60
1	0	470	C	C5-C6-N1	5.06	123.53	121.00
25	AV	915	C	N1-C2-O2	5.06	121.94	118.90
25	N	2794	C	N1-C2-O2	5.05	121.93	118.90
25	N	158	U	N1-C2-O2	5.05	126.33	122.80
25	AV	2153	C	C6-N1-C2	-5.04	118.28	120.30
1	0	442	G	C4-N9-C1'	5.04	133.06	126.50
1	AA	330	C	N1-C2-O2	5.04	121.92	118.90
56	B	472	LEU	CA-CB-CG	5.04	126.89	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	386	C	C6-N1-C1'	5.04	126.84	120.80
24	AU	72	C	N1-C2-O2	5.03	121.92	118.90
4	AD	90	LEU	CA-CB-CG	5.03	126.87	115.30
25	AV	481	G	P-O3'-C3'	5.03	125.73	119.70
29	R	115	GLN	CA-CB-CG	5.03	124.46	113.40
1	AA	439	U	C2-N1-C1'	5.03	123.73	117.70
25	N	2832	U	P-O3'-C3'	5.02	125.72	119.70
25	N	784	G	P-O3'-C3'	5.01	125.72	119.70
7	6	13	LEU	CA-CB-CG	5.01	126.82	115.30
25	N	2072	C	C5-C6-N1	5.01	123.50	121.00
24	AU	59	U	N3-C2-O2	-5.01	118.70	122.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

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	
2	1	216/241 (90%)	203 (94%)	13 (6%)	0	100	100
2	AB	216/241 (90%)	203 (94%)	13 (6%)	0	100	100
3	2	204/233 (88%)	197 (97%)	7 (3%)	0	100	100
3	AC	204/233 (88%)	198 (97%)	6 (3%)	0	100	100
4	3	203/206 (98%)	195 (96%)	8 (4%)	0	100	100
4	AD	203/206 (98%)	191 (94%)	12 (6%)	0	100	100
5	4	148/167 (89%)	139 (94%)	9 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	AE	148/167 (89%)	135 (91%)	12 (8%)	1 (1%)	19	51
6	5	98/135 (73%)	90 (92%)	8 (8%)	0	100	100
6	AF	98/135 (73%)	94 (96%)	4 (4%)	0	100	100
7	6	149/179 (83%)	145 (97%)	4 (3%)	0	100	100
7	AG	149/179 (83%)	142 (95%)	7 (5%)	0	100	100
8	7	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
8	AH	127/130 (98%)	123 (97%)	3 (2%)	1 (1%)	16	48
9	8	125/130 (96%)	113 (90%)	11 (9%)	1 (1%)	16	48
9	AI	125/130 (96%)	118 (94%)	7 (6%)	0	100	100
10	9	96/103 (93%)	86 (90%)	9 (9%)	1 (1%)	13	42
10	AJ	96/103 (93%)	83 (86%)	13 (14%)	0	100	100
12	A1	64/71 (90%)	64 (100%)	0	0	100	100
12	v	68/71 (96%)	66 (97%)	2 (3%)	0	100	100
14	AK	130/234 (56%)	126 (97%)	4 (3%)	0	100	100
14	C	130/234 (56%)	129 (99%)	1 (1%)	0	100	100
15	AL	112/118 (95%)	103 (92%)	9 (8%)	0	100	100
15	F	112/118 (95%)	108 (96%)	4 (4%)	0	100	100
16	AM	92/101 (91%)	79 (86%)	13 (14%)	0	100	100
16	G	96/101 (95%)	87 (91%)	8 (8%)	1 (1%)	13	42
17	AN	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
17	H	85/89 (96%)	83 (98%)	2 (2%)	0	100	100
18	AO	80/82 (98%)	74 (92%)	6 (8%)	0	100	100
18	I	80/82 (98%)	73 (91%)	7 (9%)	0	100	100
19	AP	78/84 (93%)	68 (87%)	10 (13%)	0	100	100
19	J	78/84 (93%)	74 (95%)	4 (5%)	0	100	100
20	AQ	64/75 (85%)	58 (91%)	6 (9%)	0	100	100
20	K	63/75 (84%)	62 (98%)	1 (2%)	0	100	100
21	AR	73/92 (79%)	69 (94%)	4 (6%)	0	100	100
21	t	75/92 (82%)	70 (93%)	5 (7%)	0	100	100
22	AS	83/87 (95%)	80 (96%)	3 (4%)	0	100	100
22	u	83/87 (95%)	82 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	AT	56/70 (80%)	52 (93%)	4 (7%)	0	100	100
23	L	58/70 (83%)	54 (93%)	4 (7%)	0	100	100
27	AX	269/273 (98%)	255 (95%)	14 (5%)	0	100	100
27	P	269/273 (98%)	256 (95%)	13 (5%)	0	100	100
28	AY	207/209 (99%)	190 (92%)	17 (8%)	0	100	100
28	Q	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
29	AZ	199/201 (99%)	194 (98%)	5 (2%)	0	100	100
29	R	199/201 (99%)	193 (97%)	6 (3%)	0	100	100
30	Aa	175/179 (98%)	168 (96%)	7 (4%)	0	100	100
30	S	175/179 (98%)	162 (93%)	13 (7%)	0	100	100
31	Ab	174/177 (98%)	167 (96%)	7 (4%)	0	100	100
31	T	173/177 (98%)	167 (96%)	6 (4%)	0	100	100
32	Ac	147/149 (99%)	133 (90%)	14 (10%)	0	100	100
32	U	147/149 (99%)	136 (92%)	11 (8%)	0	100	100
33	Ad	139/142 (98%)	120 (86%)	18 (13%)	1 (1%)	19	51
33	V	132/142 (93%)	119 (90%)	13 (10%)	0	100	100
34	Ae	140/142 (99%)	132 (94%)	8 (6%)	0	100	100
34	W	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
35	Af	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
35	X	120/123 (98%)	114 (95%)	6 (5%)	0	100	100
36	Ag	140/144 (97%)	134 (96%)	6 (4%)	0	100	100
36	Y	141/144 (98%)	133 (94%)	8 (6%)	0	100	100
37	Ah	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
37	Z	134/136 (98%)	132 (98%)	2 (2%)	0	100	100
38	Ai	116/127 (91%)	112 (97%)	4 (3%)	0	100	100
38	a	117/127 (92%)	111 (95%)	6 (5%)	0	100	100
39	Aj	114/117 (97%)	113 (99%)	1 (1%)	0	100	100
39	b	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
40	Ak	112/115 (97%)	106 (95%)	6 (5%)	0	100	100
40	c	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
41	Al	115/118 (98%)	113 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	d	115/118 (98%)	115 (100%)	0	0	100	100
42	Am	101/103 (98%)	96 (95%)	5 (5%)	0	100	100
42	e	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
43	An	108/110 (98%)	103 (95%)	5 (5%)	0	100	100
43	f	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
44	Ao	91/100 (91%)	89 (98%)	2 (2%)	0	100	100
44	g	91/100 (91%)	83 (91%)	8 (9%)	0	100	100
45	Ap	100/104 (96%)	92 (92%)	8 (8%)	0	100	100
45	h	100/104 (96%)	93 (93%)	7 (7%)	0	100	100
46	Aq	92/94 (98%)	88 (96%)	3 (3%)	1 (1%)	12	39
46	i	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
47	Ar	73/85 (86%)	69 (94%)	4 (6%)	0	100	100
47	j	73/85 (86%)	72 (99%)	1 (1%)	0	100	100
48	As	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
48	k	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
49	At	61/63 (97%)	59 (97%)	2 (3%)	0	100	100
49	l	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
50	Au	54/59 (92%)	50 (93%)	4 (7%)	0	100	100
50	m	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
51	Av	54/57 (95%)	50 (93%)	4 (7%)	0	100	100
52	Aw	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
52	o	48/55 (87%)	45 (94%)	3 (6%)	0	100	100
53	Ax	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
53	p	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
54	Ay	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
54	q	62/65 (95%)	60 (97%)	1 (2%)	1 (2%)	8	31
55	Az	36/38 (95%)	29 (81%)	7 (19%)	0	100	100
55	r	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
56	B	1291/1326 (97%)	1247 (97%)	44 (3%)	0	100	100
57	D	115/129 (89%)	107 (93%)	8 (7%)	0	100	100
57	y	115/129 (89%)	104 (90%)	11 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
58	E	121/124 (98%)	109 (90%)	12 (10%)	0	100	100
58	z	121/124 (98%)	115 (95%)	6 (5%)	0	100	100
60	n	52/56 (93%)	49 (94%)	3 (6%)	0	100	100
61	s	35/179 (20%)	33 (94%)	2 (6%)	0	100	100
63	x	125/165 (76%)	118 (94%)	7 (6%)	0	100	100
All	All	13095/14247 (92%)	12440 (95%)	647 (5%)	8 (0%)	50	79

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
33	Ad	47	ASP
9	8	39	PHE
5	AE	90	THR
8	AH	66	PHE
16	G	33	ASP
46	Aq	84	PRO
10	9	57	VAL
54	q	32	ILE

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	
2	1	180/199 (90%)	173 (96%)	7 (4%)	27	58
2	AB	180/199 (90%)	172 (96%)	8 (4%)	24	54
3	2	170/190 (90%)	166 (98%)	4 (2%)	44	70
3	AC	170/190 (90%)	164 (96%)	6 (4%)	31	61
4	3	172/173 (99%)	166 (96%)	6 (4%)	31	61
4	AD	172/173 (99%)	160 (93%)	12 (7%)	12	39
5	4	113/126 (90%)	104 (92%)	9 (8%)	10	34
5	AE	113/126 (90%)	102 (90%)	11 (10%)	6	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	5	87/116 (75%)	81 (93%)	6 (7%)	13	39
6	AF	87/116 (75%)	80 (92%)	7 (8%)	10	34
7	6	124/147 (84%)	120 (97%)	4 (3%)	34	63
7	AG	124/147 (84%)	121 (98%)	3 (2%)	44	70
8	7	104/105 (99%)	102 (98%)	2 (2%)	52	75
8	AH	104/105 (99%)	97 (93%)	7 (7%)	13	40
9	8	105/107 (98%)	98 (93%)	7 (7%)	13	40
9	AI	105/107 (98%)	100 (95%)	5 (5%)	21	51
10	9	86/90 (96%)	77 (90%)	9 (10%)	5	22
10	AJ	86/90 (96%)	83 (96%)	3 (4%)	31	61
12	A1	56/61 (92%)	56 (100%)	0	100	100
12	v	60/61 (98%)	60 (100%)	0	100	100
14	AK	110/181 (61%)	105 (96%)	5 (4%)	23	53
14	C	110/181 (61%)	107 (97%)	3 (3%)	40	67
15	AL	92/96 (96%)	86 (94%)	6 (6%)	14	41
15	F	92/96 (96%)	90 (98%)	2 (2%)	47	71
16	AM	79/84 (94%)	78 (99%)	1 (1%)	65	82
16	G	82/84 (98%)	82 (100%)	0	100	100
17	AN	76/77 (99%)	73 (96%)	3 (4%)	27	58
17	H	75/77 (97%)	72 (96%)	3 (4%)	27	58
18	AO	65/65 (100%)	60 (92%)	5 (8%)	10	35
18	I	65/65 (100%)	63 (97%)	2 (3%)	35	63
19	AP	74/78 (95%)	72 (97%)	2 (3%)	40	67
19	J	74/78 (95%)	73 (99%)	1 (1%)	62	81
20	AQ	57/65 (88%)	53 (93%)	4 (7%)	12	39
20	K	56/65 (86%)	54 (96%)	2 (4%)	30	60
21	AR	66/79 (84%)	63 (96%)	3 (4%)	23	53
21	t	68/79 (86%)	66 (97%)	2 (3%)	37	65
22	AS	65/66 (98%)	59 (91%)	6 (9%)	7	28
22	u	65/66 (98%)	64 (98%)	1 (2%)	60	80
23	AT	55/62 (89%)	51 (93%)	4 (7%)	11	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	L	57/62 (92%)	56 (98%)	1 (2%)	54	76
27	AX	216/218 (99%)	210 (97%)	6 (3%)	38	66
27	P	216/218 (99%)	211 (98%)	5 (2%)	45	70
28	AY	164/164 (100%)	155 (94%)	9 (6%)	18	47
28	Q	164/164 (100%)	158 (96%)	6 (4%)	29	59
29	AZ	165/165 (100%)	154 (93%)	11 (7%)	13	40
29	R	165/165 (100%)	157 (95%)	8 (5%)	21	51
30	Aa	148/150 (99%)	144 (97%)	4 (3%)	40	67
30	S	148/150 (99%)	139 (94%)	9 (6%)	15	43
31	Ab	137/138 (99%)	134 (98%)	3 (2%)	47	71
31	T	136/138 (99%)	131 (96%)	5 (4%)	29	59
32	Ac	114/114 (100%)	110 (96%)	4 (4%)	31	61
32	U	114/114 (100%)	108 (95%)	6 (5%)	19	48
33	Ad	109/110 (99%)	106 (97%)	3 (3%)	38	66
33	V	104/110 (94%)	99 (95%)	5 (5%)	21	51
34	Ae	116/116 (100%)	113 (97%)	3 (3%)	41	68
34	W	116/116 (100%)	113 (97%)	3 (3%)	41	68
35	Af	103/104 (99%)	92 (89%)	11 (11%)	5	21
35	X	103/104 (99%)	99 (96%)	4 (4%)	27	58
36	Ag	101/103 (98%)	97 (96%)	4 (4%)	27	58
36	Y	102/103 (99%)	98 (96%)	4 (4%)	27	58
37	Ah	109/109 (100%)	105 (96%)	4 (4%)	29	59
37	Z	109/109 (100%)	105 (96%)	4 (4%)	29	59
38	Ai	98/103 (95%)	95 (97%)	3 (3%)	35	63
38	a	99/103 (96%)	94 (95%)	5 (5%)	20	49
39	Aj	86/87 (99%)	80 (93%)	6 (7%)	12	39
39	b	86/87 (99%)	81 (94%)	5 (6%)	17	45
40	Ak	99/100 (99%)	95 (96%)	4 (4%)	27	58
40	c	99/100 (99%)	98 (99%)	1 (1%)	73	86
41	Al	89/90 (99%)	84 (94%)	5 (6%)	17	46
41	d	89/90 (99%)	87 (98%)	2 (2%)	47	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	Am	84/84 (100%)	83 (99%)	1 (1%)	67	83
42	e	84/84 (100%)	80 (95%)	4 (5%)	21	51
43	An	93/93 (100%)	90 (97%)	3 (3%)	34	63
43	f	93/93 (100%)	91 (98%)	2 (2%)	47	71
44	Ao	80/84 (95%)	76 (95%)	4 (5%)	20	50
44	g	80/84 (95%)	73 (91%)	7 (9%)	8	30
45	Ap	83/85 (98%)	81 (98%)	2 (2%)	44	70
45	h	83/85 (98%)	79 (95%)	4 (5%)	21	51
46	Aq	78/78 (100%)	76 (97%)	2 (3%)	41	68
46	i	78/78 (100%)	74 (95%)	4 (5%)	20	49
47	Ar	57/63 (90%)	55 (96%)	2 (4%)	31	61
47	j	57/63 (90%)	54 (95%)	3 (5%)	19	48
48	As	67/68 (98%)	64 (96%)	3 (4%)	23	53
48	k	67/68 (98%)	62 (92%)	5 (8%)	11	36
49	At	55/55 (100%)	53 (96%)	2 (4%)	30	60
49	l	55/55 (100%)	53 (96%)	2 (4%)	30	60
50	Au	47/49 (96%)	44 (94%)	3 (6%)	14	42
50	m	48/49 (98%)	47 (98%)	1 (2%)	48	72
51	Av	47/48 (98%)	44 (94%)	3 (6%)	14	42
52	Aw	45/49 (92%)	44 (98%)	1 (2%)	47	71
52	o	45/49 (92%)	44 (98%)	1 (2%)	47	71
53	Ax	38/38 (100%)	37 (97%)	1 (3%)	41	68
53	p	38/38 (100%)	37 (97%)	1 (3%)	41	68
54	Ay	51/52 (98%)	47 (92%)	4 (8%)	10	35
54	q	51/52 (98%)	49 (96%)	2 (4%)	27	58
55	Az	34/34 (100%)	33 (97%)	1 (3%)	37	65
55	r	34/34 (100%)	32 (94%)	2 (6%)	16	44
56	B	1130/1158 (98%)	1097 (97%)	33 (3%)	37	65
57	D	90/99 (91%)	87 (97%)	3 (3%)	33	62
57	y	90/99 (91%)	81 (90%)	9 (10%)	6	24
58	E	103/104 (99%)	98 (95%)	5 (5%)	21	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
58	z	103/104 (99%)	96 (93%)	7 (7%)	13	40
60	n	46/47 (98%)	42 (91%)	4 (9%)	8	31
61	s	34/158 (22%)	32 (94%)	2 (6%)	16	44
63	x	96/123 (78%)	94 (98%)	2 (2%)	48	72
All	All	10949/11680 (94%)	10490 (96%)	459 (4%)	27	56

All (459) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	22	TYR
2	1	32	PHE
2	1	59	LYS
2	1	77	SER
2	1	127	ASP
2	1	192	ASP
2	1	197	ASP
3	2	36	ASP
3	2	70	THR
3	2	118	ASP
3	2	181	ASP
4	3	4	TYR
4	3	71	GLN
4	3	76	TYR
4	3	85	ASN
4	3	178	MET
4	3	203	LEU
5	4	10	GLU
5	4	11	LEU
5	4	76	LEU
5	4	78	ASN
5	4	97	GLN
5	4	135	ASN
5	4	142	ASP
5	4	149	SER
5	4	157	ARG
6	5	13	ASP
6	5	35	LYS
6	5	39	LEU
6	5	40	GLU
6	5	47	LEU
6	5	81	ASN

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Mol	Chain	Res	Type
7	6	20	SER
7	6	60	GLU
7	6	75	VAL
7	6	140	ASP
8	7	32	LEU
8	7	113	ASP
9	8	6	TYR
9	8	34	SER
9	8	37	GLN
9	8	63	LEU
9	8	87	LEU
9	8	89	GLU
9	8	106	ARG
10	9	10	LEU
10	9	57	VAL
10	9	63	ASP
10	9	65	TYR
10	9	71	LEU
10	9	80	THR
10	9	91	ASP
10	9	92	LEU
10	9	101	SER
2	AB	30	PHE
2	AB	90	PHE
2	AB	109	GLN
2	AB	121	SER
2	AB	127	ASP
2	AB	144	LEU
2	AB	170	HIS
2	AB	213	TYR
3	AC	29	PHE
3	AC	31	ASP
3	AC	32	ASN
3	AC	38	LYS
3	AC	88	ARG
3	AC	130	PHE
4	AD	3	ARG
4	AD	5	LEU
4	AD	50	ASP
4	AD	72	PHE
4	AD	74	ASN
4	AD	81	ARG

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Mol	Chain	Res	Type
4	AD	85	ASN
4	AD	134	SER
4	AD	179	GLU
4	AD	187	GLU
4	AD	190	ASP
4	AD	191	LEU
5	AE	11	LEU
5	AE	15	LEU
5	AE	62	LYS
5	AE	69	ARG
5	AE	73	ASN
5	AE	81	LEU
5	AE	100	SER
5	AE	115	LEU
5	AE	122	ASN
5	AE	135	ASN
5	AE	149	SER
6	AF	8	PHE
6	AF	11	HIS
6	AF	44	ARG
6	AF	52	ASN
6	AF	59	TYR
6	AF	72	ASP
6	AF	82	ASP
7	AG	15	ASP
7	AG	26	PHE
7	AG	115	SER
8	AH	12	THR
8	AH	55	THR
8	AH	63	LEU
8	AH	79	SER
8	AH	111	MET
8	AH	112	THR
8	AH	128	TYR
9	AI	6	TYR
9	AI	46	MET
9	AI	49	ARG
9	AI	88	MET
9	AI	94	LEU
10	AJ	35	GLN
10	AJ	60	ASP
10	AJ	71	LEU

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Mol	Chain	Res	Type
14	AK	42	VAL
14	AK	172	HIS
14	AK	188	ASN
14	AK	208	TYR
14	AK	216	THR
15	AL	11	ASP
15	AL	19	LEU
15	AL	34	LEU
15	AL	52	GLN
15	AL	58	ASP
15	AL	83	LEU
16	AM	11	VAL
17	AN	20	ASN
17	AN	22	THR
17	AN	48	LYS
18	AO	1	MET
18	AO	14	ARG
18	AO	39	PHE
18	AO	53	ASP
18	AO	79	ASN
19	AP	68	SER
19	AP	69	LYS
20	AQ	11	CYS
20	AQ	31	ASN
20	AQ	64	TYR
20	AQ	73	ARG
21	AR	36	ARG
21	AR	44	MET
21	AR	55	ARG
22	AS	3	ASN
22	AS	13	GLN
22	AS	36	TYR
22	AS	40	GLU
22	AS	61	GLN
22	AS	66	LEU
23	AT	26	SER
23	AT	34	LEU
23	AT	45	THR
23	AT	65	ASN
27	AX	20	VAL
27	AX	35	GLU
27	AX	203	ARG

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Mol	Chain	Res	Type
27	AX	213	TRP
27	AX	251	GLN
27	AX	266	PHE
28	AY	30	GLU
28	AY	45	TYR
28	AY	73	VAL
28	AY	82	PHE
28	AY	105	LYS
28	AY	137	SER
28	AY	161	MET
28	AY	169	ARG
28	AY	189	VAL
29	AZ	12	LEU
29	AZ	19	PHE
29	AZ	30	GLN
29	AZ	90	GLN
29	AZ	116	ASP
29	AZ	124	PHE
29	AZ	144	GLU
29	AZ	171	ASP
29	AZ	183	PHE
29	AZ	198	GLU
29	AZ	199	MET
30	Aa	5	HIS
30	Aa	38	MET
30	Aa	96	MET
30	Aa	162	SER
31	Ab	20	ASN
31	Ab	166	ASP
31	Ab	170	ARG
32	Ac	28	ASN
32	Ac	51	ARG
32	Ac	101	ASP
32	Ac	147	VAL
33	Ad	57	VAL
33	Ad	79	LEU
33	Ad	135	SER
34	Ae	14	ASP
34	Ae	32	LEU
34	Ae	128	ASN
35	Af	1	MET
35	Af	9	ASN

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Mol	Chain	Res	Type
35	Af	21	CYS
35	Af	23	LYS
35	Af	25	LEU
35	Af	37	ASP
35	Af	40	LYS
35	Af	49	ARG
35	Af	58	LEU
35	Af	80	ASP
35	Af	109	SER
36	Ag	12	SER
36	Ag	54	GLN
36	Ag	69	ARG
36	Ag	81	ASP
37	Ah	7	THR
37	Ah	88	ASN
37	Ah	90	GLU
37	Ah	93	VAL
38	Ai	1	MET
38	Ai	16	HIS
38	Ai	51	LEU
39	Aj	32	PRO
39	Aj	47	VAL
39	Aj	89	ASP
39	Aj	95	SER
39	Aj	98	GLN
39	Aj	103	VAL
40	Ak	41	GLN
40	Ak	65	SER
40	Ak	74	PHE
40	Ak	99	TYR
41	Al	51	ARG
41	Al	56	GLN
41	Al	76	TYR
41	Al	79	PHE
41	Al	109	LEU
42	Am	39	LEU
43	An	1	MET
43	An	7	HIS
43	An	34	ASP
44	Ao	32	LEU
44	Ao	36	LYS
44	Ao	51	PHE

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Mol	Chain	Res	Type
44	Ao	87	LEU
45	Ap	27	ASN
45	Ap	81	ASP
46	Aq	1	MET
46	Aq	42	LEU
47	Ar	21	LEU
47	Ar	53	CYS
48	As	44	LYS
48	As	60	ASP
48	As	65	ASP
49	At	31	GLN
49	At	49	ASP
50	Au	6	LYS
50	Au	25	LEU
50	Au	40	ASP
51	Av	6	ASN
51	Av	22	LEU
51	Av	27	SER
52	Aw	7	GLU
53	Ax	43	THR
54	Ay	28	ASN
54	Ay	31	HIS
54	Ay	47	LYS
54	Ay	62	LEU
55	Az	12	ARG
56	B	9	PHE
56	B	76	ASN
56	B	85	ASP
56	B	132	ARG
56	B	172	LEU
56	B	173	MET
56	B	208	PHE
56	B	209	LEU
56	B	250	SER
56	B	269	ASP
56	B	660	LEU
56	B	669	MET
56	B	677	SER
56	B	723	THR
56	B	758	ASP
56	B	851	PHE
56	B	860	ARG

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Mol	Chain	Res	Type
56	B	891	PHE
56	B	898	LEU
56	B	953	VAL
56	B	1086	HIS
56	B	1089	LEU
56	B	1099	PHE
56	B	1115	CYS
56	B	1128	VAL
56	B	1129	TRP
56	B	1132	GLU
56	B	1160	LEU
56	B	1175	ASP
56	B	1194	TYR
56	B	1265	ARG
56	B	1288	ASP
56	B	1292	LEU
14	C	41	SER
14	C	174	THR
14	C	196	LEU
57	D	34	ILE
57	D	82	LEU
57	D	119	ASN
58	E	14	ARG
58	E	44	LYS
58	E	64	THR
58	E	72	HIS
58	E	93	VAL
15	F	54	ASP
15	F	83	LEU
17	H	4	SER
17	H	20	ASN
17	H	66	LEU
18	I	48	GLU
18	I	69	ASP
19	J	50	ASN
20	K	25	ASP
20	K	42	SER
23	L	34	LEU
27	P	10	SER
27	P	72	ASP
27	P	130	LEU
27	P	213	TRP

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Mol	Chain	Res	Type
27	P	259	SER
28	Q	80	TRP
28	Q	84	LEU
28	Q	113	SER
28	Q	118	PHE
28	Q	185	ASN
28	Q	200	ASP
29	R	75	SER
29	R	115	GLN
29	R	124	PHE
29	R	141	MET
29	R	150	THR
29	R	156	ASN
29	R	165	HIS
29	R	166	LYS
30	S	5	HIS
30	S	17	MET
30	S	52	ASN
30	S	68	THR
30	S	80	ARG
30	S	83	TYR
30	S	115	ARG
30	S	121	SER
30	S	164	GLU
31	T	50	LEU
31	T	60	ASP
31	T	155	GLU
31	T	164	TYR
31	T	166	ASP
32	U	9	VAL
32	U	21	VAL
32	U	25	TYR
32	U	53	GLU
32	U	62	LEU
32	U	90	LEU
33	V	28	LEU
33	V	60	THR
33	V	69	PHE
33	V	80	LEU
33	V	97	LYS
34	W	28	LEU
34	W	60	ASP

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Mol	Chain	Res	Type
34	W	90	GLU
35	X	25	LEU
35	X	56	ASP
35	X	84	CYS
35	X	88	ASN
36	Y	12	SER
36	Y	60	ARG
36	Y	74	THR
36	Y	93	ASN
37	Z	24	THR
37	Z	30	SER
37	Z	54	THR
37	Z	88	ASN
38	a	2	ARG
38	a	4	ARG
38	a	8	ARG
38	a	23	ASN
38	a	60	VAL
39	b	2	ASP
39	b	48	LEU
39	b	58	ILE
39	b	64	TYR
39	b	67	ASN
40	c	109	ARG
41	d	79	PHE
41	d	102	ASP
42	e	2	TYR
42	e	5	PHE
42	e	15	SER
42	e	86	GLN
43	f	59	GLU
43	f	61	ASN
44	g	17	SER
44	g	24	MET
44	g	25	GLU
44	g	32	LEU
44	g	37	ASP
44	g	62	VAL
44	g	69	ARG
45	h	8	ASP
45	h	14	LEU
45	h	68	SER

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Mol	Chain	Res	Type
45	h	81	ASP
46	i	42	LEU
46	i	69	GLU
46	i	73	LYS
46	i	75	GLN
47	j	12	ASN
47	j	19	LYS
47	j	32	LEU
48	k	4	VAL
48	k	45	ARG
48	k	46	PHE
48	k	47	VAL
48	k	48	THR
49	l	40	SER
49	l	58	ASN
50	m	29	LEU
60	n	22	LEU
60	n	27	SER
60	n	28	LEU
60	n	46	ASP
52	o	49	TYR
53	p	25	LYS
54	q	31	HIS
54	q	47	LYS
55	r	4	ARG
55	r	11	CYS
61	s	127	ASN
61	s	136	SER
21	t	31	LEU
21	t	32	ARG
22	u	59	ASP
63	x	72	LEU
63	x	99	PHE
57	y	18	ASP
57	y	36	ASP
57	y	42	LEU
57	y	58	SER
57	y	95	SER
57	y	107	ILE
57	y	119	ASN
57	y	121	CYS
57	y	126	LYS

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Mol	Chain	Res	Type
58	z	19	SER
58	z	46	ASN
58	z	66	TYR
58	z	81	LEU
58	z	89	ASP
58	z	93	VAL
58	z	108	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	94	HIS
2	AB	15	HIS
2	AB	109	GLN
6	AF	81	ASN
7	AG	122	ASN
18	AO	9	HIS
22	AS	82	GLN
29	AZ	24	ASN
36	Ag	104	GLN
37	Ah	45	GLN
38	Ai	62	ASN
47	Ar	12	ASN
56	B	600	GLN
16	G	35	ASN
30	S	21	ASN
32	U	66	ASN
33	V	43	ASN
39	b	43	ASN
46	i	75	GLN
58	z	77	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	1532/1542 (99%)	232 (15%)	14 (0%)
1	AA	1538/1542 (99%)	250 (16%)	14 (0%)
11	A	75/76 (98%)	20 (26%)	5 (6%)
13	A3	76/77 (98%)	28 (36%)	6 (7%)
24	AU	75/76 (98%)	13 (17%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
25	AV	2895/2903 (99%)	498 (17%)	21 (0%)
25	N	2895/2903 (99%)	439 (15%)	15 (0%)
26	AW	117/120 (97%)	23 (19%)	0
26	O	117/120 (97%)	18 (15%)	1 (0%)
59	M	74/75 (98%)	14 (18%)	1 (1%)
62	w	56/698 (8%)	27 (48%)	0
All	All	9450/10132 (93%)	1562 (16%)	77 (0%)

All (1562) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	4	U
1	0	5	U
1	0	9	G
1	0	32	A
1	0	39	G
1	0	47	C
1	0	48	C
1	0	51	A
1	0	52	C
1	0	65	A
1	0	66	A
1	0	72	A
1	0	81	A
1	0	83	C
1	0	88	U
1	0	95	C
1	0	97	G
1	0	108	G
1	0	116	A
1	0	121	U
1	0	122	G
1	0	131	A
1	0	144	G
1	0	163	C
1	0	173	U
1	0	174	A
1	0	177	G
1	0	182	A
1	0	183	C
1	0	191	G
1	0	197	A

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Mol	Chain	Res	Type
1	0	226	G
1	0	245	U
1	0	247	G
1	0	251	G
1	0	262	A
1	0	266	G
1	0	267	C
1	0	279	A
1	0	280	C
1	0	281	G
1	0	289	G
1	0	306	A
1	0	328	C
1	0	330	C
1	0	332	G
1	0	338	A
1	0	351	G
1	0	352	C
1	0	354	G
1	0	367	U
1	0	372	C
1	0	373	A
1	0	388	G
1	0	397	A
1	0	406	G
1	0	411	A
1	0	412	A
1	0	413	G
1	0	421	U
1	0	422	C
1	0	424	G
1	0	429	U
1	0	435	A
1	0	436	C
1	0	439	U
1	0	440	C
1	0	441	A
1	0	451	A
1	0	458	U
1	0	467	U
1	0	468	A
1	0	479	U

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Mol	Chain	Res	Type
1	0	484	G
1	0	492	C
1	0	493	A
1	0	495	A
1	0	496	A
1	0	497	G
1	0	509	A
1	0	510	A
1	0	511	C
1	0	517	G
1	0	518	C
1	0	521	G
1	0	527	G
1	0	531	U
1	0	532	A
1	0	547	A
1	0	562	U
1	0	564	C
1	0	572	A
1	0	573	A
1	0	576	C
1	0	577	G
1	0	584	G
1	0	618	C
1	0	619	U
1	0	621	A
1	0	633	G
1	0	653	U
1	0	665	A
1	0	666	G
1	0	687	A
1	0	701	U
1	0	702	A
1	0	703	G
1	0	723	U
1	0	724	G
1	0	731	G
1	0	755	G
1	0	793	U
1	0	794	A
1	0	808	C
1	0	813	U

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Mol	Chain	Res	Type
1	0	815	A
1	0	817	C
1	0	819	A
1	0	821	G
1	0	828	U
1	0	829	G
1	0	832	G
1	0	841	C
1	0	842	U
1	0	843	U
1	0	844	G
1	0	845	A
1	0	846	G
1	0	849	G
1	0	885	G
1	0	889	A
1	0	914	A
1	0	934	C
1	0	935	A
1	0	958	A
1	0	960	U
1	0	966	G
1	0	969	A
1	0	971	G
1	0	972	C
1	0	975	A
1	0	976	G
1	0	977	A
1	0	992	U
1	0	993	G
1	0	996	A
1	0	1004	A
1	0	1005	A
1	0	1006	G
1	0	1016	A
1	0	1017	U
1	0	1022	A
1	0	1026	G
1	0	1029	U
1	0	1030	U
1	0	1031	C
1	0	1032	G

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Mol	Chain	Res	Type
1	0	1045	C
1	0	1046	A
1	0	1064	G
1	0	1065	U
1	0	1066	C
1	0	1085	U
1	0	1094	G
1	0	1095	U
1	0	1101	A
1	0	1108	G
1	0	1125	U
1	0	1133	G
1	0	1137	C
1	0	1139	G
1	0	1143	G
1	0	1154	G
1	0	1158	C
1	0	1159	U
1	0	1182	G
1	0	1183	U
1	0	1184	G
1	0	1191	A
1	0	1196	A
1	0	1197	A
1	0	1198	G
1	0	1202	U
1	0	1206	G
1	0	1213	A
1	0	1226	C
1	0	1227	A
1	0	1241	G
1	0	1257	A
1	0	1258	G
1	0	1260	G
1	0	1268	G
1	0	1270	G
1	0	1280	A
1	0	1285	A
1	0	1286	U
1	0	1287	A
1	0	1297	G
1	0	1298	U

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Mol	Chain	Res	Type
1	0	1300	G
1	0	1301	U
1	0	1302	C
1	0	1305	G
1	0	1312	G
1	0	1317	C
1	0	1318	A
1	0	1322	C
1	0	1323	G
1	0	1332	A
1	0	1340	A
1	0	1346	A
1	0	1362	A
1	0	1363	A
1	0	1364	U
1	0	1370	G
1	0	1379	G
1	0	1401	G
1	0	1419	G
1	0	1432	G
1	0	1441	A
1	0	1452	C
1	0	1487	G
1	0	1491	G
1	0	1492	A
1	0	1494	G
1	0	1497	G
1	0	1499	A
1	0	1503	A
1	0	1506	U
1	0	1517	G
1	0	1529	G
1	0	1530	G
11	A	7	A
11	A	8	U
11	A	9	A
11	A	10	G
11	A	13	C
11	A	17	C
11	A	18	G
11	A	19	G
11	A	20	U

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Mol	Chain	Res	Type
11	A	21	A
11	A	22	G
11	A	45	U
11	A	47	U
11	A	52	G
11	A	53	G
11	A	54	U
11	A	55	U
11	A	56	C
11	A	74	C
11	A	75	C
13	A3	7	G
13	A3	13	C
13	A3	16	U
13	A3	17	U
13	A3	19	G
13	A3	21	U
13	A3	23	G
13	A3	35	C
13	A3	42	A
13	A3	46	G
13	A3	47	G
13	A3	48	U
13	A3	49	C
13	A3	50	A
13	A3	51	C
13	A3	52	A
13	A3	53	G
13	A3	58	G
13	A3	59	A
13	A3	62	C
13	A3	63	C
13	A3	64	C
13	A3	66	U
13	A3	67	C
13	A3	72	C
13	A3	73	C
13	A3	75	C
13	A3	77	A
1	AA	4	U
1	AA	6	G
1	AA	9	G

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Mol	Chain	Res	Type
1	AA	22	G
1	AA	32	A
1	AA	39	G
1	AA	47	C
1	AA	48	C
1	AA	51	A
1	AA	65	A
1	AA	71	A
1	AA	82	G
1	AA	83	C
1	AA	86	G
1	AA	95	C
1	AA	97	G
1	AA	108	G
1	AA	116	A
1	AA	121	U
1	AA	122	G
1	AA	130	A
1	AA	143	A
1	AA	144	G
1	AA	148	G
1	AA	149	A
1	AA	163	C
1	AA	174	A
1	AA	183	C
1	AA	197	A
1	AA	210	C
1	AA	211	G
1	AA	226	G
1	AA	245	U
1	AA	246	A
1	AA	247	G
1	AA	251	G
1	AA	253	A
1	AA	266	G
1	AA	267	C
1	AA	279	A
1	AA	281	G
1	AA	289	G
1	AA	301	G
1	AA	306	A
1	AA	328	C

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Mol	Chain	Res	Type
1	AA	330	C
1	AA	332	G
1	AA	346	G
1	AA	347	G
1	AA	351	G
1	AA	352	C
1	AA	354	G
1	AA	363	A
1	AA	367	U
1	AA	372	C
1	AA	389	A
1	AA	397	A
1	AA	406	G
1	AA	411	A
1	AA	412	A
1	AA	413	G
1	AA	421	U
1	AA	422	C
1	AA	423	G
1	AA	424	G
1	AA	429	U
1	AA	439	U
1	AA	458	U
1	AA	467	U
1	AA	468	A
1	AA	478	A
1	AA	479	U
1	AA	481	G
1	AA	484	G
1	AA	494	G
1	AA	496	A
1	AA	497	G
1	AA	509	A
1	AA	510	A
1	AA	511	C
1	AA	517	G
1	AA	518	C
1	AA	519	C
1	AA	521	G
1	AA	527	G
1	AA	531	U
1	AA	532	A

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Mol	Chain	Res	Type
1	AA	533	A
1	AA	547	A
1	AA	559	A
1	AA	562	U
1	AA	564	C
1	AA	572	A
1	AA	573	A
1	AA	576	C
1	AA	577	G
1	AA	596	A
1	AA	619	U
1	AA	633	G
1	AA	653	U
1	AA	665	A
1	AA	687	A
1	AA	688	G
1	AA	695	A
1	AA	702	A
1	AA	703	G
1	AA	718	A
1	AA	721	G
1	AA	723	U
1	AA	724	G
1	AA	731	G
1	AA	747	A
1	AA	752	G
1	AA	755	G
1	AA	793	U
1	AA	794	A
1	AA	799	G
1	AA	813	U
1	AA	814	A
1	AA	815	A
1	AA	817	C
1	AA	818	G
1	AA	819	A
1	AA	821	G
1	AA	828	U
1	AA	836	G
1	AA	843	U
1	AA	844	G
1	AA	845	A

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Mol	Chain	Res	Type
1	AA	846	G
1	AA	885	G
1	AA	889	A
1	AA	890	G
1	AA	891	U
1	AA	902	G
1	AA	914	A
1	AA	922	G
1	AA	926	G
1	AA	934	C
1	AA	935	A
1	AA	958	A
1	AA	960	U
1	AA	965	U
1	AA	966	G
1	AA	969	A
1	AA	971	G
1	AA	972	C
1	AA	975	A
1	AA	976	G
1	AA	977	A
1	AA	982	U
1	AA	992	U
1	AA	993	G
1	AA	999	C
1	AA	1004	A
1	AA	1008	U
1	AA	1014	A
1	AA	1015	G
1	AA	1016	A
1	AA	1017	U
1	AA	1022	A
1	AA	1024	G
1	AA	1025	U
1	AA	1026	G
1	AA	1027	C
1	AA	1030	U
1	AA	1031	C
1	AA	1043	G
1	AA	1056	U
1	AA	1064	G
1	AA	1065	U

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Mol	Chain	Res	Type
1	AA	1066	C
1	AA	1085	U
1	AA	1094	G
1	AA	1095	U
1	AA	1101	A
1	AA	1104	G
1	AA	1108	G
1	AA	1125	U
1	AA	1133	G
1	AA	1136	C
1	AA	1137	C
1	AA	1138	G
1	AA	1139	G
1	AA	1157	A
1	AA	1158	C
1	AA	1159	U
1	AA	1160	G
1	AA	1167	A
1	AA	1169	A
1	AA	1183	U
1	AA	1184	G
1	AA	1196	A
1	AA	1202	U
1	AA	1212	U
1	AA	1226	C
1	AA	1227	A
1	AA	1238	A
1	AA	1250	A
1	AA	1258	G
1	AA	1260	G
1	AA	1275	A
1	AA	1280	A
1	AA	1285	A
1	AA	1287	A
1	AA	1297	G
1	AA	1298	U
1	AA	1300	G
1	AA	1301	U
1	AA	1305	G
1	AA	1317	C
1	AA	1319	A
1	AA	1320	C

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Mol	Chain	Res	Type
1	AA	1322	C
1	AA	1323	G
1	AA	1324	A
1	AA	1328	C
1	AA	1331	G
1	AA	1332	A
1	AA	1337	G
1	AA	1338	G
1	AA	1340	A
1	AA	1346	A
1	AA	1347	G
1	AA	1348	U
1	AA	1353	G
1	AA	1362	A
1	AA	1363	A
1	AA	1364	U
1	AA	1370	G
1	AA	1379	G
1	AA	1398	A
1	AA	1419	G
1	AA	1429	A
1	AA	1432	G
1	AA	1442	G
1	AA	1451	U
1	AA	1452	C
1	AA	1454	G
1	AA	1487	G
1	AA	1492	A
1	AA	1497	G
1	AA	1503	A
1	AA	1506	U
1	AA	1517	G
1	AA	1529	G
1	AA	1530	G
1	AA	1534	A
1	AA	1535	C
1	AA	1538	C
24	AU	9	A
24	AU	16	C
24	AU	17	U
24	AU	18	G
24	AU	19	G

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Mol	Chain	Res	Type
24	AU	20	G
24	AU	21	A
24	AU	22	G
24	AU	43	G
24	AU	46	G
24	AU	55	U
24	AU	59	U
24	AU	76	A
25	AV	2	G
25	AV	10	A
25	AV	15	G
25	AV	27	G
25	AV	34	U
25	AV	35	G
25	AV	42	A
25	AV	46	G
25	AV	49	A
25	AV	50	U
25	AV	51	G
25	AV	60	G
25	AV	63	A
25	AV	71	A
25	AV	72	U
25	AV	74	A
25	AV	75	G
25	AV	84	A
25	AV	96	C
25	AV	100	U
25	AV	101	A
25	AV	102	U
25	AV	103	A
25	AV	118	A
25	AV	119	A
25	AV	120	U
25	AV	125	A
25	AV	138	U
25	AV	139	U
25	AV	140	C
25	AV	141	G
25	AV	142	A
25	AV	160	A
25	AV	162	U

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Mol	Chain	Res	Type
25	AV	196	A
25	AV	199	A
25	AV	215	G
25	AV	216	A
25	AV	222	A
25	AV	223	A
25	AV	228	C
25	AV	233	A
25	AV	241	A
25	AV	243	U
25	AV	248	G
25	AV	250	G
25	AV	255	A
25	AV	266	G
25	AV	271	G
25	AV	276	U
25	AV	277	G
25	AV	278	A
25	AV	281	C
25	AV	284	U
25	AV	301	G
25	AV	310	A
25	AV	323	C
25	AV	329	G
25	AV	330	A
25	AV	331	C
25	AV	332	A
25	AV	333	G
25	AV	338	G
25	AV	354	A
25	AV	361	G
25	AV	362	A
25	AV	368	A
25	AV	371	A
25	AV	372	G
25	AV	373	U
25	AV	386	G
25	AV	388	G
25	AV	396	G
25	AV	405	U
25	AV	411	G
25	AV	422	A

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Mol	Chain	Res	Type
25	AV	424	G
25	AV	429	A
25	AV	435	C
25	AV	451	U
25	AV	455	C
25	AV	456	C
25	AV	457	A
25	AV	479	A
25	AV	480	A
25	AV	481	G
25	AV	482	A
25	AV	491	G
25	AV	503	A
25	AV	504	A
25	AV	505	A
25	AV	509	C
25	AV	529	A
25	AV	530	G
25	AV	532	A
25	AV	533	G
25	AV	544	C
25	AV	546	U
25	AV	547	A
25	AV	548	G
25	AV	549	G
25	AV	550	C
25	AV	563	A
25	AV	572	A
25	AV	573	U
25	AV	575	A
25	AV	586	A
25	AV	603	A
25	AV	613	A
25	AV	614	A
25	AV	622	G
25	AV	627	A
25	AV	637	A
25	AV	646	U
25	AV	647	G
25	AV	648	G
25	AV	654	A
25	AV	655	A

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Mol	Chain	Res	Type
25	AV	669	G
25	AV	670	A
25	AV	671	C
25	AV	686	U
25	AV	712	G
25	AV	726	G
25	AV	729	G
25	AV	730	A
25	AV	739	A
25	AV	740	C
25	AV	747	U
25	AV	757	G
25	AV	764	A
25	AV	765	C
25	AV	774	G
25	AV	776	G
25	AV	782	A
25	AV	783	A
25	AV	784	G
25	AV	785	G
25	AV	800	A
25	AV	805	G
25	AV	811	U
25	AV	812	C
25	AV	819	A
25	AV	827	U
25	AV	828	U
25	AV	831	G
25	AV	844	A
25	AV	845	A
25	AV	846	U
25	AV	847	U
25	AV	859	G
25	AV	860	U
25	AV	894	U
25	AV	896	A
25	AV	897	C
25	AV	910	A
25	AV	914	G
25	AV	931	U
25	AV	934	U
25	AV	941	A

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Mol	Chain	Res	Type
25	AV	945	A
25	AV	946	C
25	AV	960	A
25	AV	961	C
25	AV	973	A
25	AV	974	G
25	AV	980	A
25	AV	983	A
25	AV	995	C
25	AV	996	A
25	AV	1005	C
25	AV	1009	A
25	AV	1010	A
25	AV	1012	U
25	AV	1013	C
25	AV	1022	G
25	AV	1026	G
25	AV	1033	U
25	AV	1040	A
25	AV	1046	A
25	AV	1047	G
25	AV	1056	G
25	AV	1060	U
25	AV	1062	G
25	AV	1065	U
25	AV	1066	U
25	AV	1067	A
25	AV	1068	G
25	AV	1070	A
25	AV	1071	G
25	AV	1075	C
25	AV	1078	U
25	AV	1083	U
25	AV	1084	A
25	AV	1087	G
25	AV	1088	A
25	AV	1089	A
25	AV	1090	A
25	AV	1094	U
25	AV	1095	A
25	AV	1096	A
25	AV	1097	U

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Mol	Chain	Res	Type
25	AV	1100	C
25	AV	1103	A
25	AV	1104	C
25	AV	1110	G
25	AV	1112	G
25	AV	1130	U
25	AV	1131	G
25	AV	1132	U
25	AV	1133	A
25	AV	1135	C
25	AV	1136	G
25	AV	1139	G
25	AV	1142	A
25	AV	1143	A
25	AV	1157	G
25	AV	1172	C
25	AV	1173	U
25	AV	1174	U
25	AV	1175	A
25	AV	1176	U
25	AV	1180	U
25	AV	1181	U
25	AV	1204	A
25	AV	1206	G
25	AV	1210	G
25	AV	1211	C
25	AV	1223	G
25	AV	1224	U
25	AV	1227	G
25	AV	1237	A
25	AV	1238	G
25	AV	1251	C
25	AV	1253	A
25	AV	1256	G
25	AV	1266	G
25	AV	1271	G
25	AV	1272	A
25	AV	1274	A
25	AV	1293	C
25	AV	1300	G
25	AV	1301	A
25	AV	1306	C

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Mol	Chain	Res	Type
25	AV	1321	A
25	AV	1345	C
25	AV	1346	G
25	AV	1360	G
25	AV	1365	A
25	AV	1368	G
25	AV	1376	C
25	AV	1378	A
25	AV	1379	U
25	AV	1380	G
25	AV	1383	A
25	AV	1416	G
25	AV	1419	A
25	AV	1420	A
25	AV	1427	A
25	AV	1437	C
25	AV	1451	C
25	AV	1458	U
25	AV	1459	G
25	AV	1475	G
25	AV	1478	G
25	AV	1482	G
25	AV	1496	A
25	AV	1497	U
25	AV	1504	A
25	AV	1515	A
25	AV	1524	G
25	AV	1530	G
25	AV	1533	C
25	AV	1535	A
25	AV	1536	C
25	AV	1537	G
25	AV	1546	G
25	AV	1566	A
25	AV	1583	A
25	AV	1584	U
25	AV	1585	C
25	AV	1587	G
25	AV	1588	G
25	AV	1603	A
25	AV	1608	A
25	AV	1613	G

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Mol	Chain	Res	Type
25	AV	1616	A
25	AV	1634	A
25	AV	1646	C
25	AV	1647	U
25	AV	1648	U
25	AV	1660	G
25	AV	1665	A
25	AV	1667	G
25	AV	1674	G
25	AV	1675	C
25	AV	1682	G
25	AV	1698	A
25	AV	1714	U
25	AV	1715	G
25	AV	1729	U
25	AV	1730	C
25	AV	1738	G
25	AV	1744	A
25	AV	1752	C
25	AV	1756	G
25	AV	1757	A
25	AV	1758	U
25	AV	1764	C
25	AV	1773	A
25	AV	1784	A
25	AV	1790	C
25	AV	1800	C
25	AV	1808	A
25	AV	1816	C
25	AV	1829	A
25	AV	1835	G
25	AV	1847	A
25	AV	1852	U
25	AV	1869	G
25	AV	1870	C
25	AV	1881	C
25	AV	1884	G
25	AV	1901	A
25	AV	1906	G
25	AV	1913	A
25	AV	1926	U
25	AV	1927	A

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Mol	Chain	Res	Type
25	AV	1929	G
25	AV	1930	G
25	AV	1937	A
25	AV	1938	A
25	AV	1955	U
25	AV	1967	C
25	AV	1970	A
25	AV	1971	U
25	AV	1972	G
25	AV	1991	U
25	AV	1992	G
25	AV	1993	U
25	AV	1997	C
25	AV	2020	A
25	AV	2022	U
25	AV	2023	C
25	AV	2030	A
25	AV	2031	A
25	AV	2033	A
25	AV	2043	C
25	AV	2052	A
25	AV	2055	C
25	AV	2056	G
25	AV	2057	G
25	AV	2060	A
25	AV	2061	G
25	AV	2062	A
25	AV	2069	G
25	AV	2096	C
25	AV	2097	A
25	AV	2104	C
25	AV	2107	G
25	AV	2110	G
25	AV	2111	U
25	AV	2112	G
25	AV	2113	U
25	AV	2115	G
25	AV	2119	A
25	AV	2120	G
25	AV	2125	G
25	AV	2126	A
25	AV	2131	U

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Mol	Chain	Res	Type
25	AV	2132	U
25	AV	2133	G
25	AV	2134	A
25	AV	2144	G
25	AV	2145	C
25	AV	2157	G
25	AV	2161	C
25	AV	2162	G
25	AV	2163	A
25	AV	2165	C
25	AV	2172	U
25	AV	2173	A
25	AV	2178	C
25	AV	2198	A
25	AV	2199	A
25	AV	2204	G
25	AV	2210	U
25	AV	2211	A
25	AV	2214	C
25	AV	2225	A
25	AV	2226	C
25	AV	2238	G
25	AV	2239	G
25	AV	2250	G
25	AV	2266	A
25	AV	2269	G
25	AV	2278	A
25	AV	2283	C
25	AV	2286	G
25	AV	2287	A
25	AV	2288	A
25	AV	2305	U
25	AV	2307	G
25	AV	2309	A
25	AV	2312	U
25	AV	2319	G
25	AV	2321	U
25	AV	2325	G
25	AV	2333	A
25	AV	2347	C
25	AV	2350	C
25	AV	2352	A

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Mol	Chain	Res	Type
25	AV	2357	G
25	AV	2361	G
25	AV	2383	G
25	AV	2385	C
25	AV	2402	U
25	AV	2406	A
25	AV	2423	U
25	AV	2425	A
25	AV	2426	A
25	AV	2428	G
25	AV	2429	G
25	AV	2430	A
25	AV	2431	U
25	AV	2441	U
25	AV	2447	G
25	AV	2448	A
25	AV	2460	U
25	AV	2476	A
25	AV	2478	A
25	AV	2487	G
25	AV	2491	U
25	AV	2494	G
25	AV	2498	C
25	AV	2502	G
25	AV	2503	A
25	AV	2504	U
25	AV	2518	A
25	AV	2520	C
25	AV	2529	G
25	AV	2535	G
25	AV	2547	A
25	AV	2554	U
25	AV	2566	A
25	AV	2567	G
25	AV	2572	A
25	AV	2576	G
25	AV	2578	G
25	AV	2602	A
25	AV	2609	U
25	AV	2613	U
25	AV	2615	U
25	AV	2621	G

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Mol	Chain	Res	Type
25	AV	2629	U
25	AV	2630	G
25	AV	2642	G
25	AV	2646	C
25	AV	2655	G
25	AV	2656	U
25	AV	2682	A
25	AV	2685	G
25	AV	2686	G
25	AV	2689	U
25	AV	2690	U
25	AV	2714	G
25	AV	2716	C
25	AV	2726	A
25	AV	2733	A
25	AV	2744	G
25	AV	2748	A
25	AV	2750	A
25	AV	2757	A
25	AV	2758	A
25	AV	2765	A
25	AV	2769	U
25	AV	2777	G
25	AV	2778	A
25	AV	2779	U
25	AV	2798	U
25	AV	2808	G
25	AV	2809	A
25	AV	2818	U
25	AV	2820	A
25	AV	2823	A
25	AV	2832	U
25	AV	2833	U
25	AV	2834	G
25	AV	2849	U
25	AV	2872	A
25	AV	2873	A
25	AV	2877	G
25	AV	2880	C
25	AV	2884	U
25	AV	2886	A
25	AV	2891	U

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Mol	Chain	Res	Type
25	AV	2893	A
25	AV	2903	U
26	AW	9	G
26	AW	13	G
26	AW	23	G
26	AW	25	U
26	AW	30	C
26	AW	35	C
26	AW	37	C
26	AW	41	G
26	AW	42	C
26	AW	44	G
26	AW	52	A
26	AW	56	G
26	AW	66	A
26	AW	67	G
26	AW	87	U
26	AW	88	C
26	AW	89	U
26	AW	90	C
26	AW	91	C
26	AW	99	A
26	AW	105	G
26	AW	108	A
26	AW	109	A
59	M	9	C
59	M	10	G
59	M	14	A
59	M	16	C
59	M	17	G
59	M	19	U
59	M	20	A
59	M	41	G
59	M	42	G
59	M	45	U
59	M	46	U
59	M	47	C
59	M	55	C
59	M	75	A
25	N	10	A
25	N	15	G
25	N	34	U

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Mol	Chain	Res	Type
25	N	35	G
25	N	46	G
25	N	51	G
25	N	60	G
25	N	63	A
25	N	71	A
25	N	74	A
25	N	75	G
25	N	85	G
25	N	91	A
25	N	96	C
25	N	102	U
25	N	103	A
25	N	114	U
25	N	118	A
25	N	119	A
25	N	120	U
25	N	131	A
25	N	138	U
25	N	139	U
25	N	140	C
25	N	141	G
25	N	162	U
25	N	163	C
25	N	181	A
25	N	196	A
25	N	199	A
25	N	215	G
25	N	216	A
25	N	222	A
25	N	229	C
25	N	241	A
25	N	248	G
25	N	255	A
25	N	266	G
25	N	267	C
25	N	272	A
25	N	276	U
25	N	278	A
25	N	281	C
25	N	285	G
25	N	301	G

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Mol	Chain	Res	Type
25	N	310	A
25	N	329	G
25	N	330	A
25	N	331	C
25	N	346	A
25	N	361	G
25	N	362	A
25	N	370	G
25	N	371	A
25	N	372	G
25	N	386	G
25	N	396	G
25	N	403	U
25	N	405	U
25	N	406	G
25	N	407	G
25	N	411	G
25	N	422	A
25	N	424	G
25	N	435	C
25	N	457	A
25	N	467	G
25	N	477	A
25	N	481	G
25	N	482	A
25	N	489	G
25	N	491	G
25	N	504	A
25	N	505	A
25	N	509	C
25	N	510	C
25	N	529	A
25	N	530	G
25	N	532	A
25	N	533	G
25	N	539	G
25	N	540	C
25	N	543	G
25	N	544	C
25	N	546	U
25	N	548	G
25	N	549	G

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Mol	Chain	Res	Type
25	N	563	A
25	N	573	U
25	N	575	A
25	N	577	G
25	N	586	A
25	N	603	A
25	N	614	A
25	N	622	G
25	N	627	A
25	N	637	A
25	N	646	U
25	N	647	G
25	N	654	A
25	N	664	G
25	N	668	A
25	N	669	G
25	N	670	A
25	N	671	C
25	N	677	A
25	N	686	U
25	N	704	G
25	N	715	A
25	N	717	C
25	N	726	G
25	N	730	A
25	N	747	U
25	N	764	A
25	N	765	C
25	N	776	G
25	N	782	A
25	N	784	G
25	N	785	G
25	N	805	G
25	N	811	U
25	N	812	C
25	N	819	A
25	N	827	U
25	N	828	U
25	N	845	A
25	N	846	U
25	N	847	U
25	N	858	G

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Mol	Chain	Res	Type
25	N	869	G
25	N	878	A
25	N	882	G
25	N	883	G
25	N	884	U
25	N	895	U
25	N	897	C
25	N	907	G
25	N	910	A
25	N	941	A
25	N	946	C
25	N	957	C
25	N	961	C
25	N	973	A
25	N	974	G
25	N	980	A
25	N	983	A
25	N	995	C
25	N	996	A
25	N	1009	A
25	N	1012	U
25	N	1013	C
25	N	1020	A
25	N	1022	G
25	N	1026	G
25	N	1033	U
25	N	1046	A
25	N	1047	G
25	N	1060	U
25	N	1062	G
25	N	1063	G
25	N	1070	A
25	N	1071	G
25	N	1083	U
25	N	1084	A
25	N	1087	G
25	N	1088	A
25	N	1090	A
25	N	1110	G
25	N	1111	A
25	N	1112	G
25	N	1132	U

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Mol	Chain	Res	Type
25	N	1133	A
25	N	1135	C
25	N	1136	G
25	N	1139	G
25	N	1142	A
25	N	1155	A
25	N	1168	G
25	N	1174	U
25	N	1175	A
25	N	1176	U
25	N	1180	U
25	N	1186	G
25	N	1206	G
25	N	1208	C
25	N	1212	G
25	N	1237	A
25	N	1238	G
25	N	1247	A
25	N	1250	G
25	N	1252	G
25	N	1253	A
25	N	1256	G
25	N	1265	A
25	N	1266	G
25	N	1272	A
25	N	1273	U
25	N	1300	G
25	N	1301	A
25	N	1314	C
25	N	1321	A
25	N	1332	G
25	N	1345	C
25	N	1352	U
25	N	1365	A
25	N	1368	G
25	N	1378	A
25	N	1379	U
25	N	1380	G
25	N	1383	A
25	N	1386	C
25	N	1395	A
25	N	1403	A

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Mol	Chain	Res	Type
25	N	1416	G
25	N	1419	A
25	N	1427	A
25	N	1428	C
25	N	1437	C
25	N	1453	A
25	N	1458	U
25	N	1461	C
25	N	1478	G
25	N	1482	G
25	N	1493	C
25	N	1504	A
25	N	1509	A
25	N	1515	A
25	N	1522	A
25	N	1524	G
25	N	1529	G
25	N	1530	G
25	N	1535	A
25	N	1536	C
25	N	1537	G
25	N	1558	C
25	N	1560	G
25	N	1566	A
25	N	1569	A
25	N	1578	U
25	N	1583	A
25	N	1584	U
25	N	1585	C
25	N	1607	C
25	N	1608	A
25	N	1610	A
25	N	1618	A
25	N	1619	G
25	N	1646	C
25	N	1647	U
25	N	1648	U
25	N	1654	A
25	N	1665	A
25	N	1674	G
25	N	1715	G
25	N	1729	U

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Mol	Chain	Res	Type
25	N	1730	C
25	N	1732	C
25	N	1733	G
25	N	1738	G
25	N	1756	G
25	N	1758	U
25	N	1764	C
25	N	1773	A
25	N	1781	U
25	N	1786	A
25	N	1800	C
25	N	1807	G
25	N	1808	A
25	N	1816	C
25	N	1829	A
25	N	1857	G
25	N	1866	A
25	N	1870	C
25	N	1901	A
25	N	1906	G
25	N	1913	A
25	N	1914	C
25	N	1927	A
25	N	1929	G
25	N	1930	G
25	N	1936	A
25	N	1937	A
25	N	1938	A
25	N	1955	U
25	N	1964	G
25	N	1967	C
25	N	1970	A
25	N	1971	U
25	N	1972	G
25	N	1991	U
25	N	1992	G
25	N	1996	C
25	N	1997	C
25	N	2020	A
25	N	2021	C
25	N	2022	U
25	N	2023	C

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Mol	Chain	Res	Type
25	N	2030	A
25	N	2031	A
25	N	2033	A
25	N	2043	C
25	N	2055	C
25	N	2056	G
25	N	2059	A
25	N	2060	A
25	N	2061	G
25	N	2062	A
25	N	2069	G
25	N	2072	C
25	N	2093	G
25	N	2097	A
25	N	2098	U
25	N	2110	G
25	N	2111	U
25	N	2112	G
25	N	2113	U
25	N	2114	A
25	N	2115	G
25	N	2118	U
25	N	2119	A
25	N	2125	G
25	N	2126	A
25	N	2128	G
25	N	2132	U
25	N	2133	G
25	N	2136	G
25	N	2145	C
25	N	2149	U
25	N	2158	A
25	N	2162	G
25	N	2167	U
25	N	2168	G
25	N	2171	A
25	N	2172	U
25	N	2173	A
25	N	2178	C
25	N	2194	U
25	N	2198	A
25	N	2204	G

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Mol	Chain	Res	Type
25	N	2211	A
25	N	2214	C
25	N	2225	A
25	N	2226	C
25	N	2238	G
25	N	2239	G
25	N	2250	G
25	N	2266	A
25	N	2278	A
25	N	2283	C
25	N	2286	G
25	N	2287	A
25	N	2288	A
25	N	2305	U
25	N	2307	G
25	N	2309	A
25	N	2312	U
25	N	2320	U
25	N	2325	G
25	N	2333	A
25	N	2336	A
25	N	2347	C
25	N	2350	C
25	N	2354	C
25	N	2357	G
25	N	2361	G
25	N	2383	G
25	N	2385	C
25	N	2402	U
25	N	2406	A
25	N	2422	C
25	N	2423	U
25	N	2425	A
25	N	2429	G
25	N	2430	A
25	N	2441	U
25	N	2447	G
25	N	2448	A
25	N	2473	U
25	N	2476	A
25	N	2484	G
25	N	2494	G

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Mol	Chain	Res	Type
25	N	2498	C
25	N	2502	G
25	N	2503	A
25	N	2504	U
25	N	2518	A
25	N	2520	C
25	N	2529	G
25	N	2547	A
25	N	2554	U
25	N	2566	A
25	N	2567	G
25	N	2572	A
25	N	2585	U
25	N	2602	A
25	N	2609	U
25	N	2613	U
25	N	2615	U
25	N	2621	G
25	N	2629	U
25	N	2630	G
25	N	2635	A
25	N	2645	G
25	N	2646	C
25	N	2655	G
25	N	2656	U
25	N	2663	G
25	N	2689	U
25	N	2690	U
25	N	2714	G
25	N	2726	A
25	N	2729	G
25	N	2732	G
25	N	2733	A
25	N	2739	U
25	N	2744	G
25	N	2748	A
25	N	2757	A
25	N	2777	G
25	N	2778	A
25	N	2779	U
25	N	2780	G
25	N	2794	C

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Mol	Chain	Res	Type
25	N	2798	U
25	N	2800	A
25	N	2818	U
25	N	2820	A
25	N	2833	U
25	N	2834	G
25	N	2849	U
25	N	2871	U
25	N	2872	A
25	N	2873	A
25	N	2880	C
25	N	2883	A
25	N	2884	U
25	N	2891	U
25	N	2895	G
25	N	2903	U
26	O	13	G
26	O	15	A
26	O	16	G
26	O	24	G
26	O	25	U
26	O	35	C
26	O	41	G
26	O	42	C
26	O	44	G
26	O	67	G
26	O	87	U
26	O	88	C
26	O	89	U
26	O	90	C
26	O	99	A
26	O	108	A
26	O	109	A
26	O	112	G
62	w	525	A
62	w	529	A
62	w	530	C
62	w	531	G
62	w	532	U
62	w	533	C
62	w	534	G
62	w	535	C

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Mol	Chain	Res	Type
62	w	538	U
62	w	540	A
62	w	541	A
62	w	542	U
62	w	543	A
62	w	544	G
62	w	545	U
62	w	555	G
62	w	556	U
62	w	558	U
62	w	559	U
62	w	560	U
62	w	561	U
62	w	563	U
62	w	564	U
62	w	569	U
62	w	571	U
62	w	572	U
62	w	573	U

All (77) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	96	U
1	0	115	G
1	0	439	U
1	0	517	G
1	0	620	C
1	0	812	G
1	0	1182	G
1	0	1190	G
1	0	1197	A
1	0	1201	A
1	0	1300	G
1	0	1345	U
1	0	1491	G
1	0	1493	A
11	A	16	U
11	A	19	G
11	A	21	A
11	A	46	G
11	A	54	U

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Mol	Chain	Res	Type
13	A3	16	U
13	A3	22	A
13	A3	50	A
13	A3	51	C
13	A3	66	U
13	A3	76	C
1	AA	96	U
1	AA	115	G
1	AA	388	G
1	AA	518	C
1	AA	812	G
1	AA	890	G
1	AA	965	U
1	AA	1026	G
1	AA	1182	G
1	AA	1201	A
1	AA	1300	G
1	AA	1345	U
1	AA	1347	G
1	AA	1451	U
25	AV	227	A
25	AV	242	G
25	AV	372	G
25	AV	404	A
25	AV	421	C
25	AV	481	G
25	AV	670	A
25	AV	746	U
25	AV	784	G
25	AV	859	G
25	AV	960	A
25	AV	1095	A
25	AV	1142	A
25	AV	1900	A
25	AV	2125	G
25	AV	2225	A
25	AV	2286	G
25	AV	2311	A
25	AV	2655	G
25	AV	2756	U
25	AV	2776	A
59	M	44	A

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Mol	Chain	Res	Type
25	N	84	A
25	N	277	G
25	N	404	A
25	N	421	C
25	N	481	G
25	N	670	A
25	N	784	G
25	N	1109	C
25	N	1900	A
25	N	2225	A
25	N	2311	A
25	N	2655	G
25	N	2756	U
25	N	2776	A
25	N	2832	U
26	O	24	G

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

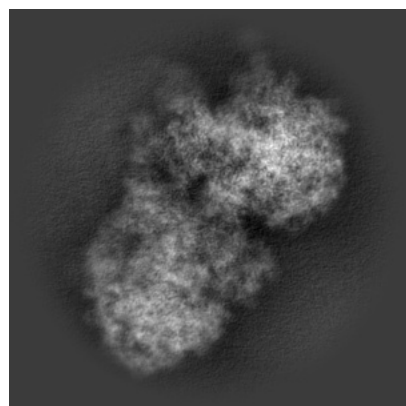
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51318. These allow visual inspection of the internal detail of the map and identification of artifacts.

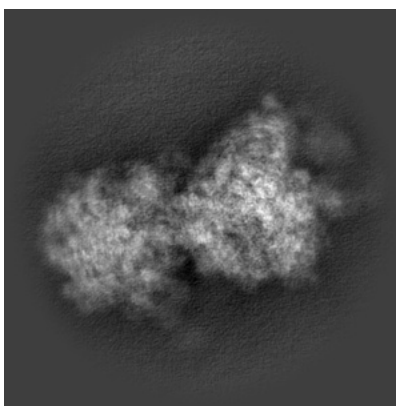
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

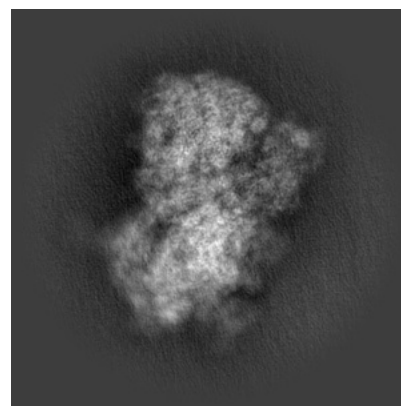
6.1.1 Primary map



X

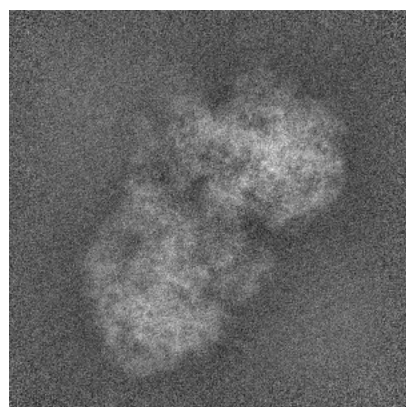


Y

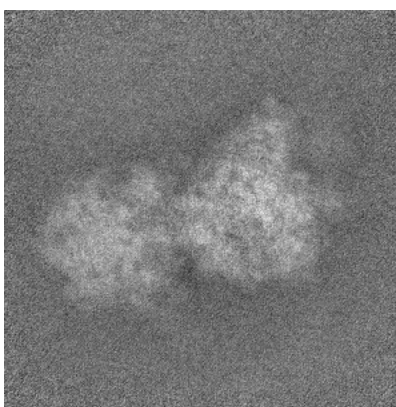


Z

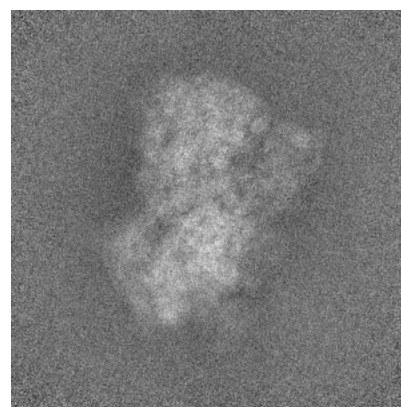
6.1.2 Raw map



X



Y

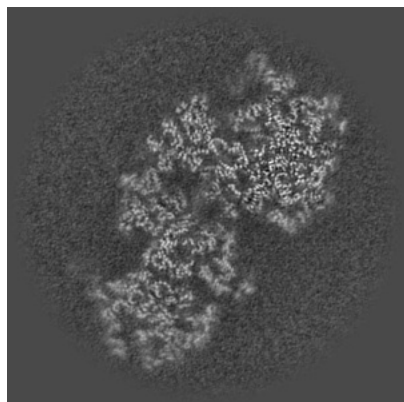


Z

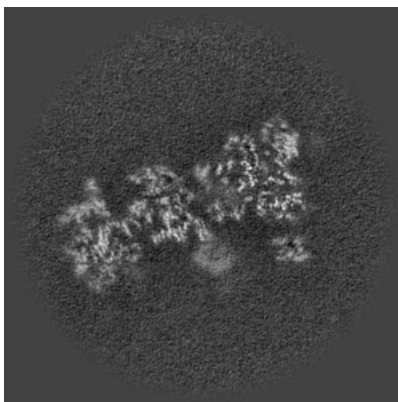
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

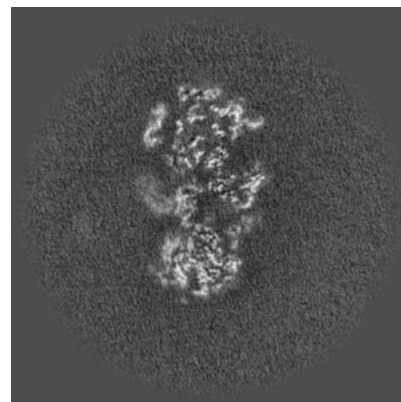
6.2.1 Primary map



X Index: 350

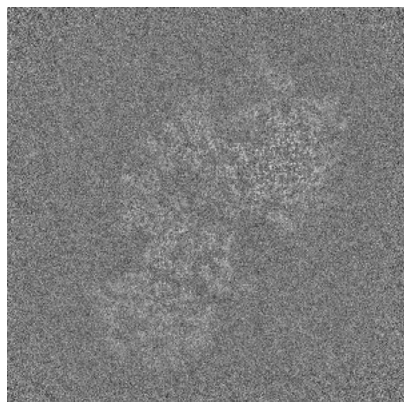


Y Index: 350

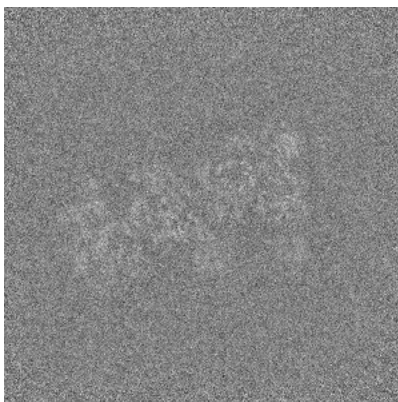


Z Index: 350

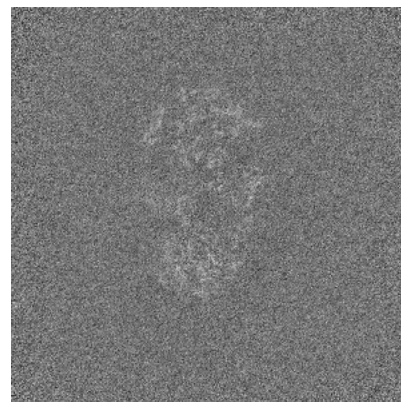
6.2.2 Raw map



X Index: 350



Y Index: 350

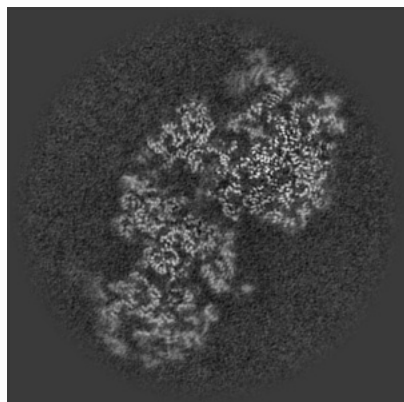


Z Index: 350

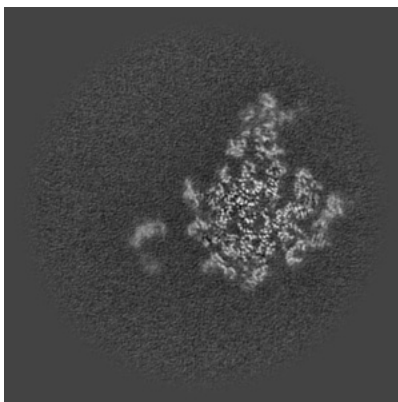
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

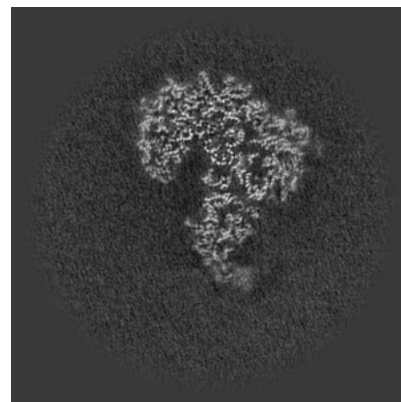
6.3.1 Primary map



X Index: 355

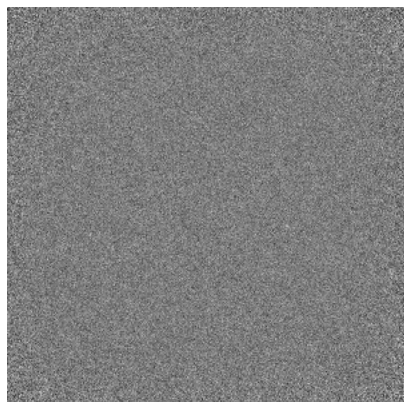


Y Index: 457

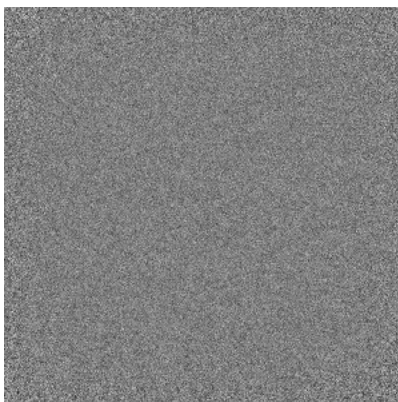


Z Index: 446

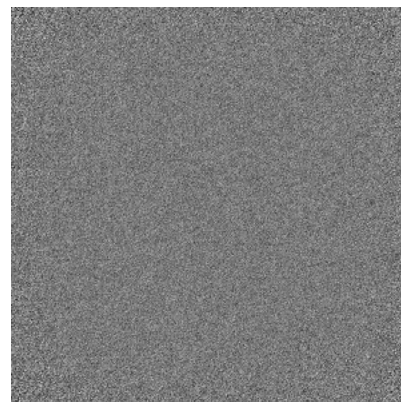
6.3.2 Raw map



X Index: 0



Y Index: 0

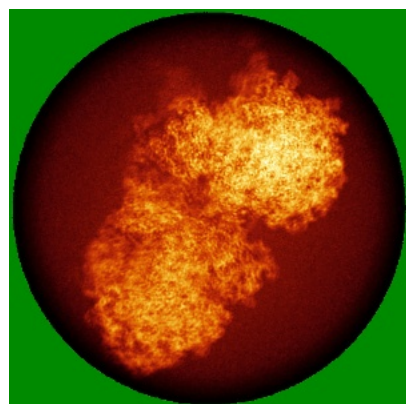


Z Index: 0

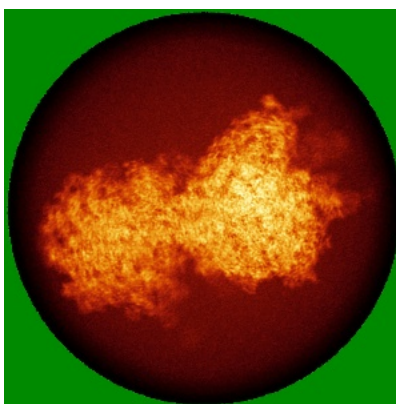
The images above show the largest variance slices of the map in three orthogonal directions.

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

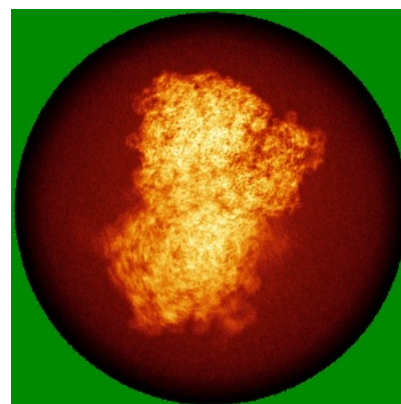
6.4.1 Primary map



X

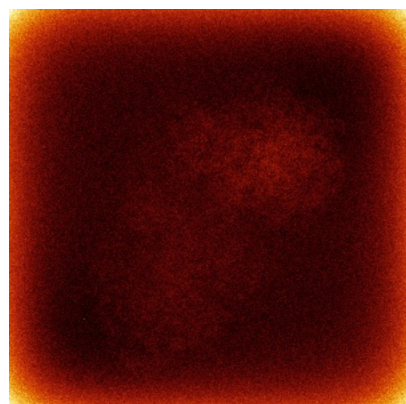


Y

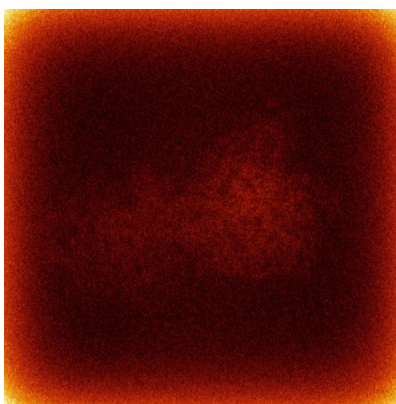


Z

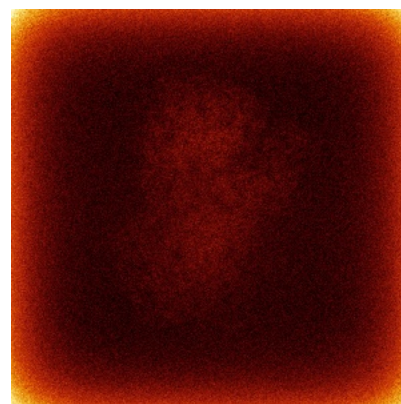
6.4.2 Raw map



X



Y

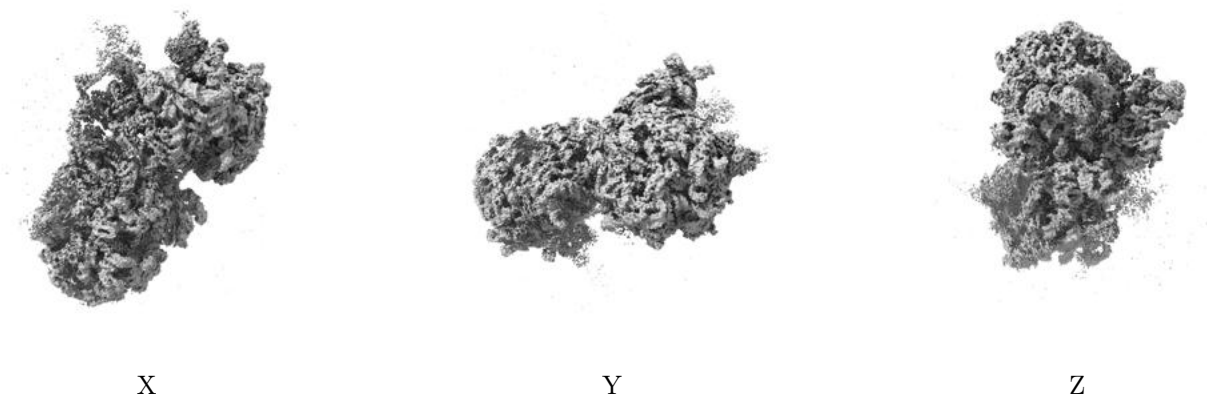


Z

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.

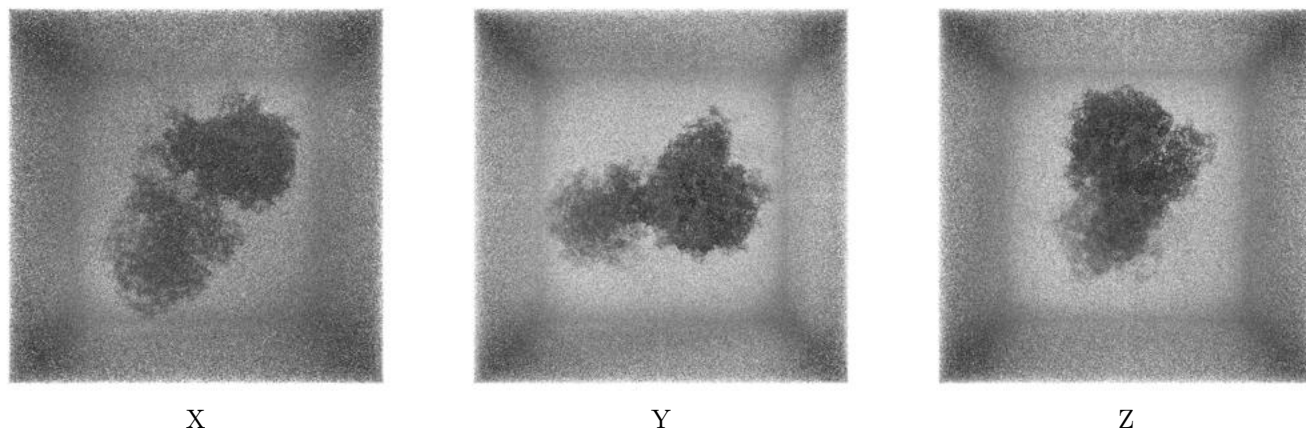
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.165. 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.

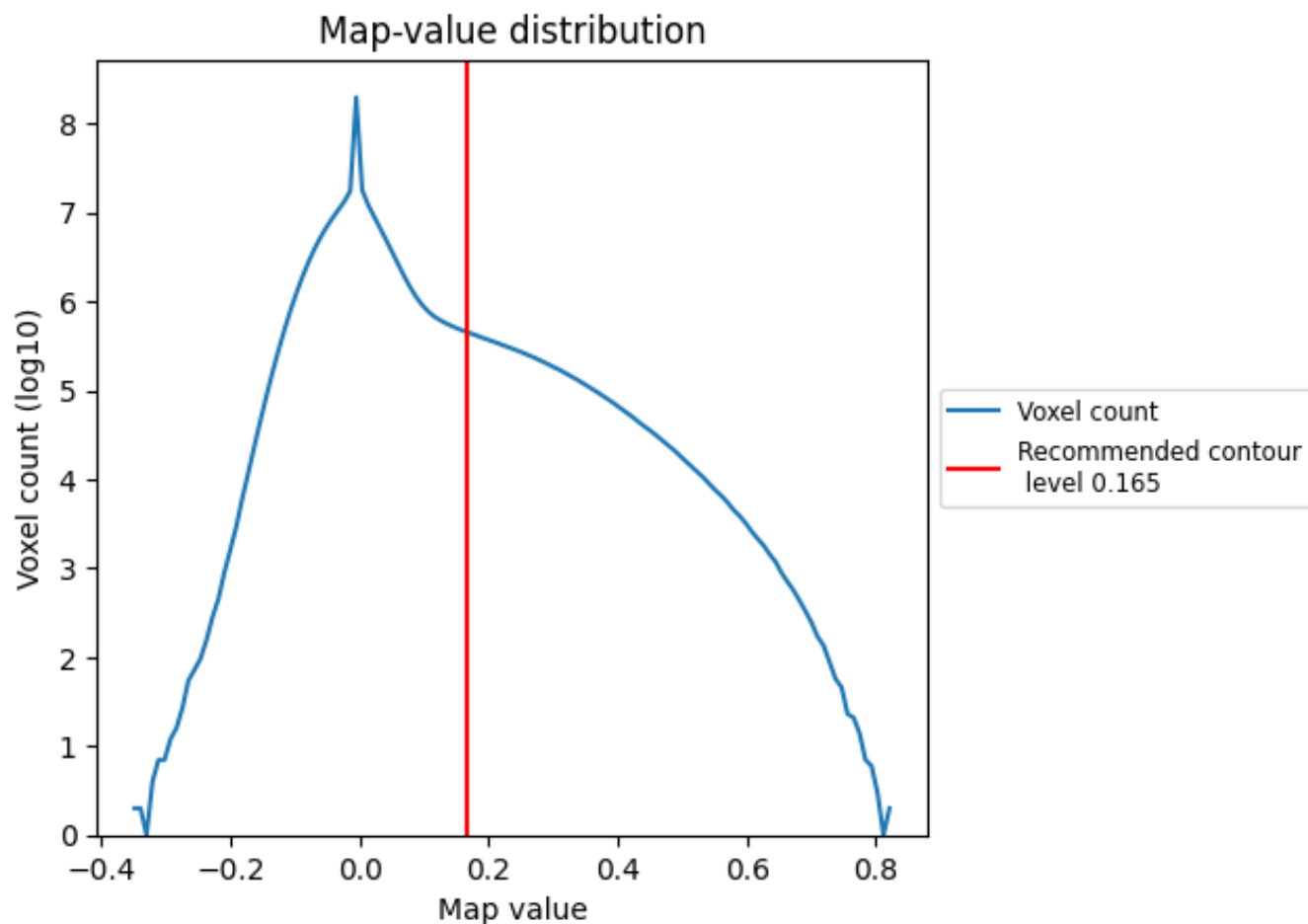
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

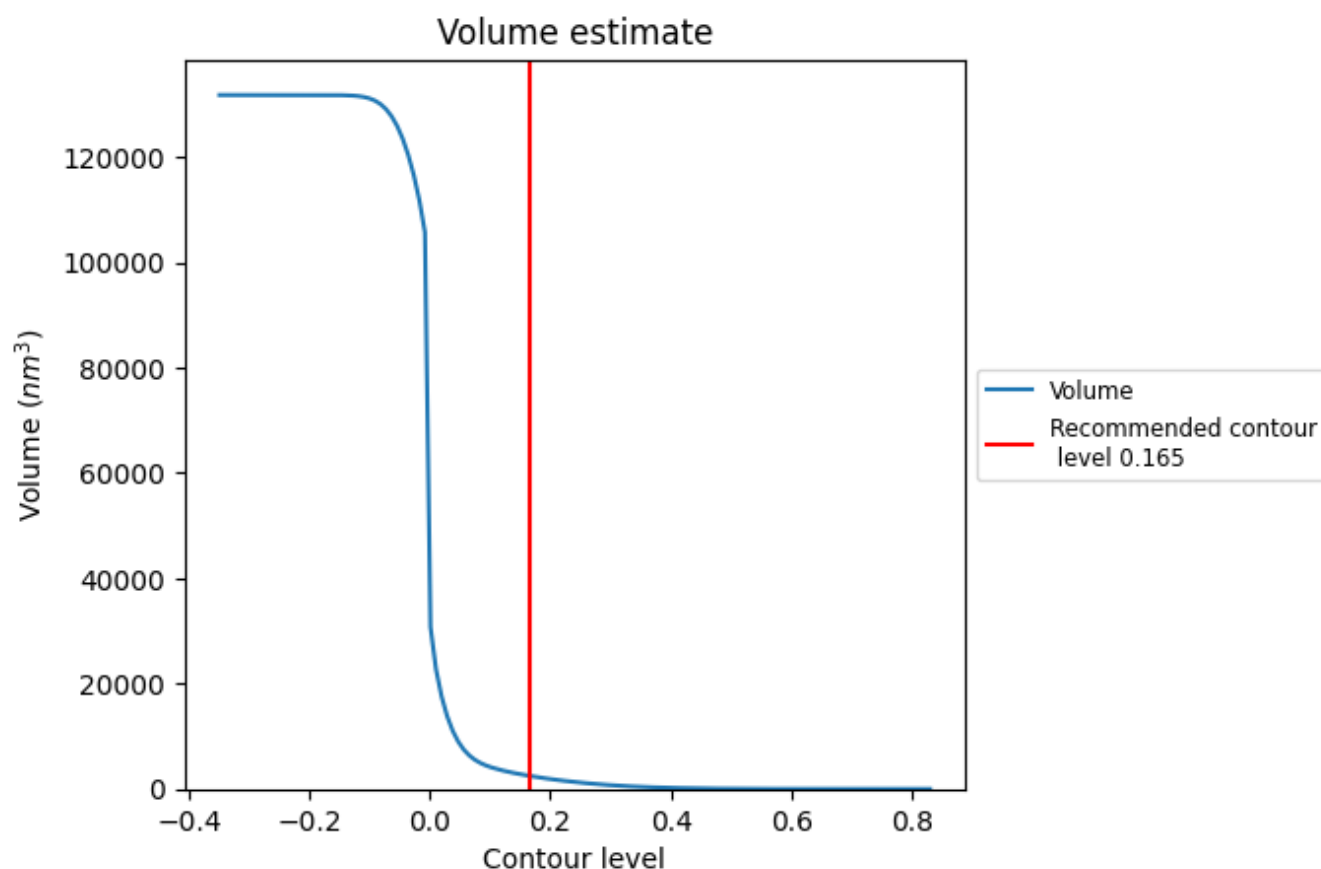
This section contains the results of statistical analysis of the map.

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.

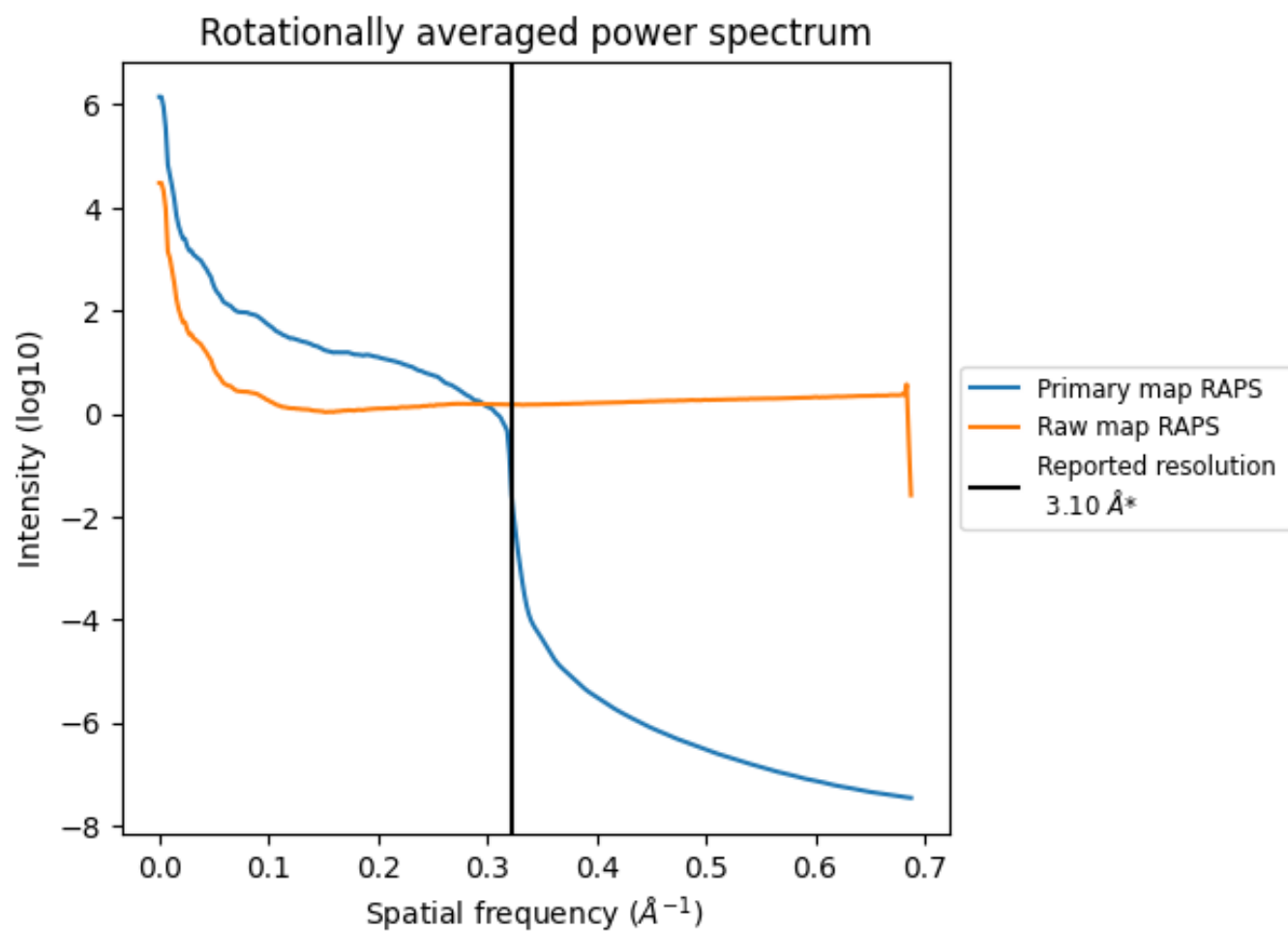
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2494 nm³; this corresponds to an approximate mass of 2253 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 ⓘ

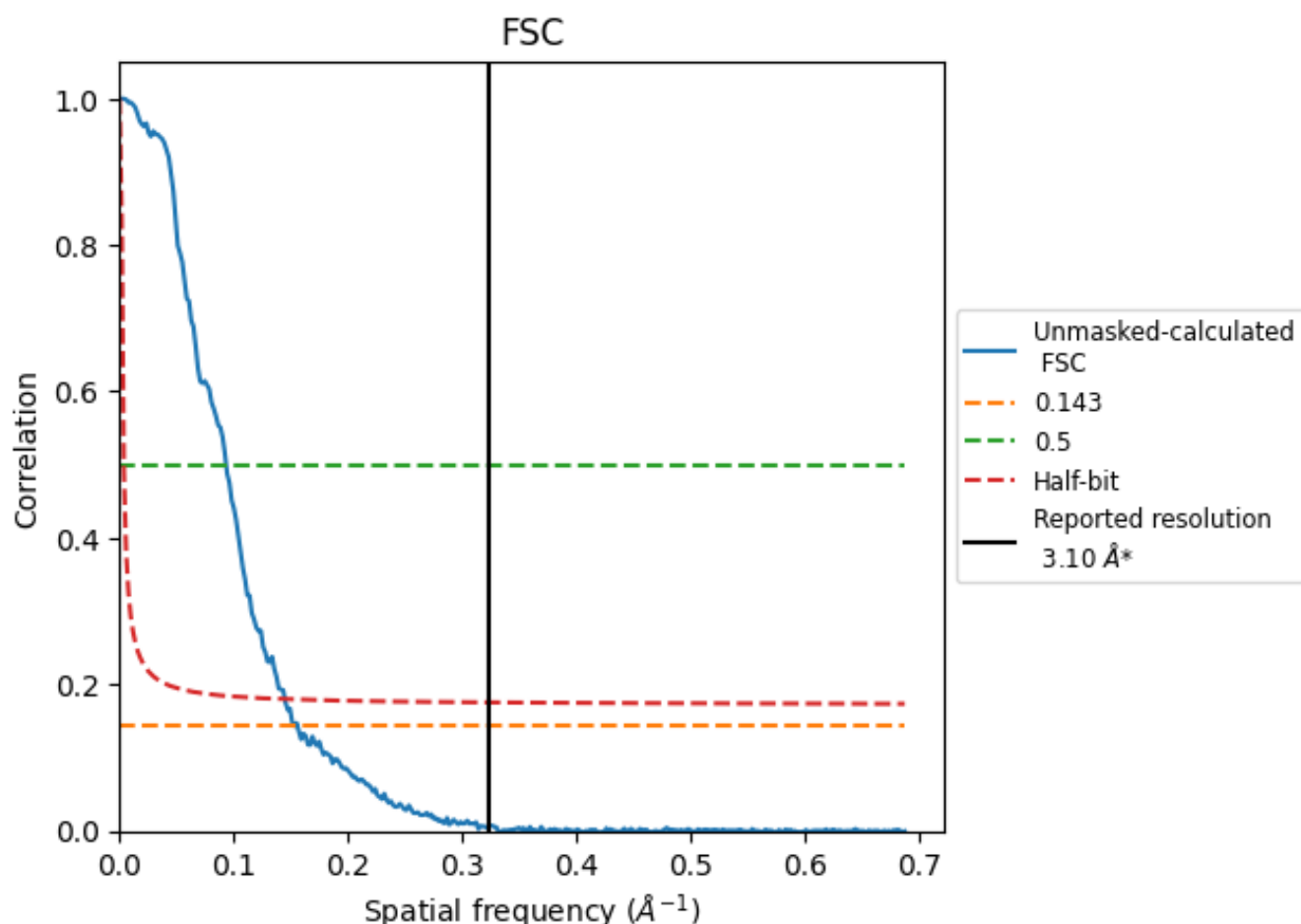


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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](#)

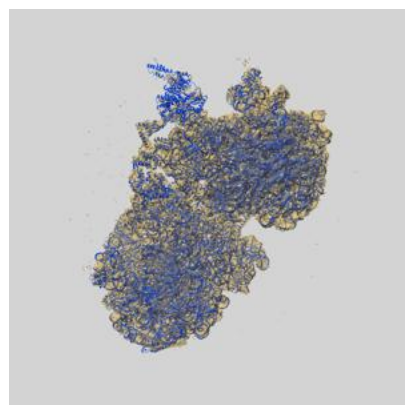
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.53	10.71	6.90

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.53 differs from the reported value 3.1 by more than 10 %

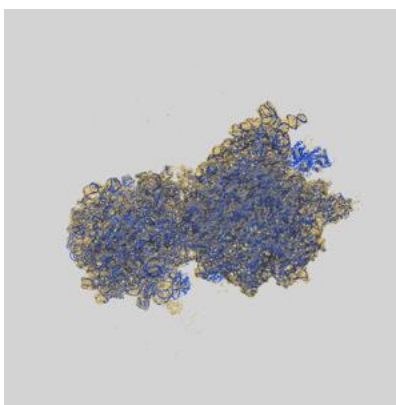
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51318 and PDB model 9GFT. Per-residue inclusion information can be found in section 3 on page 21.

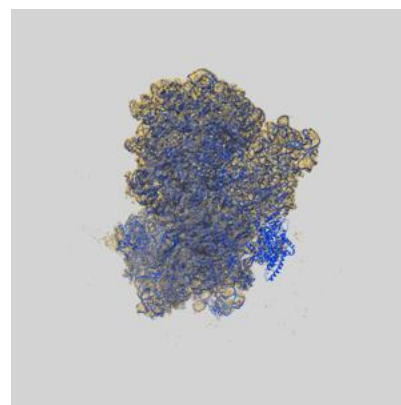
9.1 Map-model overlay [i](#)



X



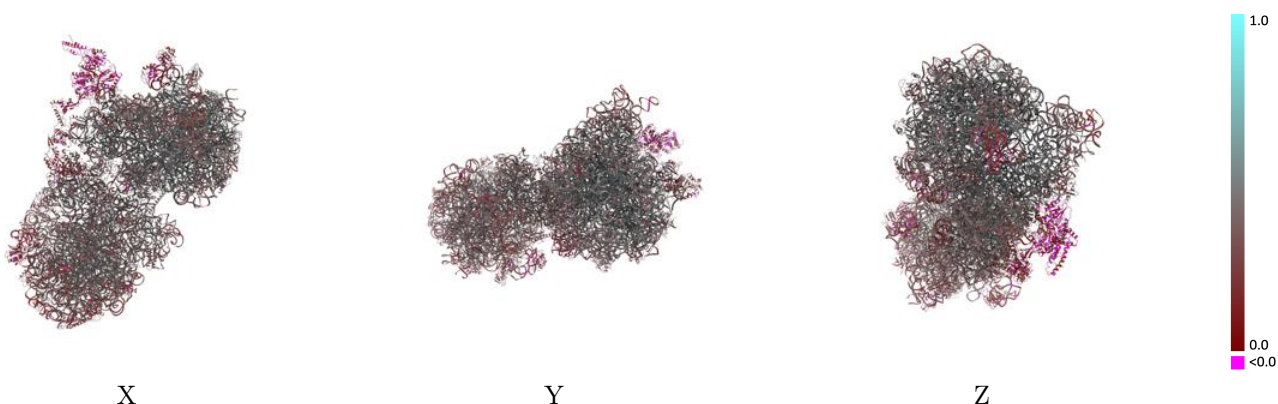
Y



Z

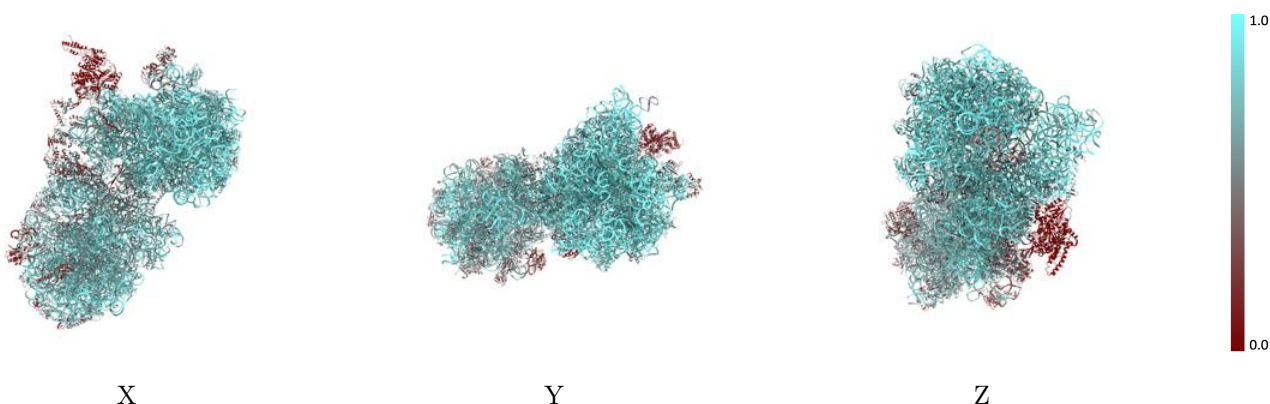
The images above show the 3D surface view of the map at the recommended contour level 0.165 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



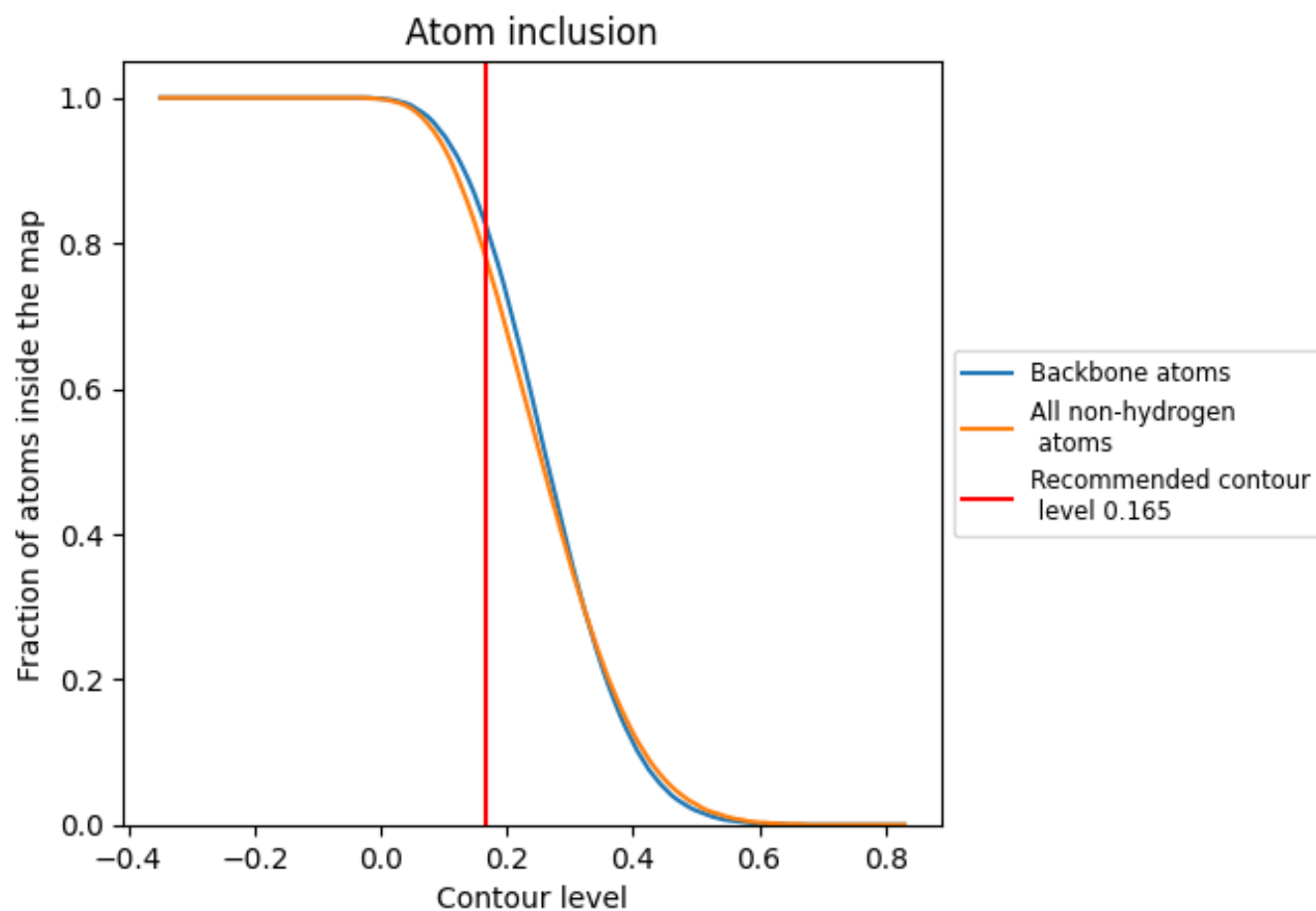
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.165).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 78% 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 (0.165) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7850	 0.3850
0	 0.9350	 0.4290
1	 0.6270	 0.3960
2	 0.6800	 0.4380
3	 0.6550	 0.3780
4	 0.7290	 0.4460
5	 0.7000	 0.4350
6	 0.6630	 0.4130
7	 0.7240	 0.4480
8	 0.7050	 0.4210
9	 0.5660	 0.4050
A	 0.8770	 0.4200
A1	 0.4960	 0.3940
A3	 0.6190	 0.3180
AA	 0.8990	 0.3990
AB	 0.5230	 0.3490
AC	 0.5870	 0.4120
AD	 0.5790	 0.4140
AE	 0.5890	 0.4050
AF	 0.5890	 0.3590
AG	 0.6480	 0.3750
AH	 0.5800	 0.3680
AI	 0.6320	 0.3690
AJ	 0.6030	 0.4190
AK	 0.1120	 0.1620
AL	 0.5970	 0.3250
AM	 0.6060	 0.3700
AN	 0.6250	 0.3540
AO	 0.6240	 0.3910
AP	 0.5970	 0.3730
AQ	 0.5990	 0.3760
AR	 0.5890	 0.3300
AS	 0.6090	 0.3140
AT	 0.4690	 0.3030
AU	 0.7460	 0.3420



















































































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Chain	Atom inclusion	Q-score
AV	 0.8490	 0.3450
AW	 0.7780	 0.2440
AX	 0.6080	 0.4290
AY	 0.5270	 0.3630
AZ	 0.3710	 0.3120
Aa	 0.4650	 0.2850
Ab	 0.3150	 0.2550
Ac	 0.2020	 0.2500
Ad	 0.0810	 0.1470
Ae	 0.5090	 0.3040
Af	 0.5290	 0.4120
Ag	 0.5430	 0.3420
Ah	 0.4580	 0.3460
Ai	 0.6700	 0.3670
Aj	 0.4700	 0.2680
Ak	 0.5040	 0.3570
Al	 0.5660	 0.2940
Am	 0.4440	 0.2700
An	 0.6380	 0.3840
Ao	 0.5620	 0.3390
Ap	 0.2530	 0.2670
Aq	 0.4590	 0.2570
Ar	 0.6100	 0.2990
As	 0.6140	 0.3800
At	 0.5710	 0.2760
Au	 0.5440	 0.3220
Av	 0.6990	 0.3690
Aw	 0.5610	 0.3330
Ax	 0.6870	 0.4140
Ay	 0.6050	 0.3870
Az	 0.5620	 0.3460
B	 0.1950	 0.1830
C	 0.0920	 0.1490
D	 0.6690	 0.4580
E	 0.7590	 0.4890
F	 0.7520	 0.4030
G	 0.7210	 0.4080
H	 0.7540	 0.4430
I	 0.7010	 0.4090
J	 0.7250	 0.4380
K	 0.6980	 0.4560
L	 0.6310	 0.3590

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Chain	Atom inclusion	Q-score
M	 0.8960	 0.4310
N	 0.9340	 0.4420
O	 0.9470	 0.3970
P	 0.7830	 0.5070
Q	 0.8050	 0.4730
R	 0.7450	 0.4310
S	 0.6690	 0.3770
T	 0.7650	 0.3990
U	 0.6200	 0.3700
V	 0.1950	 0.1520
W	 0.8310	 0.4510
X	 0.7590	 0.4910
Y	 0.7690	 0.4550
Z	 0.7950	 0.4950
a	 0.8340	 0.4380
b	 0.7290	 0.3770
c	 0.7790	 0.4550
d	 0.8120	 0.4590
e	 0.7790	 0.4440
f	 0.7740	 0.4700
g	 0.7380	 0.4310
h	 0.7410	 0.4060
i	 0.7630	 0.4060
j	 0.8160	 0.4780
k	 0.7540	 0.4720
l	 0.7060	 0.3630
m	 0.8080	 0.4560
n	 0.8140	 0.4590
o	 0.6660	 0.4190
p	 0.7910	 0.5110
q	 0.7880	 0.4950
r	 0.7880	 0.4700
s	 0.7920	 0.4990
t	 0.8000	 0.4300
u	 0.7060	 0.3500
v	 0.5470	 0.4110
w	 0.3900	 0.2920
x	 0.3530	 0.2100
y	 0.6440	 0.4020
z	 0.6430	 0.4370