Full wwPDB EM Validation Report ⓘ

Feb 10, 2025 – 07:34 am GMT

PDB ID	:	9GGR
EMDB ID	:	EMD-51340
Title	:	Structure of the HrpA-bound E. coli disome, Class II
Authors	:	Esser, H.F.; Berninghausen, O.; Becker, T.; Beckmann, R.
Deposited on	:	2024-08-14
Resolution	:	3.20 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:

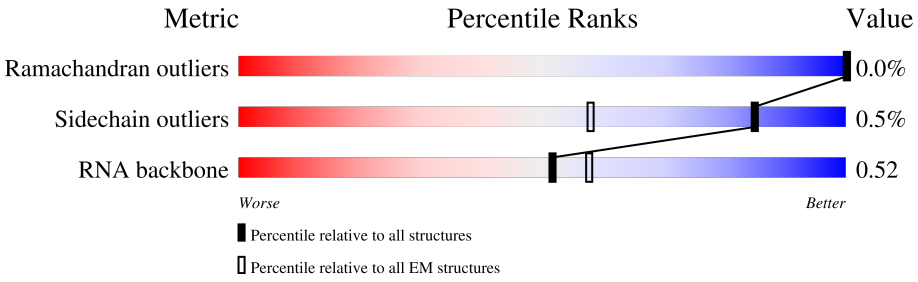
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 Å.

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



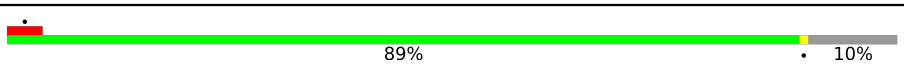
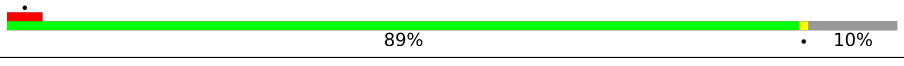
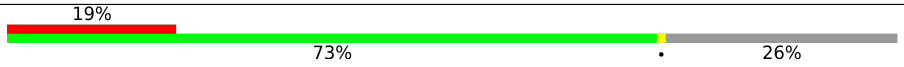
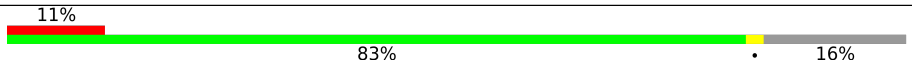
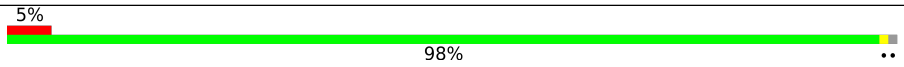
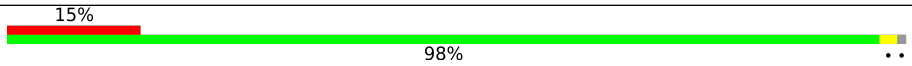
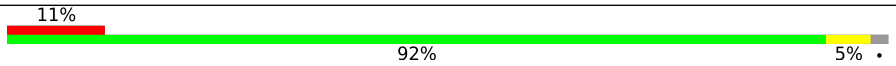
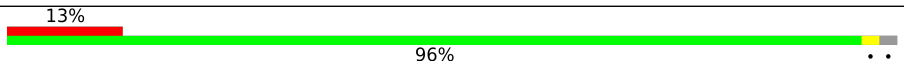
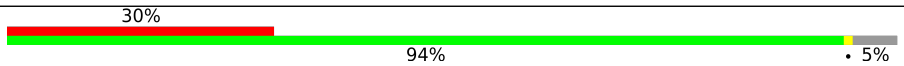
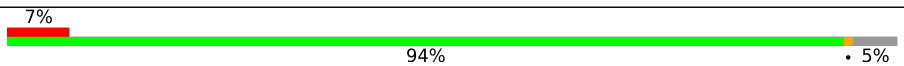
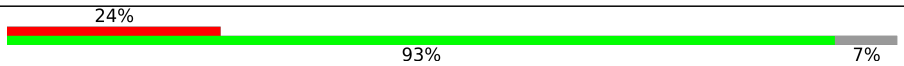
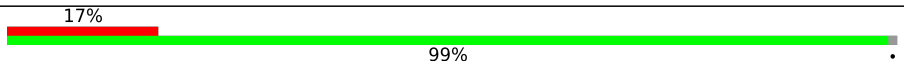
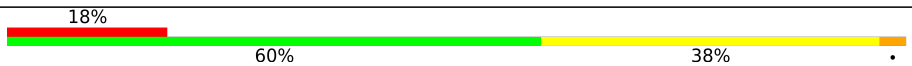
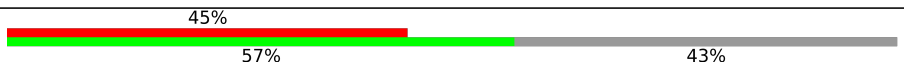
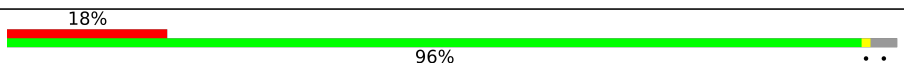
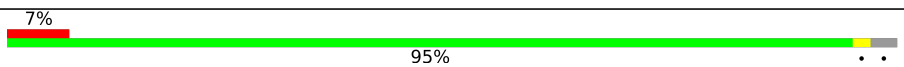
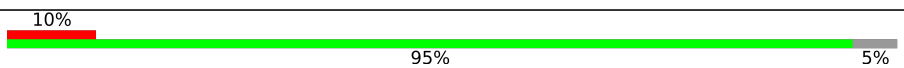
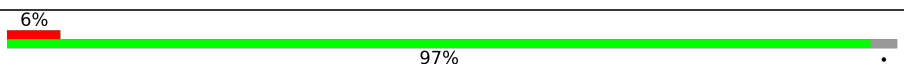
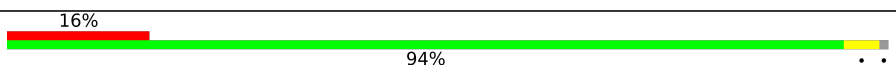
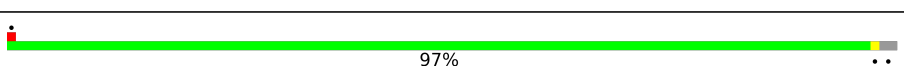
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	0	1542	80% 19%
1	AA	1542	80% 18%
2	1	241	8% 88% 10%
2	AB	241	12% 90% 10%
3	2	233	7% 88% 12%
3	AC	233	9% 88% 12%
4	3	206	14% 99%
4	AD	206	12% 98%

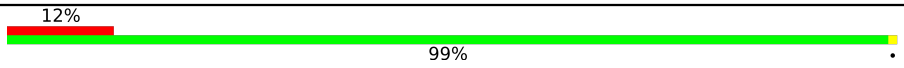
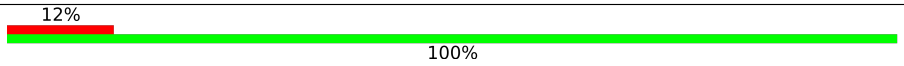
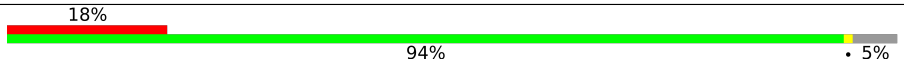
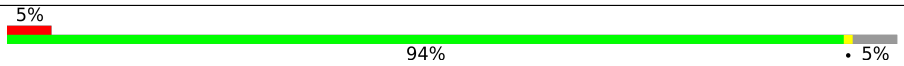
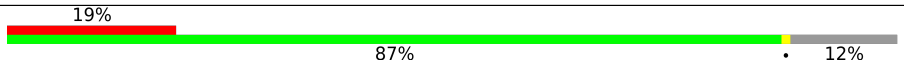
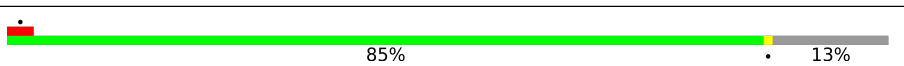
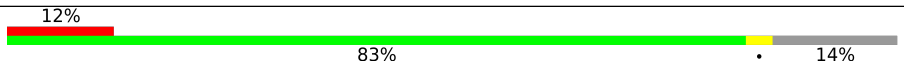
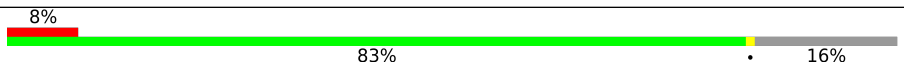
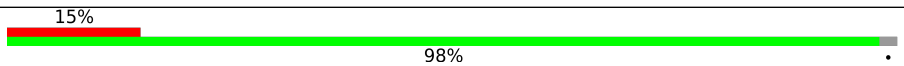
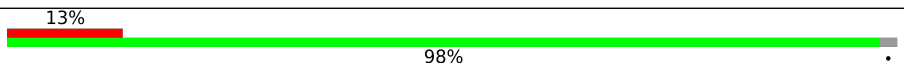
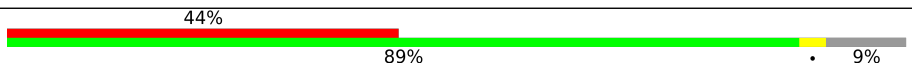
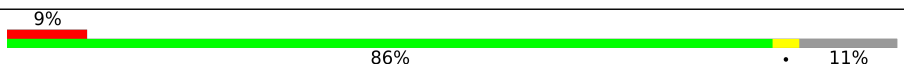
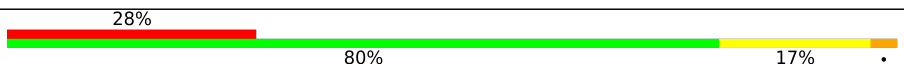
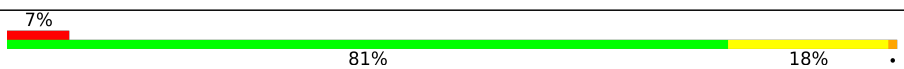
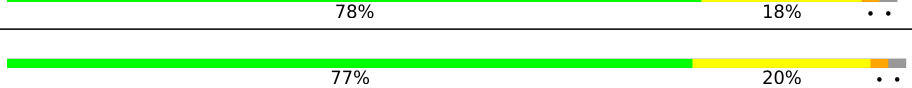
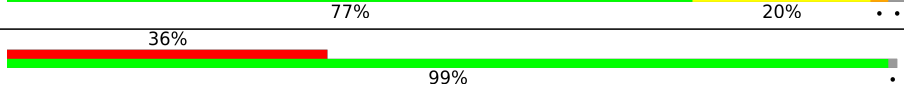
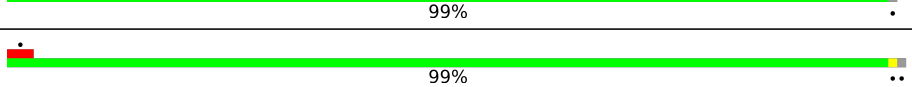
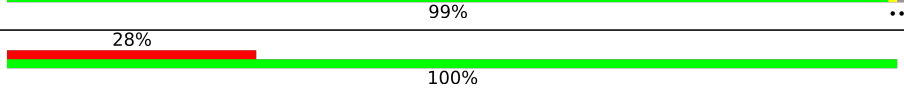
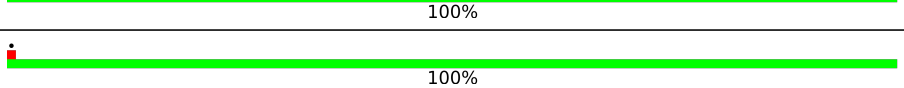
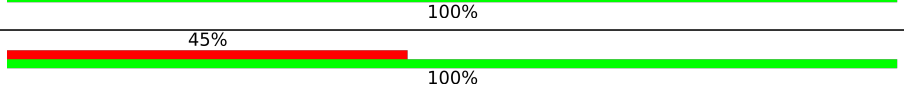
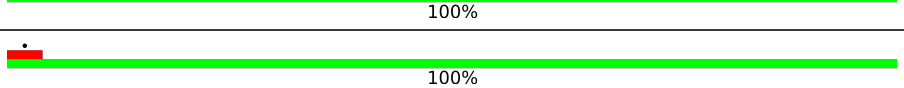
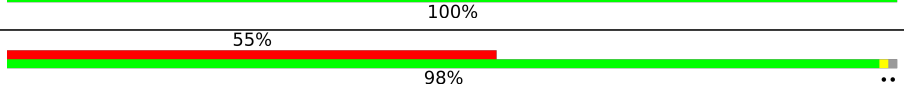
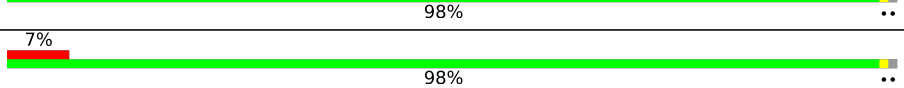
Continued on next page...

Continued from previous page...

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	A2	1300	
14	A3	77	
15	AK	234	
15	C	234	
16	AL	118	
16	F	118	
17	AM	101	
17	G	101	
18	AN	89	
18	H	89	

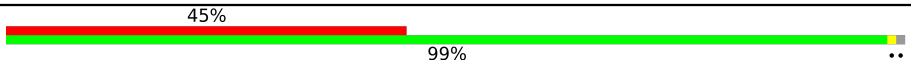
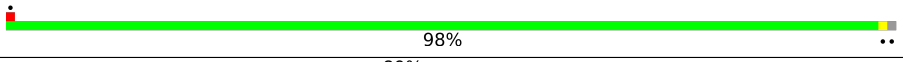
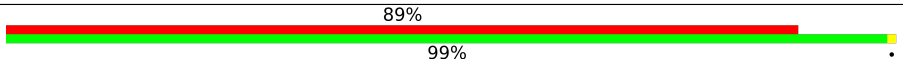
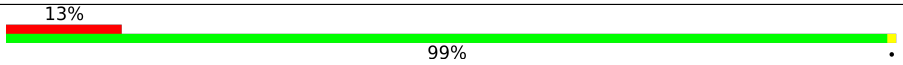
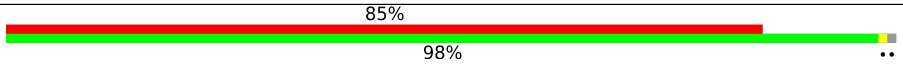
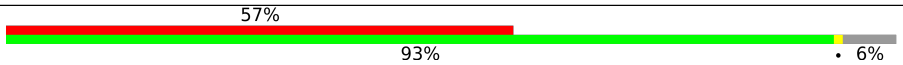
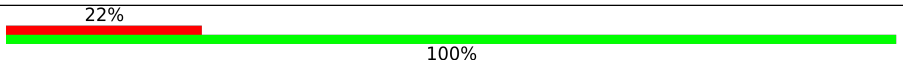
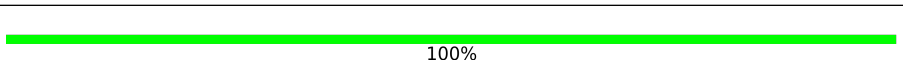
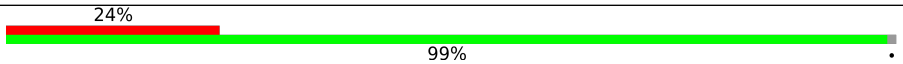
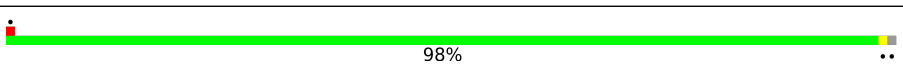
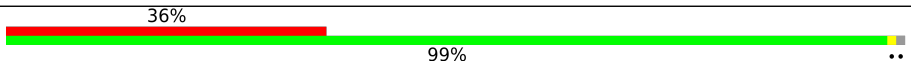
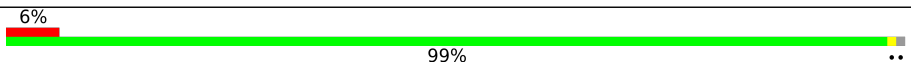
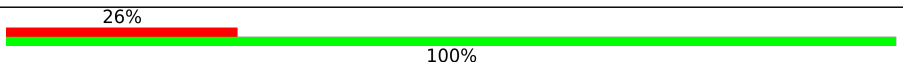
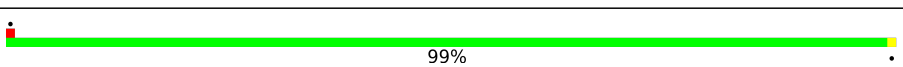
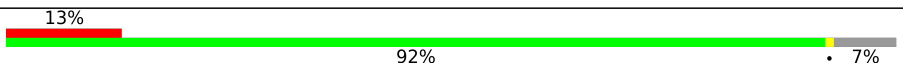
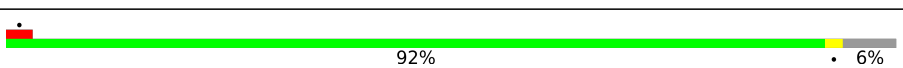
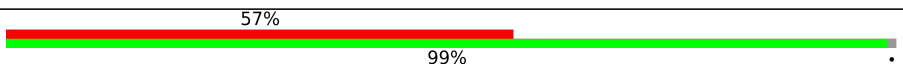
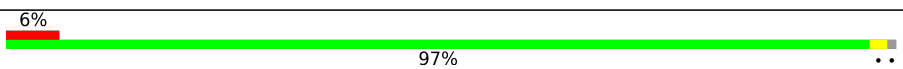
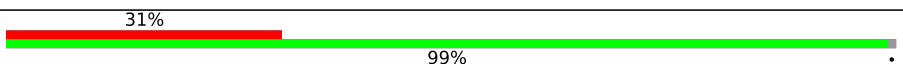
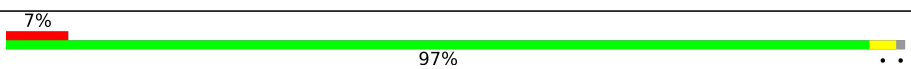
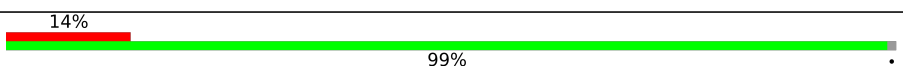
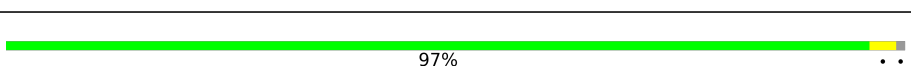
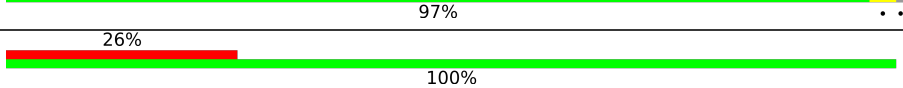
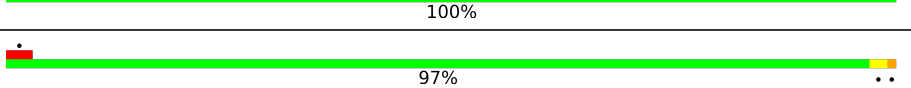
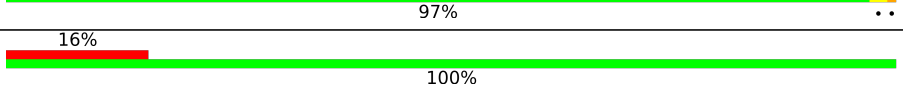
Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

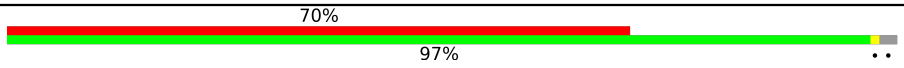
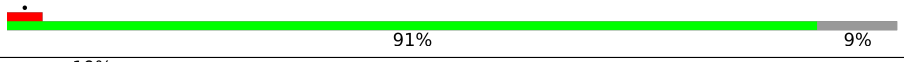
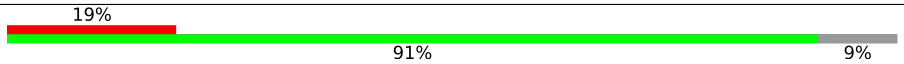
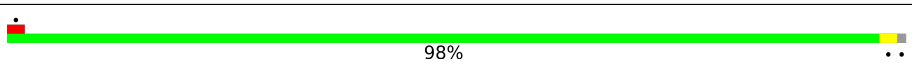
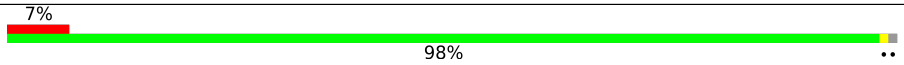
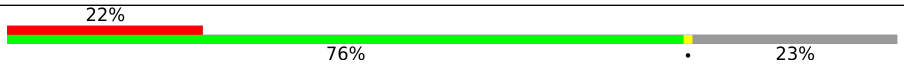
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
44	f	110	6% 99%
45	Ao	100	31% 93% 7%
45	g	100	9% 92% 7%
46	Ap	104	73% 98%
46	h	104	13% 98%
47	Aq	94	24% 100%
47	i	94	100%
48	Ar	85	15% 88% 12%
48	j	85	88% 12%
49	As	78	13% 97%
49	k	78	96%
50	At	63	37% 100%
50	l	63	11% 100%
51	Au	59	25% 95% 5%
51	m	59	97%
52	Av	57	11% 98%
52	n	57	95% 5%
53	Aw	55	55% 91% 9%
53	o	55	87% 9%
54	Ax	46	17% 98%
54	p	46	98%
55	Ay	65	25% 98%
55	q	65	97%
56	Az	38	21% 100%
56	r	38	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
57	B	1326	
58	D	129	
58	y	129	
59	E	124	
59	z	124	
60	M	75	
61	s	179	
62	w	57	
63	x	165	

2 Entry composition (i)

There are 63 unique types of molecules in this entry. The entry contains 309783 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 32895	C 14671	N 6036	O 10655	P 1533	0	0
1	AA	1539	Total 33015	C 14725	N 6052	O 10699	P 1539	0	0

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

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

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

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

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

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

- 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		

Continued on next page...

Continued from previous page...

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 protein called ATP-dependent RNA helicase HrpA.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A2	290	Total	C	N	O	S	0	0
			2340	1494	413	424	9		

- Molecule 14 is a RNA chain called A-site tRNA.

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

- Molecule 15 is a protein called Large ribosomal subunit protein uL1.

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

- Molecule 16 is a protein called Small ribosomal subunit protein uS13.

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

Continued on next page...

Continued from previous page...

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

- Molecule 17 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 18 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AN	88	Total 710	C 437	N 143	O 129	S 1	0	0
18	H	87	Total 702	C 433	N 140	O 128	S 1	0	0

- Molecule 19 is a protein called Small ribosomal subunit protein bS16.

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

- Molecule 20 is a protein called Small ribosomal subunit protein uS17.

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

- Molecule 21 is a protein called Small ribosomal subunit protein bS18.

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

- Molecule 22 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AR	79	Total	C	N	O	S	0	0
			637	408	120	107	2		
22	t	77	Total	C	N	O	S	0	0
			620	399	115	104	2		

- Molecule 23 is a protein called Small ribosomal subunit protein bS20.

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

- Molecule 24 is a protein called Large ribosomal subunit protein bL31A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AT	64	Total	C	N	O	S	0	0
			511	317	97	91	6		
24	L	62	Total	C	N	O	S	0	0
			499	309	95	89	6		

- Molecule 25 is a RNA chain called P-site tRNA.

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

- Molecule 26 is a RNA chain called 23S ribosomal RNA.

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

- Molecule 27 is a RNA chain called 5S ribosomal RNA.

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

Continued on next page...

Continued from previous page...

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

- Molecule 28 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 29 is a protein called 50S ribosomal protein L3.

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

- Molecule 30 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 31 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 32 is a protein called Large ribosomal subunit protein uL6.

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

- Molecule 33 is a protein called Large ribosomal subunit protein bL9.

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

- Molecule 34 is a protein called 50S ribosomal protein L11.

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

- Molecule 35 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 36 is a protein called Large ribosomal subunit protein uL14.

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

- Molecule 37 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Ag	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		
37	Y	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 38 is a protein called 50S ribosomal protein L16.

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

- Molecule 39 is a protein called Large ribosomal subunit protein bL17.

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

- Molecule 40 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 41 is a protein called Large ribosomal subunit protein bL19.

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

- Molecule 42 is a protein called Large ribosomal subunit protein bL20.

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

- Molecule 43 is a protein called Large ribosomal subunit protein bL21.

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

Continued on next page...

Continued from previous page...

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

- Molecule 44 is a protein called Large ribosomal subunit protein uL22.

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

- Molecule 45 is a protein called Large ribosomal subunit protein uL23.

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

- Molecule 46 is a protein called Large ribosomal subunit protein uL24.

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

- Molecule 47 is a protein called Large ribosomal subunit protein bL25.

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

- Molecule 48 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Ar	75	Total 569	C 353	N 113	O 102	S 1	0	0
48	j	75	Total 575	C 356	N 116	O 102	S 1	0	0

- Molecule 49 is a protein called Large ribosomal subunit protein bL28.

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

- Molecule 50 is a protein called Large ribosomal subunit protein uL29.

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

- Molecule 51 is a protein called Large ribosomal subunit protein uL30.

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

- Molecule 52 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Av	56	Total	C	N	O	S	0	0
			444	269	94	80	1		
52	n	54	Total	C	N	O	S	0	0
			429	260	91	77	1		

- Molecule 53 is a protein called Large ribosomal subunit protein bL33.

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

- Molecule 54 is a protein called Large ribosomal subunit protein bL34.

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

- Molecule 55 is a protein called Large ribosomal subunit protein bL35.

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

- Molecule 56 is a protein called Large ribosomal subunit protein bL36A.

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

- Molecule 57 is a protein called ATP-dependent RNA helicase HrpA.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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
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 58 is a protein called Small ribosomal subunit protein uS11.

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

- Molecule 59 is a protein called Small ribosomal subunit protein uS12.

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

- Molecule 60 is a RNA chain called P-site tRNA.

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

- 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		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
w	556	U	-	expression tag	GB 1895674257
w	557	U	-	expression tag	GB 1895674257
w	558	U	-	expression tag	GB 1895674257
w	559	U	-	expression tag	GB 1895674257
w	560	U	-	expression tag	GB 1895674257
w	561	U	-	expression tag	GB 1895674257
w	562	U	-	expression tag	GB 1895674257
w	563	U	-	expression tag	GB 1895674257
w	564	U	-	expression tag	GB 1895674257
w	565	U	-	expression tag	GB 1895674257
w	566	U	-	expression tag	GB 1895674257
w	567	U	-	expression tag	GB 1895674257
w	568	U	-	expression tag	GB 1895674257
w	569	U	-	expression tag	GB 1895674257
w	570	U	-	expression tag	GB 1895674257
w	571	U	-	expression tag	GB 1895674257
w	572	U	-	expression tag	GB 1895674257
w	573	U	-	expression tag	GB 1895674257
w	574	U	-	expression tag	GB 1895674257
w	575	U	-	expression tag	GB 1895674257
w	576	U	-	expression tag	GB 1895674257
w	577	U	-	expression tag	GB 1895674257

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

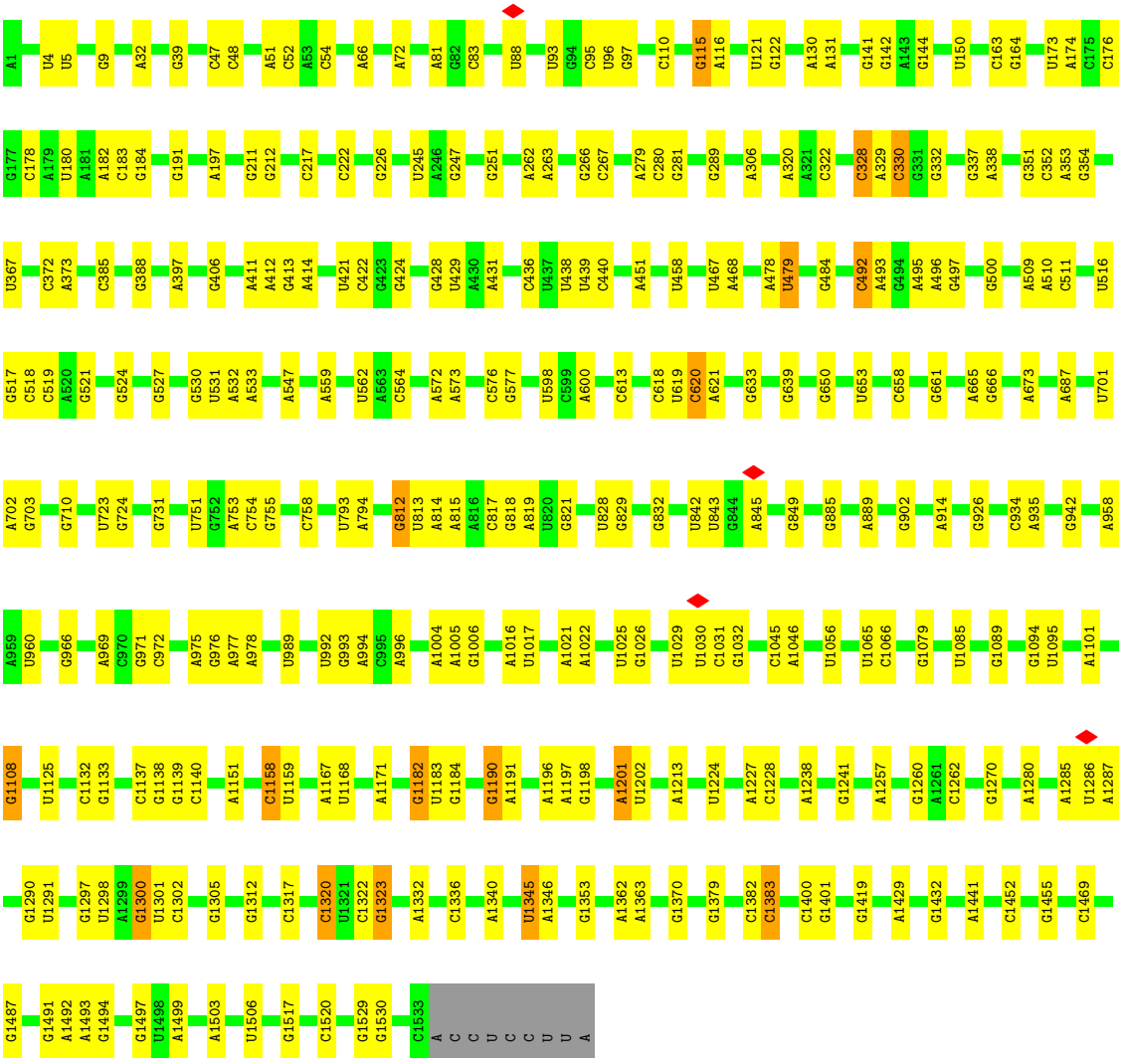
Mol	Chain	Residues	Atoms					AltConf	Trace
63	x	127	Total	C	N	O	S	0	0
			958	605	171	178	4		

3 Residue-property plots (i)

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

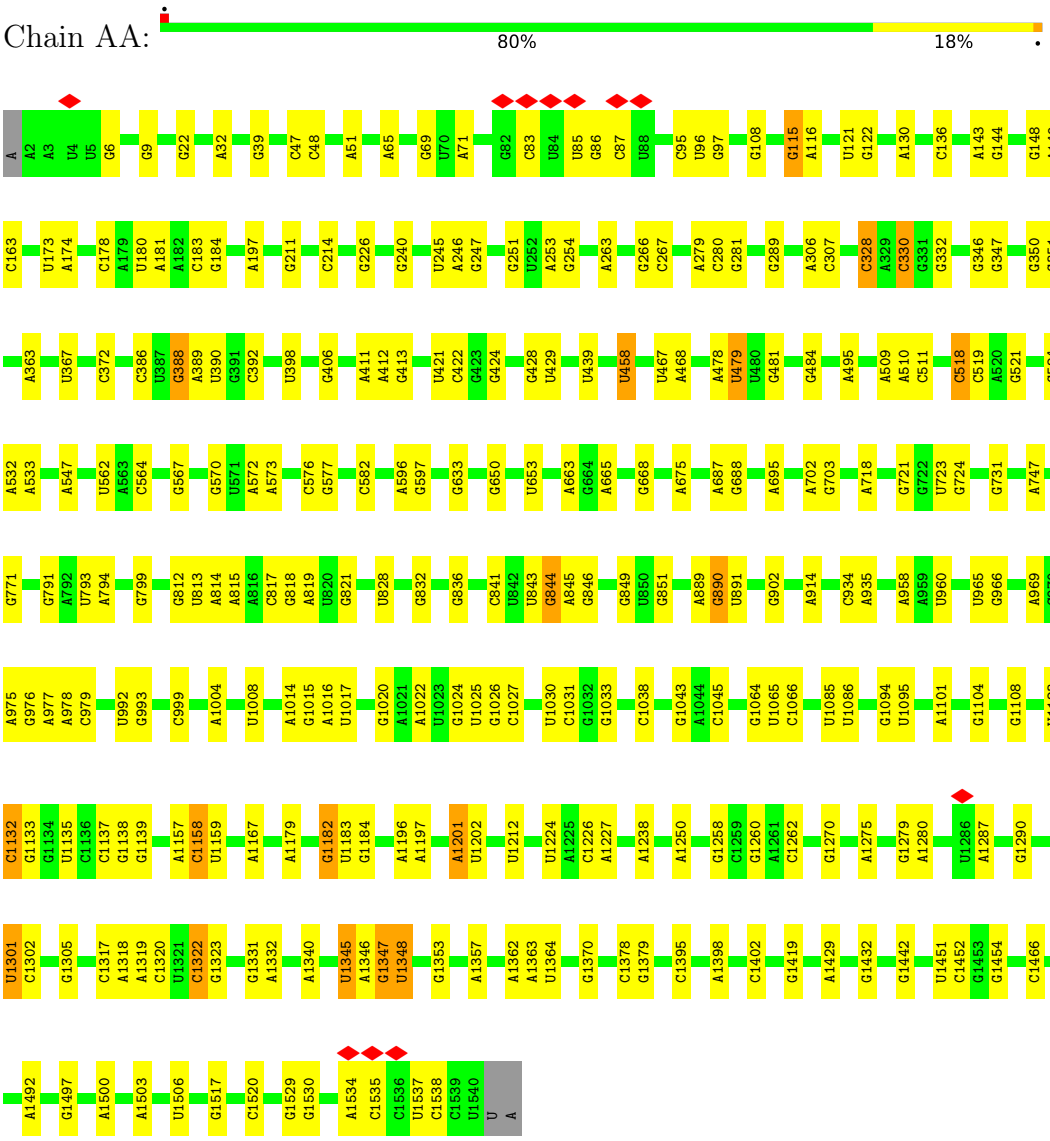
- Molecule 1: 16S ribosomal RNA

Chain 0:



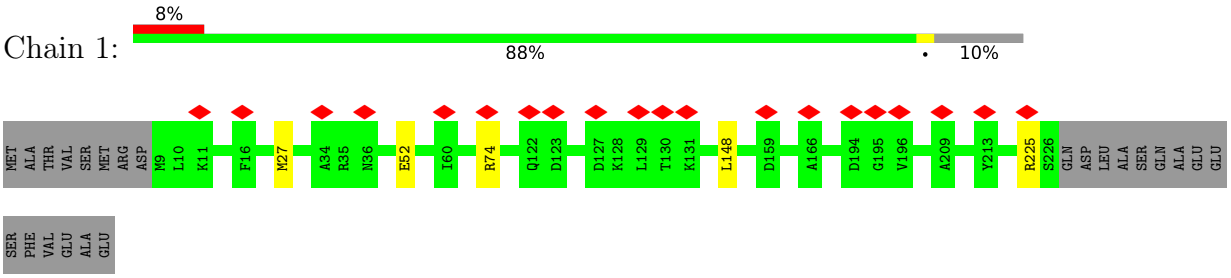
- Molecule 1: 16S ribosomal RNA

Chain AA:



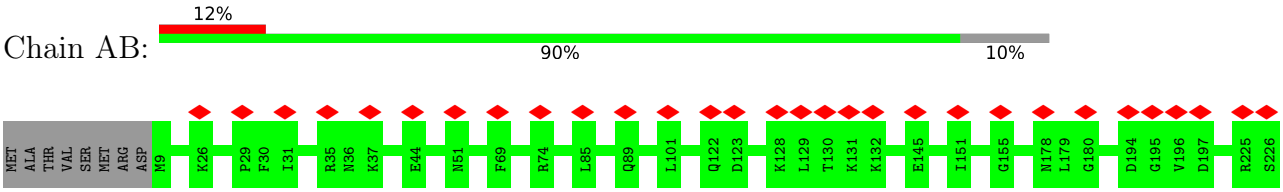
• Molecule 2: Small ribosomal subunit protein uS2

Chain 1:



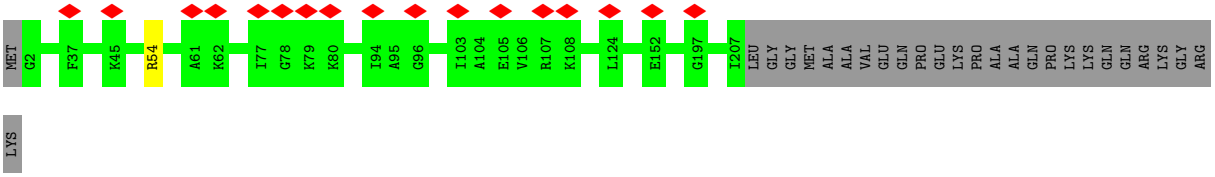
• Molecule 2: Small ribosomal subunit protein uS2

Chain AB:



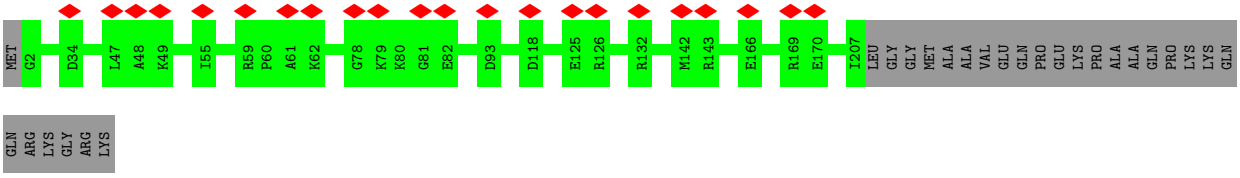
• Molecule 3: Small ribosomal subunit protein uS3

Chain 2:



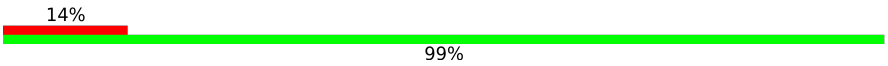
• Molecule 3: Small ribosomal subunit protein uS3

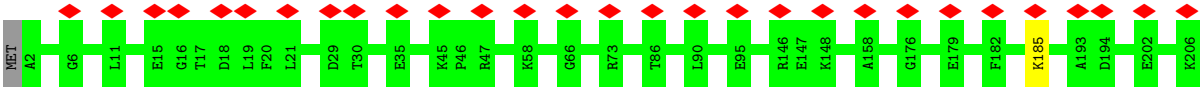
Chain AC:



• Molecule 4: Small ribosomal subunit protein uS4

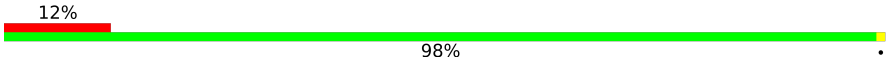
Chain 3:





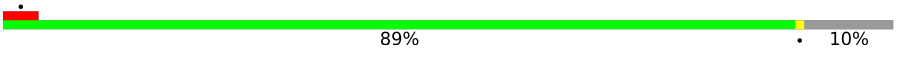
• Molecule 4: Small ribosomal subunit protein uS4

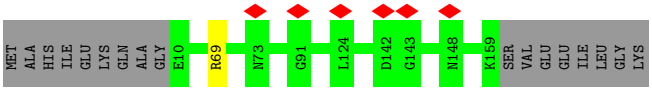
Chain AD:



• Molecule 5: Small ribosomal subunit protein uS5

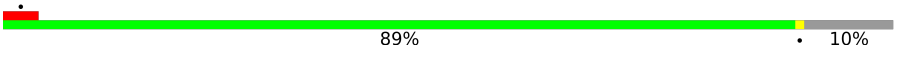
Chain 4:

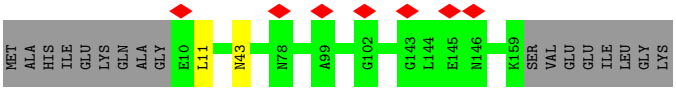




• Molecule 5: Small ribosomal subunit protein uS5

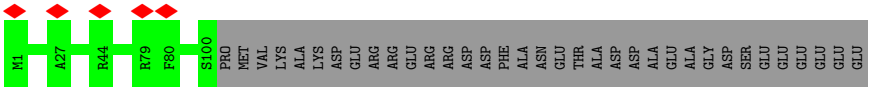
Chain AE:





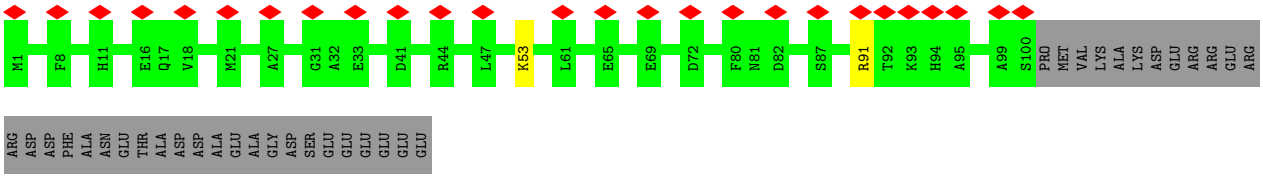
• Molecule 6: Small ribosomal subunit protein bS6, fully modified isoform

Chain 5:



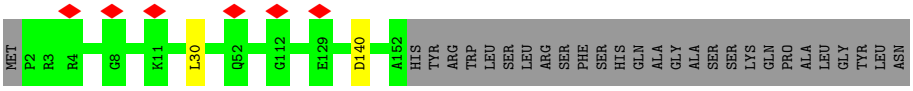
• Molecule 6: Small ribosomal subunit protein bS6, fully modified isoform

Chain AF:



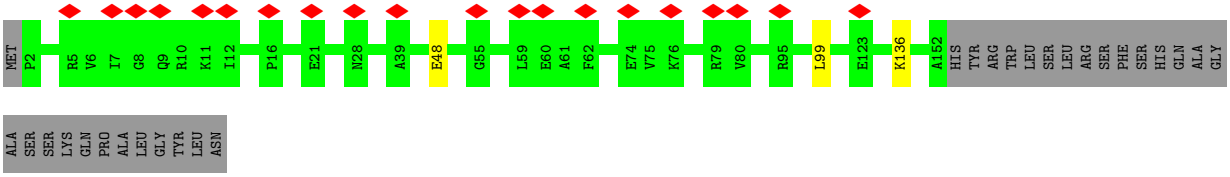
• Molecule 7: Small ribosomal subunit protein uS7

Chain 6:



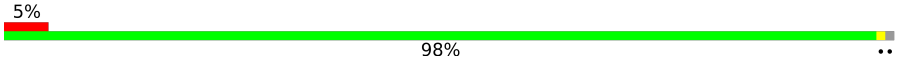
• Molecule 7: Small ribosomal subunit protein uS7

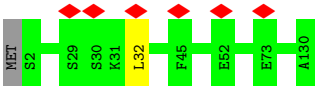
Chain AG:



• Molecule 8: Small ribosomal subunit protein uS8

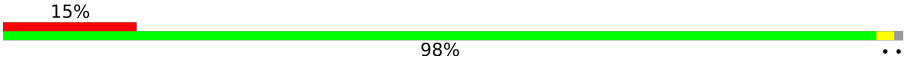
Chain 7:

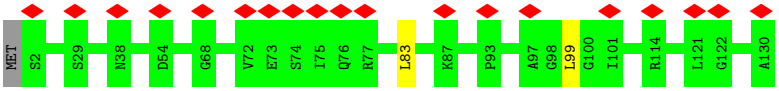




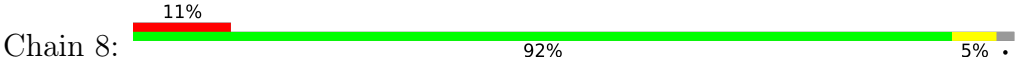
• Molecule 8: Small ribosomal subunit protein uS8

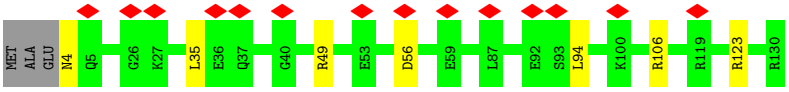
Chain AH:



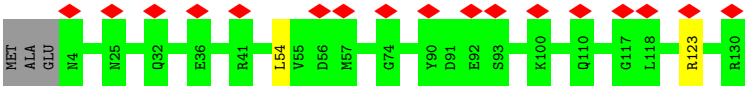


• Molecule 9: Small ribosomal subunit protein uS9

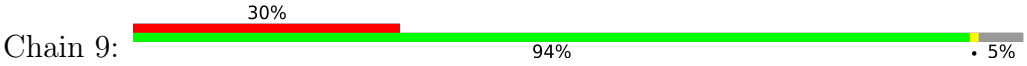


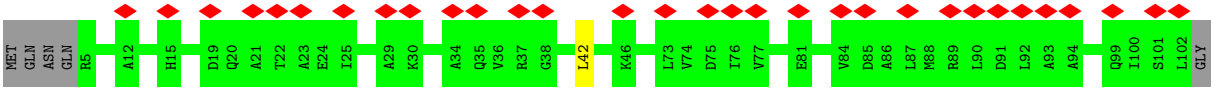


• Molecule 9: Small ribosomal subunit protein uS9

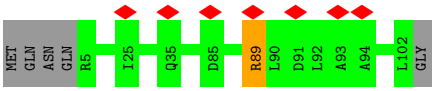


• Molecule 10: Small ribosomal subunit protein uS10

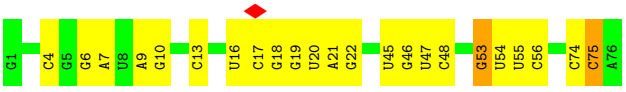




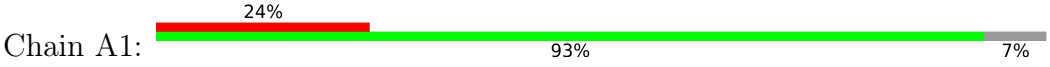
• Molecule 10: Small ribosomal subunit protein uS10

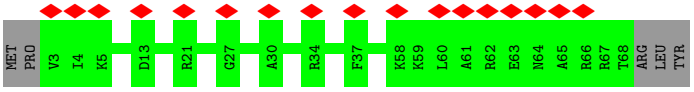


• Molecule 11: A-site tRNA



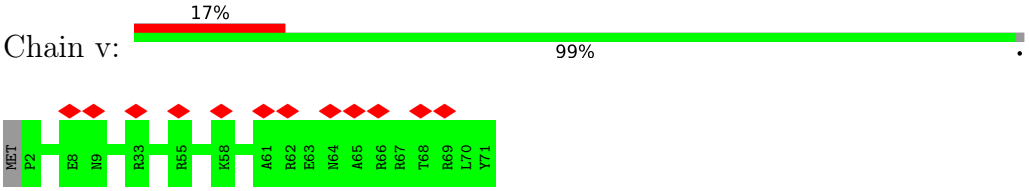
• Molecule 12: Small ribosomal subunit protein bS21





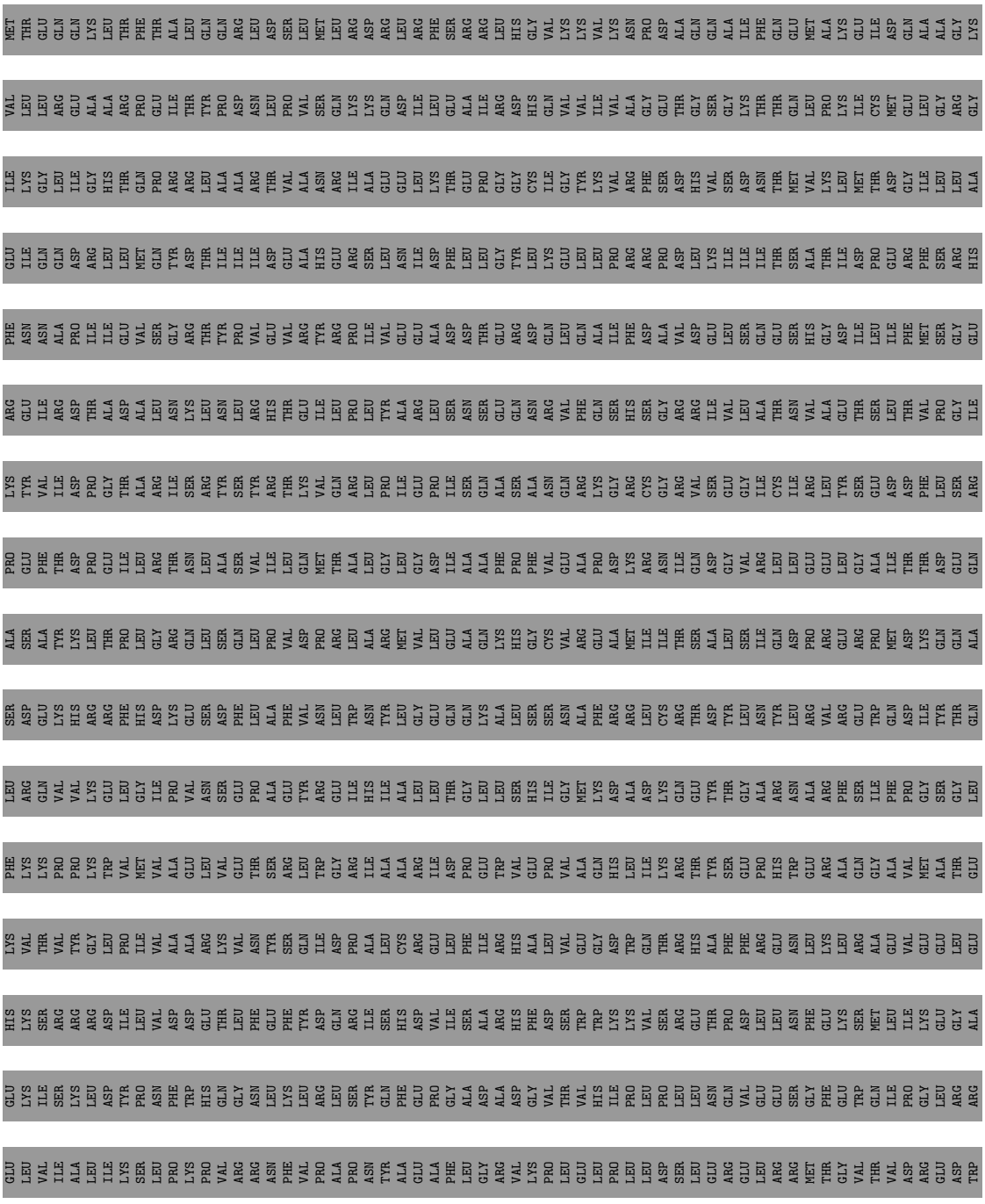
• Molecule 12: Small ribosomal subunit protein bS21

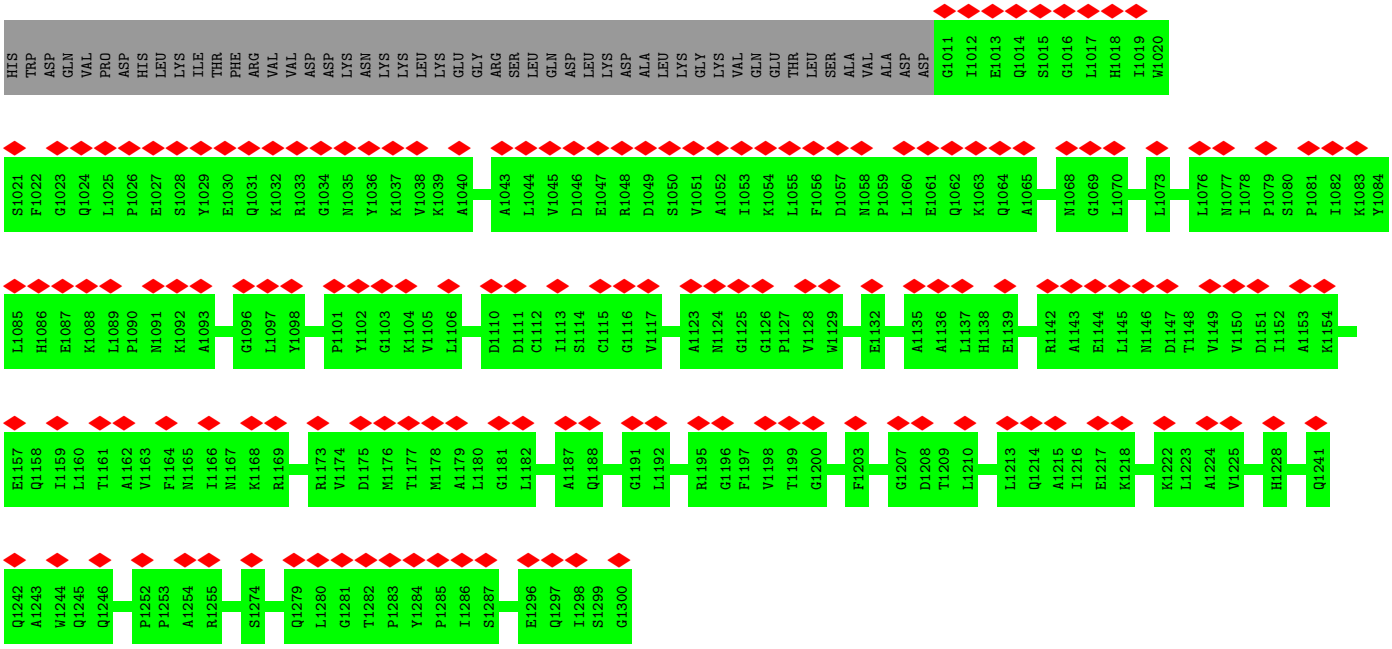
Chain v:



• Molecule 13: ATP-dependent RNA helicase HrpA

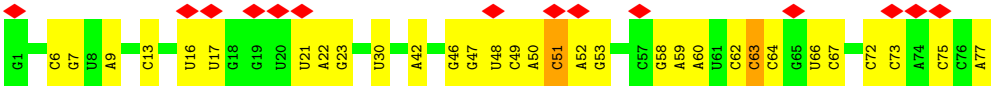
Chain A2:





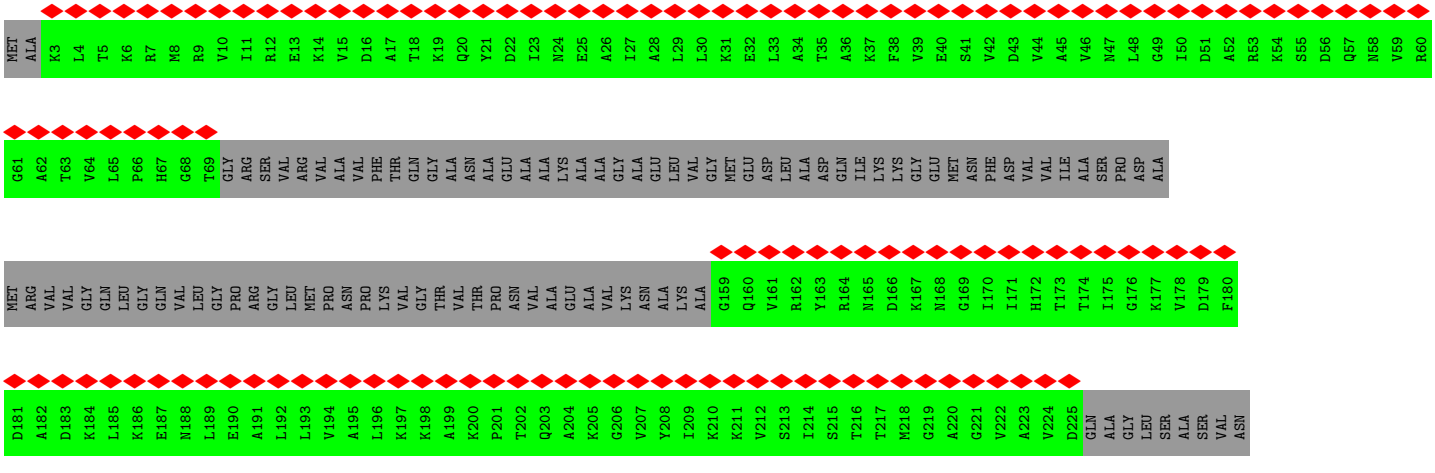
• Molecule 14: A-site tRNA

Chain A3:



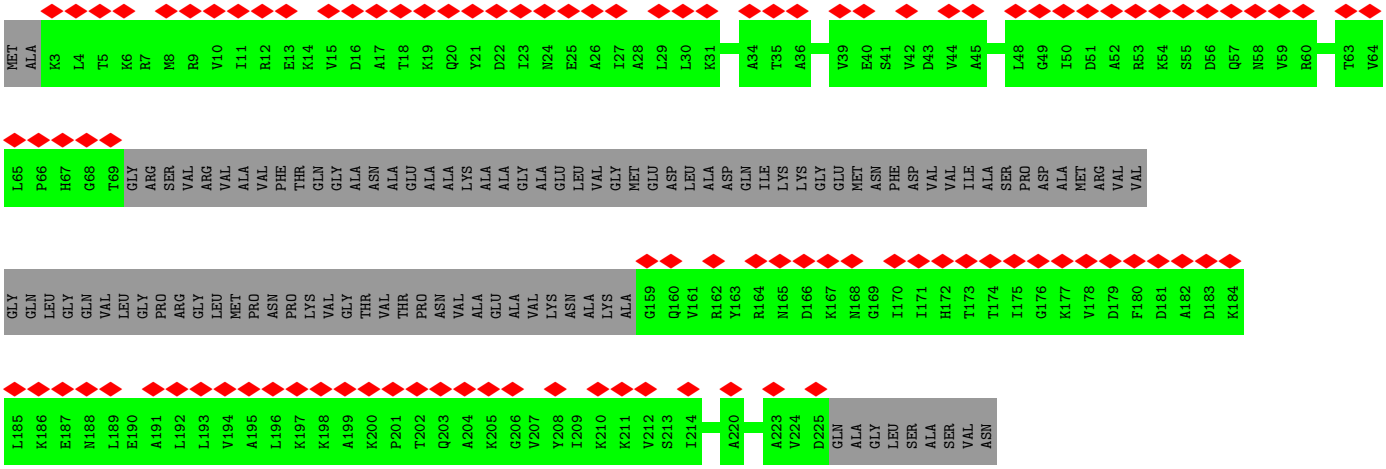
• Molecule 15: Large ribosomal subunit protein uL1

Chain AK:



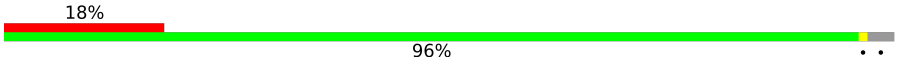
• Molecule 15: Large ribosomal subunit protein uL1

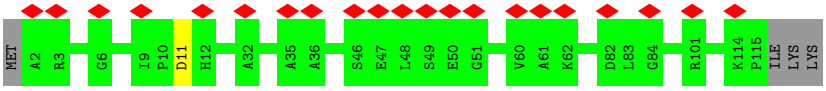
Chain C:



• Molecule 16: Small ribosomal subunit protein uS13

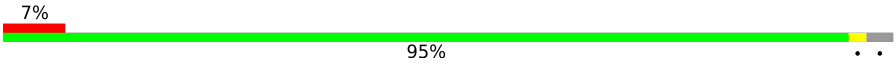
Chain AL:

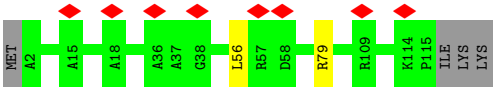




• Molecule 16: Small ribosomal subunit protein uS13

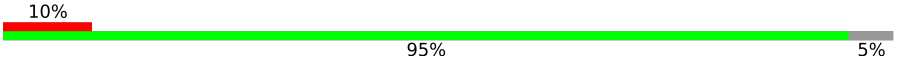
Chain F:

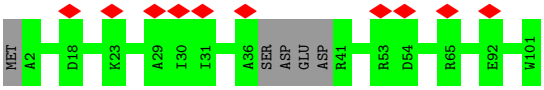




• Molecule 17: Small ribosomal subunit protein uS14

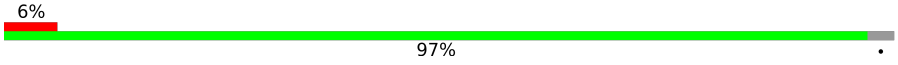
Chain AM:

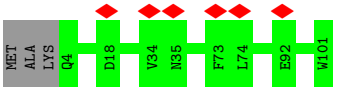




• Molecule 17: Small ribosomal subunit protein uS14

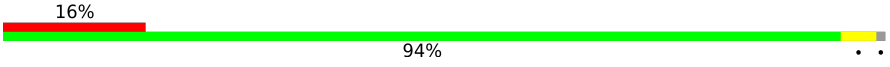
Chain G:

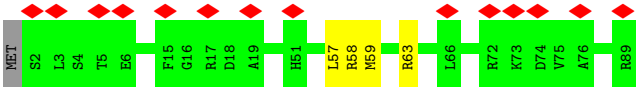




• Molecule 18: Small ribosomal subunit protein uS15

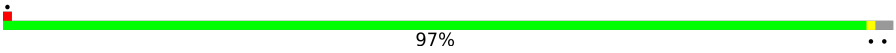
Chain AN:





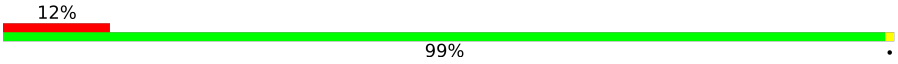
• Molecule 18: Small ribosomal subunit protein uS15

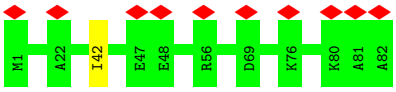
Chain H:



• Molecule 19: Small ribosomal subunit protein bS16

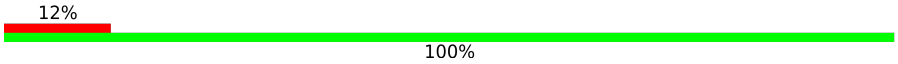
Chain AO:

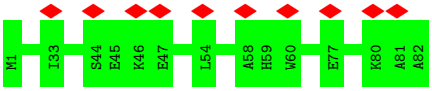




• Molecule 19: Small ribosomal subunit protein bS16

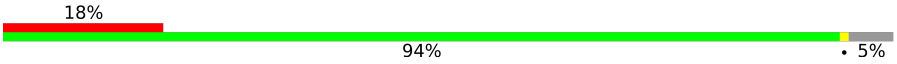
Chain I:

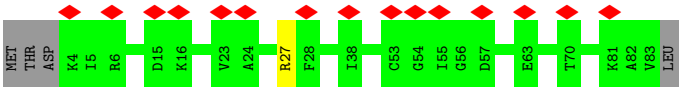




• Molecule 20: Small ribosomal subunit protein uS17

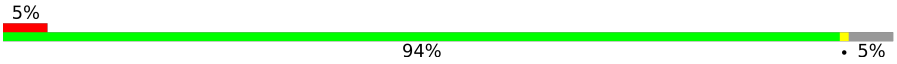
Chain AP:

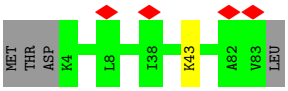




• Molecule 20: Small ribosomal subunit protein uS17

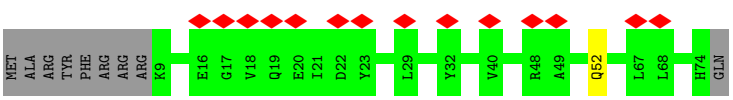
Chain J:





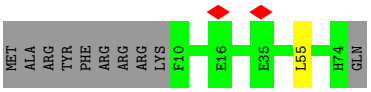
• Molecule 21: Small ribosomal subunit protein bS18

Chain AQ:



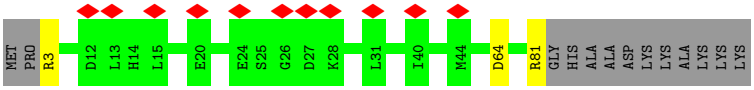
• Molecule 21: Small ribosomal subunit protein bS18

Chain K:



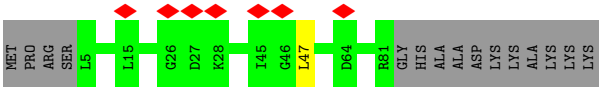
• Molecule 22: Small ribosomal subunit protein uS19

Chain AR:



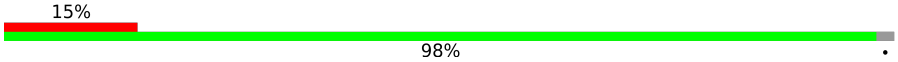
• Molecule 22: Small ribosomal subunit protein uS19

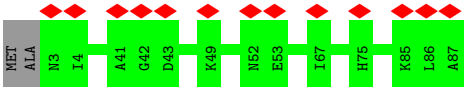
Chain t:



• Molecule 23: Small ribosomal subunit protein bS20

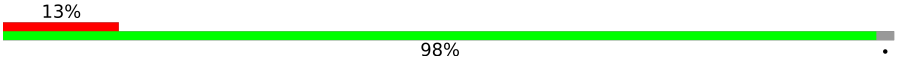
Chain AS:

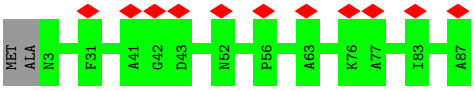




• Molecule 23: Small ribosomal subunit protein bS20

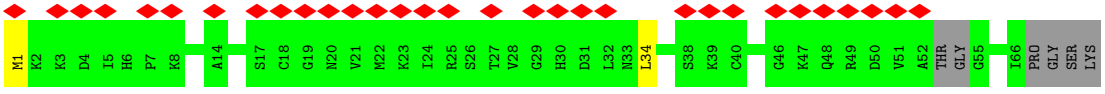
Chain u:





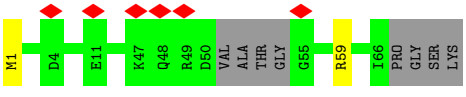
• Molecule 24: Large ribosomal subunit protein bL31A

Chain AT:



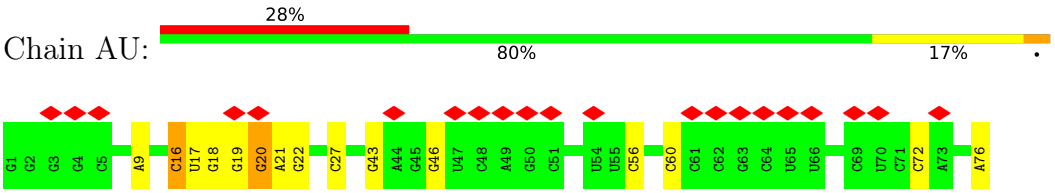
• Molecule 24: Large ribosomal subunit protein bL31A

Chain L:



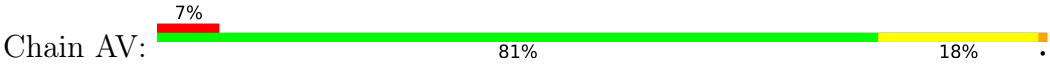
• Molecule 25: P-site tRNA

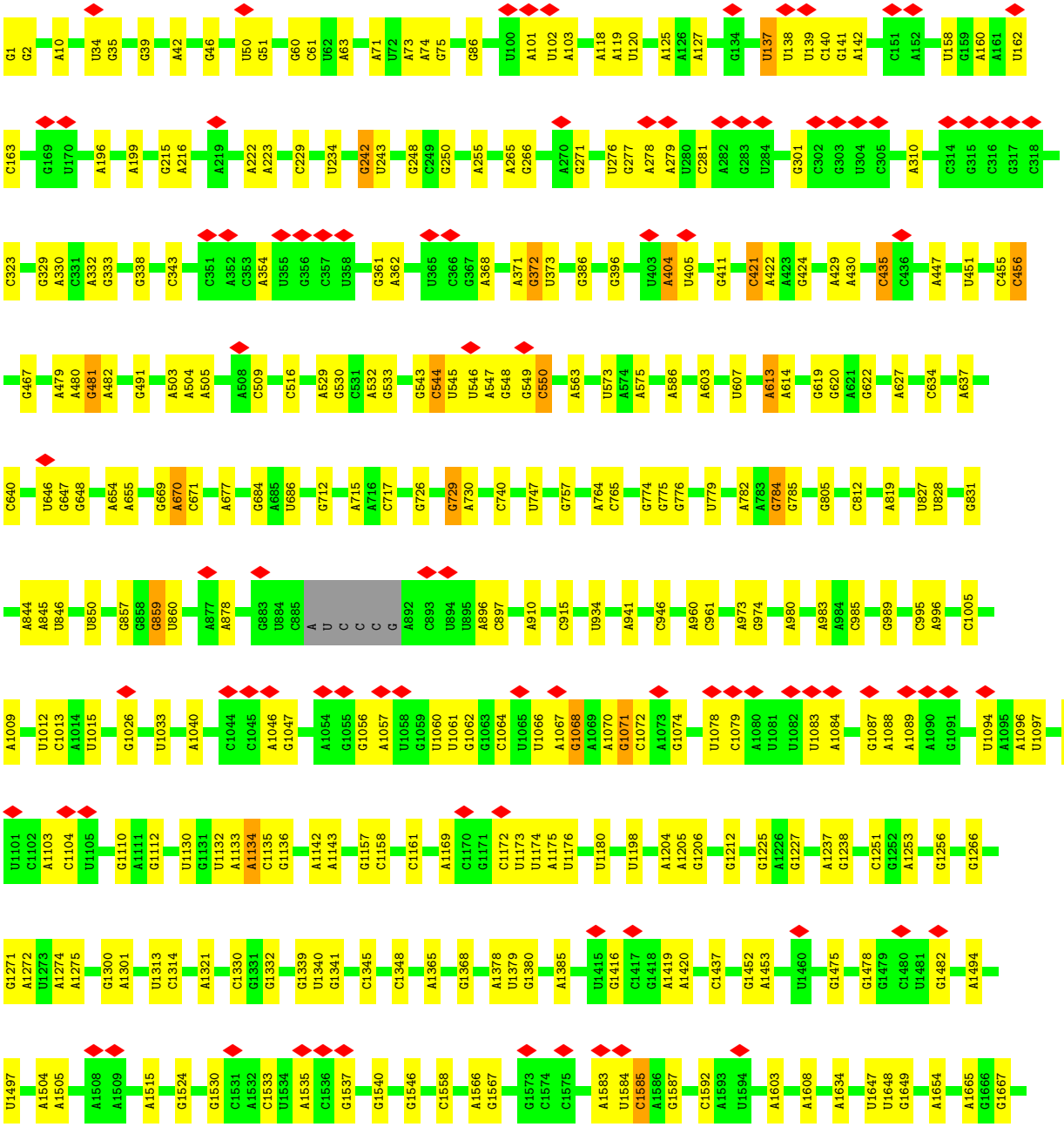
Chain AU:

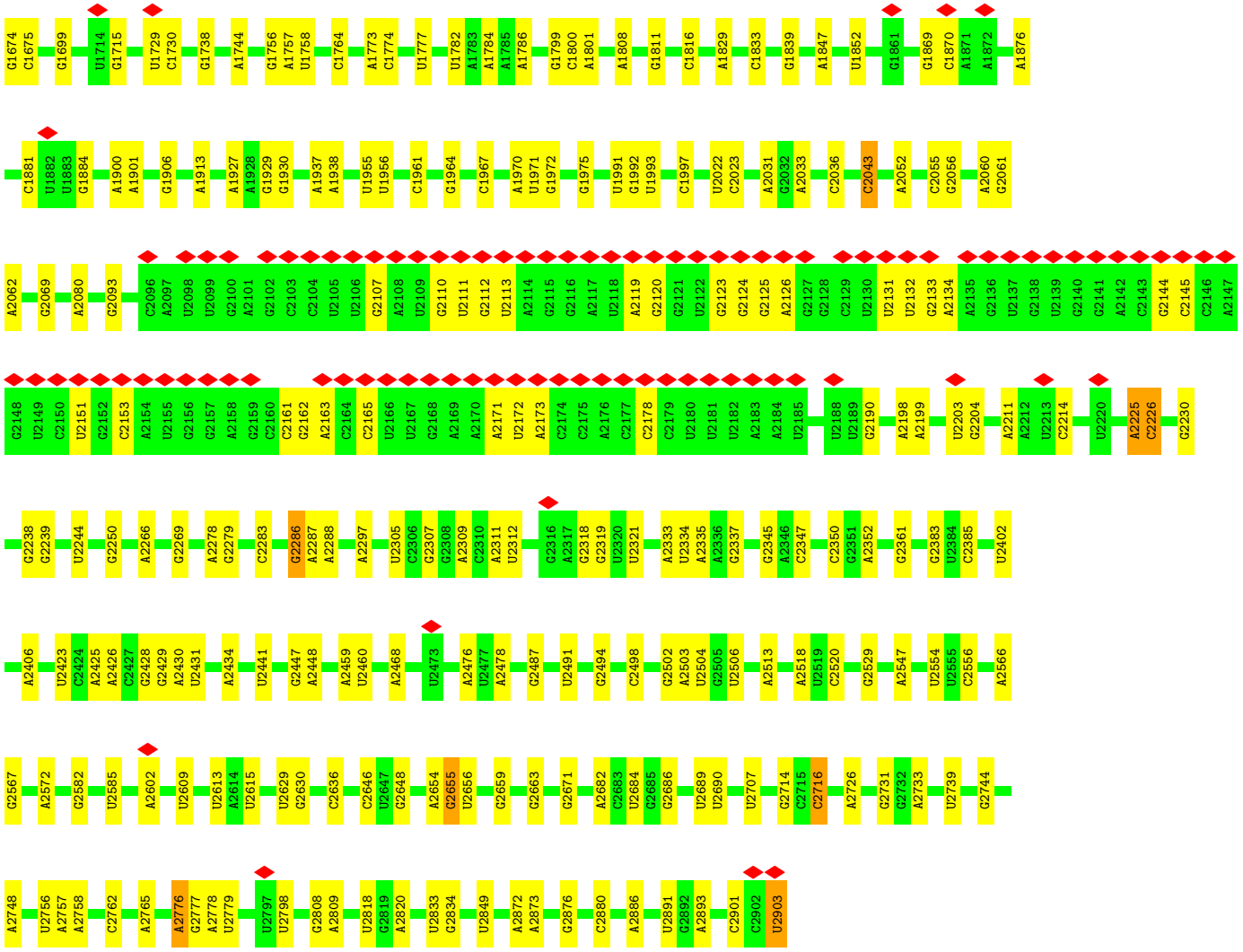


• Molecule 26: 23S ribosomal RNA

Chain AV:

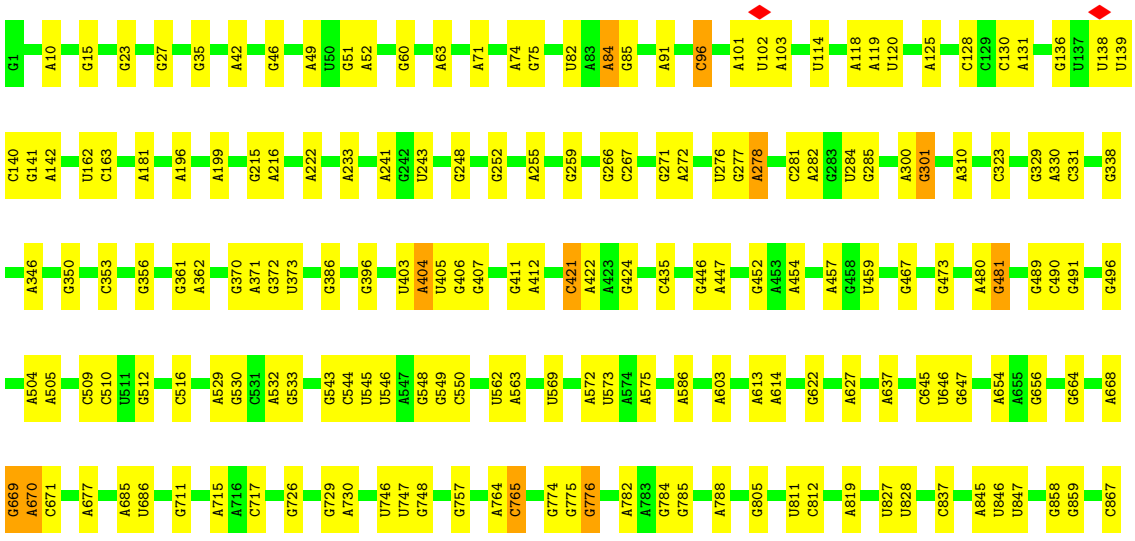


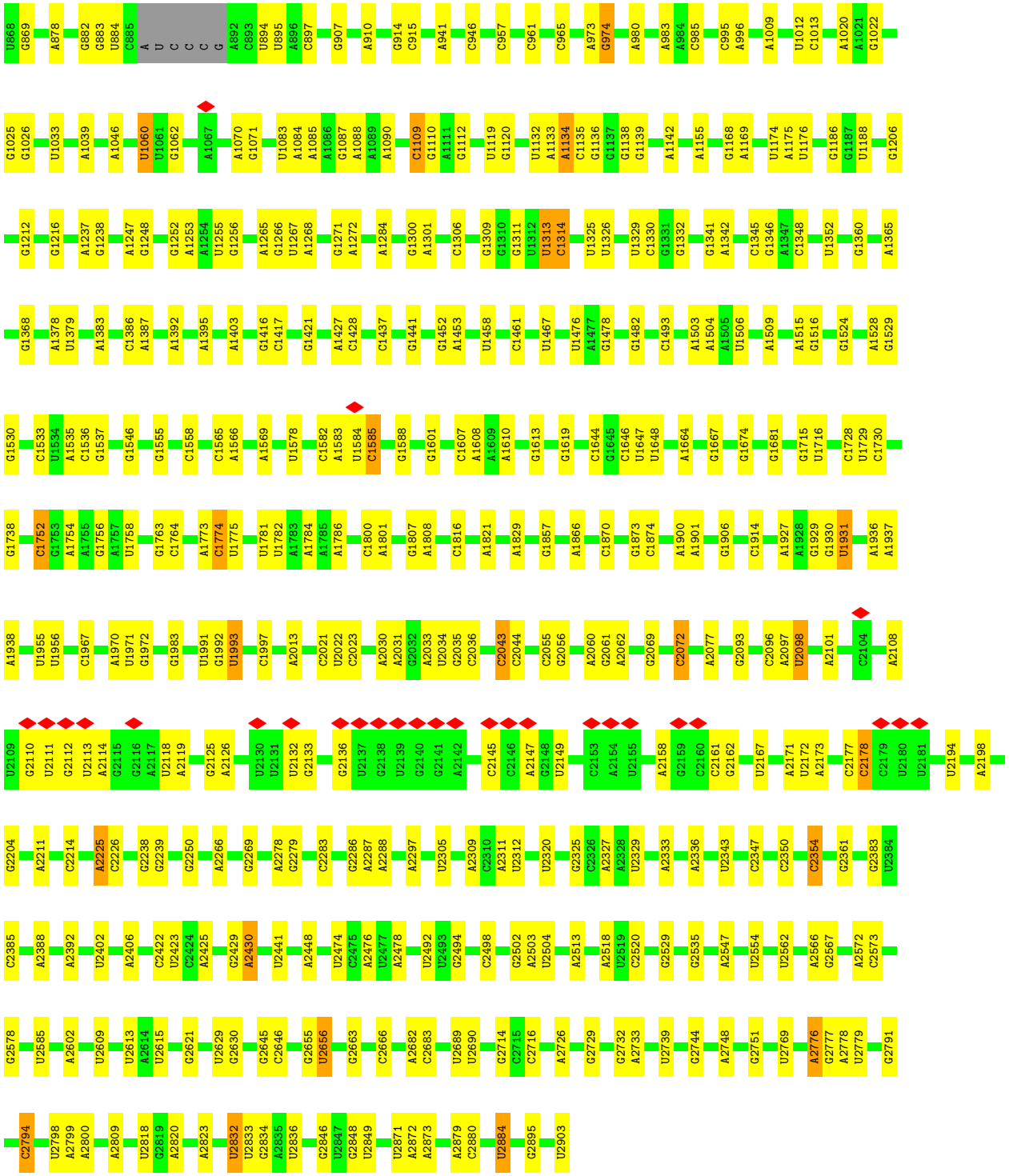




• Molecule 26: 23S ribosomal RNA

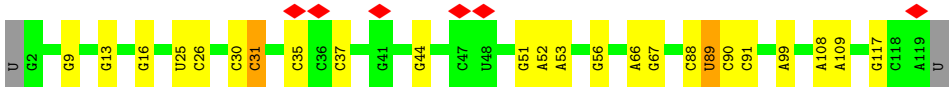
Chain N:





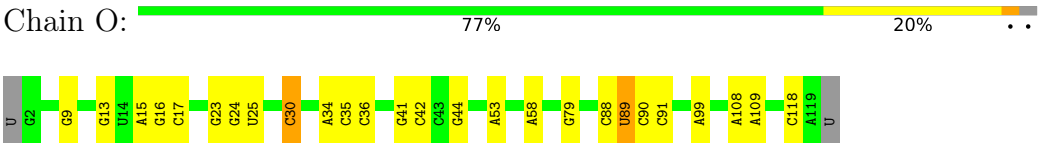
• Molecule 27: 5S ribosomal RNA

Chain AW:



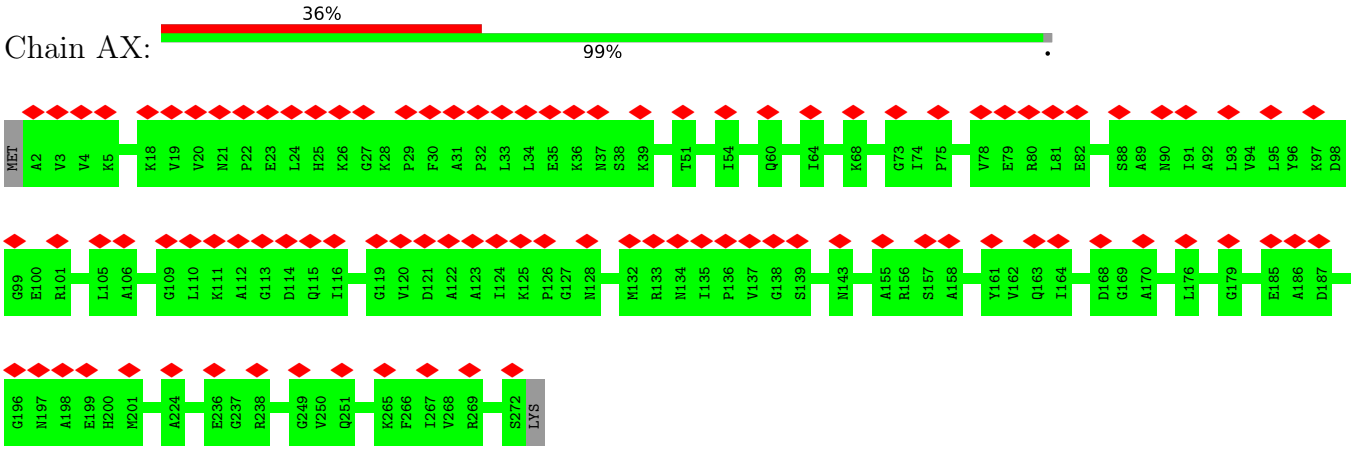
• Molecule 27: 5S ribosomal RNA

Chain O:



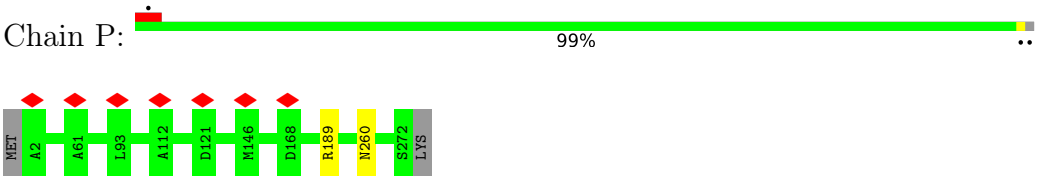
• Molecule 28: Large ribosomal subunit protein uL2

Chain AX:



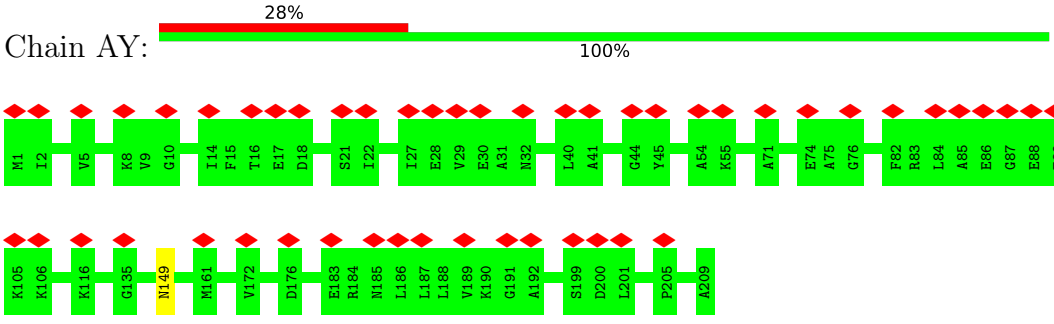
• Molecule 28: Large ribosomal subunit protein uL2

Chain P:



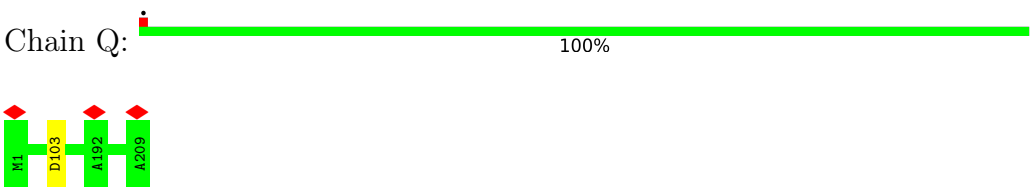
• Molecule 29: 50S ribosomal protein L3

Chain AY:



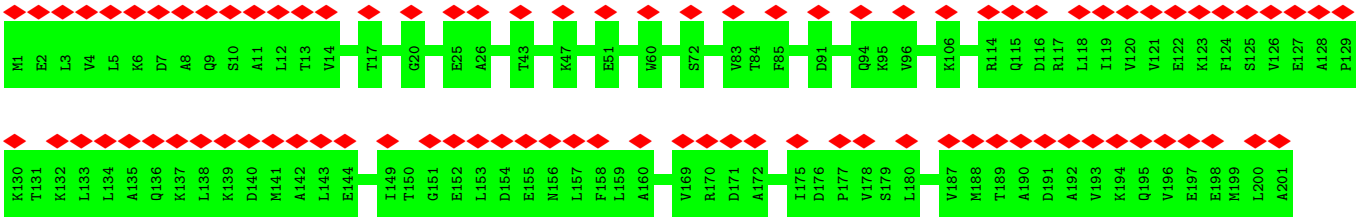
• Molecule 29: 50S ribosomal protein L3

Chain Q:



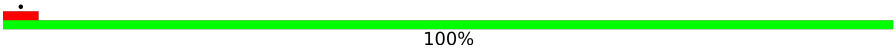
• Molecule 30: Large ribosomal subunit protein uL4

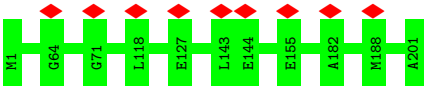
Chain AZ:



• Molecule 30: Large ribosomal subunit protein uL4

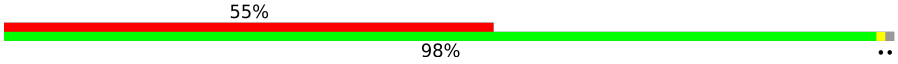
Chain R:





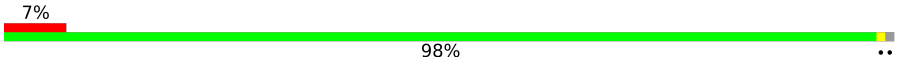
• Molecule 31: Large ribosomal subunit protein uL5

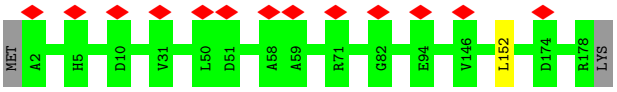
Chain Aa:



• Molecule 31: Large ribosomal subunit protein uL5

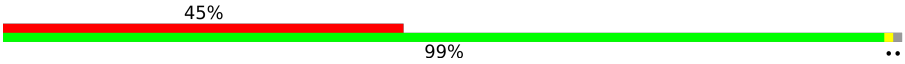
Chain S:

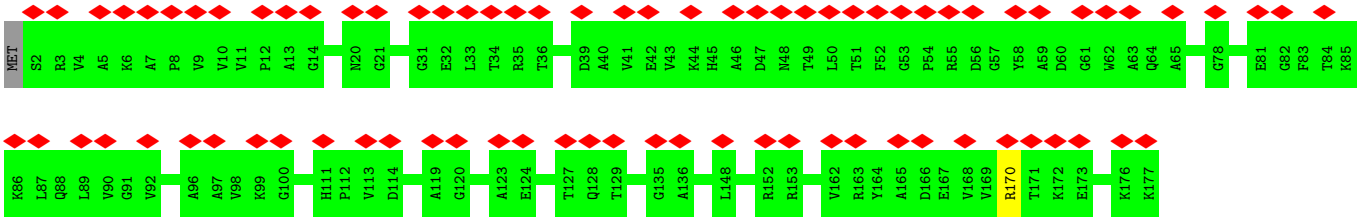




• Molecule 32: Large ribosomal subunit protein uL6

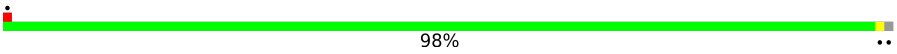
Chain Ab:

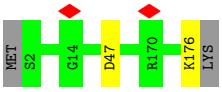




• Molecule 32: Large ribosomal subunit protein uL6

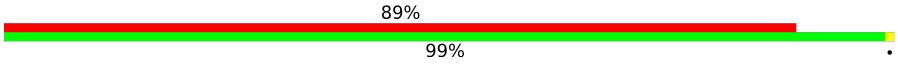
Chain T:

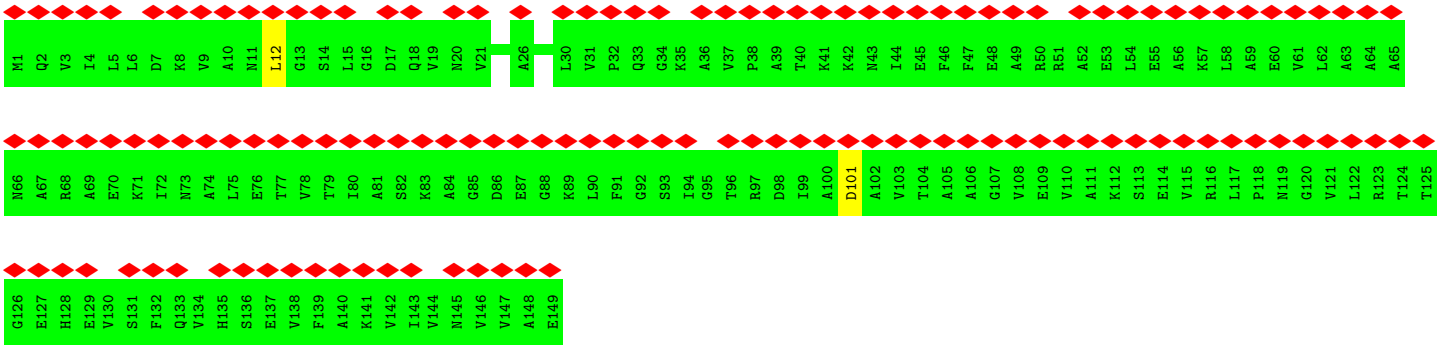




• Molecule 33: Large ribosomal subunit protein bL9

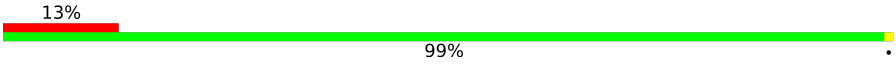
Chain Ac:

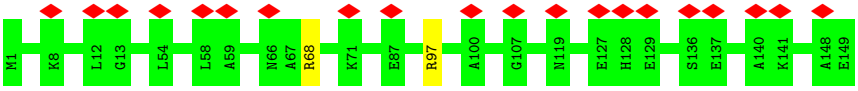




• Molecule 33: Large ribosomal subunit protein bL9

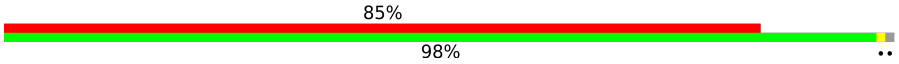
Chain U:

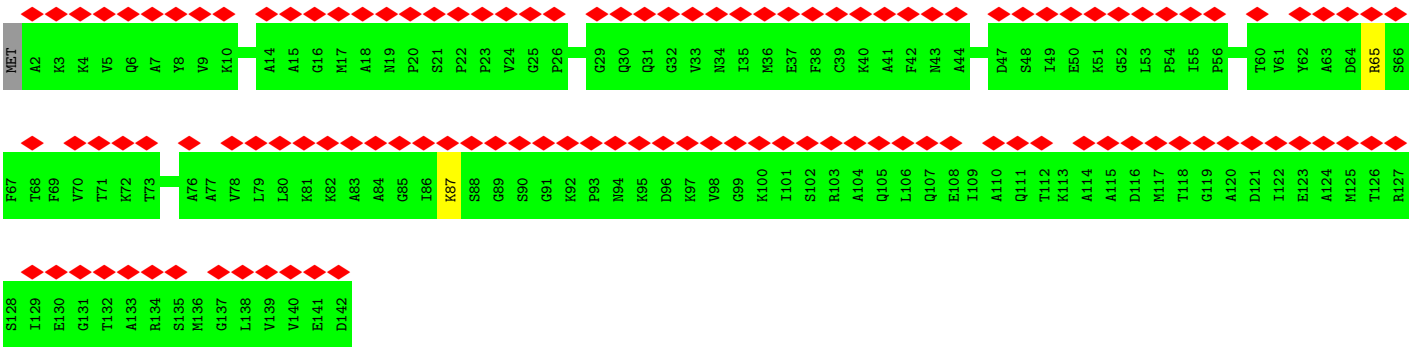




• Molecule 34: 50S ribosomal protein L11

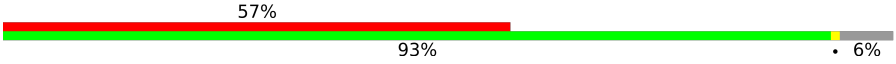
Chain Ad:

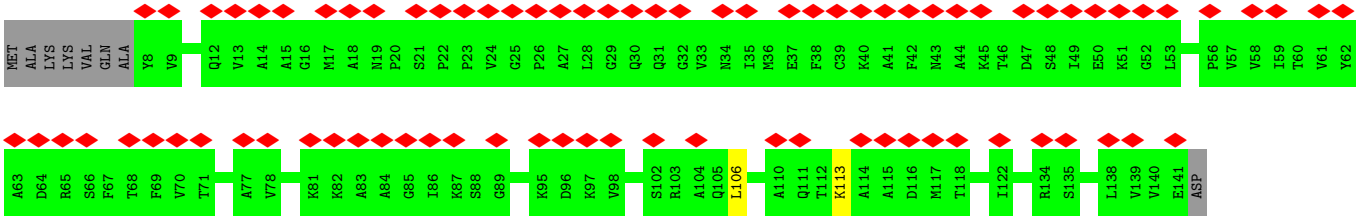




• Molecule 34: 50S ribosomal protein L11

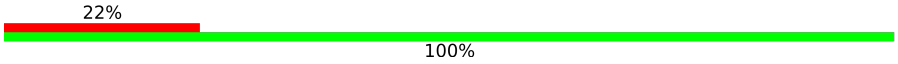
Chain V:

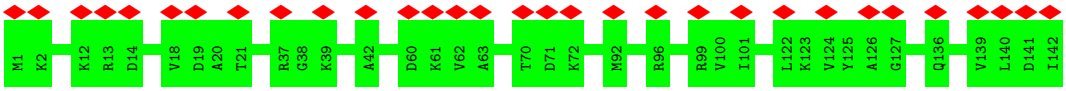




• Molecule 35: Large ribosomal subunit protein uL13

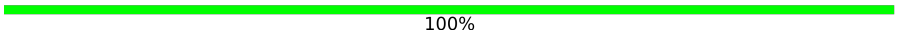
Chain Ae:





• Molecule 35: Large ribosomal subunit protein uL13

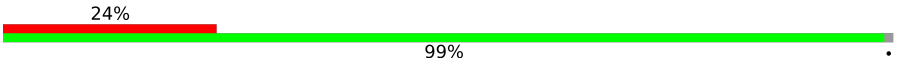
Chain W:

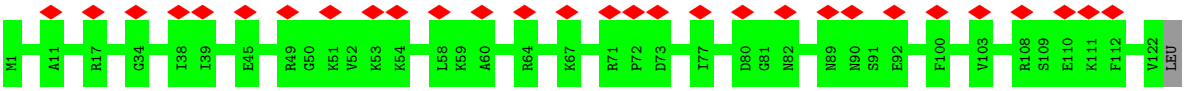


There are no outlier residues recorded for this chain.

• Molecule 36: Large ribosomal subunit protein uL14

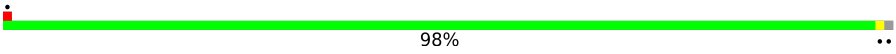
Chain Af:

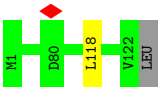




• Molecule 36: Large ribosomal subunit protein uL14

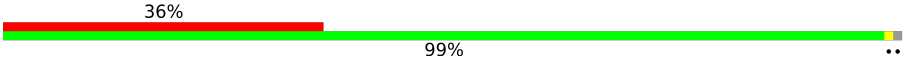
Chain X:

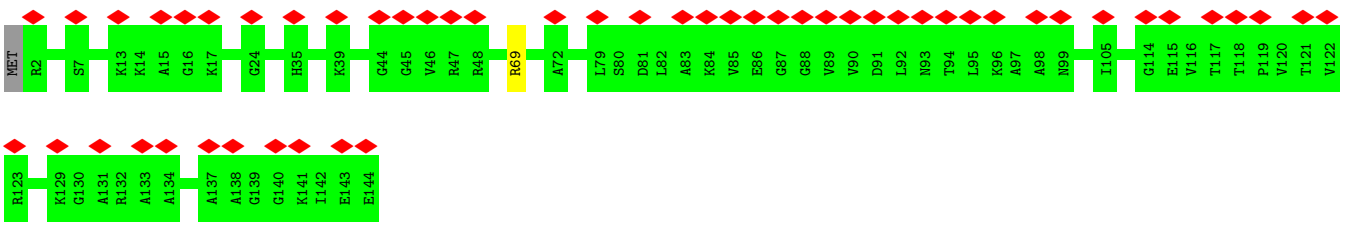




• Molecule 37: Large ribosomal subunit protein uL15

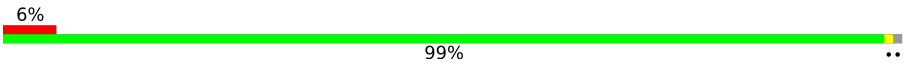
Chain Ag:

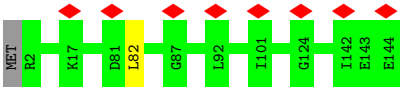




• Molecule 37: Large ribosomal subunit protein uL15

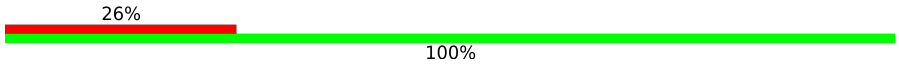
Chain Y:

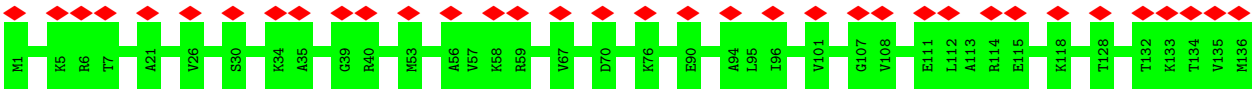




• Molecule 38: 50S ribosomal protein L16

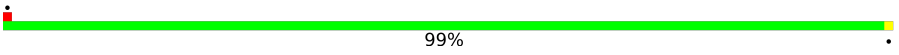
Chain Ah:

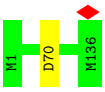




• Molecule 38: 50S ribosomal protein L16

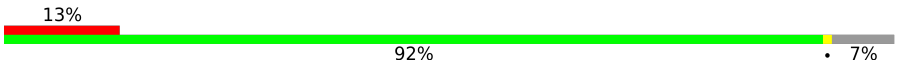
Chain Z:

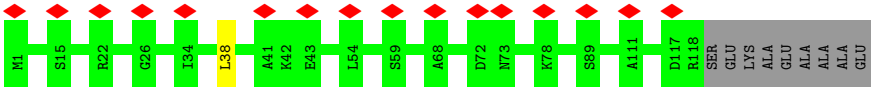




• Molecule 39: Large ribosomal subunit protein bL17

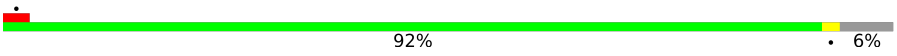
Chain Ai:





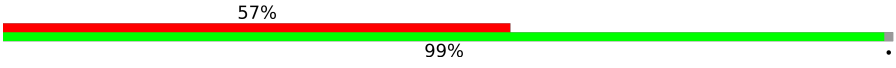
• Molecule 39: Large ribosomal subunit protein bL17

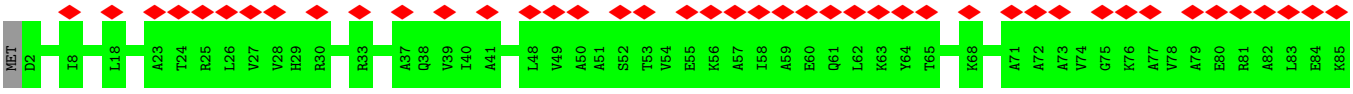
Chain a:

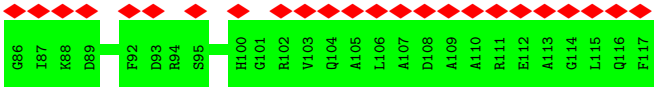


• Molecule 40: Large ribosomal subunit protein uL18

Chain Aj:

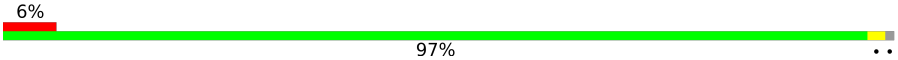


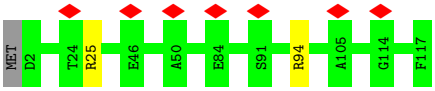




• Molecule 40: Large ribosomal subunit protein uL18

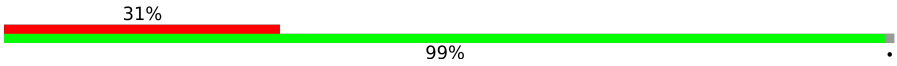
Chain b:

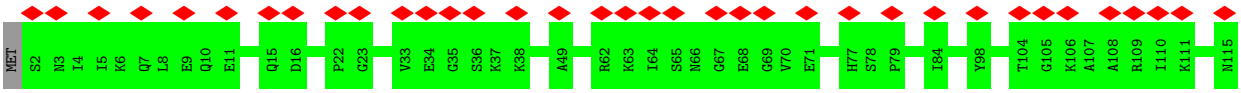




• Molecule 41: Large ribosomal subunit protein bL19

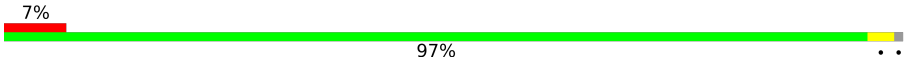
Chain Ak:

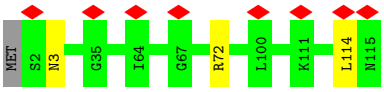




• Molecule 41: Large ribosomal subunit protein bL19

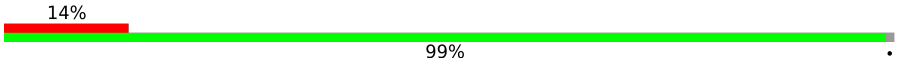
Chain c:

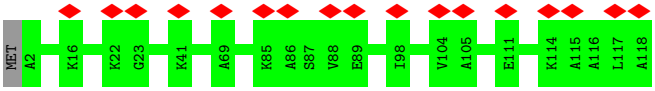




• Molecule 42: Large ribosomal subunit protein bL20

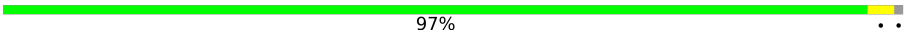
Chain Al:





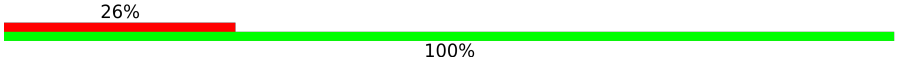
• Molecule 42: Large ribosomal subunit protein bL20

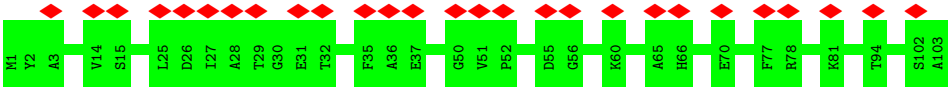
Chain d:



• Molecule 43: Large ribosomal subunit protein bL21

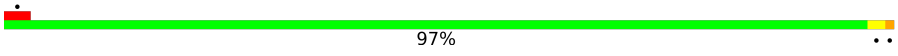
Chain Am:





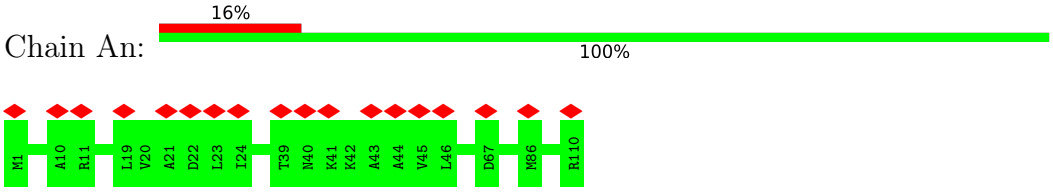
• Molecule 43: Large ribosomal subunit protein bL21

Chain e:



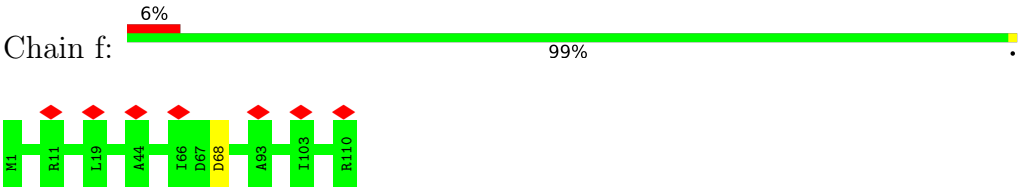
• Molecule 44: Large ribosomal subunit protein uL22

Chain An:



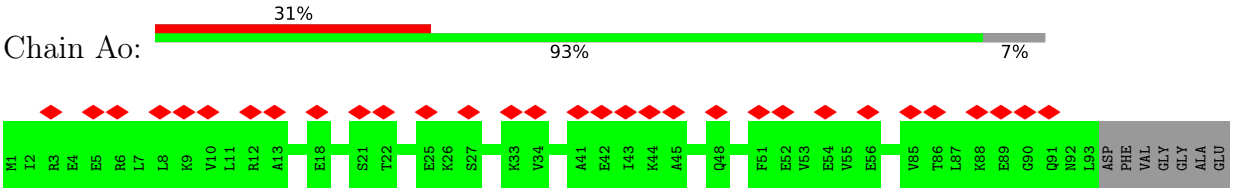
• Molecule 44: Large ribosomal subunit protein uL22

Chain f:



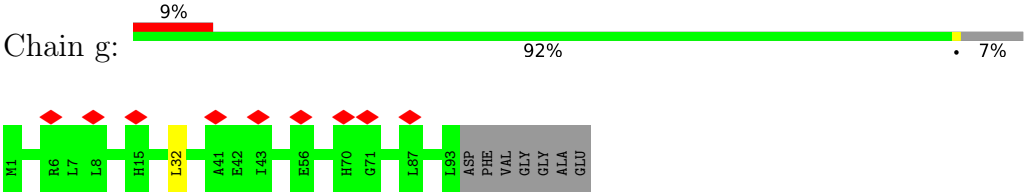
• Molecule 45: Large ribosomal subunit protein uL23

Chain Ao:



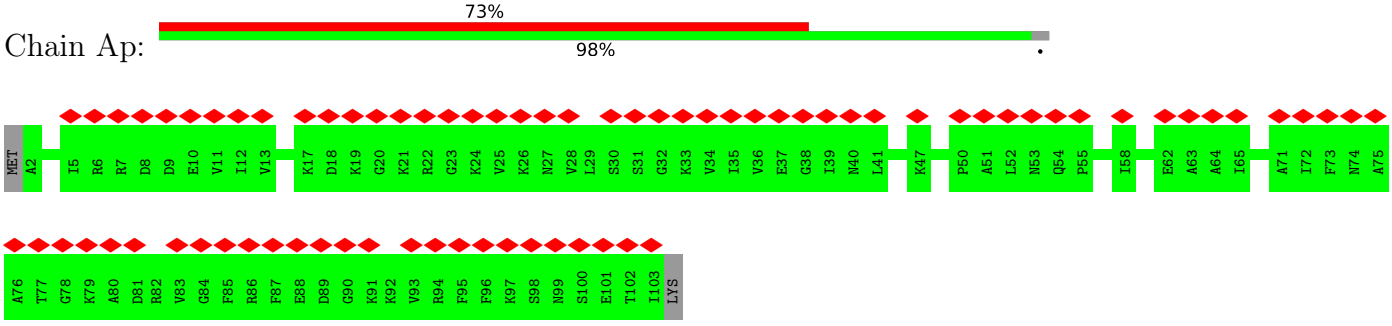
• Molecule 45: Large ribosomal subunit protein uL23

Chain g:



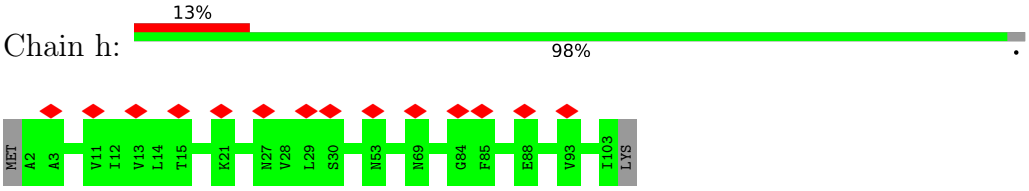
• Molecule 46: Large ribosomal subunit protein uL24

Chain Ap:



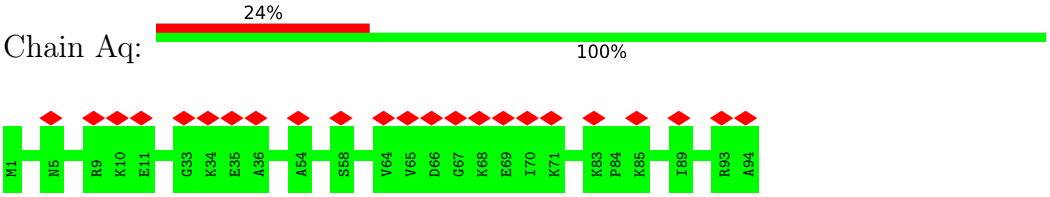
• Molecule 46: Large ribosomal subunit protein uL24

Chain h:



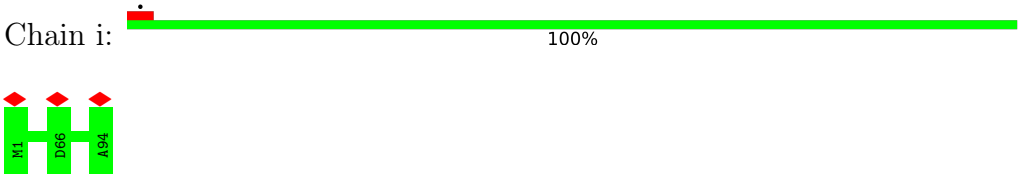
• Molecule 47: Large ribosomal subunit protein bL25

Chain Aq:



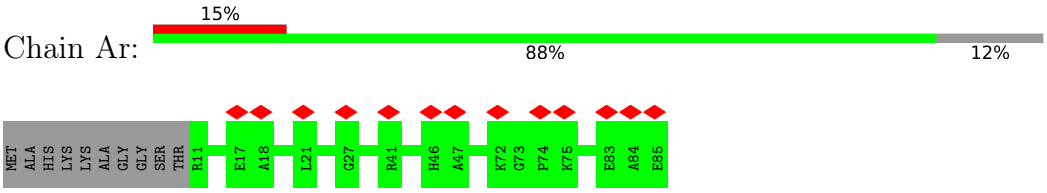
• Molecule 47: Large ribosomal subunit protein bL25

Chain i:



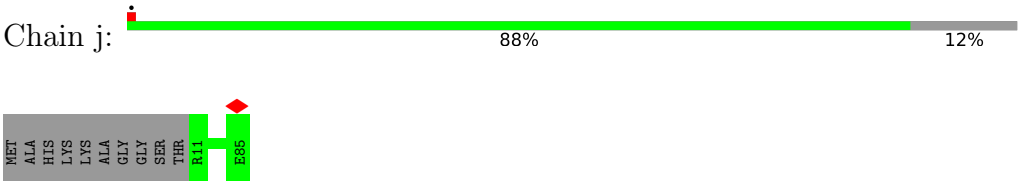
• Molecule 48: Large ribosomal subunit protein bL27

Chain Ar:



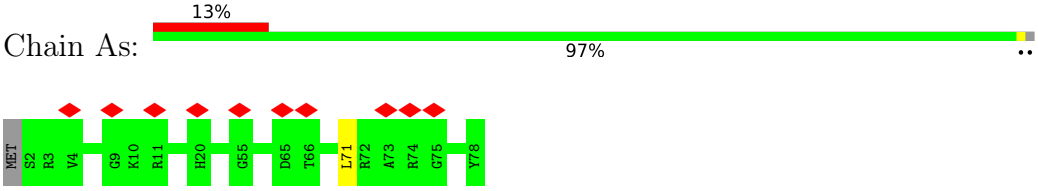
• Molecule 48: Large ribosomal subunit protein bL27

Chain j:



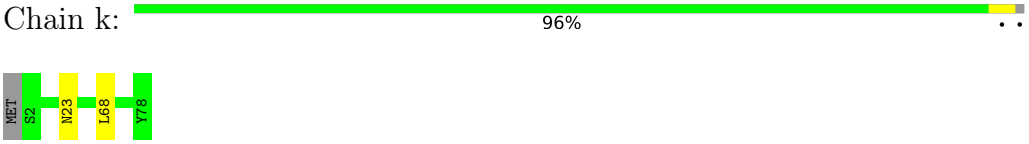
• Molecule 49: Large ribosomal subunit protein bL28

Chain As:



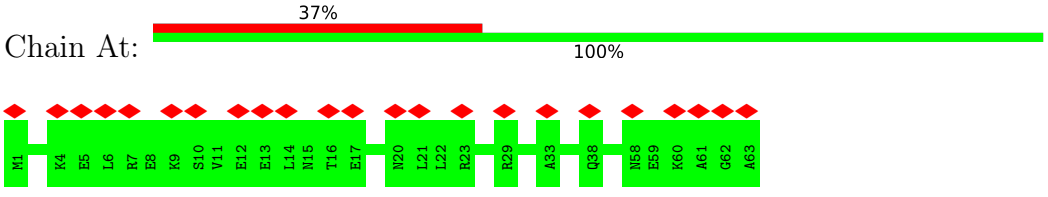
• Molecule 49: Large ribosomal subunit protein bL28

Chain k:



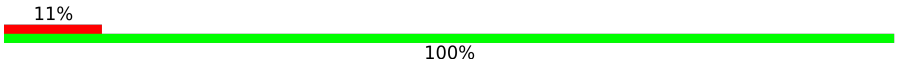
• Molecule 50: Large ribosomal subunit protein uL29

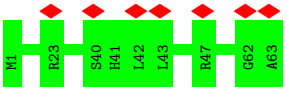
Chain At:



• Molecule 50: Large ribosomal subunit protein uL29

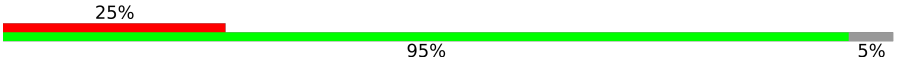
Chain l:

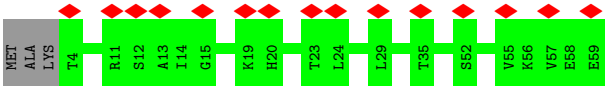




• Molecule 51: Large ribosomal subunit protein uL30

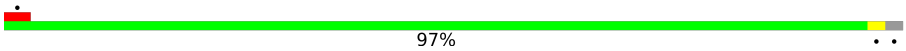
Chain Au:

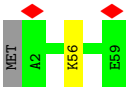




• Molecule 51: Large ribosomal subunit protein uL30

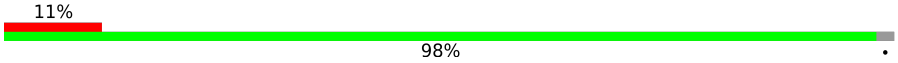
Chain m:

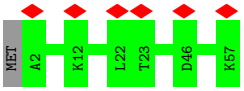




• Molecule 52: Large ribosomal subunit protein bL32

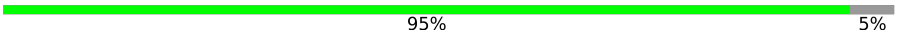
Chain Av:

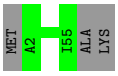




• Molecule 52: Large ribosomal subunit protein bL32

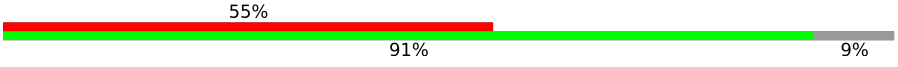
Chain n:

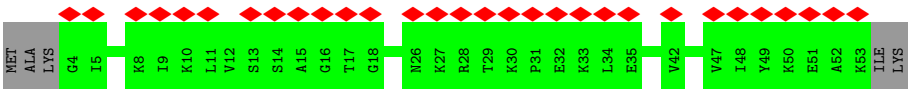




• Molecule 53: Large ribosomal subunit protein bL33

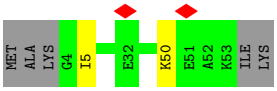
Chain Aw:





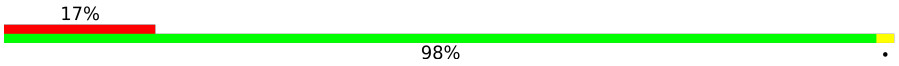
• Molecule 53: Large ribosomal subunit protein bL33

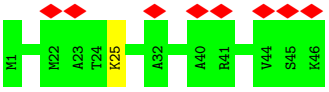
Chain o:



• Molecule 54: Large ribosomal subunit protein bL34

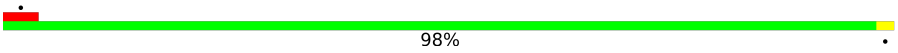
Chain Ax:

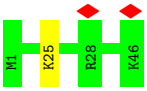




• Molecule 54: Large ribosomal subunit protein bL34

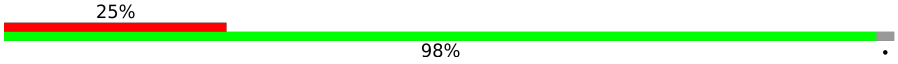
Chain p:

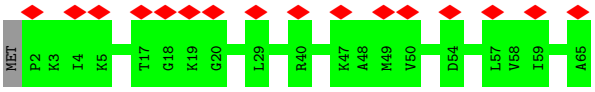




• Molecule 55: Large ribosomal subunit protein bL35

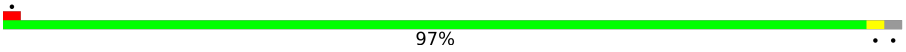
Chain Ay:

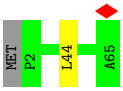




• Molecule 55: Large ribosomal subunit protein bL35

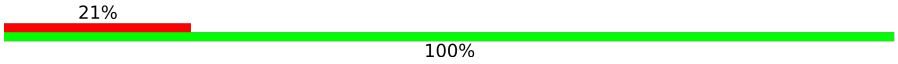
Chain q:

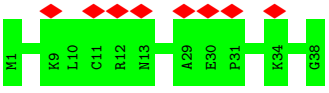




• Molecule 56: Large ribosomal subunit protein bL36A

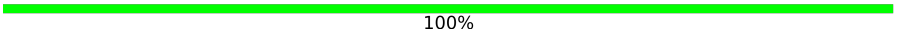
Chain Az:





• Molecule 56: Large ribosomal subunit protein bL36A

Chain r:

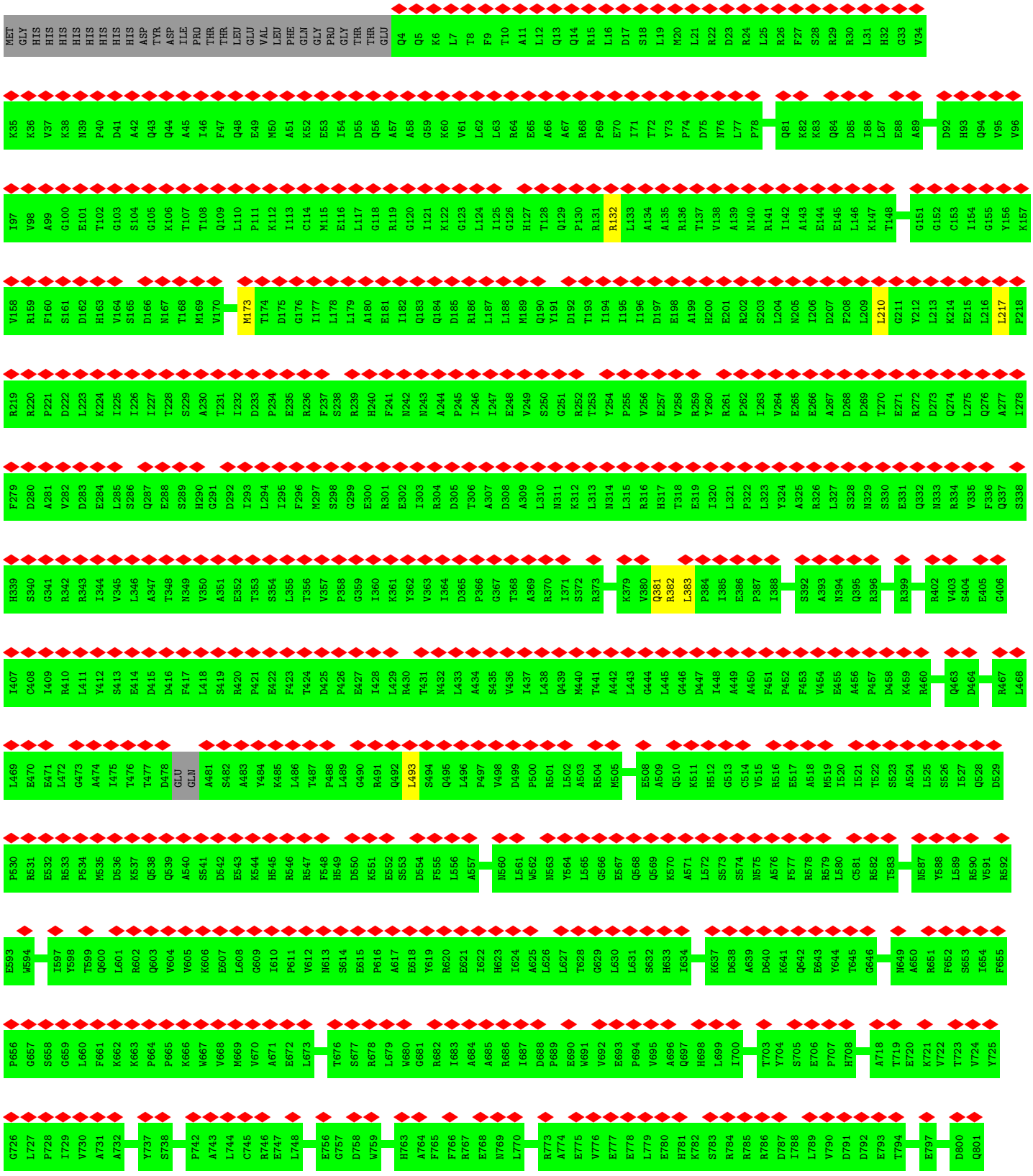


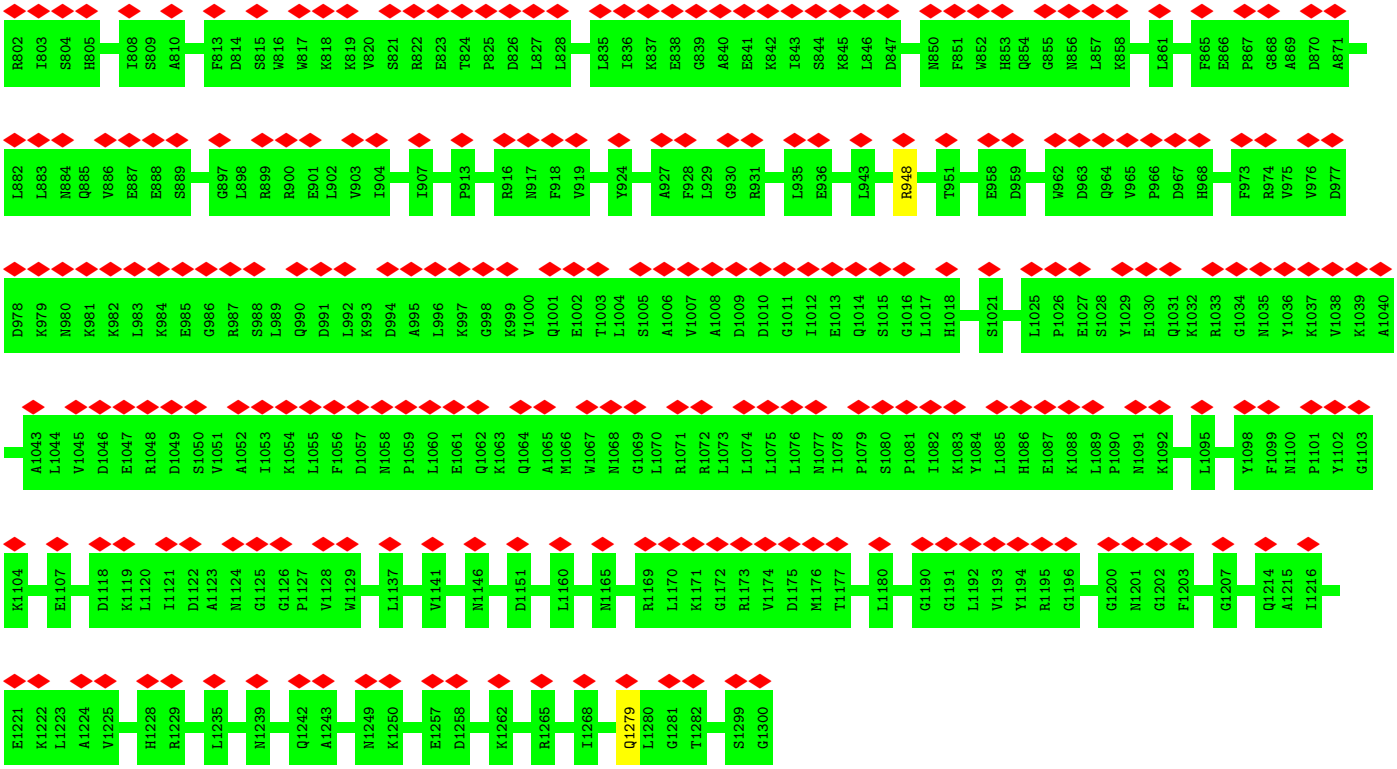
There are no outlier residues recorded for this chain.

• Molecule 57: ATP-dependent RNA helicase HrpA

Chain B:

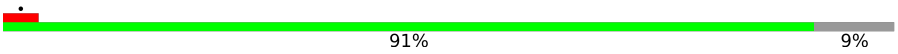
70%
97%

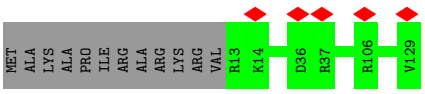

MET GLY HIS HIS HIS HIS HIS HIS HIS ASP TYR ASP ILE PRO THR THR LEU GLU VAL LEU PHE GLN GLY PRO GLY THR THR GLU Q4 Q5 K6 L7 T8 F9 T10 A11 L12 Q13 Q14 R15 L16 D17 S18 L19 M20 L21 R22 D23 R24 L25 R26 F27 S28 R29 R30 L31 H32 G33 V34
K35 K36 V37 K38 N39 P40 D41 A42 Q43 Q44 A45 I46 F47 Q48 E49 M50 A51 K52 E53 I54 D55 Q56 A57 A58 G59 K60 V61 L62 L63 R64 E65 A66 A67 R68 P69 E70 I71 T72 Y73 P74 D75 N76 L77 P78 Q81 K82 K83 Q84 D85 I86 L87 E88 A89 D92 H93 Q94 V95 V96
I97 V98 A99 G100 E101 T102 G103 S104 G105 K106 T107 T108 Q109 L110 P111 K112 I113 C114 M115 E116 L117 G118 R119 G120 I121 K122 G123 L124 I125 G126 H127 T128 Q129 P130 R131 R132 L133 A134 A135 R136 T137 V138 A139 N140 R141 I142 A143 E144 E145 L146 K147 T148 G151 G152 C153 I154 G155 Y156 K157
V158 R159 F160 S161 D162 H163 V164 S165 D166 N167 T168 M169 V170 M173 T174 D175 G176 I177 L178 L179 A180 E181 I182 Q183 Q184 D185 R186 L187 L188 M189 Q190 Y191 D192 T193 I194 I195 I196 D197 E198 A199 H200 E201 R202 S203 L204 N205 I206 D207 F208 L209 L210 G211 Y212 L213 K214 E215 L216 L217 P218
R219 R220 P221 D222 L223 K224 I225 I226 I227 T228 S229 A230 T231 I232 D233 P234 E235 R236 F237 S238 R239 H240 F241 N242 N243 A244 P245 I246 I247 E248 V249 S250 G251 R252 T253 Y254 P255 V256 E257 V258 R259 Y260 R261 P262 I263 V264 E265 E266 A267 D268 D269 T270 E271 R272 D273 Q274 L275 Q276 A277 I278
F279 D280 A281 V282 D283 E284 L285 S286 Q287 E288 S289 H290 G291 D292 I293 L294 I295 F296 M297 S298 G299 E300 R301 E302 I303 R304 D305 T306 A307 D308 A309 L310 N311 K312 L313 N314 L315 R316 H317 T318 E319 I320 L321 P322 L323 Y324 A325 R326 L327 S328 N329 S330 E331 Q332 N333 R334 V335 F336 Q337 S338
H339 S340 G341 R342 R343 I344 V345 L346 A347 T348 N349 V350 A351 E352 T353 S354 L355 T356 V357 P358 G359 I360 K361 Y362 V363 I364 D365 P366 G367 T368 A369 R370 I371 S372 R373 K379 V380 Q381 R382 L383 P384 I385 E386 P387 I388 S392 A393 N394 Q395 R396 R399 R402 V403 S404 E405 G406
I407 C408 I409 R410 L411 Y412 S413 E414 D415 D416 F417 L418 S419 R420 P421 E422 F423 T424 D425 P426 E427 I428 L429 R430 T431 N432 L433 A434 S435 V436 I437 L438 Q439 M440 T441 A442 L443 G444 L445 G446 D447 I448 A449 A450 F451 P452 F453 V454 E455 A456 P457 D458 K459 R460 Q463 D464 R467 L468
L469 E470 E471 L472 G473 A474 I475 T476 T477 D478 GLU GLN A481 S482 A483 Y484 K485 L486 T487 P488 L489 G490 R491 Q492 L493 S494 Q495 L496 P497 V498 D499 P500 R501 L502 A503 R504 M505 E508 A509 Q510 K511 H512 G513 C514 V515 R516 E517 A518 M519 I520 I521 T522 S523 A524 L525 S526 I527 Q528 D529
P530 R531 E532 R533 P534 M535 D536 K537 Q538 Q539 A540 S541 D542 E543 K544 H545 R546 R547 F548 H549 D550 K551 E552 S553 D554 F555 L556 A557 N560 L561 W562 N563 Y564 L565 G566 E567 Q568 Q569 K570 A571 L572 S573 S574 N575 A576 F577 R578 R579 L580 C581 R582 T583 N587 Y588 L589 R590 V591 R592
E593 W594 I597 Y598 T599 Q600 L601 R602 Q603 V604 V605 K606 E607 L608 G609 I610 P611 V612 N613 S614 E615 P616 A617 E618 Y619 R620 E621 I622 H623 I624 A625 L626 L627 T628 G629 L630 L631 S632 H633 I634 K637 D638 A639 D640 K641 Q642 E643 Y644 T645 G646 N649 A650 R651 F652 S653 I654 F655
P656 G657 S658 G659 L660 F661 K662 K663 P664 P665 K666 W667 V668 M669 V670 A671 E672 L673 T676 S677 R678 L679 W680 G681 R682 I683 A684 A685 R686 I687 D688 P689 E690 W691 V692 E693 P694 V695 A696 Q697 H698 L699 I700 T703 Y704 S705 E706 P707 H708 A718 T719 E720 K721 V722 T723 V724 Y725
G726 L727 P728 I729 V730 A731 A732 Y737 S738 P742 A743 L744 C745 R746 E747 L748 E756 G757 D758 W759 H763 A764 F765 F766 R767 E768 N769 L770 R773 A774 E775 V776 E777 E778 L779 E780 H781 K782 S783 R784 R785 R786 D787 I788 L789 V790 D791 D792 E793 T794 E797 D800 Q801



• Molecule 58: Small ribosomal subunit protein uS11

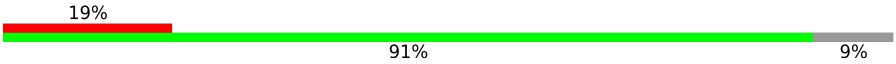
Chain D:

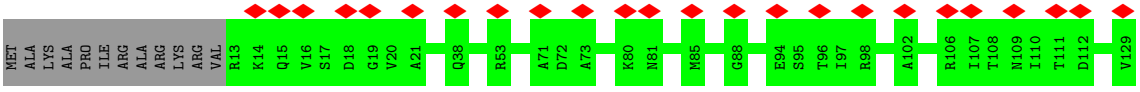




• Molecule 58: Small ribosomal subunit protein uS11

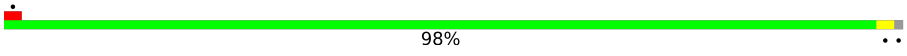
Chain y:

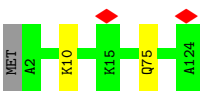




• Molecule 59: Small ribosomal subunit protein uS12

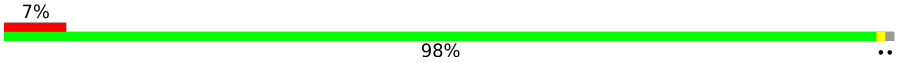
Chain E:

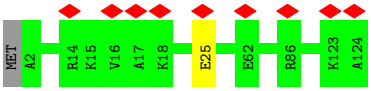




• Molecule 59: Small ribosomal subunit protein uS12

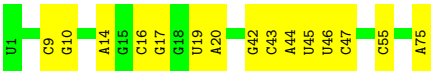
Chain z:





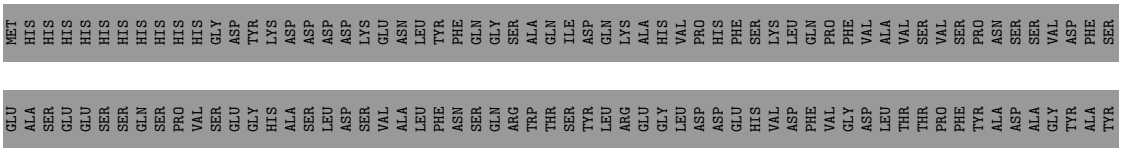
• Molecule 60: P-site tRNA

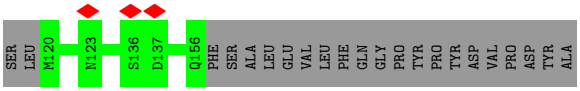
Chain M:



• Molecule 61: VemP nascent chain

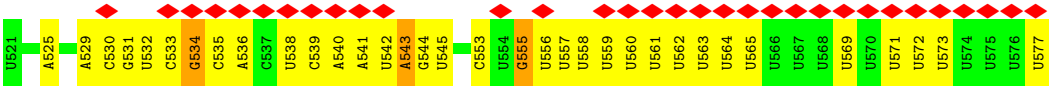
Chain s:





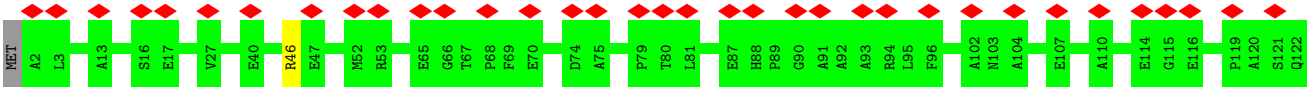
• Molecule 62: messenger RNA

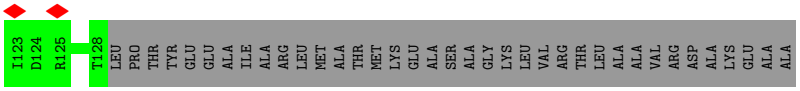
Chain w:



• Molecule 63: Large ribosomal subunit protein uL10

Chain x:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	17805	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 ($e^-/Å^2$)	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	2.044	Depositor
Minimum map value	-0.926	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.118	Depositor
Recommended contour level	0.32	Depositor
Map size (Å)	508.9, 508.9, 508.9	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.454, 1.454, 1.454	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	0.42	0/36834	0.96	56/57462 (0.1%)
1	AA	0.37	0/36966	0.95	50/57666 (0.1%)
2	1	0.36	0/1735	0.73	3/2338 (0.1%)
2	AB	0.32	0/1735	0.68	0/2338
3	2	0.33	0/1651	0.68	0/2225
3	AC	0.31	0/1651	0.69	0/2225
4	3	0.31	0/1665	0.64	0/2227
4	AD	0.31	0/1665	0.71	2/2227 (0.1%)
5	4	0.34	0/1118	0.72	0/1504
5	AE	0.34	0/1118	0.74	1/1504 (0.1%)
6	5	0.35	0/835	0.76	0/1128
6	AF	0.33	0/835	0.75	1/1128 (0.1%)
7	6	0.33	0/1195	0.71	2/1602 (0.1%)
7	AG	0.35	0/1195	0.80	3/1602 (0.2%)
8	7	0.32	0/989	0.69	1/1326 (0.1%)
8	AH	0.32	0/989	0.71	2/1326 (0.2%)
9	8	0.33	0/1034	0.80	3/1375 (0.2%)
9	AI	0.31	0/1034	0.79	1/1375 (0.1%)
10	9	0.30	0/796	0.79	1/1077 (0.1%)
10	AJ	0.34	0/796	0.79	0/1077
11	A	0.38	0/1812	1.02	9/2823 (0.3%)
12	A1	0.30	0/557	0.66	0/738
12	v	0.31	0/597	0.69	0/792
13	A2	0.29	0/2387	0.61	0/3221
14	A3	0.35	0/1830	1.10	8/2849 (0.3%)
15	AK	0.27	0/1033	0.59	0/1387
15	C	0.26	0/1033	0.58	0/1387
16	AL	0.29	0/892	0.78	1/1193 (0.1%)
16	F	0.33	0/892	0.79	1/1193 (0.1%)
17	AM	0.31	0/785	0.72	0/1043
17	G	0.29	0/803	0.65	0/1070
18	AN	0.35	0/718	0.87	3/959 (0.3%)
18	H	0.48	0/710	0.89	1/950 (0.1%)
19	AO	0.33	0/659	0.73	1/884 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
19	I	0.30	0/658	0.72	0/884
20	AP	0.38	0/657	0.82	0/881
20	J	0.32	0/657	0.69	0/881
21	AQ	0.32	0/553	0.71	0/742
21	K	0.34	0/544	0.68	1/731 (0.1%)
22	AR	0.31	0/652	0.70	1/877 (0.1%)
22	t	0.31	0/635	0.67	1/855 (0.1%)
23	AS	0.33	0/671	0.66	0/888
23	u	0.35	0/671	0.73	0/888
24	AT	0.27	0/519	0.65	1/691 (0.1%)
24	L	0.33	0/507	0.70	0/674
25	AU	0.33	0/1816	1.06	10/2830 (0.4%)
26	AV	0.31	0/69659	0.93	90/108672 (0.1%)
26	N	0.43	0/69659	0.96	115/108672 (0.1%)
27	AW	0.29	0/2828	0.99	9/4410 (0.2%)
27	O	0.36	0/2828	0.95	8/4410 (0.2%)
28	AX	0.29	0/2121	0.65	0/2852
28	P	0.33	0/2121	0.69	0/2852
29	AY	0.30	0/1586	0.63	1/2134 (0.0%)
29	Q	0.32	0/1586	0.65	1/2134 (0.0%)
30	AZ	0.28	0/1571	0.57	0/2113
30	R	0.30	0/1571	0.64	0/2113
31	Aa	0.28	0/1434	0.69	2/1926 (0.1%)
31	S	0.32	0/1434	0.68	1/1926 (0.1%)
32	Ab	0.27	0/1343	0.60	0/1816
32	T	0.31	0/1333	0.67	1/1805 (0.1%)
33	Ac	0.29	0/1122	0.67	2/1515 (0.1%)
33	U	0.33	0/1122	0.65	0/1515
34	Ad	0.28	0/1046	0.62	1/1410 (0.1%)
34	V	0.32	0/993	0.63	1/1341 (0.1%)
35	Ae	0.27	0/1152	0.60	0/1551
35	W	0.31	0/1152	0.62	0/1551
36	Af	0.29	0/947	0.70	0/1268
36	X	0.34	0/947	0.76	1/1268 (0.1%)
37	Ag	0.27	0/1054	0.66	0/1403
37	Y	0.34	0/1054	0.73	1/1403 (0.1%)
38	Ah	0.31	0/1093	0.67	0/1460
38	Z	0.34	0/1093	0.75	1/1460 (0.1%)
39	Ai	0.28	0/958	0.74	1/1281 (0.1%)
39	a	0.33	0/964	0.77	1/1289 (0.1%)
40	Aj	0.26	0/902	0.61	0/1209
40	b	0.34	0/902	0.73	0/1209
41	Ak	0.29	0/929	0.69	0/1242

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
41	c	0.37	0/929	0.72	1/1242 (0.1%)
42	Al	0.29	0/960	0.62	0/1278
42	d	0.32	0/960	0.67	1/1278 (0.1%)
43	Am	0.30	0/829	0.71	0/1107
43	e	0.35	0/829	0.74	3/1107 (0.3%)
44	An	0.28	0/864	0.66	0/1156
44	f	0.31	0/864	0.78	1/1156 (0.1%)
45	Ao	0.28	0/744	0.65	0/994
45	g	0.33	0/744	0.73	1/994 (0.1%)
46	Ap	0.27	0/787	0.59	0/1051
46	h	0.31	0/787	0.63	0/1051
47	Aq	0.31	0/766	0.64	0/1025
47	i	0.30	0/766	0.62	0/1025
48	Ar	0.28	0/576	0.60	0/762
48	j	0.31	0/582	0.70	0/769
49	As	0.26	0/635	0.69	1/848 (0.1%)
49	k	0.34	0/635	0.79	1/848 (0.1%)
50	At	0.26	0/510	0.66	0/677
50	l	0.38	0/510	0.77	0/677
51	Au	0.29	0/439	0.74	0/587
51	m	0.30	0/453	0.75	0/605
52	Av	0.25	0/450	0.66	0/599
52	n	0.28	0/435	0.68	0/581
53	Aw	0.26	0/416	0.58	0/554
53	o	0.34	0/416	0.76	2/554 (0.4%)
54	Ax	0.27	0/380	0.72	0/498
54	p	0.28	0/380	0.77	0/498
55	Ay	0.26	0/513	0.61	0/676
55	q	0.34	0/513	0.76	1/676 (0.1%)
56	Az	0.27	0/303	0.68	0/397
56	r	0.36	0/303	0.73	0/397
57	B	0.29	0/10668	0.63	4/14419 (0.0%)
58	D	0.31	0/893	0.63	0/1205
58	y	0.31	0/893	0.72	0/1205
59	E	0.35	0/969	0.71	0/1300
59	z	0.31	0/969	0.74	0/1300
60	M	0.38	0/1778	0.94	0/2768
61	s	0.30	0/326	0.51	0/441
62	w	0.37	0/1302	1.09	12/2018 (0.6%)
63	x	0.30	0/970	0.65	0/1307
All	All	0.36	0/335634	0.88	429/499883 (0.1%)

There are no bond length outliers.

All (429) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	AV	613	A	O4'-C1'-N9	10.25	116.40	108.20
27	AW	89	U	N1-C2-O2	10.14	129.90	122.80
27	AW	89	U	C2-N1-C1'	9.97	129.67	117.70
26	N	1313	U	C2-N1-C1'	9.68	129.32	117.70
27	AW	89	U	N3-C2-O2	-9.62	115.47	122.20
26	AV	545	U	C2-N1-C1'	9.42	129.00	117.70
26	AV	2506	U	C2-N1-C1'	9.38	128.96	117.70
26	N	1774	C	N3-C2-O2	-8.93	115.65	121.90
1	0	1125	U	C2-N1-C1'	8.90	128.38	117.70
10	9	42	LEU	CA-CB-CG	8.89	135.75	115.30
26	AV	1774	C	N3-C2-O2	-8.66	115.84	121.90
1	AA	386	C	N3-C2-O2	-8.64	115.85	121.90
38	Z	70	ASP	CB-CG-OD1	8.61	126.05	118.30
26	AV	2903	U	C2-N1-C1'	8.59	128.01	117.70
26	N	1313	U	N1-C2-O2	8.58	128.81	122.80
26	AV	2903	U	N1-C2-O2	8.54	128.78	122.80
1	0	1322	C	N1-C2-O2	8.52	124.01	118.90
26	AV	545	U	N1-C2-O2	8.52	128.76	122.80
26	AV	2506	U	N1-C2-O2	8.51	128.75	122.80
26	N	1313	U	N3-C2-O2	-8.46	116.27	122.20
26	N	2656	U	C2-N1-C1'	8.46	127.85	117.70
26	AV	2903	U	N3-C2-O2	-8.34	116.36	122.20
26	AV	1313	U	C2-N1-C1'	8.33	127.70	117.70
22	AR	64	ASP	CB-CG-OD1	8.29	125.76	118.30
57	B	383	LEU	CA-CB-CG	8.02	133.75	115.30
26	N	510	C	N1-C2-O2	8.02	123.71	118.90
26	N	2656	U	C5-C6-N1	7.97	126.69	122.70
27	O	89	U	C2-N1-C1'	7.97	127.26	117.70
1	AA	979	C	N1-C2-O2	7.94	123.67	118.90
32	T	47	ASP	CB-CG-OD1	7.92	125.43	118.30
26	AV	545	U	N3-C2-O2	-7.87	116.69	122.20
26	N	1774	C	N1-C2-O2	7.87	123.62	118.90
1	0	754	C	N3-C2-O2	-7.85	116.40	121.90
26	AV	1774	C	N1-C2-O2	7.73	123.54	118.90
29	Q	103	ASP	CB-CG-OD1	7.66	125.19	118.30
26	N	510	C	C2-N1-C1'	7.66	127.22	118.80
26	AV	2506	U	N3-C2-O2	-7.61	116.87	122.20
1	0	1322	C	C2-N1-C1'	7.60	127.16	118.80
26	N	1774	C	C6-N1-C2	-7.58	117.27	120.30
14	A3	30	U	C2-N1-C1'	7.51	126.71	117.70
11	A	75	C	C2-N1-C1'	7.50	127.04	118.80
25	AU	72	C	C2-N1-C1'	7.40	126.94	118.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	AG	99	LEU	CA-CB-CG	7.38	132.27	115.30
26	AV	1071	G	C4-N9-C1'	7.37	136.08	126.50
27	O	89	U	N1-C2-O2	7.31	127.92	122.80
1	AA	1125	U	C2-N1-C1'	7.30	126.46	117.70
26	N	837	C	N1-C2-O2	7.29	123.27	118.90
4	AD	191	LEU	CA-CB-CG	7.28	132.05	115.30
26	N	2178	C	N3-C2-O2	-7.27	116.81	121.90
31	S	152	LEU	CA-CB-CG	7.21	131.90	115.30
26	AV	729	G	O4'-C1'-N9	7.21	113.97	108.20
26	AV	1068	G	N3-C4-C5	-7.18	125.01	128.60
26	N	2656	U	N1-C2-O2	7.18	127.82	122.80
1	0	620	C	N1-C2-O2	7.17	123.20	118.90
42	d	97	ASP	CB-CG-OD1	7.17	124.75	118.30
16	AL	11	ASP	CB-CG-OD1	7.14	124.72	118.30
41	c	114	LEU	CA-CB-CG	7.07	131.56	115.30
18	AN	59	MET	CB-CG-SD	7.03	133.49	112.40
1	AA	979	C	N3-C2-O2	-7.01	116.99	121.90
26	N	1138	G	N9-C4-C5	6.98	108.19	105.40
62	w	534	G	C4-N9-C1'	6.97	135.56	126.50
1	0	1322	C	N3-C2-O2	-6.96	117.03	121.90
14	A3	30	U	N1-C2-O2	6.91	127.63	122.80
26	AV	1068	G	N3-C4-N9	6.85	130.11	126.00
1	0	431	A	N1-C6-N6	-6.84	114.50	118.60
44	f	68	ASP	CB-CG-OD1	6.84	124.45	118.30
26	AV	1961	C	N3-C2-O2	-6.82	117.12	121.90
33	Ac	12	LEU	CA-CB-CG	6.82	130.98	115.30
1	0	110	C	N1-C2-O2	6.80	122.98	118.90
39	a	79	LEU	CA-CB-CG	6.77	130.87	115.30
14	A3	30	U	N3-C2-O2	-6.76	117.47	122.20
26	AV	1068	G	C4-N9-C1'	6.76	135.29	126.50
1	AA	1301	U	C2-N1-C1'	6.74	125.78	117.70
26	N	1348	C	N1-C2-O2	6.73	122.94	118.90
1	0	1320	C	N1-C2-O2	6.71	122.92	118.90
26	N	1716	U	C2-N1-C1'	6.69	125.73	117.70
1	AA	1132	C	C2-N1-C1'	6.69	126.15	118.80
49	As	71	LEU	CA-CB-CG	6.68	130.66	115.30
1	0	110	C	N3-C2-O2	-6.67	117.23	121.90
25	AU	20	G	N3-C4-C5	-6.65	125.27	128.60
1	AA	386	C	C6-N1-C2	-6.65	117.64	120.30
26	N	2043	C	C2-N1-C1'	6.63	126.10	118.80
1	AA	1395	C	C2-N1-C1'	6.62	126.08	118.80
26	AV	234	U	N3-C2-O2	-6.62	117.57	122.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	N	1993	U	N1-C2-O2	6.59	127.41	122.80
27	O	89	U	N3-C2-O2	-6.58	117.59	122.20
62	w	555	G	C4-N9-C1'	6.58	135.06	126.50
27	AW	26	C	N1-C2-O2	6.58	122.85	118.90
26	N	1956	U	N3-C2-O2	-6.58	117.59	122.20
26	N	1993	U	N3-C2-O2	-6.56	117.61	122.20
57	B	493	LEU	CA-CB-CG	6.54	130.33	115.30
1	0	1320	C	C2-N1-C1'	6.52	125.97	118.80
1	0	598	U	N3-C2-O2	-6.51	117.64	122.20
31	Aa	152	LEU	CA-CB-CG	6.48	130.21	115.30
1	AA	1322	C	C2-N1-C1'	6.48	125.92	118.80
57	B	217	LEU	CA-CB-CG	6.48	130.19	115.30
26	N	2177	C	N3-C2-O2	-6.46	117.38	121.90
1	AA	979	C	C2-N1-C1'	6.44	125.88	118.80
26	N	2072	C	C6-N1-C2	-6.43	117.73	120.30
26	AV	1071	G	C8-N9-C1'	-6.42	118.66	127.00
62	w	534	G	N3-C4-N9	6.42	129.85	126.00
62	w	543	A	P-O3'-C3'	6.41	127.39	119.70
62	w	555	G	P-O3'-C3'	6.41	127.39	119.70
26	N	404	A	P-O3'-C3'	6.41	127.39	119.70
11	A	75	C	N1-C2-O2	6.41	122.74	118.90
26	AV	544	C	N1-C2-O2	6.41	122.74	118.90
26	AV	1313	U	N1-C2-O2	6.40	127.28	122.80
62	w	555	G	N3-C4-C5	-6.39	125.40	128.60
26	AV	2043	C	C2-N1-C1'	6.38	125.82	118.80
26	N	974	G	C4-N9-C1'	6.38	134.79	126.50
26	N	669	G	C4-N9-C1'	6.37	134.78	126.50
1	AA	1470	U	N3-C2-O2	-6.36	117.75	122.20
1	0	1201	A	P-O3'-C3'	6.36	127.33	119.70
25	AU	20	G	C4-N9-C1'	6.35	134.76	126.50
22	t	47	LEU	CA-CB-CG	6.34	129.89	115.30
26	N	1716	U	C5-C6-N1	6.34	125.87	122.70
11	A	53	G	C4-N9-C1'	6.33	134.73	126.50
26	AV	1072	C	N1-C2-O2	6.33	122.70	118.90
27	AW	89	U	C6-N1-C1'	-6.33	112.34	121.20
1	AA	1322	C	N1-C2-O2	6.30	122.68	118.90
26	N	84	A	P-O3'-C3'	6.29	127.25	119.70
26	AV	1961	C	N1-C2-O2	6.29	122.67	118.90
27	O	30	C	N1-C2-O2	6.28	122.67	118.90
1	AA	1125	U	N1-C2-O2	6.27	127.19	122.80
26	N	2072	C	C2-N1-C1'	6.27	125.69	118.80
1	0	330	C	N1-C2-O2	6.26	122.66	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1201	A	P-O3'-C3'	6.25	127.20	119.70
26	N	1993	U	C2-N1-C1'	6.25	125.19	117.70
26	N	1313	U	C6-N1-C1'	-6.24	112.46	121.20
62	w	534	G	N3-C4-C5	-6.21	125.50	128.60
26	AV	2225	A	P-O3'-C3'	6.19	127.13	119.70
26	AV	2776	A	P-O3'-C3'	6.19	127.12	119.70
14	A3	51	C	P-O3'-C3'	6.18	127.12	119.70
26	AV	421	C	P-O3'-C3'	6.18	127.11	119.70
26	N	421	C	P-O3'-C3'	6.18	127.11	119.70
26	AV	2506	U	C6-N1-C1'	-6.17	112.56	121.20
26	AV	545	U	C5-C6-N1	6.14	125.77	122.70
25	AU	20	G	N3-C4-N9	6.14	129.68	126.00
31	Aa	152	LEU	CB-CG-CD1	-6.14	100.57	111.00
26	N	2666	C	N1-C2-O2	6.13	122.58	118.90
62	w	555	G	N3-C4-N9	6.13	129.68	126.00
26	AV	242	G	P-O3'-C3'	6.12	127.04	119.70
26	AV	1061	U	C2-N1-C1'	6.11	125.03	117.70
26	N	1109	C	P-O3'-C3'	6.09	127.01	119.70
26	N	837	C	N3-C2-O2	-6.09	117.64	121.90
2	1	52	GLU	CA-CB-CG	6.08	126.78	113.40
1	AA	307	C	N1-C2-O2	6.07	122.54	118.90
26	AV	1348	C	N1-C2-O2	6.07	122.54	118.90
62	w	534	G	C8-N9-C1'	-6.06	119.12	127.00
26	AV	1314	C	C2-N1-C1'	6.06	125.46	118.80
1	0	754	C	N1-C2-O2	6.04	122.53	118.90
1	AA	479	U	N1-C2-O2	6.04	127.03	122.80
26	N	2794	C	C2-N1-C1'	6.04	125.44	118.80
1	0	658	C	N1-C2-O2	6.03	122.52	118.90
1	0	751	U	C2-N1-C1'	6.02	124.92	117.70
1	0	492	C	N3-C2-O2	-6.02	117.69	121.90
11	A	53	G	C8-N9-C1'	-6.00	119.20	127.00
26	AV	545	U	C6-N1-C1'	-5.99	112.82	121.20
26	N	1716	U	N1-C2-O2	5.98	126.99	122.80
57	B	210	LEU	CA-CB-CG	5.96	129.00	115.30
26	AV	1071	G	N3-C4-N9	5.95	129.57	126.00
26	AV	670	A	P-O3'-C3'	5.93	126.82	119.70
7	AG	48	GLU	CA-CB-CG	5.93	126.45	113.40
26	N	1752	C	C6-N1-C2	-5.92	117.93	120.30
1	0	812	G	P-O3'-C3'	5.92	126.81	119.70
26	N	2225	A	P-O3'-C3'	5.92	126.80	119.70
1	0	598	U	N1-C2-O2	5.91	126.94	122.80
26	N	96	C	C2-N1-C1'	5.91	125.30	118.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	N	510	C	C6-N1-C2	-5.91	117.94	120.30
7	6	140	ASP	CB-CG-OD1	5.90	123.61	118.30
26	N	2776	A	P-O3'-C3'	5.90	126.78	119.70
27	O	17	C	C2-N1-C1'	5.90	125.29	118.80
1	AA	844	G	C4-N9-C1'	5.89	134.16	126.50
1	AA	1466	C	N3-C2-O2	-5.89	117.78	121.90
1	AA	1086	U	N1-C2-O2	5.88	126.92	122.80
1	AA	115	G	P-O3'-C3'	5.88	126.75	119.70
1	0	658	C	N3-C2-O2	-5.88	117.78	121.90
5	AE	11	LEU	CA-CB-CG	5.87	128.80	115.30
53	o	50	LYS	CA-CB-CG	5.86	126.29	113.40
14	A3	63	C	O4'-C1'-N1	5.86	112.89	108.20
62	w	553	C	C2-N1-C1'	5.86	125.24	118.80
26	AV	404	A	P-O3'-C3'	5.85	126.72	119.70
1	0	115	G	P-O3'-C3'	5.85	126.72	119.70
4	AD	5	LEU	CA-CB-CG	5.85	128.75	115.30
26	N	748	G	O4'-C1'-N9	5.84	112.87	108.20
26	N	1774	C	C2-N1-C1'	5.84	125.22	118.80
26	N	1931	U	C2-N1-C1'	5.83	124.70	117.70
26	N	1931	U	N1-C2-O2	5.83	126.88	122.80
26	N	670	A	P-O3'-C3'	5.83	126.69	119.70
14	A3	63	C	C2-N1-C1'	-5.83	112.39	118.80
1	AA	582	C	N1-C2-O2	5.83	122.39	118.90
26	AV	1	G	C4-N9-C1'	5.82	134.07	126.50
1	0	1125	U	N3-C2-O2	-5.79	118.14	122.20
1	0	1125	U	C6-N1-C1'	-5.79	113.10	121.20
26	AV	1313	U	N3-C2-O2	-5.78	118.15	122.20
1	AA	890	G	P-O3'-C3'	5.77	126.63	119.70
1	AA	1301	U	N1-C2-O2	5.75	126.83	122.80
1	AA	979	C	C6-N1-C2	-5.74	118.01	120.30
1	0	1132	C	N1-C2-O2	5.73	122.34	118.90
26	AV	2244	U	N3-C4-O4	5.73	123.41	119.40
26	N	1582	C	N3-C2-O2	-5.73	117.89	121.90
18	AN	57	LEU	CA-CB-CG	5.73	128.47	115.30
11	A	75	C	N3-C2-O2	-5.72	117.89	121.90
26	N	2354	C	C2-N1-C1'	5.72	125.09	118.80
26	N	2683	C	N1-C2-O2	5.72	122.33	118.90
26	N	2177	C	N1-C2-O2	5.69	122.32	118.90
26	N	2098	U	C2-N1-C1'	5.69	124.53	117.70
26	AV	1064	C	N3-C4-N4	-5.69	114.02	118.00
26	AV	61	C	N1-C2-O2	5.68	122.31	118.90
33	Ac	101	ASP	CB-CG-OD1	5.68	123.41	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	N	510	C	N3-C2-O2	-5.68	117.92	121.90
26	N	82	U	N1-C2-O2	5.67	126.77	122.80
26	N	2656	U	N3-C2-O2	-5.67	118.23	122.20
26	N	323	C	C2-N1-C1'	5.66	125.03	118.80
1	AA	1348	U	N1-C2-O2	5.66	126.76	122.80
26	AV	2739	U	N3-C2-O2	-5.66	118.24	122.20
26	AV	1071	G	N3-C4-C5	-5.65	125.77	128.60
26	AV	2153	C	N3-C2-O2	-5.64	117.95	121.90
1	0	1125	U	N3-C4-O4	5.64	123.35	119.40
26	N	243	U	C2-N1-C1'	5.63	124.46	117.70
26	N	1138	G	C8-N9-C4	-5.62	104.15	106.40
27	AW	89	U	C5-C6-N1	5.62	125.51	122.70
1	0	1158	C	C2-N1-C1'	5.61	124.98	118.80
26	N	974	G	C8-N9-C1'	-5.61	119.70	127.00
1	0	479	U	N1-C2-O2	5.61	126.72	122.80
45	g	32	LEU	CA-CB-CG	5.61	128.20	115.30
1	0	1262	C	N1-C2-O2	5.60	122.26	118.90
26	AV	2506	U	C5-C6-N1	5.60	125.50	122.70
26	N	1314	C	C2-N1-C1'	5.60	124.96	118.80
26	N	1138	G	N1-C6-O6	-5.59	116.54	119.90
26	AV	2286	G	P-O3'-C3'	5.59	126.41	119.70
1	AA	1125	U	N3-C2-O2	-5.58	118.29	122.20
18	H	77	ARG	NE-CZ-NH2	5.58	123.09	120.30
26	N	669	G	C8-N9-C1'	-5.57	119.76	127.00
1	AA	1279	G	C4-N9-C1'	5.57	133.74	126.50
26	AV	1585	C	N1-C2-O2	5.57	122.24	118.90
26	N	1348	C	C2-N1-C1'	5.57	124.92	118.80
1	0	1125	U	N1-C2-O2	5.56	126.69	122.80
1	0	613	C	O5'-P-OP1	-5.55	100.70	105.70
1	0	438	U	C2-N1-C1'	5.54	124.35	117.70
55	q	44	LEU	CA-CB-CG	5.54	128.03	115.30
9	8	56	ASP	CB-CG-OD1	5.53	123.28	118.30
26	N	1644	C	N3-C2-O2	-5.53	118.03	121.90
1	AA	1086	U	N3-C2-O2	-5.53	118.33	122.20
1	0	110	C	C6-N1-C2	-5.52	118.09	120.30
1	AA	1520	C	C2-N1-C1'	5.52	124.87	118.80
26	N	2098	U	N1-C2-O2	5.52	126.67	122.80
43	e	50	GLY	N-CA-C	-5.52	99.30	113.10
1	0	54	C	N3-C2-O2	-5.52	118.04	121.90
26	N	765	C	C2-N1-C1'	5.52	124.87	118.80
26	N	2161	C	N1-C2-O2	5.51	122.21	118.90
26	N	2072	C	C5-C6-N1	5.51	123.75	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A3	63	C	C6-N1-C1'	5.50	127.40	120.80
1	AA	1347	G	P-O3'-C3'	5.49	126.29	119.70
26	N	1956	U	N1-C2-O2	5.49	126.64	122.80
2	1	52	GLU	N-CA-CB	5.48	120.47	110.60
25	AU	72	C	N1-C2-O2	5.48	122.19	118.90
26	N	2474	U	N1-C2-O2	5.48	126.64	122.80
26	AV	1068	G	C8-N9-C1'	-5.48	119.88	127.00
26	AV	2762	C	C2-N1-C1'	5.48	124.83	118.80
26	AV	607	U	N3-C2-O2	-5.47	118.37	122.20
26	AV	550	C	N1-C2-O2	5.47	122.18	118.90
26	AV	456	C	C2-N1-C1'	5.46	124.81	118.80
26	N	867	C	N1-C2-O2	5.46	122.18	118.90
26	AV	784	G	P-O3'-C3'	5.46	126.25	119.70
1	0	217	C	C5-C6-N1	5.46	123.73	121.00
26	AV	544	C	C2-N1-C1'	5.45	124.80	118.80
1	AA	1182	G	P-O3'-C3'	5.45	126.24	119.70
34	V	106	LEU	CA-CB-CG	5.45	127.84	115.30
11	A	53	G	N3-C4-N9	5.45	129.27	126.00
26	N	1644	C	N1-C2-O2	5.45	122.17	118.90
26	AV	859	G	P-O3'-C3'	5.45	126.24	119.70
1	0	1190	G	P-O3'-C3'	5.44	126.23	119.70
26	AV	2244	U	C5-C4-O4	-5.44	122.64	125.90
1	0	1323	G	N3-C4-N9	5.44	129.26	126.00
1	0	1520	C	C2-N1-C1'	5.43	124.78	118.80
26	AV	915	C	N1-C2-O2	5.43	122.16	118.90
26	N	1060	U	N3-C4-O4	5.42	123.20	119.40
26	N	2474	U	C2-N1-C1'	5.42	124.21	117.70
53	o	5	ILE	CG1-CB-CG2	-5.42	99.47	111.40
7	AG	48	GLU	N-CA-CB	5.42	120.36	110.60
26	N	1314	C	C6-N1-C2	-5.41	118.14	120.30
1	AA	844	G	C8-N9-C1'	-5.41	119.97	127.00
25	AU	16	C	N1-C2-O2	5.41	122.14	118.90
26	N	510	C	C5-C6-N1	5.40	123.70	121.00
26	N	1752	C	C5-C6-N1	5.37	123.69	121.00
9	8	94	LEU	CB-CG-CD1	5.37	120.13	111.00
26	N	1348	C	N3-C2-O2	-5.37	118.14	121.90
62	w	555	G	C8-N9-C1'	-5.37	120.02	127.00
1	0	1300	G	P-O3'-C3'	5.36	126.14	119.70
25	AU	72	C	C6-N1-C1'	-5.36	114.36	120.80
26	AV	2318	G	C8-N9-C4	-5.36	104.25	106.40
1	AA	458	U	C2-N1-C1'	5.36	124.13	117.70
26	AV	2716	C	C2-N1-C1'	5.36	124.70	118.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	AV	234	U	N1-C2-O2	5.36	126.55	122.80
26	N	1267	U	N3-C2-O2	-5.36	118.45	122.20
26	AV	2903	U	C6-N1-C1'	-5.36	113.70	121.20
26	N	776	G	C4-N9-C1'	5.36	133.47	126.50
39	Ai	38	LEU	CA-CB-CG	5.36	127.62	115.30
26	AV	1313	U	C6-N1-C1'	-5.35	113.71	121.20
27	O	118	C	N3-C2-O2	-5.35	118.15	121.90
25	AU	27	C	N1-C2-O2	5.35	122.11	118.90
43	e	51	VAL	N-CA-C	-5.35	96.56	111.00
26	AV	2739	U	C2-N1-C1'	5.34	124.10	117.70
27	O	89	U	C6-N1-C1'	-5.34	113.73	121.20
36	X	118	LEU	CB-CG-CD1	5.34	120.07	111.00
26	N	2098	U	N3-C2-O2	-5.33	118.47	122.20
26	AV	158	U	C2-N1-C1'	5.33	124.09	117.70
1	AA	479	U	C2-N1-C1'	5.32	124.09	117.70
26	AV	435	C	N1-C2-O2	5.32	122.09	118.90
1	0	1320	C	C6-N1-C1'	-5.31	114.43	120.80
18	AN	59	MET	CA-CB-CG	5.29	122.30	113.30
26	AV	717	C	N1-C2-O2	5.29	122.08	118.90
1	AA	1300	G	P-O3'-C3'	5.29	126.05	119.70
62	w	539	C	P-O3'-C3'	5.29	126.05	119.70
1	0	1108	G	C4-N9-C1'	5.29	133.38	126.50
26	AV	2153	C	C6-N1-C2	-5.29	118.18	120.30
24	AT	34	LEU	CA-CB-CG	5.29	127.45	115.30
26	N	545	U	C2-N1-C1'	5.28	124.04	117.70
8	7	32	LEU	CB-CG-CD2	5.28	119.98	111.00
26	N	1267	U	N1-C2-O2	5.28	126.49	122.80
1	0	1345	U	P-O3'-C3'	5.27	126.03	119.70
1	0	1322	C	C6-N1-C1'	-5.27	114.48	120.80
1	AA	1262	C	N1-C2-O2	5.26	122.06	118.90
19	AO	42	ILE	CG1-CB-CG2	-5.26	99.82	111.40
26	AV	1956	U	N1-C2-O2	5.26	126.48	122.80
1	0	178	C	N3-C2-O2	-5.25	118.22	121.90
26	N	965	C	C2-N1-C1'	5.25	124.58	118.80
37	Y	82	LEU	CA-CB-CG	5.24	127.36	115.30
26	N	271	G	C4-N9-C1'	-5.24	119.69	126.50
27	O	30	C	N3-C2-O2	-5.23	118.24	121.90
26	N	2043	C	C6-N1-C1'	-5.22	114.53	120.80
1	0	492	C	N1-C2-O2	5.22	122.03	118.90
11	A	75	C	C6-N1-C1'	-5.22	114.53	120.80
26	AV	640	C	C5-C6-N1	5.22	123.61	121.00
1	0	530	G	C4-N9-C1'	5.22	133.29	126.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	N	481	G	OP2-P-O3'	5.22	116.69	105.20
1	0	1469	C	N1-C2-O2	5.22	122.03	118.90
26	AV	2901	C	N1-C2-O2	5.21	122.03	118.90
1	AA	1345	U	P-O3'-C3'	5.21	125.95	119.70
27	AW	26	C	N3-C2-O2	-5.21	118.26	121.90
26	N	2329	U	C5-C6-N1	5.20	125.30	122.70
26	N	1417	C	C2-N1-C1'	5.20	124.52	118.80
1	0	1182	G	P-O3'-C3'	5.20	125.94	119.70
26	N	1313	U	C5-C6-N1	5.19	125.30	122.70
26	N	2562	U	N3-C2-O2	-5.19	118.56	122.20
26	N	2832	U	P-O3'-C3'	5.19	125.93	119.70
1	AA	1301	U	N3-C2-O2	-5.19	118.57	122.20
26	N	301	G	C4-N9-C1'	-5.19	119.75	126.50
7	6	30	LEU	CA-CB-CG	5.19	127.23	115.30
1	AA	156	C	C2-N1-C1'	5.19	124.51	118.80
26	AV	137	U	N3-C2-O2	-5.19	118.57	122.20
1	AA	518	C	P-O3'-C3'	5.19	125.92	119.70
1	AA	1158	C	C2-N1-C1'	5.19	124.50	118.80
26	AV	550	C	N3-C2-O2	-5.18	118.28	121.90
26	N	1188	U	N1-C2-O2	5.18	126.43	122.80
1	0	328	C	N1-C2-O2	5.17	122.00	118.90
26	N	669	G	N3-C4-N9	5.17	129.10	126.00
6	AF	53	LYS	CA-CB-CG	5.17	124.77	113.40
26	AV	1956	U	N3-C2-O2	-5.16	118.59	122.20
43	e	55	ASP	CB-CG-OD1	5.16	122.94	118.30
1	AA	458	U	N3-C2-O2	-5.16	118.59	122.20
1	0	1383	C	N1-C2-O2	5.16	121.99	118.90
9	8	35	LEU	CA-CB-CG	5.15	127.16	115.30
2	1	148	LEU	CA-CB-CG	5.15	127.14	115.30
1	AA	1395	C	C6-N1-C2	-5.15	118.24	120.30
25	AU	56	C	C2-N1-C1'	5.15	124.47	118.80
26	N	435	C	N1-C2-O2	5.15	121.99	118.90
1	0	530	G	N7-C8-N9	5.14	115.67	113.10
26	AV	2226	C	N1-C2-O2	5.14	121.99	118.90
26	N	1931	U	N3-C2-O2	-5.14	118.60	122.20
26	N	2884	U	C2-N1-C1'	5.14	123.87	117.70
26	N	2430	A	C2-N3-C4	5.14	113.17	110.60
26	AV	1134	A	OP2-P-O3'	5.14	116.51	105.20
1	AA	386	C	N1-C2-N3	5.14	122.80	119.20
1	AA	754	C	C2-N1-C1'	5.13	124.45	118.80
29	AY	149	ASN	CB-CA-C	5.13	120.66	110.40
26	N	550	C	C2-N1-C1'	5.13	124.44	118.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	AH	99	LEU	CA-CB-CG	5.13	127.09	115.30
1	0	322	C	C6-N1-C2	-5.13	118.25	120.30
1	AA	328	C	N1-C2-O2	5.13	121.98	118.90
26	AV	544	C	N3-C2-O2	-5.13	118.31	121.90
26	N	2656	U	C6-N1-C1'	-5.13	114.02	121.20
14	A3	6	C	C2-N1-C1'	5.12	124.44	118.80
26	N	1326	U	N3-C2-O2	-5.12	118.61	122.20
1	AA	388	G	P-O3'-C3'	5.12	125.84	119.70
1	0	620	C	C2-N1-C1'	5.12	124.43	118.80
26	N	2096	C	C2-N1-C1'	5.12	124.43	118.80
1	AA	330	C	N1-C2-O2	5.11	121.97	118.90
16	F	56	LEU	CA-CB-CG	5.11	127.05	115.30
8	AH	83	LEU	CA-CB-CG	5.11	127.05	115.30
25	AU	20	G	C8-N9-C1'	-5.10	120.36	127.00
26	AV	481	G	P-O3'-C3'	5.10	125.82	119.70
26	N	1585	C	N1-C2-O2	5.10	121.96	118.90
26	AV	1774	C	C6-N1-C2	-5.10	118.26	120.30
26	AV	2655	G	P-O3'-C3'	5.09	125.81	119.70
49	k	68	LEU	CA-CB-CG	5.09	127.01	115.30
26	N	1348	C	C6-N1-C2	-5.09	118.27	120.30
27	AW	31	C	C2-N1-C1'	5.08	124.39	118.80
26	N	1728	C	C2-N1-C1'	5.08	124.39	118.80
26	N	82	U	N3-C2-O2	-5.08	118.64	122.20
9	AI	54	LEU	CB-CG-CD2	5.08	119.63	111.00
26	AV	1072	C	N3-C2-O2	-5.08	118.35	121.90
26	N	2043	C	N1-C2-O2	5.07	121.94	118.90
11	A	4	C	C2-N1-C1'	5.07	124.37	118.80
26	AV	158	U	N3-C2-O2	-5.06	118.66	122.20
26	AV	372	G	P-O3'-C3'	5.06	125.77	119.70
1	0	1031	C	P-O3'-C3'	5.06	125.77	119.70
26	AV	61	C	N3-C2-O2	-5.06	118.36	121.90
21	K	55	LEU	CA-CB-CG	5.06	126.94	115.30
26	AV	2636	C	C2-N1-C1'	5.05	124.35	118.80
26	AV	2901	C	N3-C2-O2	-5.05	118.37	121.90
26	N	1060	U	C5-C4-O4	-5.05	122.87	125.90
26	N	2666	C	N3-C2-O2	-5.04	118.37	121.90
27	AW	89	U	C6-N1-C2	-5.04	117.97	121.00
26	N	894	U	N1-C2-O2	5.04	126.33	122.80
1	0	1228	C	C2-N1-C1'	5.04	124.34	118.80
1	AA	458	U	N1-C2-O2	5.04	126.33	122.80
26	N	2161	C	N3-C2-O2	-5.03	118.38	121.90
1	0	1323	G	C8-N9-C1'	-5.03	120.46	127.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	AV	2556	C	N1-C2-O2	5.03	121.92	118.90
34	Ad	87	LYS	CA-CB-CG	5.03	124.47	113.40
1	AA	1378	C	N1-C2-O2	5.02	121.92	118.90
26	N	1134	A	P-O3'-C3'	5.02	125.72	119.70
26	AV	669	G	N3-C4-N9	5.02	129.01	126.00
26	N	278	A	C4-N9-C1'	5.01	135.32	126.30
11	A	53	G	C6-C5-N7	-5.01	127.39	130.40
26	N	1874	C	C2-N1-C1'	5.01	124.31	118.80
26	N	82	U	C2-N1-C1'	5.01	123.71	117.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	1	216/241 (90%)	203 (94%)	13 (6%)	0	100	100
2	AB	216/241 (90%)	204 (94%)	12 (6%)	0	100	100
3	2	204/233 (88%)	197 (97%)	7 (3%)	0	100	100
3	AC	204/233 (88%)	197 (97%)	7 (3%)	0	100	100
4	3	203/206 (98%)	194 (96%)	9 (4%)	0	100	100
4	AD	203/206 (98%)	196 (97%)	7 (3%)	0	100	100
5	4	148/167 (89%)	140 (95%)	8 (5%)	0	100	100
5	AE	148/167 (89%)	137 (93%)	11 (7%)	0	100	100
6	5	98/135 (73%)	94 (96%)	4 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	AF	98/135 (73%)	91 (93%)	7 (7%)	0	100	100
7	6	149/179 (83%)	145 (97%)	4 (3%)	0	100	100
7	AG	149/179 (83%)	143 (96%)	6 (4%)	0	100	100
8	7	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
8	AH	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
9	8	125/130 (96%)	114 (91%)	11 (9%)	0	100	100
9	AI	125/130 (96%)	118 (94%)	7 (6%)	0	100	100
10	9	96/103 (93%)	89 (93%)	7 (7%)	0	100	100
10	AJ	96/103 (93%)	84 (88%)	11 (12%)	1 (1%)	13	47
12	A1	64/71 (90%)	63 (98%)	1 (2%)	0	100	100
12	v	68/71 (96%)	68 (100%)	0	0	100	100
13	A2	288/1300 (22%)	280 (97%)	8 (3%)	0	100	100
15	AK	130/234 (56%)	124 (95%)	6 (5%)	0	100	100
15	C	130/234 (56%)	128 (98%)	2 (2%)	0	100	100
16	AL	112/118 (95%)	105 (94%)	7 (6%)	0	100	100
16	F	112/118 (95%)	106 (95%)	6 (5%)	0	100	100
17	AM	92/101 (91%)	80 (87%)	12 (13%)	0	100	100
17	G	96/101 (95%)	94 (98%)	2 (2%)	0	100	100
18	AN	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
18	H	85/89 (96%)	83 (98%)	2 (2%)	0	100	100
19	AO	80/82 (98%)	73 (91%)	7 (9%)	0	100	100
19	I	80/82 (98%)	73 (91%)	7 (9%)	0	100	100
20	AP	78/84 (93%)	69 (88%)	9 (12%)	0	100	100
20	J	78/84 (93%)	71 (91%)	7 (9%)	0	100	100
21	AQ	64/75 (85%)	59 (92%)	5 (8%)	0	100	100
21	K	63/75 (84%)	62 (98%)	1 (2%)	0	100	100
22	AR	77/92 (84%)	73 (95%)	4 (5%)	0	100	100
22	t	75/92 (82%)	71 (95%)	4 (5%)	0	100	100
23	AS	83/87 (95%)	83 (100%)	0	0	100	100
23	u	83/87 (95%)	82 (99%)	1 (1%)	0	100	100
24	AT	60/70 (86%)	56 (93%)	4 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	L	58/70 (83%)	54 (93%)	4 (7%)	0	100	100
28	AX	269/273 (98%)	257 (96%)	12 (4%)	0	100	100
28	P	269/273 (98%)	252 (94%)	17 (6%)	0	100	100
29	AY	207/209 (99%)	197 (95%)	10 (5%)	0	100	100
29	Q	207/209 (99%)	198 (96%)	9 (4%)	0	100	100
30	AZ	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
30	R	199/201 (99%)	191 (96%)	8 (4%)	0	100	100
31	Aa	175/179 (98%)	168 (96%)	7 (4%)	0	100	100
31	S	175/179 (98%)	166 (95%)	9 (5%)	0	100	100
32	Ab	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
32	T	173/177 (98%)	169 (98%)	4 (2%)	0	100	100
33	Ac	147/149 (99%)	137 (93%)	10 (7%)	0	100	100
33	U	147/149 (99%)	141 (96%)	6 (4%)	0	100	100
34	Ad	139/142 (98%)	122 (88%)	17 (12%)	0	100	100
34	V	132/142 (93%)	121 (92%)	11 (8%)	0	100	100
35	Ae	140/142 (99%)	133 (95%)	7 (5%)	0	100	100
35	W	140/142 (99%)	134 (96%)	6 (4%)	0	100	100
36	Af	120/123 (98%)	114 (95%)	6 (5%)	0	100	100
36	X	120/123 (98%)	115 (96%)	5 (4%)	0	100	100
37	Ag	141/144 (98%)	134 (95%)	7 (5%)	0	100	100
37	Y	141/144 (98%)	135 (96%)	6 (4%)	0	100	100
38	Ah	134/136 (98%)	128 (96%)	6 (4%)	0	100	100
38	Z	134/136 (98%)	131 (98%)	3 (2%)	0	100	100
39	Ai	116/127 (91%)	111 (96%)	5 (4%)	0	100	100
39	a	117/127 (92%)	110 (94%)	7 (6%)	0	100	100
40	Aj	114/117 (97%)	111 (97%)	3 (3%)	0	100	100
40	b	114/117 (97%)	107 (94%)	7 (6%)	0	100	100
41	Ak	112/115 (97%)	106 (95%)	6 (5%)	0	100	100
41	c	112/115 (97%)	102 (91%)	10 (9%)	0	100	100
42	Al	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
42	d	115/118 (98%)	114 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	Am	101/103 (98%)	91 (90%)	10 (10%)	0	100	100
43	e	101/103 (98%)	96 (95%)	5 (5%)	0	100	100
44	An	108/110 (98%)	103 (95%)	5 (5%)	0	100	100
44	f	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
45	Ao	91/100 (91%)	86 (94%)	5 (6%)	0	100	100
45	g	91/100 (91%)	81 (89%)	10 (11%)	0	100	100
46	Ap	100/104 (96%)	93 (93%)	7 (7%)	0	100	100
46	h	100/104 (96%)	90 (90%)	10 (10%)	0	100	100
47	Aq	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
47	i	92/94 (98%)	85 (92%)	7 (8%)	0	100	100
48	Ar	73/85 (86%)	71 (97%)	2 (3%)	0	100	100
48	j	73/85 (86%)	68 (93%)	5 (7%)	0	100	100
49	As	75/78 (96%)	75 (100%)	0	0	100	100
49	k	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
50	At	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
50	l	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
51	Au	54/59 (92%)	53 (98%)	1 (2%)	0	100	100
51	m	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
52	Av	54/57 (95%)	50 (93%)	4 (7%)	0	100	100
52	n	52/57 (91%)	49 (94%)	3 (6%)	0	100	100
53	Aw	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
53	o	48/55 (87%)	46 (96%)	2 (4%)	0	100	100
54	Ax	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
54	p	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
55	Ay	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
55	q	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
56	Az	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
56	r	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
57	B	1291/1326 (97%)	1235 (96%)	56 (4%)	0	100	100
58	D	115/129 (89%)	110 (96%)	5 (4%)	0	100	100
58	y	115/129 (89%)	105 (91%)	10 (9%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
59	E	121/124 (98%)	111 (92%)	10 (8%)	0	100 100
59	z	121/124 (98%)	113 (93%)	7 (6%)	1 (1%)	16 51
61	s	35/179 (20%)	33 (94%)	2 (6%)	0	100 100
63	x	125/165 (76%)	119 (95%)	6 (5%)	0	100 100
All	All	13392/15548 (86%)	12714 (95%)	676 (5%)	2 (0%)	100 100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
59	z	25	GLU
10	AJ	89	ARG

5.3.2 Protein sidechains (i)

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%)	177 (98%)	3 (2%)	56 78
2	AB	180/199 (90%)	180 (100%)	0	100 100
3	2	170/190 (90%)	169 (99%)	1 (1%)	84 92
3	AC	170/190 (90%)	170 (100%)	0	100 100
4	3	172/173 (99%)	171 (99%)	1 (1%)	84 92
4	AD	172/173 (99%)	171 (99%)	1 (1%)	84 92
5	4	113/126 (90%)	112 (99%)	1 (1%)	75 89
5	AE	113/126 (90%)	112 (99%)	1 (1%)	75 89
6	5	87/116 (75%)	87 (100%)	0	100 100
6	AF	87/116 (75%)	86 (99%)	1 (1%)	70 86
7	6	124/147 (84%)	124 (100%)	0	100 100
7	AG	124/147 (84%)	123 (99%)	1 (1%)	79 90
8	7	104/105 (99%)	104 (100%)	0	100 100
8	AH	104/105 (99%)	104 (100%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
9	8	105/107 (98%)	101 (96%)	4 (4%)	28 60
9	AI	105/107 (98%)	104 (99%)	1 (1%)	73 87
10	9	86/90 (96%)	86 (100%)	0	100 100
10	AJ	86/90 (96%)	85 (99%)	1 (1%)	67 85
12	A1	56/61 (92%)	56 (100%)	0	100 100
12	v	60/61 (98%)	60 (100%)	0	100 100
13	A2	249/1135 (22%)	249 (100%)	0	100 100
15	AK	110/181 (61%)	110 (100%)	0	100 100
15	C	110/181 (61%)	110 (100%)	0	100 100
16	AL	92/96 (96%)	92 (100%)	0	100 100
16	F	92/96 (96%)	91 (99%)	1 (1%)	70 86
17	AM	79/84 (94%)	79 (100%)	0	100 100
17	G	82/84 (98%)	82 (100%)	0	100 100
18	AN	75/77 (97%)	73 (97%)	2 (3%)	40 69
18	H	75/77 (97%)	75 (100%)	0	100 100
19	AO	65/65 (100%)	65 (100%)	0	100 100
19	I	65/65 (100%)	65 (100%)	0	100 100
20	AP	74/78 (95%)	73 (99%)	1 (1%)	62 82
20	J	74/78 (95%)	73 (99%)	1 (1%)	62 82
21	AQ	57/65 (88%)	56 (98%)	1 (2%)	54 77
21	K	56/65 (86%)	56 (100%)	0	100 100
22	AR	70/79 (89%)	68 (97%)	2 (3%)	37 67
22	t	68/79 (86%)	68 (100%)	0	100 100
23	AS	65/66 (98%)	65 (100%)	0	100 100
23	u	65/66 (98%)	65 (100%)	0	100 100
24	AT	58/62 (94%)	57 (98%)	1 (2%)	56 78
24	L	57/62 (92%)	55 (96%)	2 (4%)	31 63
28	AX	216/218 (99%)	216 (100%)	0	100 100
28	P	216/218 (99%)	214 (99%)	2 (1%)	75 89
29	AY	164/164 (100%)	164 (100%)	0	100 100
29	Q	164/164 (100%)	164 (100%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	AZ	165/165 (100%)	165 (100%)	0	100	100
30	R	165/165 (100%)	165 (100%)	0	100	100
31	Aa	148/150 (99%)	147 (99%)	1 (1%)	81	92
31	S	148/150 (99%)	148 (100%)	0	100	100
32	Ab	137/138 (99%)	136 (99%)	1 (1%)	81	92
32	T	136/138 (99%)	135 (99%)	1 (1%)	81	92
33	Ac	114/114 (100%)	114 (100%)	0	100	100
33	U	114/114 (100%)	112 (98%)	2 (2%)	54	77
34	Ad	109/110 (99%)	108 (99%)	1 (1%)	75	89
34	V	104/110 (94%)	103 (99%)	1 (1%)	73	87
35	Ae	116/116 (100%)	116 (100%)	0	100	100
35	W	116/116 (100%)	116 (100%)	0	100	100
36	Af	103/104 (99%)	103 (100%)	0	100	100
36	X	103/104 (99%)	103 (100%)	0	100	100
37	Ag	102/103 (99%)	101 (99%)	1 (1%)	73	87
37	Y	102/103 (99%)	102 (100%)	0	100	100
38	Ah	109/109 (100%)	109 (100%)	0	100	100
38	Z	109/109 (100%)	109 (100%)	0	100	100
39	Ai	98/103 (95%)	98 (100%)	0	100	100
39	a	99/103 (96%)	98 (99%)	1 (1%)	73	87
40	Aj	86/87 (99%)	86 (100%)	0	100	100
40	b	86/87 (99%)	84 (98%)	2 (2%)	45	72
41	Ak	99/100 (99%)	99 (100%)	0	100	100
41	c	99/100 (99%)	97 (98%)	2 (2%)	50	75
42	Al	89/90 (99%)	89 (100%)	0	100	100
42	d	89/90 (99%)	87 (98%)	2 (2%)	47	73
43	Am	84/84 (100%)	84 (100%)	0	100	100
43	e	84/84 (100%)	83 (99%)	1 (1%)	67	85
44	An	93/93 (100%)	93 (100%)	0	100	100
44	f	93/93 (100%)	93 (100%)	0	100	100
45	Ao	80/84 (95%)	80 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
45	g	80/84 (95%)	80 (100%)	0	100 100
46	Ap	83/85 (98%)	83 (100%)	0	100 100
46	h	83/85 (98%)	83 (100%)	0	100 100
47	Aq	78/78 (100%)	78 (100%)	0	100 100
47	i	78/78 (100%)	78 (100%)	0	100 100
48	Ar	56/63 (89%)	56 (100%)	0	100 100
48	j	57/63 (90%)	57 (100%)	0	100 100
49	As	67/68 (98%)	67 (100%)	0	100 100
49	k	67/68 (98%)	66 (98%)	1 (2%)	60 81
50	At	55/55 (100%)	55 (100%)	0	100 100
50	l	55/55 (100%)	55 (100%)	0	100 100
51	Au	47/49 (96%)	47 (100%)	0	100 100
51	m	48/49 (98%)	47 (98%)	1 (2%)	48 74
52	Av	47/48 (98%)	47 (100%)	0	100 100
52	n	46/48 (96%)	46 (100%)	0	100 100
53	Aw	45/49 (92%)	45 (100%)	0	100 100
53	o	45/49 (92%)	45 (100%)	0	100 100
54	Ax	38/38 (100%)	37 (97%)	1 (3%)	41 70
54	p	38/38 (100%)	37 (97%)	1 (3%)	41 70
55	Ay	51/52 (98%)	51 (100%)	0	100 100
55	q	51/52 (98%)	51 (100%)	0	100 100
56	Az	34/34 (100%)	34 (100%)	0	100 100
56	r	34/34 (100%)	34 (100%)	0	100 100
57	B	1130/1158 (98%)	1124 (100%)	6 (0%)	86 93
58	D	90/99 (91%)	90 (100%)	0	100 100
58	y	90/99 (91%)	90 (100%)	0	100 100
59	E	103/104 (99%)	101 (98%)	2 (2%)	52 76
59	z	103/104 (99%)	103 (100%)	0	100 100
61	s	34/158 (22%)	34 (100%)	0	100 100
63	x	96/123 (78%)	95 (99%)	1 (1%)	73 87
All	All	11204/12816 (87%)	11146 (100%)	58 (0%)	85 93

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	27	MET
2	1	74	ARG
2	1	225	ARG
3	2	54	ARG
4	3	185	LYS
5	4	69	ARG
9	8	4	ASN
9	8	49	ARG
9	8	106	ARG
9	8	123	ARG
4	AD	151	LYS
5	AE	43	ASN
6	AF	91	ARG
7	AG	136	LYS
9	AI	123	ARG
10	AJ	89	ARG
18	AN	58	ARG
18	AN	63	ARG
20	AP	27	ARG
21	AQ	52	GLN
22	AR	3	ARG
22	AR	81	ARG
24	AT	1	MET
31	Aa	167	ARG
32	Ab	170	ARG
34	Ad	65	ARG
37	Ag	69	ARG
54	Ax	25	LYS
57	B	132	ARG
57	B	173	MET
57	B	381	GLN
57	B	382	ARG
57	B	948	ARG
57	B	1279	GLN
59	E	10	LYS
59	E	75	GLN
16	F	79	ARG
20	J	43	LYS
24	L	1	MET
24	L	59	ARG
28	P	189	ARG
28	P	260	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	T	176	LYS
33	U	68	ARG
33	U	97	ARG
34	V	113	LYS
39	a	107	ASN
40	b	25	ARG
40	b	94	ARG
41	c	3	ASN
41	c	72	ARG
42	d	15	LYS
42	d	30	ARG
43	e	51	VAL
49	k	23	ASN
51	m	56	LYS
54	p	25	LYS
63	x	46	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
3	2	32	ASN
7	6	68	ASN
7	6	142	HIS
6	AF	17	GLN
6	AF	46	GLN
17	AM	49	GLN
21	AQ	52	GLN
29	AY	32	ASN
31	Aa	37	ASN
32	Ab	139	GLN
37	Ag	38	GLN
38	Ah	22	GLN
40	Aj	100	HIS
42	Al	66	ASN
42	Al	72	ASN
43	Am	66	HIS
57	B	1158	GLN
57	B	1293	GLN
30	R	97	ASN
34	V	43	ASN
39	a	9	GLN
50	l	39	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	u	3	ASN
23	u	55	GLN
59	z	59	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	1532/1542 (99%)	276 (18%)	14 (0%)
1	AA	1538/1542 (99%)	276 (17%)	14 (0%)
11	A	75/76 (98%)	20 (26%)	4 (5%)
14	A3	76/77 (98%)	29 (38%)	5 (6%)
25	AU	75/76 (98%)	12 (16%)	0
26	AV	2895/2903 (99%)	509 (17%)	20 (0%)
26	N	2895/2903 (99%)	539 (18%)	14 (0%)
27	AW	117/120 (97%)	23 (19%)	0
27	O	117/120 (97%)	22 (18%)	2 (1%)
60	M	74/75 (98%)	14 (18%)	1 (1%)
62	w	56/57 (98%)	32 (57%)	0
All	All	9450/9491 (99%)	1752 (18%)	74 (0%)

All (1752) 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	66	A
1	0	72	A
1	0	81	A
1	0	83	C
1	0	88	U
1	0	93	U
1	0	95	C
1	0	97	G
1	0	116	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	0	121	U
1	0	122	G
1	0	130	A
1	0	131	A
1	0	141	G
1	0	142	G
1	0	144	G
1	0	150	U
1	0	163	C
1	0	164	G
1	0	173	U
1	0	174	A
1	0	176	C
1	0	180	U
1	0	182	A
1	0	183	C
1	0	184	G
1	0	191	G
1	0	197	A
1	0	211	G
1	0	212	G
1	0	222	C
1	0	226	G
1	0	245	U
1	0	247	G
1	0	251	G
1	0	262	A
1	0	263	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	320	A
1	0	328	C
1	0	329	A
1	0	330	C
1	0	332	G
1	0	337	G
1	0	338	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	0	351	G
1	0	352	C
1	0	353	A
1	0	354	G
1	0	367	U
1	0	372	C
1	0	373	A
1	0	385	C
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	414	A
1	0	421	U
1	0	422	C
1	0	424	G
1	0	428	G
1	0	429	U
1	0	436	C
1	0	439	U
1	0	440	C
1	0	451	A
1	0	458	U
1	0	467	U
1	0	468	A
1	0	478	A
1	0	479	U
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	500	G
1	0	509	A
1	0	510	A
1	0	511	C
1	0	516	U
1	0	517	G
1	0	518	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	0	519	C
1	0	521	G
1	0	524	G
1	0	527	G
1	0	531	U
1	0	532	A
1	0	533	A
1	0	547	A
1	0	559	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	600	A
1	0	618	C
1	0	619	U
1	0	621	A
1	0	633	G
1	0	639	G
1	0	650	G
1	0	653	U
1	0	661	G
1	0	665	A
1	0	666	G
1	0	673	A
1	0	687	A
1	0	701	U
1	0	702	A
1	0	703	G
1	0	710	G
1	0	723	U
1	0	724	G
1	0	731	G
1	0	753	A
1	0	755	G
1	0	758	C
1	0	793	U
1	0	794	A
1	0	813	U
1	0	814	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	0	815	A
1	0	817	C
1	0	818	G
1	0	819	A
1	0	821	G
1	0	828	U
1	0	829	G
1	0	832	G
1	0	842	U
1	0	843	U
1	0	845	A
1	0	849	G
1	0	885	G
1	0	889	A
1	0	902	G
1	0	914	A
1	0	926	G
1	0	934	C
1	0	935	A
1	0	942	G
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	978	A
1	0	989	U
1	0	992	U
1	0	993	G
1	0	994	A
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	1021	A
1	0	1022	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	0	1025	U
1	0	1026	G
1	0	1029	U
1	0	1030	U
1	0	1032	G
1	0	1045	C
1	0	1046	A
1	0	1056	U
1	0	1065	U
1	0	1066	C
1	0	1079	G
1	0	1085	U
1	0	1089	G
1	0	1094	G
1	0	1095	U
1	0	1101	A
1	0	1108	G
1	0	1133	G
1	0	1137	C
1	0	1138	G
1	0	1139	G
1	0	1140	C
1	0	1151	A
1	0	1158	C
1	0	1159	U
1	0	1167	A
1	0	1168	U
1	0	1171	A
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	1201	A
1	0	1202	U
1	0	1213	A
1	0	1224	U
1	0	1227	A
1	0	1238	A
1	0	1241	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	0	1257	A
1	0	1260	G
1	0	1270	G
1	0	1280	A
1	0	1285	A
1	0	1286	U
1	0	1287	A
1	0	1290	G
1	0	1291	U
1	0	1297	G
1	0	1298	U
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	1320	C
1	0	1323	G
1	0	1332	A
1	0	1336	C
1	0	1340	A
1	0	1346	A
1	0	1353	G
1	0	1362	A
1	0	1363	A
1	0	1370	G
1	0	1379	G
1	0	1382	C
1	0	1383	C
1	0	1400	C
1	0	1401	G
1	0	1419	G
1	0	1429	A
1	0	1432	G
1	0	1441	A
1	0	1452	C
1	0	1455	G
1	0	1487	G
1	0	1492	A
1	0	1494	G
1	0	1497	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	6	G
11	A	7	A
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
11	A	21	A
11	A	22	G
11	A	45	U
11	A	47	U
11	A	48	C
11	A	53	G
11	A	54	U
11	A	55	U
11	A	56	C
11	A	74	C
11	A	75	C
14	A3	7	G
14	A3	9	A
14	A3	13	C
14	A3	16	U
14	A3	17	U
14	A3	21	U
14	A3	22	A
14	A3	23	G
14	A3	42	A
14	A3	46	G
14	A3	47	G
14	A3	48	U
14	A3	49	C
14	A3	50	A
14	A3	51	C
14	A3	52	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	A3	53	G
14	A3	58	G
14	A3	59	A
14	A3	60	A
14	A3	62	C
14	A3	63	C
14	A3	64	C
14	A3	66	U
14	A3	67	C
14	A3	72	C
14	A3	73	C
14	A3	75	C
14	A3	77	A
1	AA	6	G
1	AA	9	G
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	69	G
1	AA	71	A
1	AA	83	C
1	AA	85	U
1	AA	86	G
1	AA	87	C
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	136	C
1	AA	143	A
1	AA	144	G
1	AA	148	G
1	AA	149	A
1	AA	158	G
1	AA	163	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AA	173	U
1	AA	174	A
1	AA	178	C
1	AA	180	U
1	AA	181	A
1	AA	183	C
1	AA	184	G
1	AA	197	A
1	AA	211	G
1	AA	214	C
1	AA	226	G
1	AA	240	G
1	AA	245	U
1	AA	246	A
1	AA	247	G
1	AA	251	G
1	AA	253	A
1	AA	254	G
1	AA	263	A
1	AA	266	G
1	AA	267	C
1	AA	279	A
1	AA	280	C
1	AA	281	G
1	AA	289	G
1	AA	306	A
1	AA	328	C
1	AA	330	C
1	AA	332	G
1	AA	346	G
1	AA	347	G
1	AA	350	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	390	U
1	AA	392	C
1	AA	398	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	424	G
1	AA	428	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	495	A
1	AA	509	A
1	AA	510	A
1	AA	511	C
1	AA	518	C
1	AA	519	C
1	AA	521	G
1	AA	524	G
1	AA	527	G
1	AA	532	A
1	AA	533	A
1	AA	547	A
1	AA	562	U
1	AA	564	C
1	AA	567	G
1	AA	570	G
1	AA	572	A
1	AA	573	A
1	AA	576	C
1	AA	577	G
1	AA	596	A
1	AA	597	G
1	AA	633	G
1	AA	650	G
1	AA	653	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AA	663	A
1	AA	665	A
1	AA	668	G
1	AA	675	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	755	G
1	AA	771	G
1	AA	791	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	832	G
1	AA	836	G
1	AA	841	C
1	AA	843	U
1	AA	844	G
1	AA	845	A
1	AA	846	G
1	AA	849	G
1	AA	851	G
1	AA	889	A
1	AA	890	G
1	AA	891	U
1	AA	902	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AA	914	A
1	AA	934	C
1	AA	935	A
1	AA	958	A
1	AA	960	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	978	A
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	1020	G
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	1033	G
1	AA	1038	C
1	AA	1043	G
1	AA	1045	C
1	AA	1064	G
1	AA	1065	U
1	AA	1066	C
1	AA	1085	U
1	AA	1094	G
1	AA	1095	U
1	AA	1101	A
1	AA	1104	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AA	1108	G
1	AA	1123	U
1	AA	1125	U
1	AA	1132	C
1	AA	1133	G
1	AA	1135	U
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	1167	A
1	AA	1179	A
1	AA	1183	U
1	AA	1184	G
1	AA	1196	A
1	AA	1197	A
1	AA	1202	U
1	AA	1212	U
1	AA	1224	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	1270	G
1	AA	1275	A
1	AA	1280	A
1	AA	1287	A
1	AA	1290	G
1	AA	1297	G
1	AA	1298	U
1	AA	1300	G
1	AA	1301	U
1	AA	1302	C
1	AA	1305	G
1	AA	1317	C
1	AA	1318	A
1	AA	1319	A
1	AA	1320	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AA	1322	C
1	AA	1323	G
1	AA	1331	G
1	AA	1332	A
1	AA	1340	A
1	AA	1346	A
1	AA	1347	G
1	AA	1348	U
1	AA	1353	G
1	AA	1357	A
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	1402	C
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	1500	A
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	1537	U
1	AA	1538	C
25	AU	9	A
25	AU	16	C
25	AU	17	U
25	AU	18	G
25	AU	19	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	AU	20	G
25	AU	21	A
25	AU	22	G
25	AU	43	G
25	AU	46	G
25	AU	60	C
25	AU	76	A
26	AV	2	G
26	AV	10	A
26	AV	34	U
26	AV	35	G
26	AV	39	G
26	AV	42	A
26	AV	46	G
26	AV	50	U
26	AV	51	G
26	AV	60	G
26	AV	63	A
26	AV	71	A
26	AV	73	A
26	AV	74	A
26	AV	75	G
26	AV	86	G
26	AV	101	A
26	AV	102	U
26	AV	103	A
26	AV	118	A
26	AV	119	A
26	AV	120	U
26	AV	125	A
26	AV	127	A
26	AV	137	U
26	AV	138	U
26	AV	139	U
26	AV	140	C
26	AV	141	G
26	AV	142	A
26	AV	160	A
26	AV	162	U
26	AV	163	C
26	AV	196	A
26	AV	199	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	AV	215	G
26	AV	216	A
26	AV	222	A
26	AV	223	A
26	AV	229	C
26	AV	243	U
26	AV	248	G
26	AV	250	G
26	AV	255	A
26	AV	265	A
26	AV	266	G
26	AV	271	G
26	AV	276	U
26	AV	277	G
26	AV	278	A
26	AV	279	A
26	AV	281	C
26	AV	301	G
26	AV	310	A
26	AV	323	C
26	AV	329	G
26	AV	330	A
26	AV	332	A
26	AV	333	G
26	AV	338	G
26	AV	343	C
26	AV	354	A
26	AV	361	G
26	AV	362	A
26	AV	368	A
26	AV	371	A
26	AV	372	G
26	AV	373	U
26	AV	386	G
26	AV	396	G
26	AV	404	A
26	AV	405	U
26	AV	411	G
26	AV	422	A
26	AV	424	G
26	AV	429	A
26	AV	430	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	AV	435	C
26	AV	447	A
26	AV	451	U
26	AV	455	C
26	AV	456	C
26	AV	467	G
26	AV	479	A
26	AV	480	A
26	AV	481	G
26	AV	482	A
26	AV	491	G
26	AV	503	A
26	AV	504	A
26	AV	505	A
26	AV	509	C
26	AV	516	C
26	AV	529	A
26	AV	530	G
26	AV	532	A
26	AV	533	G
26	AV	543	G
26	AV	544	C
26	AV	546	U
26	AV	547	A
26	AV	548	G
26	AV	549	G
26	AV	550	C
26	AV	563	A
26	AV	573	U
26	AV	575	A
26	AV	586	A
26	AV	603	A
26	AV	613	A
26	AV	614	A
26	AV	619	G
26	AV	620	G
26	AV	622	G
26	AV	627	A
26	AV	634	C
26	AV	637	A
26	AV	646	U
26	AV	647	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	AV	648	G
26	AV	654	A
26	AV	655	A
26	AV	670	A
26	AV	671	C
26	AV	677	A
26	AV	684	G
26	AV	686	U
26	AV	712	G
26	AV	715	A
26	AV	726	G
26	AV	729	G
26	AV	730	A
26	AV	740	C
26	AV	747	U
26	AV	757	G
26	AV	764	A
26	AV	765	C
26	AV	774	G
26	AV	775	G
26	AV	776	G
26	AV	779	U
26	AV	782	A
26	AV	784	G
26	AV	785	G
26	AV	805	G
26	AV	812	C
26	AV	819	A
26	AV	827	U
26	AV	828	U
26	AV	831	G
26	AV	844	A
26	AV	845	A
26	AV	846	U
26	AV	850	U
26	AV	857	G
26	AV	860	U
26	AV	878	A
26	AV	896	A
26	AV	897	C
26	AV	910	A
26	AV	934	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	AV	941	A
26	AV	946	C
26	AV	961	C
26	AV	973	A
26	AV	974	G
26	AV	980	A
26	AV	983	A
26	AV	985	C
26	AV	989	G
26	AV	995	C
26	AV	996	A
26	AV	1005	C
26	AV	1009	A
26	AV	1012	U
26	AV	1013	C
26	AV	1015	U
26	AV	1026	G
26	AV	1033	U
26	AV	1040	A
26	AV	1046	A
26	AV	1047	G
26	AV	1056	G
26	AV	1057	A
26	AV	1060	U
26	AV	1062	G
26	AV	1066	U
26	AV	1067	A
26	AV	1068	G
26	AV	1070	A
26	AV	1071	G
26	AV	1074	G
26	AV	1078	U
26	AV	1079	C
26	AV	1083	U
26	AV	1084	A
26	AV	1087	G
26	AV	1088	A
26	AV	1089	A
26	AV	1094	U
26	AV	1096	A
26	AV	1097	U
26	AV	1100	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	AV	1103	A
26	AV	1104	C
26	AV	1110	G
26	AV	1112	G
26	AV	1130	U
26	AV	1132	U
26	AV	1133	A
26	AV	1135	C
26	AV	1136	G
26	AV	1143	A
26	AV	1157	G
26	AV	1158	C
26	AV	1161	C
26	AV	1169	A
26	AV	1172	C
26	AV	1173	U
26	AV	1174	U
26	AV	1175	A
26	AV	1176	U
26	AV	1180	U
26	AV	1198	U
26	AV	1204	A
26	AV	1205	A
26	AV	1206	G
26	AV	1212	G
26	AV	1225	G
26	AV	1227	G
26	AV	1237	A
26	AV	1238	G
26	AV	1251	C
26	AV	1253	A
26	AV	1256	G
26	AV	1266	G
26	AV	1271	G
26	AV	1272	A
26	AV	1274	A
26	AV	1275	A
26	AV	1300	G
26	AV	1301	A
26	AV	1321	A
26	AV	1330	C
26	AV	1332	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	AV	1339	G
26	AV	1340	U
26	AV	1341	G
26	AV	1345	C
26	AV	1365	A
26	AV	1368	G
26	AV	1378	A
26	AV	1379	U
26	AV	1380	G
26	AV	1385	A
26	AV	1416	G
26	AV	1419	A
26	AV	1420	A
26	AV	1437	C
26	AV	1452	G
26	AV	1453	A
26	AV	1475	G
26	AV	1478	G
26	AV	1482	G
26	AV	1494	A
26	AV	1497	U
26	AV	1504	A
26	AV	1505	A
26	AV	1515	A
26	AV	1524	G
26	AV	1530	G
26	AV	1533	C
26	AV	1535	A
26	AV	1537	G
26	AV	1540	G
26	AV	1546	G
26	AV	1558	C
26	AV	1566	A
26	AV	1567	G
26	AV	1583	A
26	AV	1584	U
26	AV	1585	C
26	AV	1587	G
26	AV	1592	C
26	AV	1603	A
26	AV	1608	A
26	AV	1634	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	AV	1647	U
26	AV	1648	U
26	AV	1649	G
26	AV	1654	A
26	AV	1665	A
26	AV	1667	G
26	AV	1674	G
26	AV	1675	C
26	AV	1699	G
26	AV	1715	G
26	AV	1729	U
26	AV	1730	C
26	AV	1738	G
26	AV	1744	A
26	AV	1756	G
26	AV	1757	A
26	AV	1758	U
26	AV	1764	C
26	AV	1773	A
26	AV	1777	U
26	AV	1782	U
26	AV	1784	A
26	AV	1786	A
26	AV	1799	G
26	AV	1800	C
26	AV	1801	A
26	AV	1808	A
26	AV	1811	G
26	AV	1816	C
26	AV	1829	A
26	AV	1833	C
26	AV	1839	G
26	AV	1847	A
26	AV	1852	U
26	AV	1869	G
26	AV	1870	C
26	AV	1876	A
26	AV	1881	C
26	AV	1884	G
26	AV	1901	A
26	AV	1906	G
26	AV	1913	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	AV	1927	A
26	AV	1929	G
26	AV	1930	G
26	AV	1937	A
26	AV	1938	A
26	AV	1955	U
26	AV	1964	G
26	AV	1967	C
26	AV	1970	A
26	AV	1971	U
26	AV	1972	G
26	AV	1975	G
26	AV	1991	U
26	AV	1992	G
26	AV	1993	U
26	AV	1997	C
26	AV	2022	U
26	AV	2023	C
26	AV	2031	A
26	AV	2033	A
26	AV	2036	C
26	AV	2043	C
26	AV	2052	A
26	AV	2055	C
26	AV	2056	G
26	AV	2060	A
26	AV	2061	G
26	AV	2062	A
26	AV	2069	G
26	AV	2080	A
26	AV	2093	G
26	AV	2107	G
26	AV	2110	G
26	AV	2111	U
26	AV	2112	G
26	AV	2113	U
26	AV	2119	A
26	AV	2120	G
26	AV	2123	G
26	AV	2124	G
26	AV	2125	G
26	AV	2126	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	AV	2131	U
26	AV	2132	U
26	AV	2133	G
26	AV	2134	A
26	AV	2144	G
26	AV	2145	C
26	AV	2151	U
26	AV	2161	C
26	AV	2162	G
26	AV	2163	A
26	AV	2165	C
26	AV	2171	A
26	AV	2172	U
26	AV	2173	A
26	AV	2178	C
26	AV	2190	G
26	AV	2198	A
26	AV	2199	A
26	AV	2203	U
26	AV	2204	G
26	AV	2211	A
26	AV	2214	C
26	AV	2225	A
26	AV	2226	C
26	AV	2230	G
26	AV	2238	G
26	AV	2239	G
26	AV	2250	G
26	AV	2266	A
26	AV	2269	G
26	AV	2278	A
26	AV	2279	G
26	AV	2283	C
26	AV	2286	G
26	AV	2287	A
26	AV	2288	A
26	AV	2297	A
26	AV	2305	U
26	AV	2307	G
26	AV	2309	A
26	AV	2312	U
26	AV	2319	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	AV	2321	U
26	AV	2333	A
26	AV	2334	U
26	AV	2335	A
26	AV	2337	G
26	AV	2345	G
26	AV	2347	C
26	AV	2350	C
26	AV	2352	A
26	AV	2361	G
26	AV	2383	G
26	AV	2385	C
26	AV	2402	U
26	AV	2406	A
26	AV	2423	U
26	AV	2425	A
26	AV	2426	A
26	AV	2428	G
26	AV	2429	G
26	AV	2430	A
26	AV	2431	U
26	AV	2434	A
26	AV	2441	U
26	AV	2447	G
26	AV	2448	A
26	AV	2460	U
26	AV	2468	A
26	AV	2476	A
26	AV	2478	A
26	AV	2487	G
26	AV	2491	U
26	AV	2494	G
26	AV	2498	C
26	AV	2502	G
26	AV	2503	A
26	AV	2504	U
26	AV	2513	A
26	AV	2518	A
26	AV	2520	C
26	AV	2529	G
26	AV	2547	A
26	AV	2554	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	AV	2566	A
26	AV	2567	G
26	AV	2572	A
26	AV	2582	G
26	AV	2585	U
26	AV	2602	A
26	AV	2609	U
26	AV	2613	U
26	AV	2615	U
26	AV	2629	U
26	AV	2630	G
26	AV	2646	C
26	AV	2648	G
26	AV	2654	A
26	AV	2655	G
26	AV	2656	U
26	AV	2659	G
26	AV	2663	G
26	AV	2671	G
26	AV	2682	A
26	AV	2684	U
26	AV	2686	G
26	AV	2689	U
26	AV	2690	U
26	AV	2707	U
26	AV	2714	G
26	AV	2716	C
26	AV	2726	A
26	AV	2731	G
26	AV	2733	A
26	AV	2744	G
26	AV	2748	A
26	AV	2757	A
26	AV	2758	A
26	AV	2765	A
26	AV	2777	G
26	AV	2778	A
26	AV	2779	U
26	AV	2798	U
26	AV	2808	G
26	AV	2809	A
26	AV	2818	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	AV	2820	A
26	AV	2833	U
26	AV	2834	G
26	AV	2849	U
26	AV	2872	A
26	AV	2873	A
26	AV	2876	G
26	AV	2880	C
26	AV	2886	A
26	AV	2891	U
26	AV	2893	A
26	AV	2903	U
27	AW	9	G
27	AW	13	G
27	AW	16	G
27	AW	25	U
27	AW	30	C
27	AW	31	C
27	AW	35	C
27	AW	37	C
27	AW	44	G
27	AW	51	G
27	AW	52	A
27	AW	53	A
27	AW	56	G
27	AW	66	A
27	AW	67	G
27	AW	88	C
27	AW	89	U
27	AW	90	C
27	AW	91	C
27	AW	99	A
27	AW	108	A
27	AW	109	A
27	AW	117	G
60	M	9	C
60	M	10	G
60	M	14	A
60	M	16	C
60	M	17	G
60	M	19	U
60	M	20	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
60	M	42	G
60	M	43	C
60	M	45	U
60	M	46	U
60	M	47	C
60	M	55	C
60	M	75	A
26	N	10	A
26	N	15	G
26	N	23	G
26	N	27	G
26	N	35	G
26	N	42	A
26	N	46	G
26	N	49	A
26	N	51	G
26	N	52	A
26	N	60	G
26	N	63	A
26	N	71	A
26	N	74	A
26	N	75	G
26	N	85	G
26	N	91	A
26	N	96	C
26	N	101	A
26	N	102	U
26	N	103	A
26	N	114	U
26	N	118	A
26	N	119	A
26	N	120	U
26	N	125	A
26	N	128	C
26	N	130	C
26	N	131	A
26	N	136	G
26	N	138	U
26	N	139	U
26	N	140	C
26	N	141	G
26	N	142	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	N	162	U
26	N	163	C
26	N	181	A
26	N	196	A
26	N	199	A
26	N	215	G
26	N	216	A
26	N	222	A
26	N	233	A
26	N	241	A
26	N	248	G
26	N	252	G
26	N	255	A
26	N	259	G
26	N	266	G
26	N	267	C
26	N	272	A
26	N	276	U
26	N	278	A
26	N	281	C
26	N	282	A
26	N	284	U
26	N	285	G
26	N	300	A
26	N	301	G
26	N	310	A
26	N	329	G
26	N	330	A
26	N	331	C
26	N	338	G
26	N	346	A
26	N	350	G
26	N	353	C
26	N	356	G
26	N	361	G
26	N	362	A
26	N	370	G
26	N	371	A
26	N	372	G
26	N	373	U
26	N	386	G
26	N	396	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	N	403	U
26	N	405	U
26	N	406	G
26	N	407	G
26	N	411	G
26	N	412	A
26	N	422	A
26	N	424	G
26	N	446	G
26	N	447	A
26	N	452	G
26	N	454	A
26	N	457	A
26	N	459	U
26	N	467	G
26	N	473	G
26	N	480	A
26	N	481	G
26	N	489	G
26	N	490	C
26	N	491	G
26	N	496	G
26	N	504	A
26	N	505	A
26	N	509	C
26	N	512	G
26	N	516	C
26	N	529	A
26	N	530	G
26	N	532	A
26	N	533	G
26	N	543	G
26	N	544	C
26	N	546	U
26	N	548	G
26	N	549	G
26	N	562	U
26	N	563	A
26	N	569	U
26	N	572	A
26	N	573	U
26	N	575	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	N	586	A
26	N	603	A
26	N	613	A
26	N	614	A
26	N	622	G
26	N	627	A
26	N	637	A
26	N	645	C
26	N	646	U
26	N	647	G
26	N	654	A
26	N	656	G
26	N	664	G
26	N	668	A
26	N	669	G
26	N	670	A
26	N	671	C
26	N	677	A
26	N	685	A
26	N	686	U
26	N	711	G
26	N	715	A
26	N	717	C
26	N	726	G
26	N	729	G
26	N	730	A
26	N	746	U
26	N	747	U
26	N	757	G
26	N	764	A
26	N	765	C
26	N	774	G
26	N	775	G
26	N	776	G
26	N	782	A
26	N	784	G
26	N	785	G
26	N	788	A
26	N	805	G
26	N	811	U
26	N	812	C
26	N	819	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	N	827	U
26	N	828	U
26	N	845	A
26	N	846	U
26	N	847	U
26	N	858	G
26	N	859	G
26	N	869	G
26	N	878	A
26	N	882	G
26	N	883	G
26	N	884	U
26	N	895	U
26	N	897	C
26	N	907	G
26	N	910	A
26	N	914	G
26	N	915	C
26	N	941	A
26	N	946	C
26	N	957	C
26	N	961	C
26	N	973	A
26	N	974	G
26	N	980	A
26	N	983	A
26	N	985	C
26	N	995	C
26	N	996	A
26	N	1009	A
26	N	1012	U
26	N	1013	C
26	N	1020	A
26	N	1022	G
26	N	1025	G
26	N	1026	G
26	N	1033	U
26	N	1039	A
26	N	1046	A
26	N	1060	U
26	N	1062	G
26	N	1070	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	N	1071	G
26	N	1083	U
26	N	1084	A
26	N	1085	A
26	N	1087	G
26	N	1088	A
26	N	1090	A
26	N	1110	G
26	N	1112	G
26	N	1119	U
26	N	1120	G
26	N	1132	U
26	N	1133	A
26	N	1135	C
26	N	1136	G
26	N	1139	G
26	N	1142	A
26	N	1155	A
26	N	1168	G
26	N	1169	A
26	N	1174	U
26	N	1175	A
26	N	1176	U
26	N	1186	G
26	N	1206	G
26	N	1212	G
26	N	1216	G
26	N	1237	A
26	N	1238	G
26	N	1247	A
26	N	1248	G
26	N	1252	G
26	N	1253	A
26	N	1255	U
26	N	1256	G
26	N	1265	A
26	N	1266	G
26	N	1268	A
26	N	1271	G
26	N	1272	A
26	N	1284	A
26	N	1300	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	N	1301	A
26	N	1306	C
26	N	1309	G
26	N	1311	G
26	N	1313	U
26	N	1314	C
26	N	1325	U
26	N	1329	U
26	N	1330	C
26	N	1332	G
26	N	1341	G
26	N	1342	A
26	N	1345	C
26	N	1346	G
26	N	1352	U
26	N	1360	G
26	N	1365	A
26	N	1368	G
26	N	1378	A
26	N	1379	U
26	N	1383	A
26	N	1386	C
26	N	1387	A
26	N	1392	A
26	N	1395	A
26	N	1403	A
26	N	1416	G
26	N	1421	G
26	N	1427	A
26	N	1428	C
26	N	1437	C
26	N	1441	G
26	N	1452	G
26	N	1453	A
26	N	1458	U
26	N	1461	C
26	N	1467	U
26	N	1476	U
26	N	1478	G
26	N	1482	G
26	N	1493	C
26	N	1503	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	N	1504	A
26	N	1506	U
26	N	1509	A
26	N	1515	A
26	N	1516	G
26	N	1524	G
26	N	1528	A
26	N	1529	G
26	N	1530	G
26	N	1533	C
26	N	1535	A
26	N	1536	C
26	N	1537	G
26	N	1546	G
26	N	1555	G
26	N	1558	C
26	N	1565	C
26	N	1566	A
26	N	1569	A
26	N	1578	U
26	N	1583	A
26	N	1584	U
26	N	1585	C
26	N	1588	G
26	N	1601	G
26	N	1607	C
26	N	1608	A
26	N	1610	A
26	N	1613	G
26	N	1619	G
26	N	1646	C
26	N	1647	U
26	N	1648	U
26	N	1664	A
26	N	1667	G
26	N	1674	G
26	N	1681	G
26	N	1715	G
26	N	1729	U
26	N	1730	C
26	N	1738	G
26	N	1752	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	N	1754	A
26	N	1756	G
26	N	1758	U
26	N	1763	G
26	N	1764	C
26	N	1773	A
26	N	1774	C
26	N	1775	U
26	N	1781	U
26	N	1782	U
26	N	1784	A
26	N	1786	A
26	N	1800	C
26	N	1801	A
26	N	1807	G
26	N	1808	A
26	N	1816	C
26	N	1821	A
26	N	1829	A
26	N	1857	G
26	N	1866	A
26	N	1870	C
26	N	1873	G
26	N	1900	A
26	N	1901	A
26	N	1906	G
26	N	1914	C
26	N	1927	A
26	N	1929	G
26	N	1930	G
26	N	1931	U
26	N	1936	A
26	N	1937	A
26	N	1938	A
26	N	1955	U
26	N	1967	C
26	N	1970	A
26	N	1971	U
26	N	1972	G
26	N	1983	G
26	N	1991	U
26	N	1992	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	N	1993	U
26	N	1997	C
26	N	2013	A
26	N	2021	C
26	N	2022	U
26	N	2023	C
26	N	2030	A
26	N	2031	A
26	N	2033	A
26	N	2034	U
26	N	2035	G
26	N	2036	C
26	N	2043	C
26	N	2044	C
26	N	2055	C
26	N	2056	G
26	N	2060	A
26	N	2061	G
26	N	2062	A
26	N	2069	G
26	N	2072	C
26	N	2077	A
26	N	2093	G
26	N	2097	A
26	N	2098	U
26	N	2101	A
26	N	2108	A
26	N	2110	G
26	N	2111	U
26	N	2112	G
26	N	2113	U
26	N	2114	A
26	N	2118	U
26	N	2119	A
26	N	2125	G
26	N	2126	A
26	N	2132	U
26	N	2133	G
26	N	2136	G
26	N	2145	C
26	N	2147	A
26	N	2149	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	N	2158	A
26	N	2162	G
26	N	2167	U
26	N	2171	A
26	N	2172	U
26	N	2173	A
26	N	2178	C
26	N	2194	U
26	N	2198	A
26	N	2204	G
26	N	2211	A
26	N	2214	C
26	N	2225	A
26	N	2226	C
26	N	2238	G
26	N	2239	G
26	N	2250	G
26	N	2266	A
26	N	2269	G
26	N	2278	A
26	N	2279	G
26	N	2283	C
26	N	2286	G
26	N	2287	A
26	N	2288	A
26	N	2297	A
26	N	2305	U
26	N	2309	A
26	N	2312	U
26	N	2320	U
26	N	2325	G
26	N	2327	A
26	N	2333	A
26	N	2336	A
26	N	2343	U
26	N	2347	C
26	N	2350	C
26	N	2354	C
26	N	2361	G
26	N	2383	G
26	N	2385	C
26	N	2388	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	N	2392	A
26	N	2402	U
26	N	2406	A
26	N	2422	C
26	N	2423	U
26	N	2425	A
26	N	2429	G
26	N	2430	A
26	N	2441	U
26	N	2448	A
26	N	2476	A
26	N	2478	A
26	N	2492	U
26	N	2494	G
26	N	2498	C
26	N	2502	G
26	N	2503	A
26	N	2504	U
26	N	2513	A
26	N	2518	A
26	N	2520	C
26	N	2529	G
26	N	2535	G
26	N	2547	A
26	N	2554	U
26	N	2566	A
26	N	2567	G
26	N	2572	A
26	N	2573	C
26	N	2578	G
26	N	2585	U
26	N	2602	A
26	N	2609	U
26	N	2613	U
26	N	2615	U
26	N	2621	G
26	N	2629	U
26	N	2630	G
26	N	2645	G
26	N	2646	C
26	N	2655	G
26	N	2656	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	N	2663	G
26	N	2682	A
26	N	2689	U
26	N	2690	U
26	N	2714	G
26	N	2716	C
26	N	2726	A
26	N	2729	G
26	N	2732	G
26	N	2733	A
26	N	2739	U
26	N	2744	G
26	N	2748	A
26	N	2751	G
26	N	2769	U
26	N	2777	G
26	N	2778	A
26	N	2779	U
26	N	2791	G
26	N	2794	C
26	N	2798	U
26	N	2799	A
26	N	2800	A
26	N	2809	A
26	N	2818	U
26	N	2820	A
26	N	2823	A
26	N	2832	U
26	N	2833	U
26	N	2834	G
26	N	2836	U
26	N	2846	G
26	N	2848	G
26	N	2849	U
26	N	2871	U
26	N	2872	A
26	N	2873	A
26	N	2879	A
26	N	2880	C
26	N	2884	U
26	N	2895	G
26	N	2903	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	O	9	G
27	O	13	G
27	O	15	A
27	O	16	G
27	O	23	G
27	O	25	U
27	O	30	C
27	O	35	C
27	O	36	C
27	O	41	G
27	O	42	C
27	O	44	G
27	O	53	A
27	O	58	A
27	O	79	G
27	O	88	C
27	O	89	U
27	O	90	C
27	O	91	C
27	O	99	A
27	O	108	A
27	O	109	A
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
62	w	536	A
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	557	U
62	w	558	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
62	w	559	U
62	w	560	U
62	w	561	U
62	w	562	U
62	w	563	U
62	w	564	U
62	w	565	U
62	w	569	U
62	w	571	U
62	w	572	U
62	w	573	U
62	w	577	U

All (74) 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	21	A
11	A	46	G
11	A	54	U
14	A3	16	U
14	A3	22	A
14	A3	50	A
14	A3	51	C
14	A3	66	U
1	AA	96	U
1	AA	115	G
1	AA	388	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
26	AV	242	G
26	AV	372	G
26	AV	404	A
26	AV	421	C
26	AV	481	G
26	AV	670	A
26	AV	784	G
26	AV	859	G
26	AV	960	A
26	AV	1134	A
26	AV	1142	A
26	AV	1900	A
26	AV	2125	G
26	AV	2225	A
26	AV	2286	G
26	AV	2311	A
26	AV	2459	A
26	AV	2655	G
26	AV	2756	U
26	AV	2776	A
60	M	44	A
26	N	84	A
26	N	277	G
26	N	404	A
26	N	421	C
26	N	670	A
26	N	784	G
26	N	1109	C
26	N	1134	A
26	N	1900	A
26	N	2225	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	N	2311	A
26	N	2655	G
26	N	2776	A
26	N	2832	U
27	O	24	G
27	O	34	A

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.

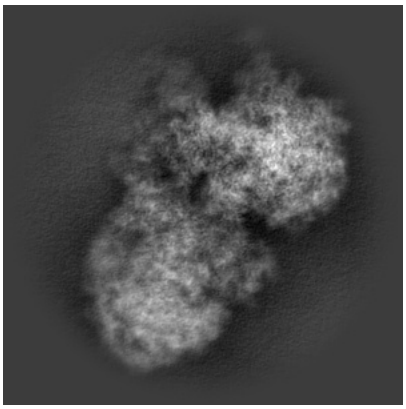
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-51340. These allow visual inspection of the internal detail of the map and identification of artifacts.

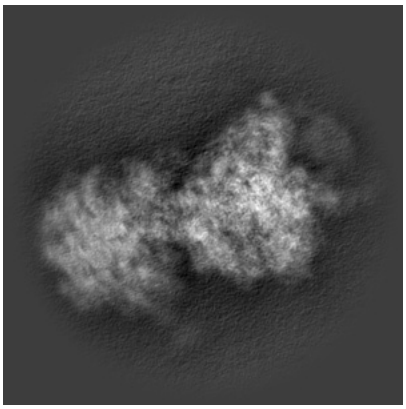
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

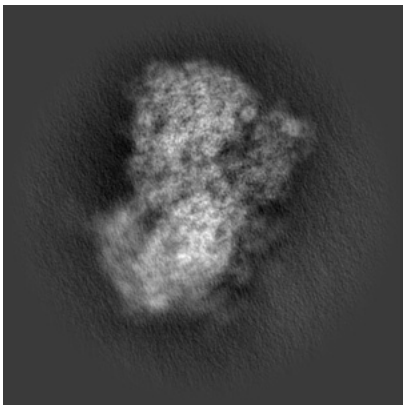
6.1.1 Primary map



X

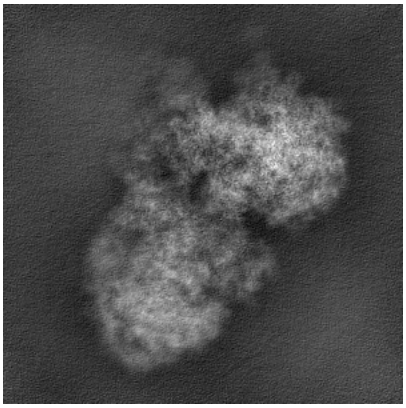


Y

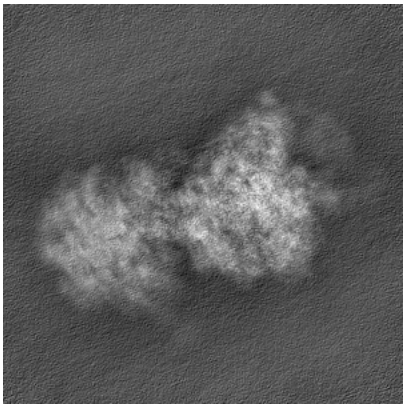


Z

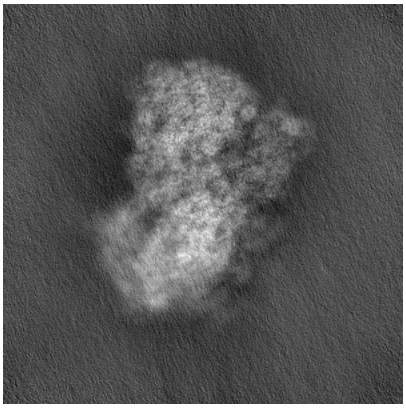
6.1.2 Raw map



X



Y

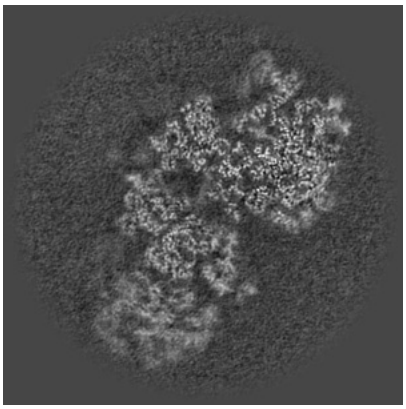


Z

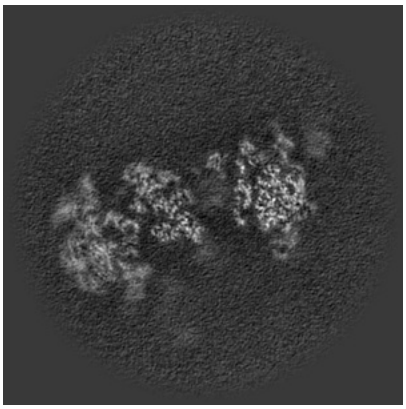
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

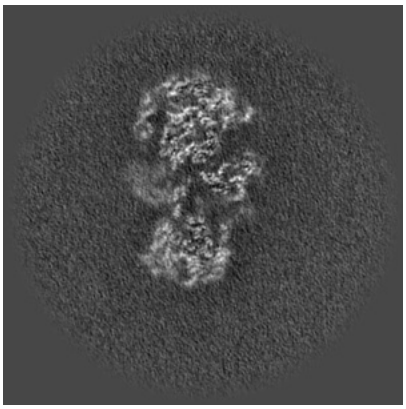
6.2.1 Primary map



X Index: 175

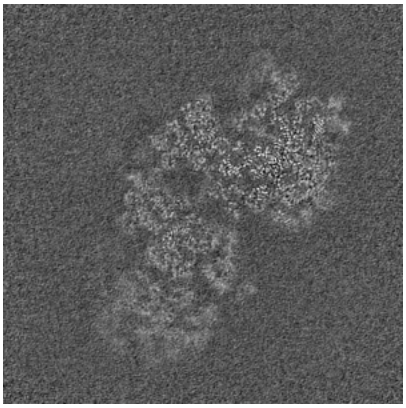


Y Index: 175

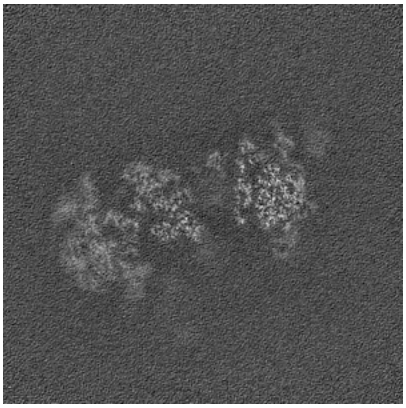


Z Index: 175

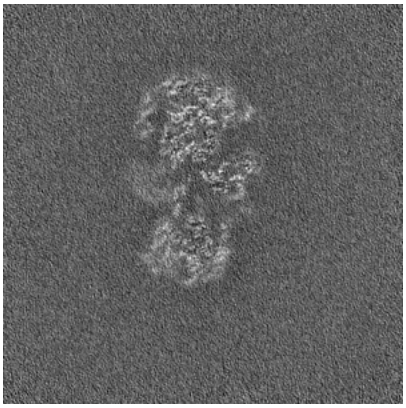
6.2.2 Raw map



X Index: 175



Y Index: 175

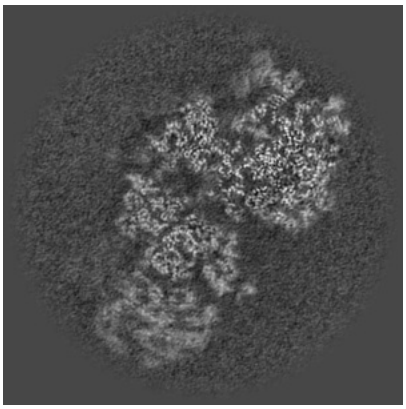


Z Index: 175

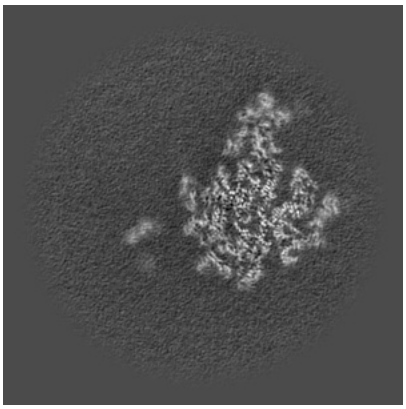
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

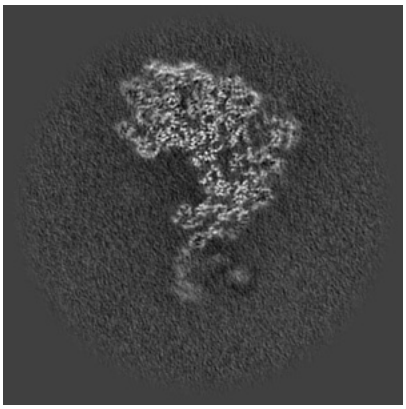
6.3.1 Primary map



X Index: 176

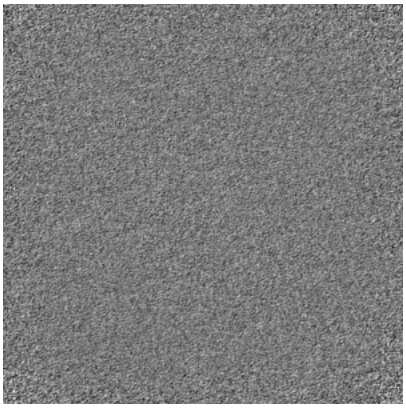


Y Index: 236

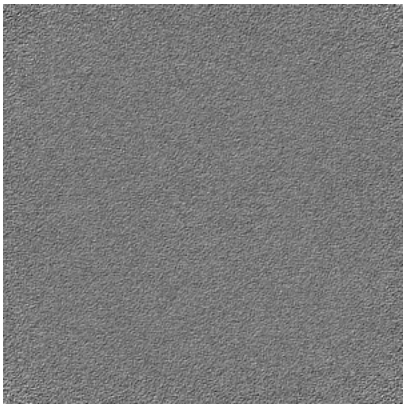


Z Index: 211

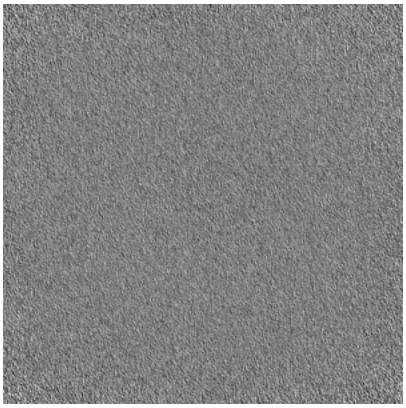
6.3.2 Raw map



X Index: 0



Y Index: 0

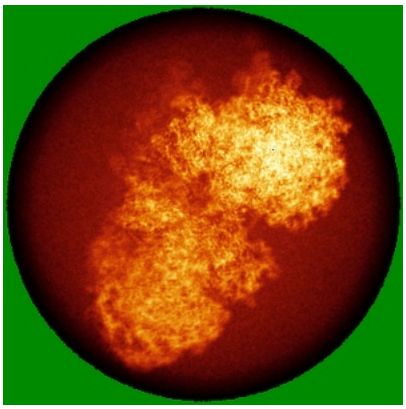


Z Index: 0

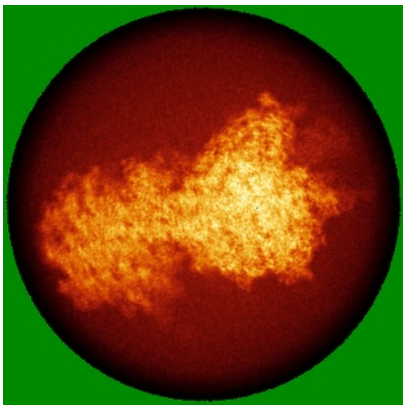
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

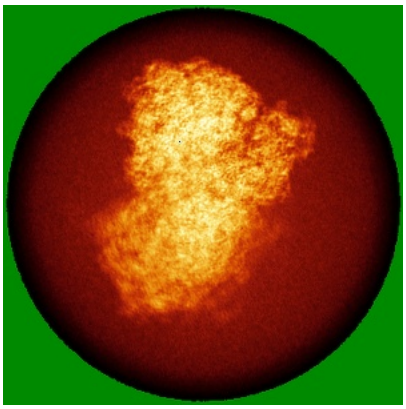
6.4.1 Primary map



X

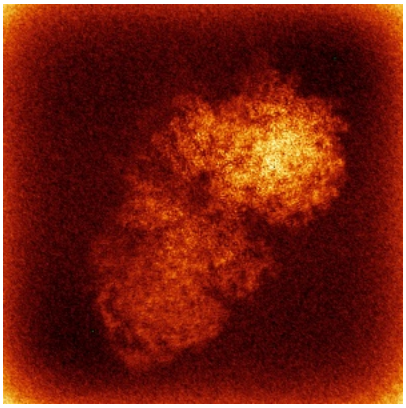


Y

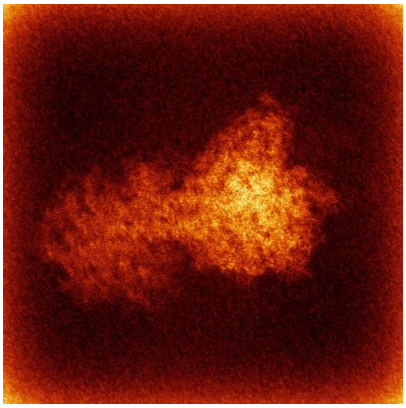


Z

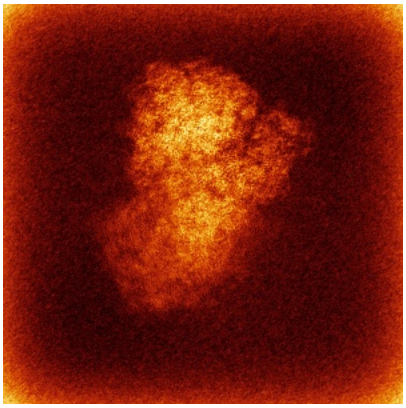
6.4.2 Raw map



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.

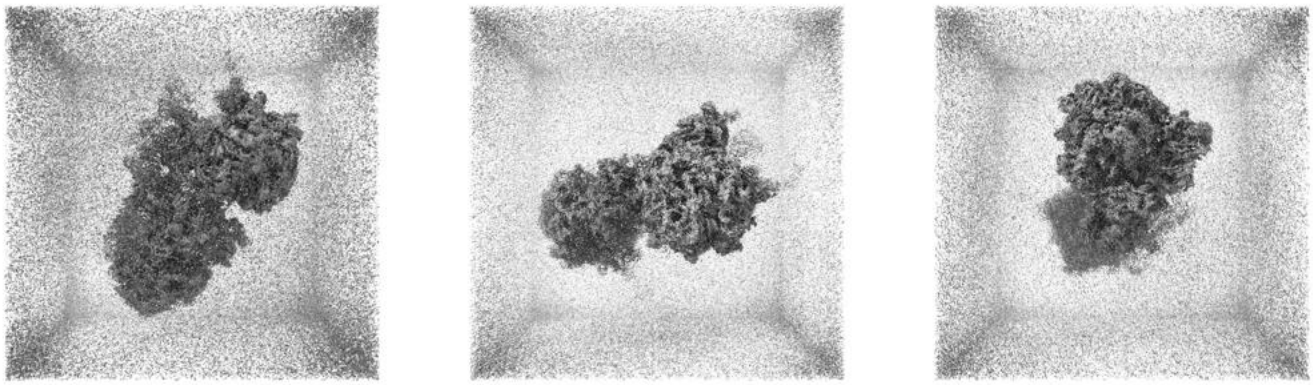
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.32. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

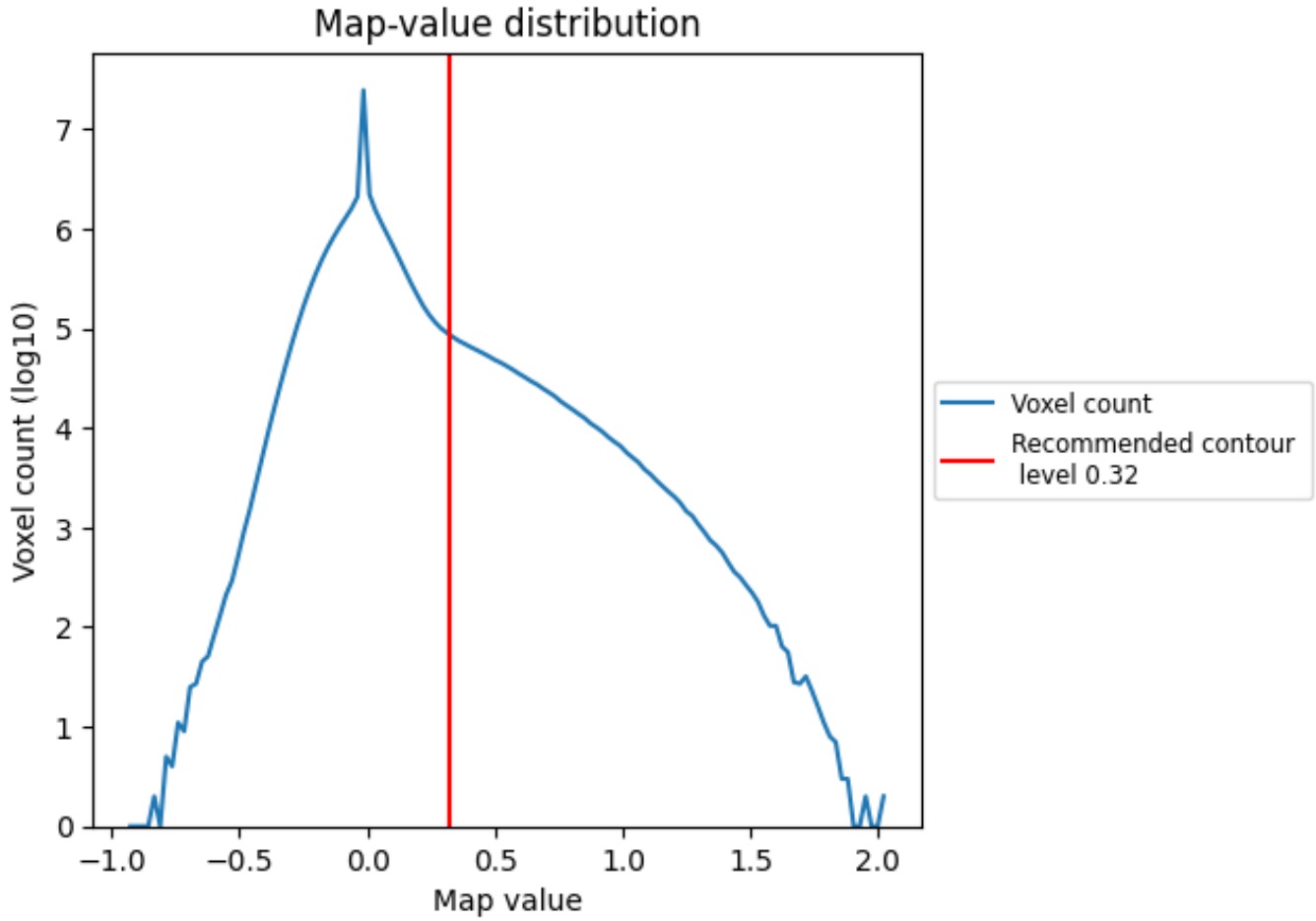
6.6 Mask visualisation (i)

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

7 Map analysis

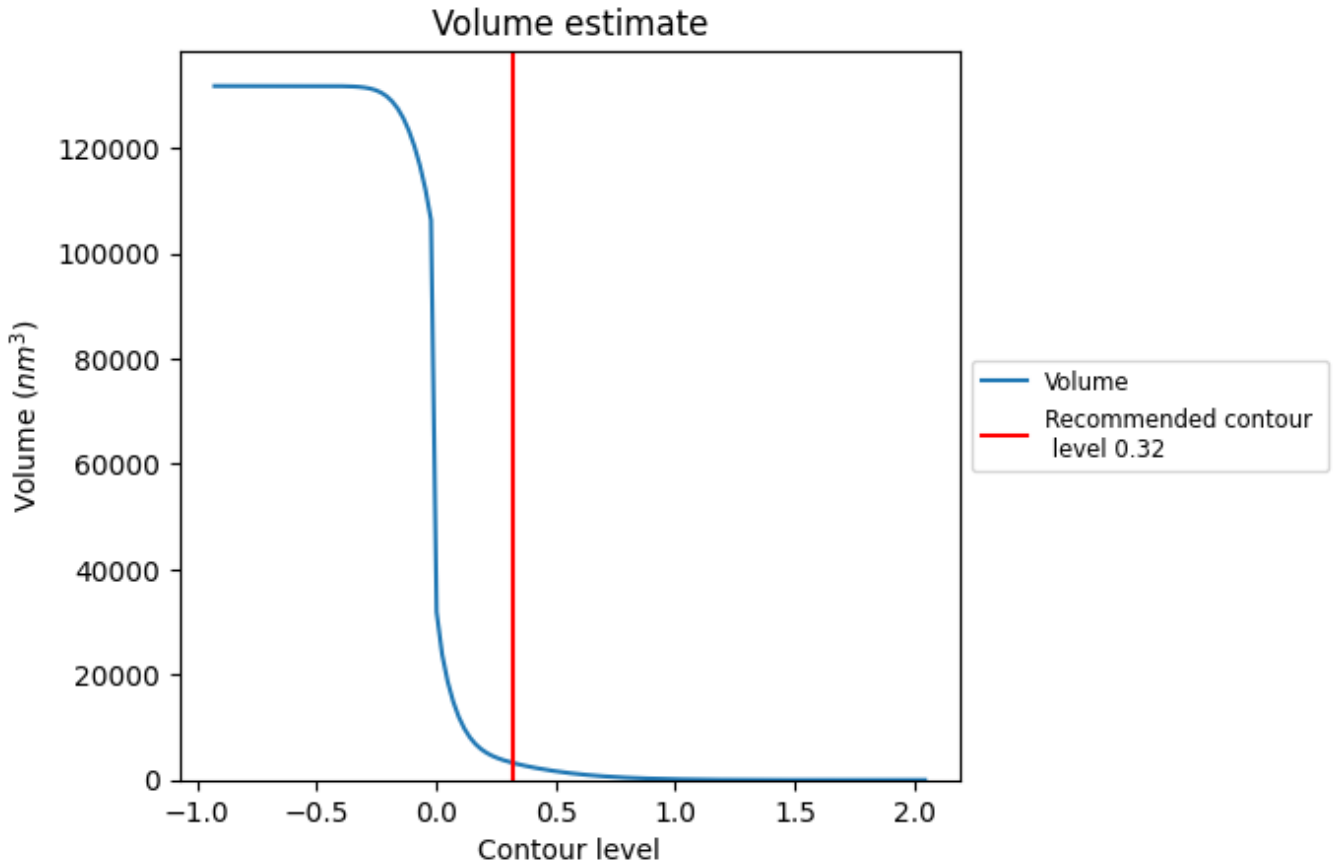
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

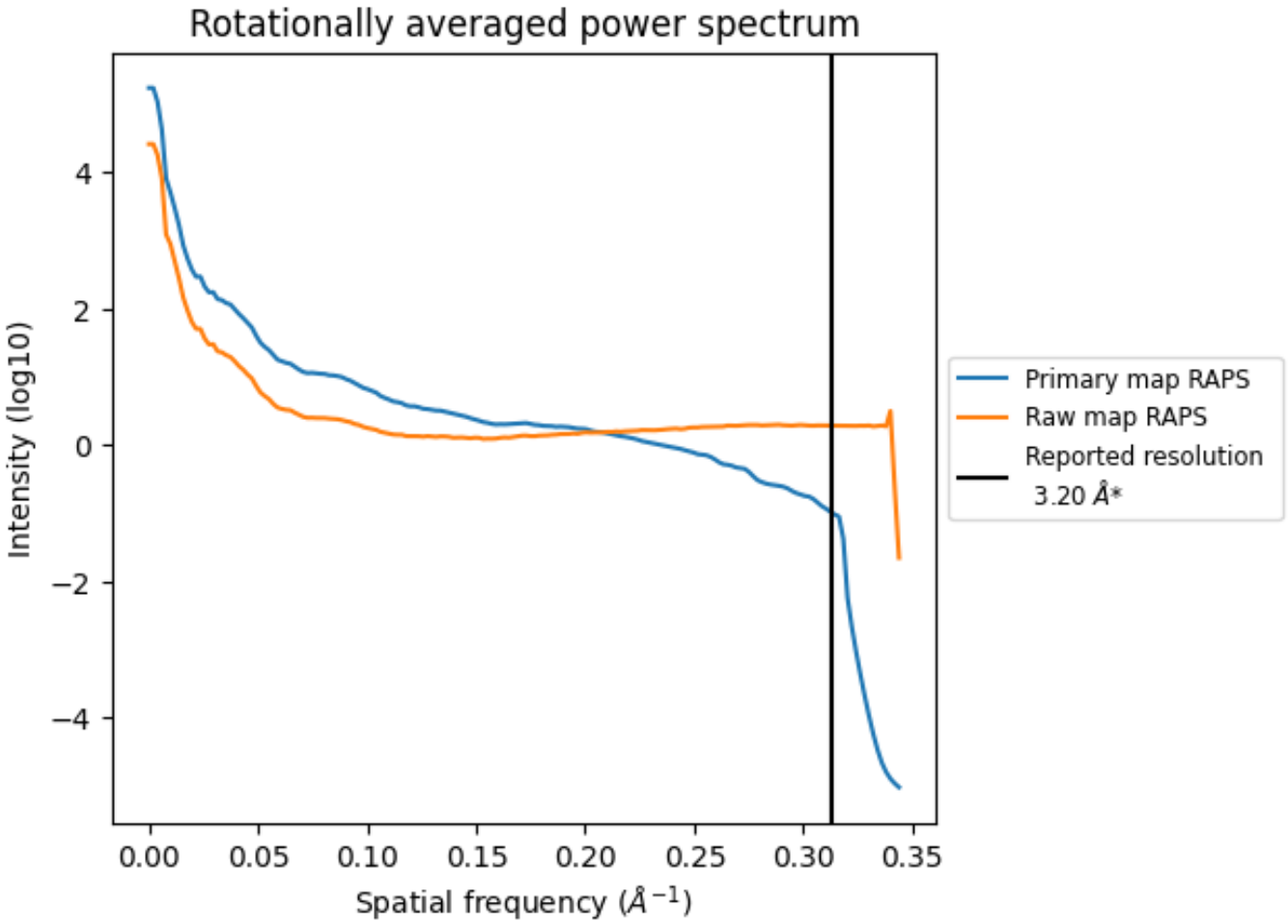
7.2 Volume estimate



The volume at the recommended contour level is 3255 nm^3; this corresponds to an approximate mass of 2940 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 (i)

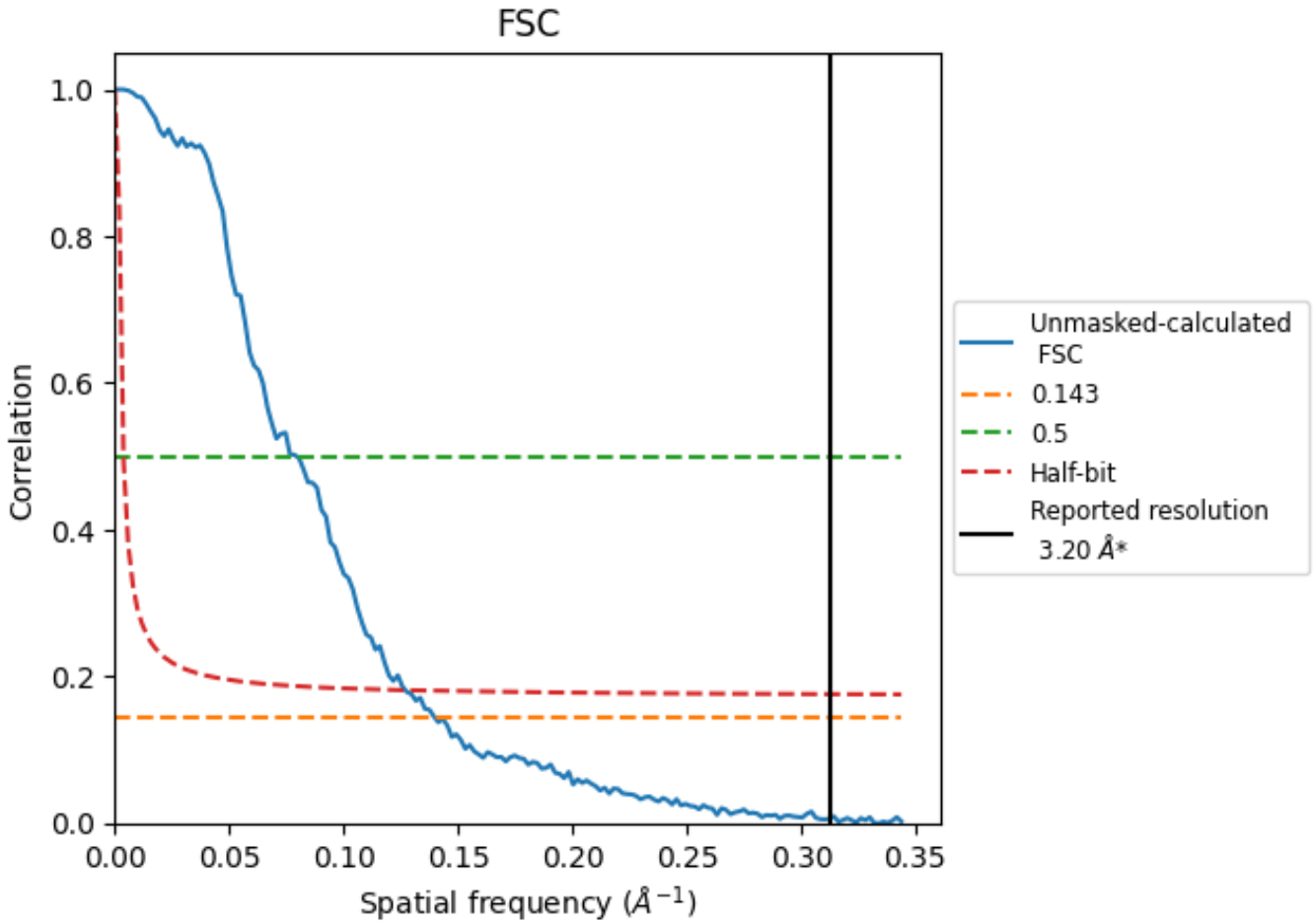


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8.2 Resolution estimates (i)

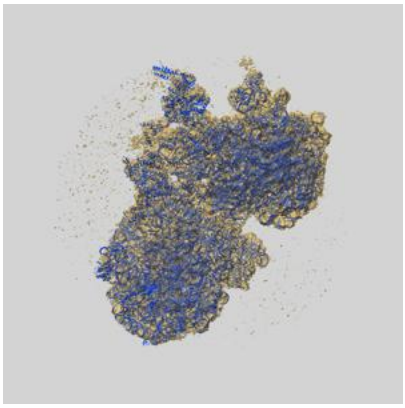
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.14	12.61	7.87

*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 7.14 differs from the reported value 3.2 by more than 10 %

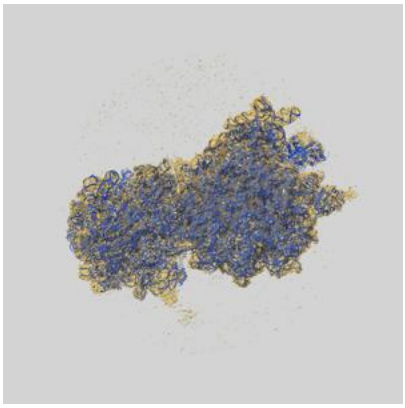
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-51340 and PDB model 9GGR. Per-residue inclusion information can be found in section 3 on page 21.

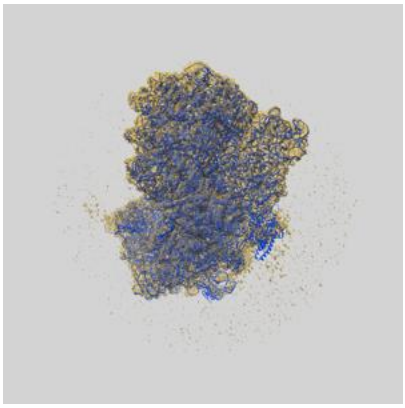
9.1 Map-model overlay



X



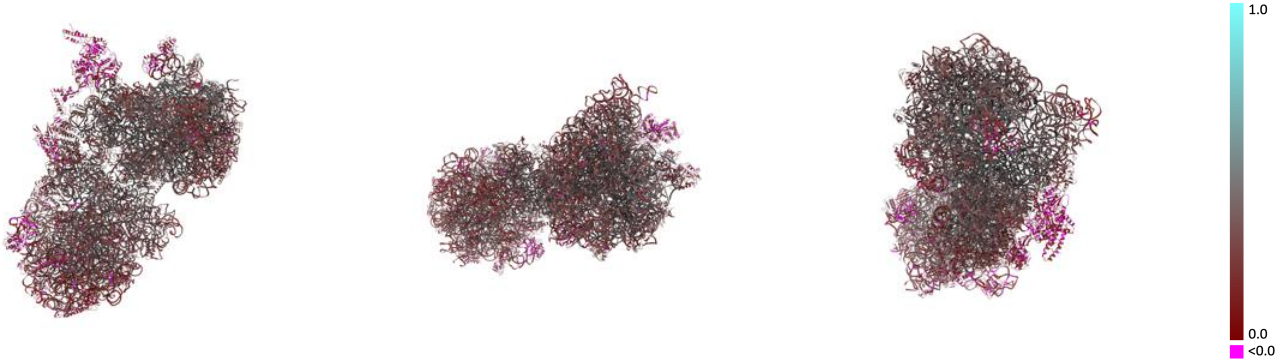
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.32 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.

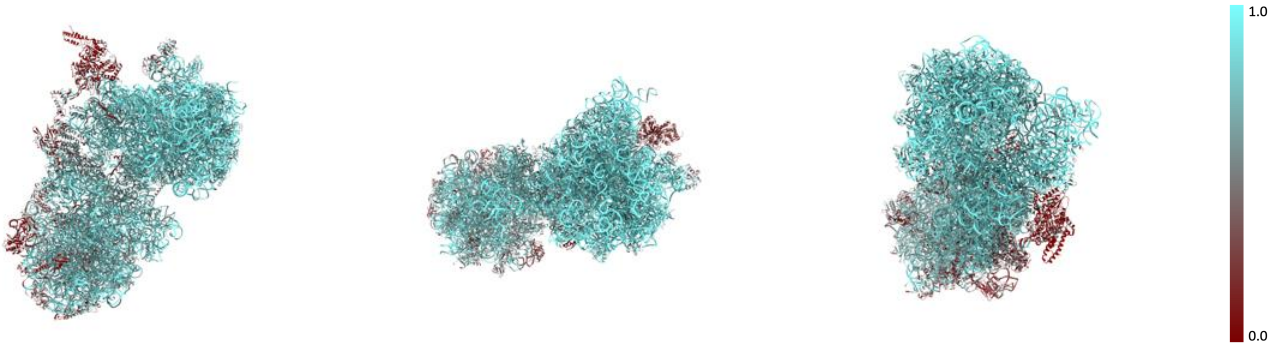
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

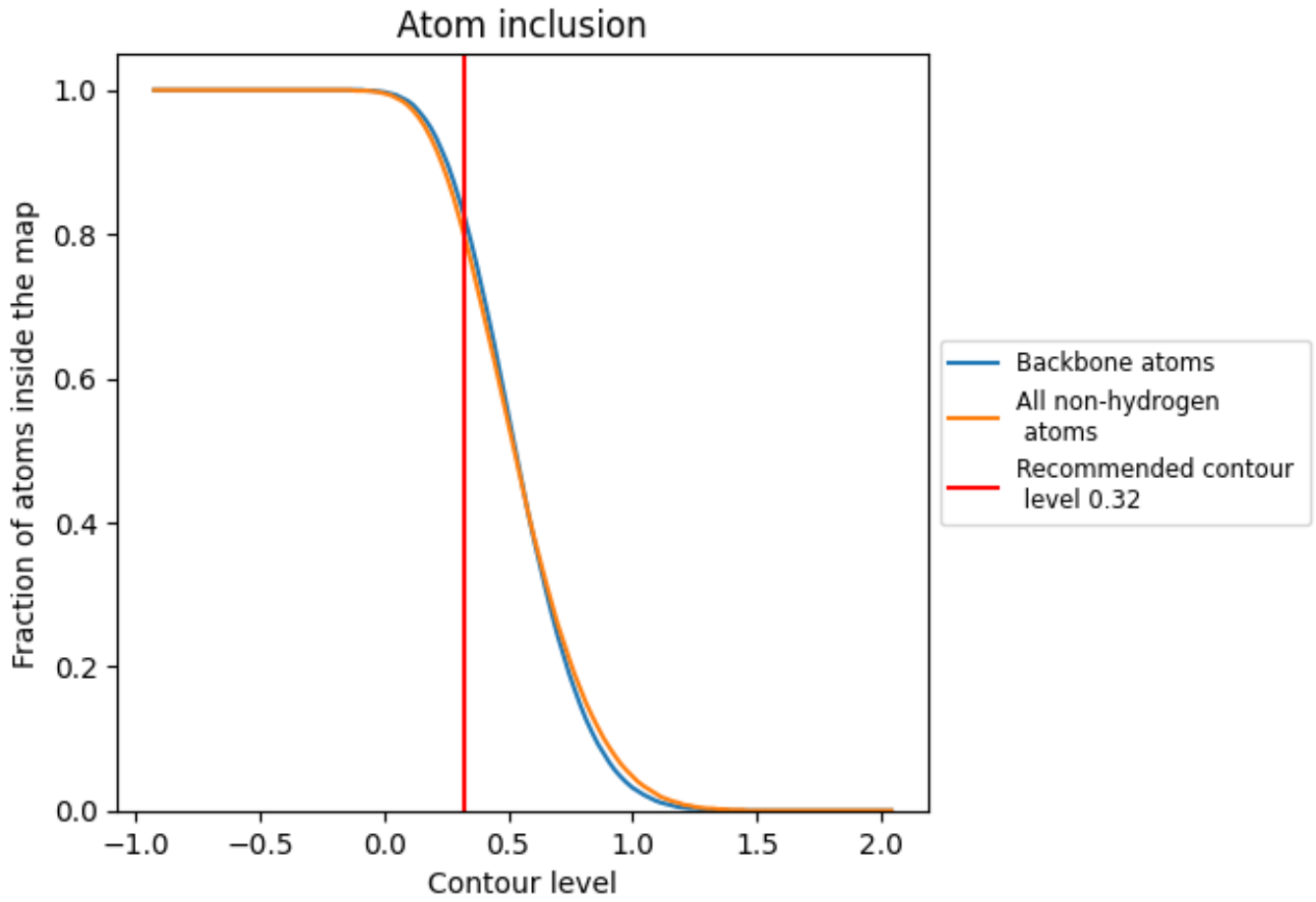
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.32).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 80% 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 (0.32) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8020	0.3110
0	0.9510	0.3720
1	0.6820	0.3260
2	0.6850	0.3590
3	0.6880	0.3110
4	0.7500	0.3820
5	0.7390	0.3720
6	0.7290	0.3850
7	0.7490	0.3500
8	0.7130	0.3610
9	0.6060	0.3570
A	0.9240	0.3910
A1	0.5590	0.2950
A2	0.4000	0.2130
A3	0.6820	0.2620
AA	0.9350	0.3460
AB	0.6460	0.3140
AC	0.6560	0.3730
AD	0.6500	0.3880
AE	0.7020	0.3890
AF	0.6220	0.2620
AG	0.6440	0.2980
AH	0.6500	0.3050
AI	0.6680	0.3000
AJ	0.6690	0.3560
AK	0.0200	0.1160
AL	0.6320	0.2510
AM	0.6880	0.3160
AN	0.6910	0.2400
AO	0.7000	0.3260
AP	0.6580	0.2750
AQ	0.6370	0.2720
AR	0.6990	0.2710
AS	0.7050	0.2320
AT	0.4440	0.2180

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
AU	0.5880	0.2780
AV	0.8350	0.2520
AW	0.7900	0.1910
AX	0.5120	0.2560
AY	0.5760	0.2580
AZ	0.4250	0.2030
Aa	0.3940	0.2120
Ab	0.4630	0.1890
Ac	0.1300	0.1490
Ad	0.1590	0.0850
Ae	0.6720	0.2260
Af	0.5510	0.3320
Ag	0.5470	0.2600
Ah	0.5830	0.2730
Ai	0.7090	0.2300
Aj	0.3910	0.1750
Ak	0.5330	0.2650
Al	0.7000	0.2100
Am	0.6260	0.1960
An	0.6720	0.2650
Ao	0.5420	0.1850
Ap	0.2360	0.1650
Aq	0.6270	0.1770
Ar	0.7050	0.2260
As	0.6340	0.2540
At	0.5110	0.1510
Au	0.6150	0.2230
Av	0.7500	0.2490
Aw	0.3740	0.2300
Ax	0.7010	0.2720
Ay	0.6640	0.2690
Az	0.6370	0.2730
B	0.2610	0.1590
C	0.1960	0.1290
D	0.7330	0.4350
E	0.8180	0.4410
F	0.7720	0.3150
G	0.7530	0.3510
H	0.7930	0.3290
I	0.7200	0.3080
J	0.7480	0.3100
K	0.7350	0.4030

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
L	0.7480	0.2670
M	0.9480	0.4000
N	0.9420	0.3650
O	0.9610	0.3170
P	0.7950	0.4250
Q	0.8560	0.4130
R	0.7850	0.3250
S	0.7530	0.3120
T	0.8350	0.3670
U	0.6810	0.3270
V	0.3590	0.1110
W	0.8930	0.4000
X	0.8010	0.4370
Y	0.7850	0.3660
Z	0.8530	0.4490
a	0.8380	0.3170
b	0.7680	0.2700
c	0.7520	0.3440
d	0.8500	0.3680
e	0.8420	0.3720
f	0.7790	0.3360
g	0.7370	0.2950
h	0.6940	0.2710
i	0.8420	0.3390
j	0.8680	0.4060
k	0.8270	0.4170
l	0.7560	0.2720
m	0.8600	0.3640
n	0.8790	0.3330
o	0.7560	0.3650
p	0.7940	0.3690
q	0.7820	0.4010
r	0.8600	0.4480
s	0.8020	0.4170
t	0.8070	0.3610
u	0.7190	0.2470
v	0.6350	0.3610
w	0.4820	0.2710
x	0.5730	0.1820
y	0.6060	0.2700
z	0.7290	0.4200