wwPDB X-ray Structure Validation Summary Report (i)

Sep 17, 2023 – 10:38 PM EDT

PDB ID	:	4XEJ
Title	:	IRES bound to bacterial Ribosome
Authors	:	Zhu, J.; Korostelev, A.; Noller, H.F.; Donohue, J.P.
Deposited on	:	2014-12-23
Resolution	:	3.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

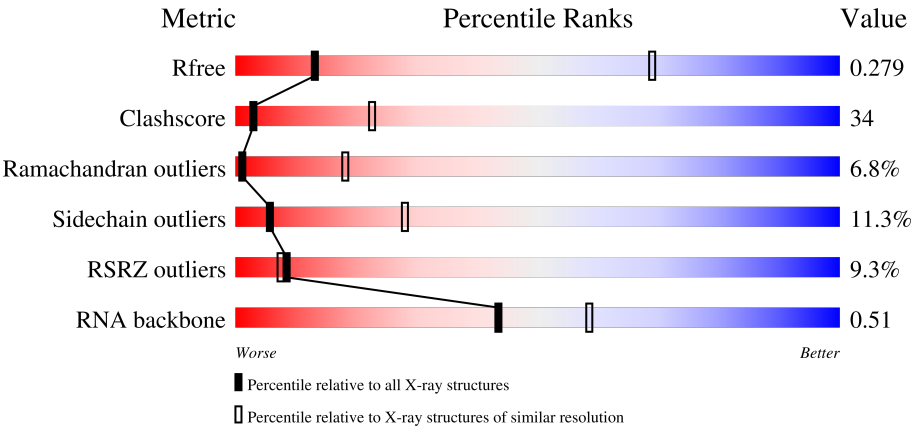
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)
RNA backbone	3102	1036 (4.60-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AL02	271	82% 17%
1	BL02	271	77% 21%
2	AL03	204	3% 80% 19%
2	BL03	204	3% 77% 21%

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Mol	Chain	Length	Quality of chain
3	AL04	202	2% 87% 13%
3	BL04	202	2% 82% 17%
4	AL05	181	30% 83% 15%
4	BL05	181	28% 82% 16%
5	AL06	159	38% 91% 9%
5	BL06	159	6% 84% 16%
6	AL09	145	30% 80% 19%
6	BL09	145	14% 81% 17%
7	AL11	147	80% 90% 10%
7	BL11	147	77% 90% 10%
8	AL13	137	6% 77% 21%
8	BL13	137	4% 77% 21%
9	AL14	122	84% 15%
9	BL14	122	2% 84% 15%
10	AL15	146	5% 64% 28% 8%
10	BL15	146	9% 68% 27% 5%
11	AL16	134	7% 86% 13%
11	BL16	134	8% 80% 18%
12	AL17	117	7% 81% 19%
12	BL17	117	2% 84% 15%
13	AL18	98	27% 81% 18%
13	BL18	98	17% 82% 16%
14	AL19	137	5% 76% 23%
14	BL19	137	3% 81% 15%
15	AL20	117	2% 84% 15%

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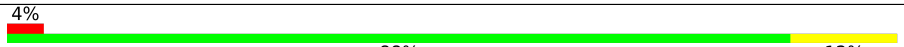
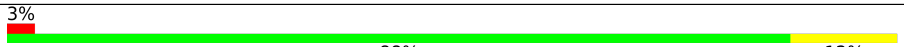
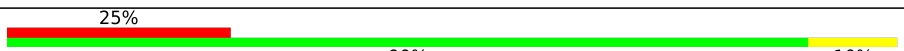
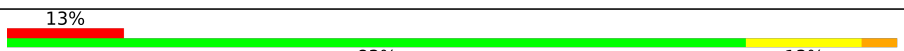
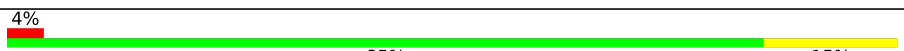
Mol	Chain	Length	Quality of chain
15	BL20	117	
16	AL21	101	
16	BL21	101	
17	AL22	112	
17	BL22	112	
18	AL23	92	
18	BL23	92	
19	AL24	100	
19	BL24	100	
20	AL25	187	
20	BL25	187	
21	AL27	76	
21	BL27	76	
22	AL28	88	
22	BL28	88	
23	AL29	62	
23	BL29	62	
24	AL30	59	
24	BL30	59	
25	AL32	52	
25	BL32	52	
26	AL33	44	
26	BL33	44	
27	AL34	48	
27	BL34	48	

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Mol	Chain	Length	Quality of chain
28	AL35	63	2% 83% 14%
28	BL35	63	2% 81% 17%
29	AS02	234	9% 88% 12%
29	BS02	234	11% 91% 8%
30	AS03	206	7% 84% 14%
30	BS03	206	6% 88% 12%
31	AS04	208	2% 87% 12%
31	BS04	208	15% 85% 15%
32	AS05	151	3% 87% 12%
32	BS05	151	3% 89% 11%
33	AS06	101	5% 88% 11%
33	BS06	101	2% 87% 13%
34	AS07	155	21% 95% 5%
34	BS07	155	19% 95% 5%
35	AS08	138	9% 88% 11%
35	BS08	138	10% 91% 9%
36	AS09	127	30% 89% 10%
36	BS09	127	24% 91% 9%
37	AS10	98	50% 88% 11%
37	BS10	98	34% 90% 10%
38	AS11	114	11% 87% 13%
38	BS11	114	3% 89% 11%
39	AS12	122	10% 88% 12%
39	BS12	122	7% 89% 10%
40	AS13	117	35% 97%

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Mol	Chain	Length	Quality of chain
40	BS13	117	26% 92% 8%
41	AS14	60	18% 93% 5%
41	BS14	60	15% 92% 8%
42	AS15	88	6% 89% 11%
42	BS15	88	6% 86% 14%
43	AS16	83	14% 83% 17%
43	BS16	83	33% 93% 7%
44	AS17	99	3% 86% 14%
44	BS17	99	3% 89% 10%
45	AS18	70	13% 90% 10%
45	BS18	70	% 84% 16%
46	AS19	78	49% 87% 12%
46	BS19	78	36% 85% 14%
47	AS20	99	9% 86% 14%
47	BS20	99	22% 92% 8%
48	ATHX	24	4% 96%
48	BTHX	24	33% 92% 8%
49	AL31	30	43% 90% 10%
49	BL31	30	37% 87% 10%
50	A16S	1506	3% 83% 17%
50	B16S	1506	4% 83% 17%
51	A23S	2879	4% 81% 19%
51	B23S	2879	4% 80% 20%
52	A5S	119	% 27% 61% 13%
52	B5S	119	% 25% 66% 9%

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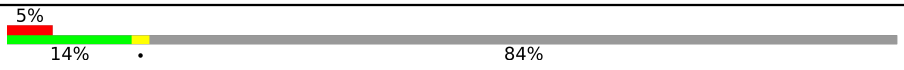
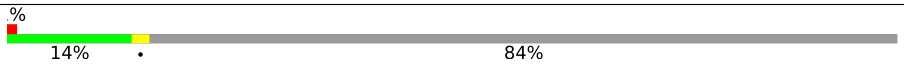
Mol	Chain	Length	Quality of chain
53	AIRE	196	
53	BIRE	196	

2 Entry composition (i)

There are 54 unique types of molecules in this entry. The entry contains 287293 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AL02	271	Total	C	N	O	S	0	0	0
			2105	1329	416	357	3			
1	BL02	271	Total	C	N	O	S	0	0	0
			2105	1329	416	357	3			

- Molecule 2 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AL03	204	Total	C	N	O	S	0	0	0
			1564	988	299	271	6			
2	BL03	204	Total	C	N	O	S	0	0	0
			1564	988	299	271	6			

- Molecule 3 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AL04	202	Total	C	N	O	S	0	0	0
			1587	1011	297	276	3			
3	BL04	202	Total	C	N	O	S	0	0	0
			1587	1011	297	276	3			

- Molecule 4 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AL05	181	Total	C	N	O	S	0	0	0
			1475	943	268	260	4			
4	BL05	181	Total	C	N	O	S	0	0	0
			1475	943	268	260	4			

- Molecule 5 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AL06	159	Total	C	N	O	S	0	0	0
			1223	773	228	221	1			
5	BL06	159	Total	C	N	O	S	0	0	0
			1223	773	228	221	1			

- Molecule 6 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AL09	145	Total	C	N	O	S	0	0	0
			1133	724	200	208	1			
6	BL09	145	Total	C	N	O	S	0	0	0
			1133	724	200	208	1			

- Molecule 7 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AL11	147	Total	C	N	O	S	0	0	0
			1088	692	191	199	6			
7	BL11	147	Total	C	N	O	S	0	0	0
			1088	692	191	199	6			

- Molecule 8 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AL13	137	Total	C	N	O	S	0	0	0
			1097	707	205	182	3			
8	BL13	137	Total	C	N	O	S	0	0	0
			1097	707	205	182	3			

- Molecule 9 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AL14	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			
9	BL14	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			

- Molecule 10 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AL15	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	BL15	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 11 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AL16	134	Total	C	N	O	S	0	0	0
			1065	680	201	179	5			
11	BL16	134	Total	C	N	O	S	0	0	0
			1065	680	201	179	5			

- Molecule 12 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	AL17	117	Total	C	N	O	0	0	0
			960	599	202	159			
12	BL17	117	Total	C	N	O	0	0	0
			960	599	202	159			

- Molecule 13 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	AL18	98	Total	C	N	O	0	0	0
			771	486	154	131			
13	BL18	98	Total	C	N	O	0	0	0
			771	486	154	131			

- Molecule 14 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AL19	137	Total	C	N	O	S	0	0	0
			1144	713	234	196	1			
14	BL19	137	Total	C	N	O	S	0	0	0
			1144	713	234	196	1			

- Molecule 15 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AL20	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
15	BL20	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 16 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AL21	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
16	BL21	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 17 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AL22	112	Total	C	N	O	S	0	0	0
			891	560	175	154	2			
17	BL22	112	Total	C	N	O	S	0	0	0
			891	560	175	154	2			

- Molecule 18 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AL23	92	Total	C	N	O	0	0	0
			726	471	131	124			
18	BL23	92	Total	C	N	O	0	0	0
			726	471	131	124			

- Molecule 19 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AL24	100	Total	C	N	O	S	0	0	0
			776	500	148	124	4			
19	BL24	100	Total	C	N	O	S	0	0	0
			776	500	148	124	4			

- Molecule 20 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AL25	187	Total	C	N	O	S	0	0	0
			1483	945	264	272	2			
20	BL25	187	Total	C	N	O	S	0	0	0
			1483	945	264	272	2			

- Molecule 21 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AL27	76	Total	C	N	O	S	0	0	0
			605	376	126	102	1			
21	BL27	76	Total	C	N	O	S	0	0	0
			605	376	126	102	1			

- Molecule 22 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	AL28	88	Total	C	N	O	0	0	0
			695	435	141	119			
22	BL28	88	Total	C	N	O	0	0	0
			695	435	141	119			

- Molecule 23 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AL29	62	Total	C	N	O	S	0	0	0
			521	325	102	92	2			
23	BL29	62	Total	C	N	O	S	0	0	0
			521	325	102	92	2			

- Molecule 24 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AL30	59	Total	C	N	O	S	0	0	0
			468	298	90	79	1			
24	BL30	59	Total	C	N	O	S	0	0	0
			468	298	90	79	1			

- Molecule 25 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	AL32	52	Total	C	N	O	S	0	0	0
			405	255	79	66	5			
25	BL32	52	Total	C	N	O	S	0	0	0
			405	255	79	66	5			

- Molecule 26 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	AL33	44	Total	C	N	O	S	0	0	0
			381	235	77	65	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BL33	44	Total	C	N	O	S	0	0	0
			381	235	77	65	4			

- Molecule 27 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	AL34	48	Total	C	N	O	S	0	0	0
			419	257	104	56	2			
27	BL34	48	Total	C	N	O	S	0	0	0
			419	257	104	56	2			

- Molecule 28 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	AL35	63	Total	C	N	O	S	0	0	0
			508	326	101	79	2			
28	BL35	63	Total	C	N	O	S	0	0	0
			508	326	101	79	2			

- Molecule 29 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	AS02	234	Total	C	N	O	S	0	0	0
			1901	1213	341	342	5			
29	BS02	234	Total	C	N	O	S	0	0	0
			1901	1213	341	342	5			

- Molecule 30 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	AS03	206	Total	C	N	O	S	0	0	0
			1613	1016	314	282	1			
30	BS03	206	Total	C	N	O	S	0	0	0
			1613	1016	314	282	1			

- Molecule 31 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	AS04	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
31	BS04	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 32 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	AS05	151	Total	C	N	O	S	0	0	0
			1156	729	218	205	4			
32	BS05	151	Total	C	N	O	S	0	0	0
			1156	729	218	205	4			

- Molecule 33 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	AS06	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
33	BS06	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 34 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	AS07	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
34	BS07	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 35 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	AS08	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
35	BS08	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 36 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
36	AS09	127	Total	C	N	O	0	0	0
			1011	639	198	174			
36	BS09	127	Total	C	N	O	0	0	0
			1011	639	198	174			

- Molecule 37 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	AS10	98	Total	C	N	O	S	0	0	0
			795	499	156	139	1			
37	BS10	98	Total	C	N	O	S	0	0	0
			795	499	156	139	1			

- Molecule 38 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	AS11	114	Total	C	N	O	S	0	0	0
			843	522	159	159	3			
38	BS11	114	Total	C	N	O	S	0	0	0
			843	522	159	159	3			

- Molecule 39 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	AS12	122	Total	C	N	O	S	0	0	0
			957	603	193	160	1			
39	BS12	122	Total	C	N	O	S	0	0	0
			957	603	193	160	1			

- Molecule 40 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	AS13	117	Total	C	N	O	S	0	0	0
			934	577	192	163	2			
40	BS13	117	Total	C	N	O	S	0	0	0
			934	577	192	163	2			

- Molecule 41 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	AS14	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
41	BS14	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 42 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	AS15	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BS15	88	Total 734	C 459	N 147	O 126	S 2	0	0	0

- Molecule 43 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	AS16	83	Total 701	C 443	N 139	O 118	S 1	0	0	0
43	BS16	83	Total 701	C 443	N 139	O 118	S 1	0	0	0

- Molecule 44 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	AS17	99	Total 824	C 528	N 152	O 142	S 2	0	0	0
44	BS17	99	Total 824	C 528	N 152	O 142	S 2	0	0	0

- Molecule 45 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
45	AS18	70	Total 574	C 367	N 112	O 95	0	0	0
45	BS18	70	Total 574	C 367	N 112	O 95	0	0	0

- Molecule 46 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	AS19	78	Total 630	C 403	N 114	O 111	S 2	0	0	0
46	BS19	78	Total 630	C 403	N 114	O 111	S 2	0	0	0

- Molecule 47 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	AS20	99	Total 762	C 469	N 162	O 129	S 2	0	0	0
47	BS20	99	Total 762	C 469	N 162	O 129	S 2	0	0	0

- Molecule 48 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
48	ATHX	24	Total	C	N	O	0	0	0
			209	128	50	31			
48	BTHX	24	Total	C	N	O	0	0	0
			209	128	50	31			

- Molecule 49 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	AL31	30	Total	C	N	O	S	0	0	0
			226	142	36	44	4			
49	BL31	30	Total	C	N	O	S	0	0	0
			226	142	36	44	4			

- Molecule 50 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	A16S	1504	Total	C	N	O	P	0	0	0
			32332	14391	5994	10444	1503			
50	B16S	1504	Total	C	N	O	P	0	0	0
			32331	14391	5994	10443	1503			

- Molecule 51 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	A23S	2876	Total	C	N	O	P	0	0	0
			61929	27563	11567	19924	2875			
51	B23S	2876	Total	C	N	O	P	0	0	0
			61931	27565	11569	19922	2875			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A23S	1141A	U	C	conflict	GB 46197919
A23S	2825	U	G	conflict	GB 46197919
B23S	1141A	U	C	conflict	GB 46197919
B23S	2825	U	G	conflict	GB 46197919

- Molecule 52 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	A5S	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			
52	B5S	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

- Molecule 53 is a RNA chain called IRES RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	AIRE	32	Total	C	N	O	P	0	0	0
			672	302	114	225	31			
53	BIRE	32	Total	C	N	O	P	0	0	0
			672	302	114	225	31			

- Molecule 54 is ZINC ION (three-letter code: ZN) (formula: Zn).

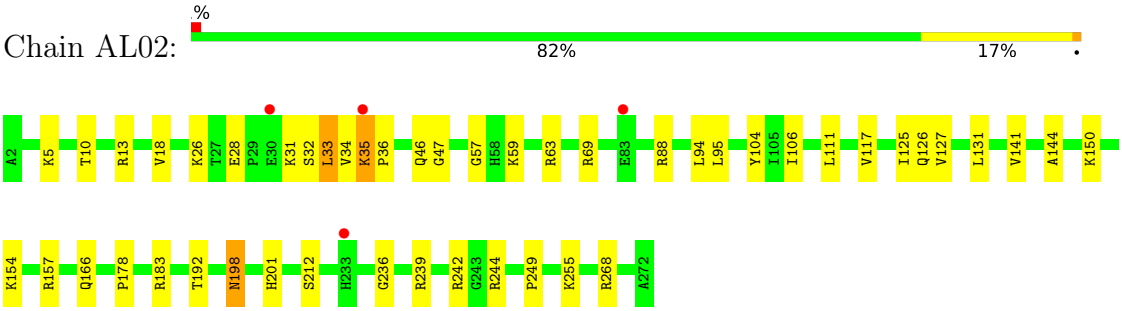
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	AS04	1	Total	Zn	0	0
			1	1		
54	AS14	1	Total	Zn	0	0
			1	1		
54	BS04	1	Total	Zn	0	0
			1	1		
54	BS14	1	Total	Zn	0	0
			1	1		

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 electron 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 dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

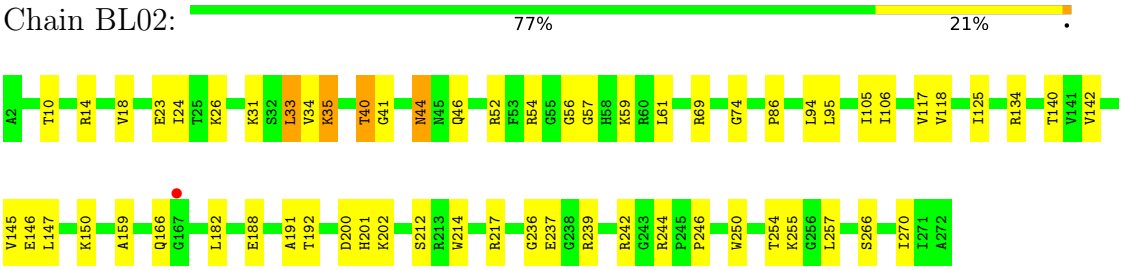
• Molecule 1: 50S ribosomal protein L2

Chain AL02:



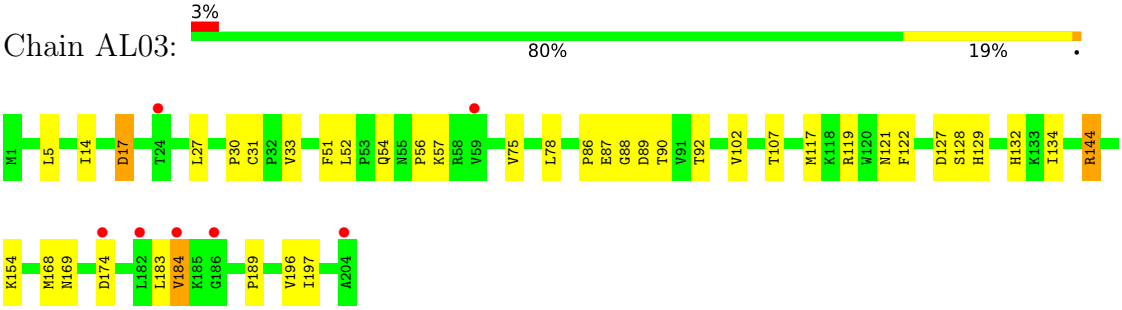
• Molecule 1: 50S ribosomal protein L2

Chain BL02:



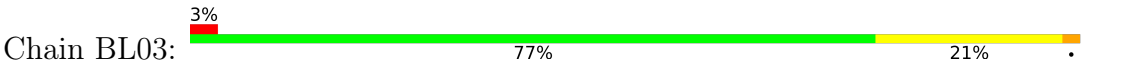
• Molecule 2: 50S ribosomal protein L3

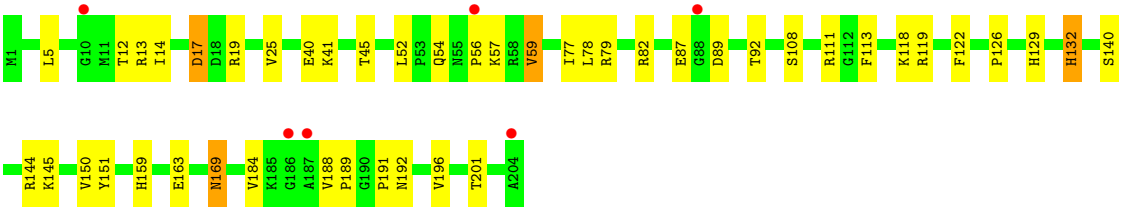
Chain AL03:



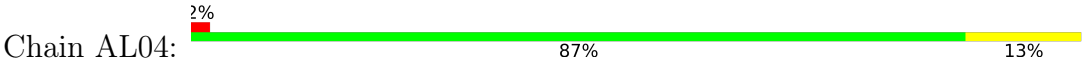
• Molecule 2: 50S ribosomal protein L3

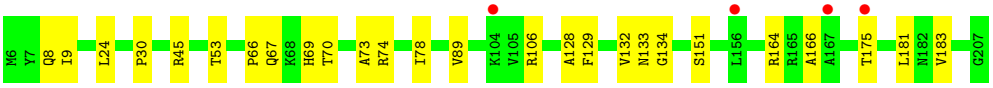
Chain BL03:



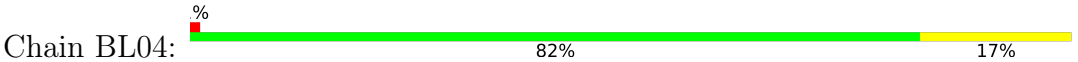


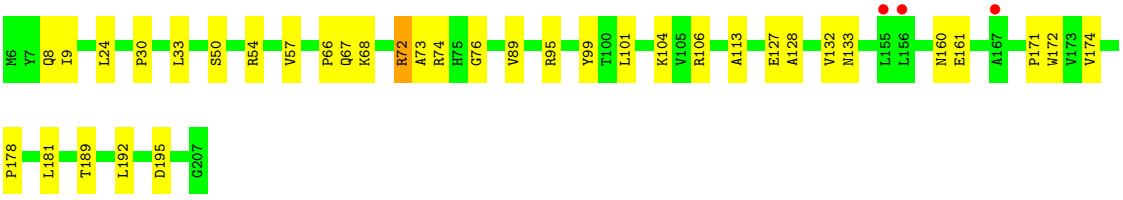
• Molecule 3: 50S ribosomal protein L4



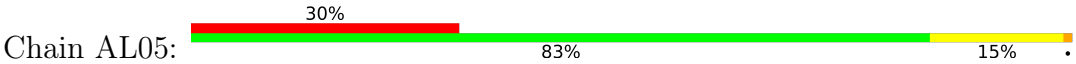


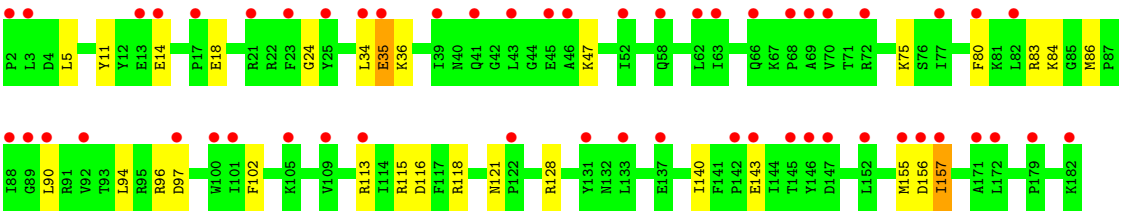
• Molecule 3: 50S ribosomal protein L4



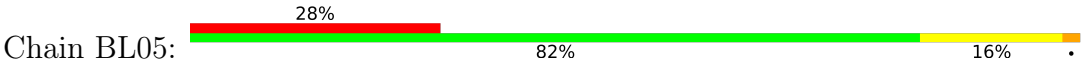


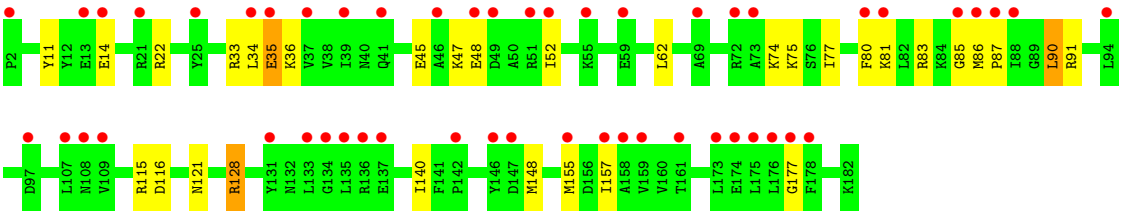
• Molecule 4: 50S ribosomal protein L5



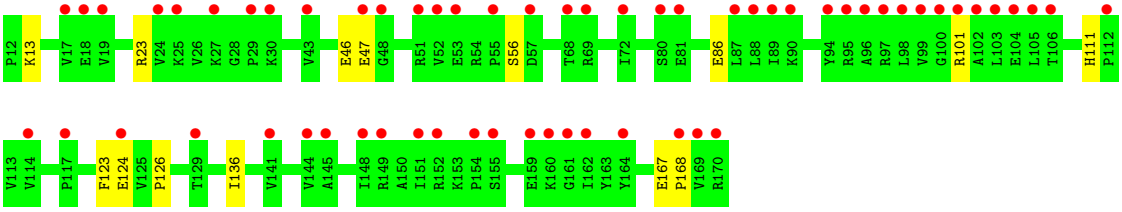


• Molecule 4: 50S ribosomal protein L5



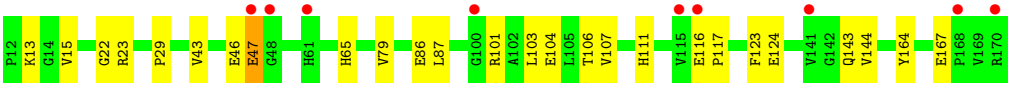


• Molecule 5: 50S ribosomal protein L6



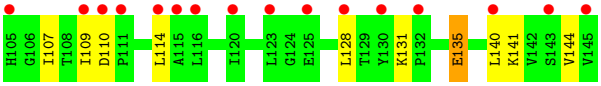
• Molecule 5: 50S ribosomal protein L6

Chain BL06:



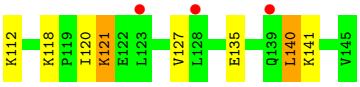
• Molecule 6: 50S ribosomal protein L9

Chain AL09:



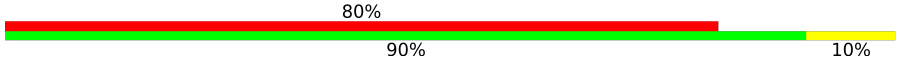
• Molecule 6: 50S ribosomal protein L9

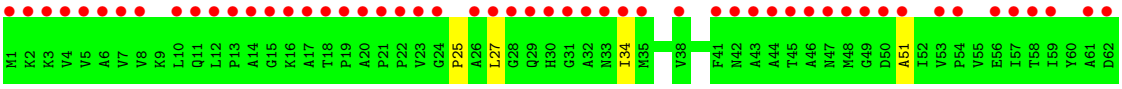
Chain BL09:

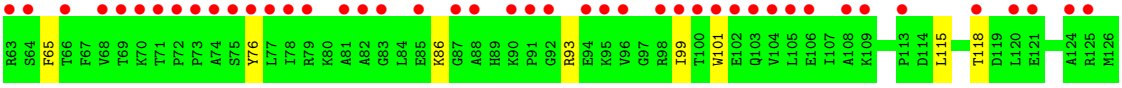


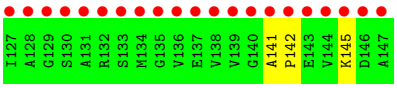
• Molecule 7: 50S ribosomal protein L11

Chain AL11:



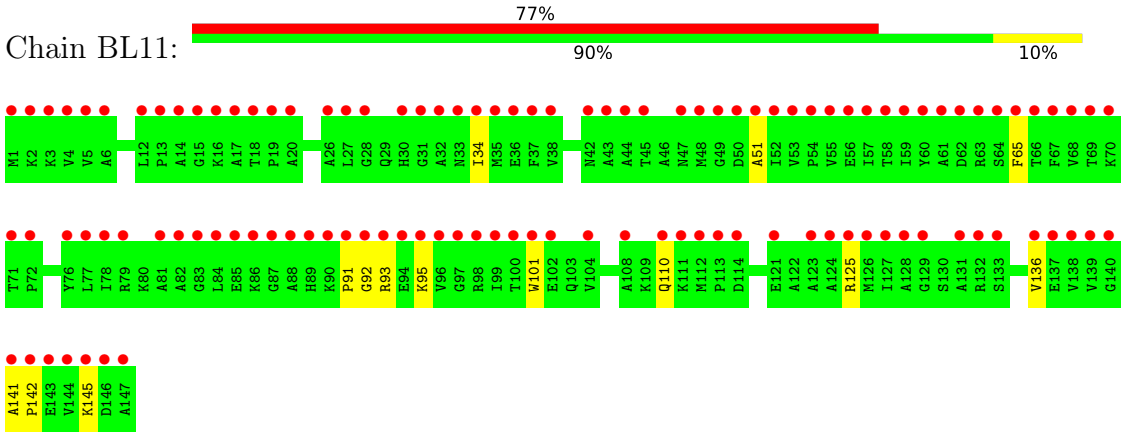






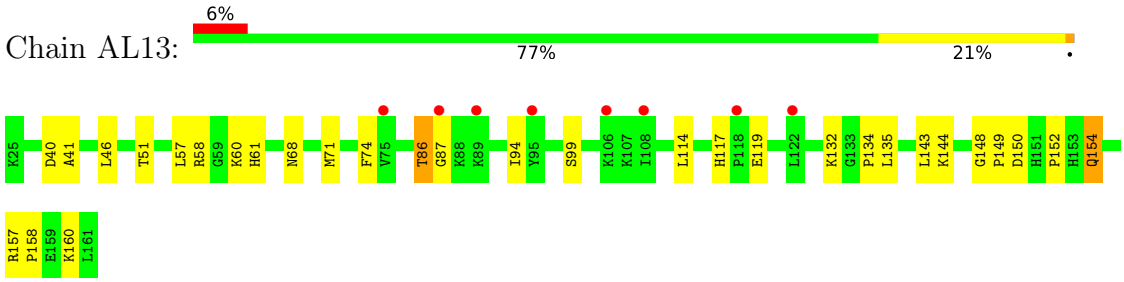
• Molecule 7: 50S ribosomal protein L11

Chain BL11:



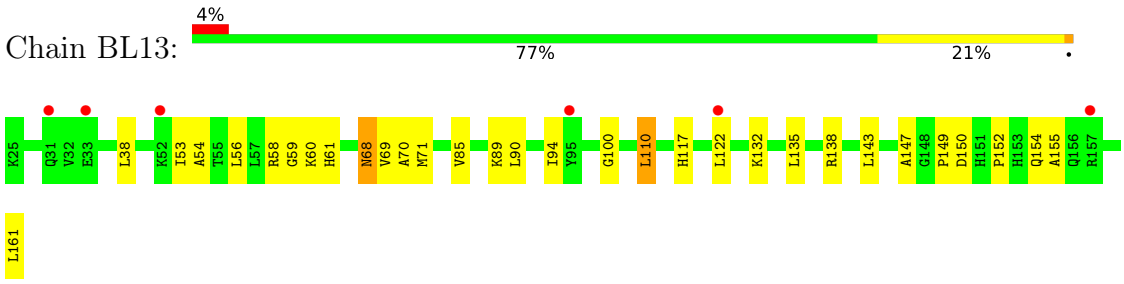
• Molecule 8: 50S ribosomal protein L13

Chain AL13:



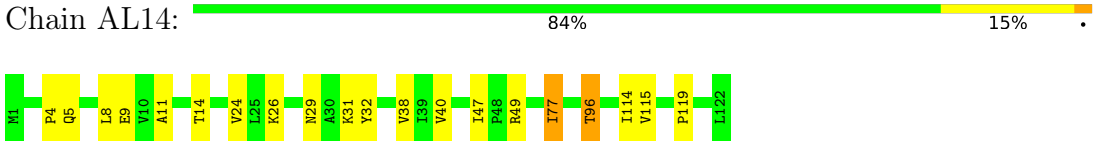
• Molecule 8: 50S ribosomal protein L13

Chain BL13:



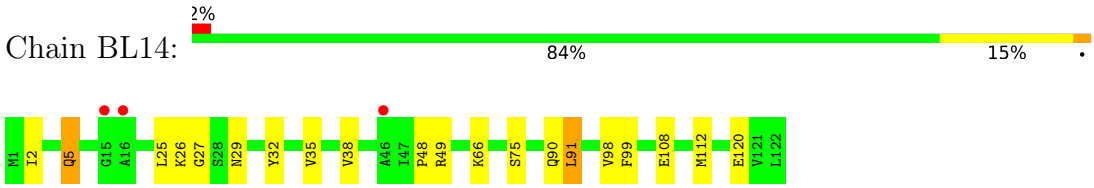
• Molecule 9: 50S ribosomal protein L14

Chain AL14:



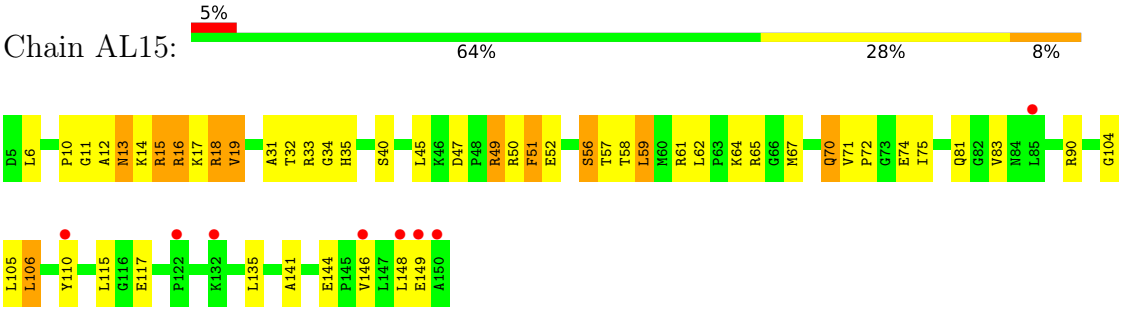
• Molecule 9: 50S ribosomal protein L14

Chain BL14:



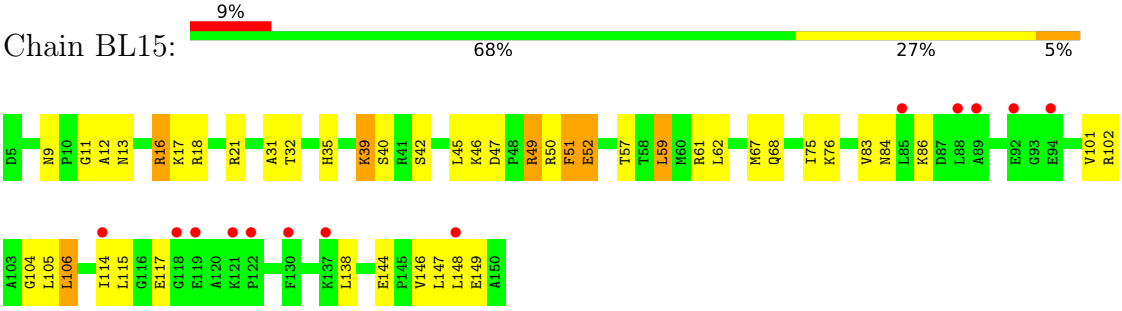
• Molecule 10: 50S ribosomal protein L15

Chain AL15:



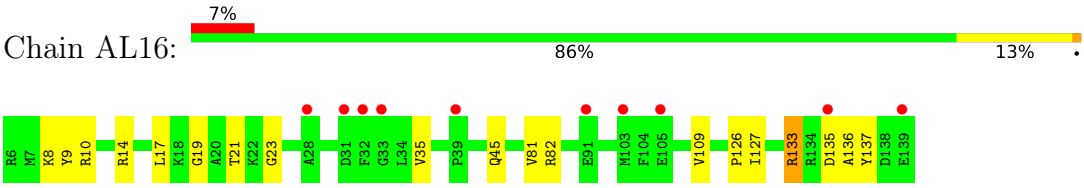
• Molecule 10: 50S ribosomal protein L15

Chain BL15:



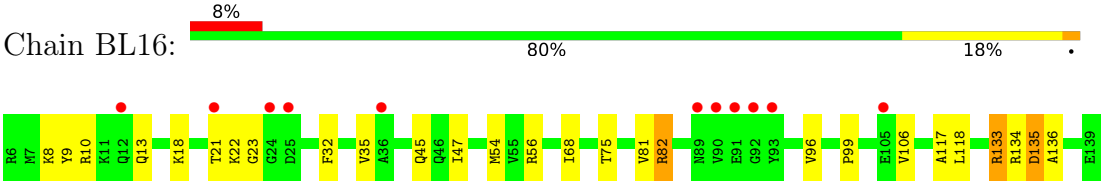
• Molecule 11: 50S ribosomal protein L16

Chain AL16:



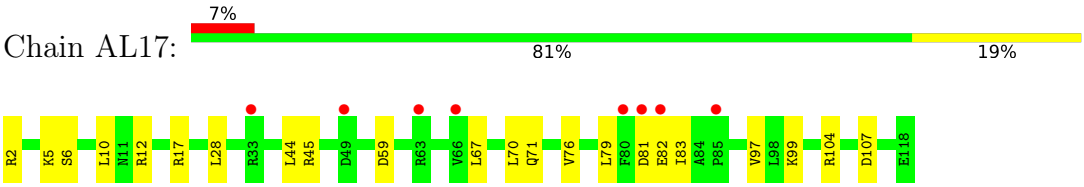
• Molecule 11: 50S ribosomal protein L16

Chain BL16:



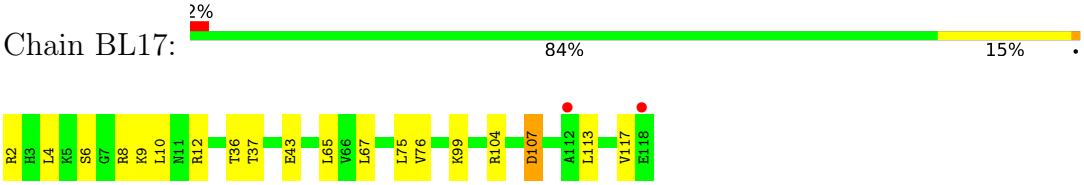
• Molecule 12: 50S ribosomal protein L17

Chain AL17:



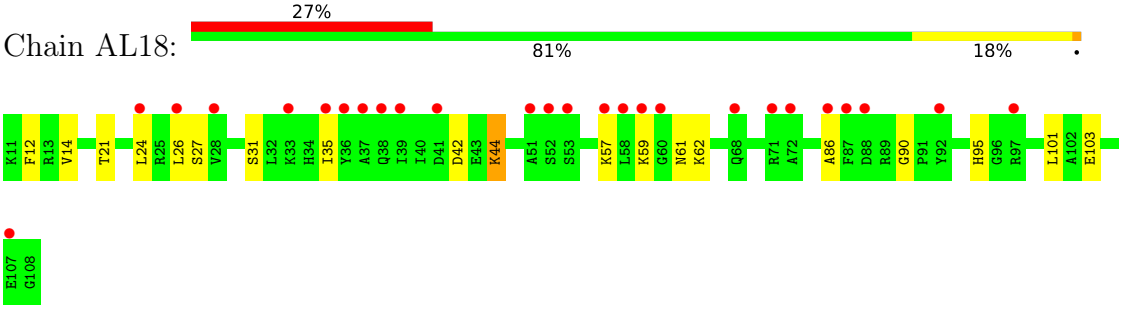
• Molecule 12: 50S ribosomal protein L17

Chain BL17:



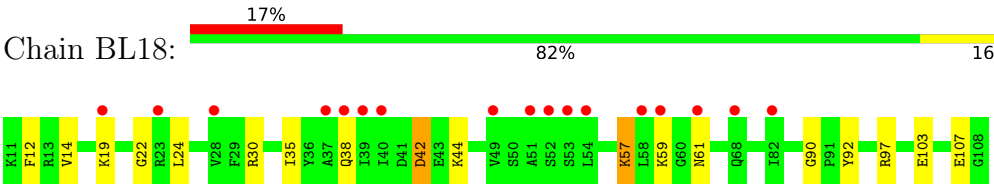
• Molecule 13: 50S ribosomal protein L18

Chain AL18:



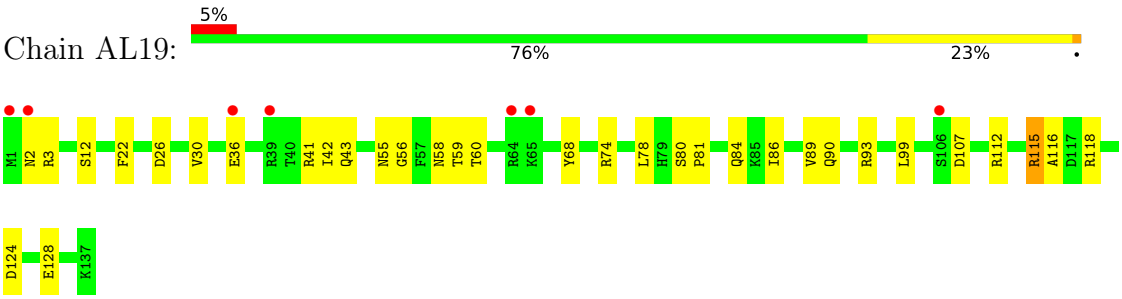
• Molecule 13: 50S ribosomal protein L18

Chain BL18:



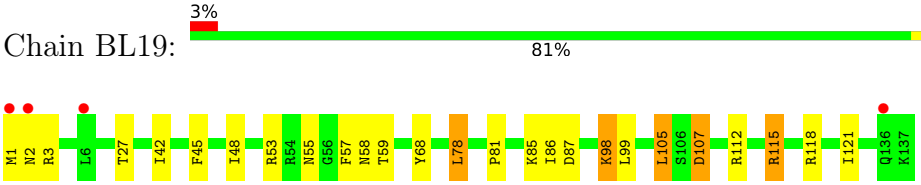
• Molecule 14: 50S ribosomal protein L19

Chain AL19:



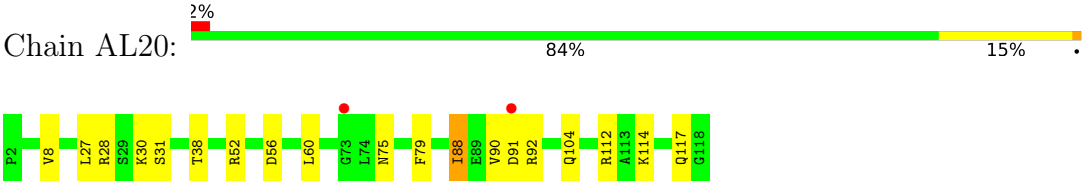
• Molecule 14: 50S ribosomal protein L19

Chain BL19:



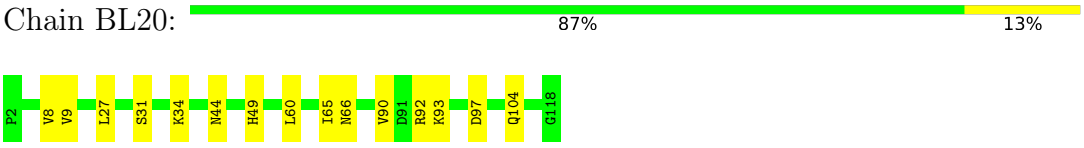
• Molecule 15: 50S ribosomal protein L20

Chain AL20:



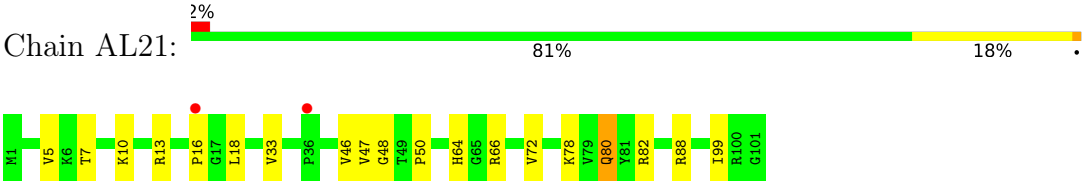
• Molecule 15: 50S ribosomal protein L20

Chain BL20:



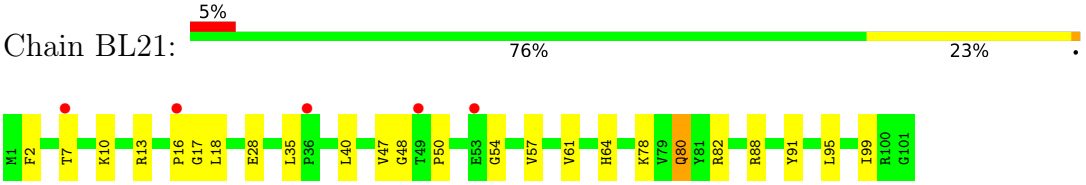
• Molecule 16: 50S ribosomal protein L21

Chain AL21:



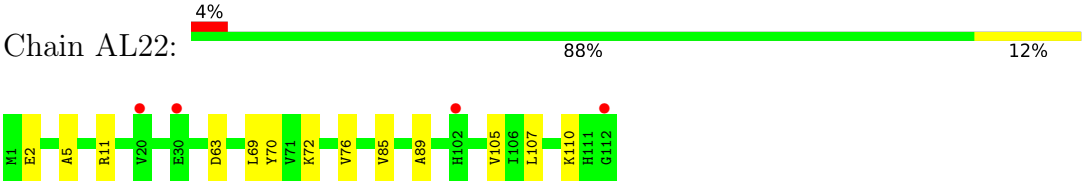
• Molecule 16: 50S ribosomal protein L21

Chain BL21:



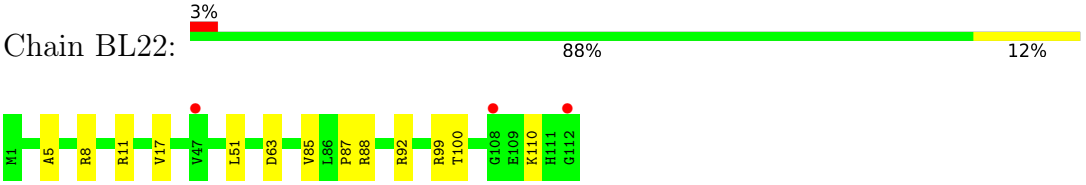
• Molecule 17: 50S ribosomal protein L22

Chain AL22:



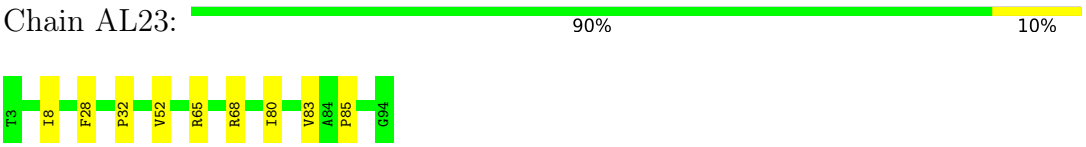
• Molecule 17: 50S ribosomal protein L22

Chain BL22:



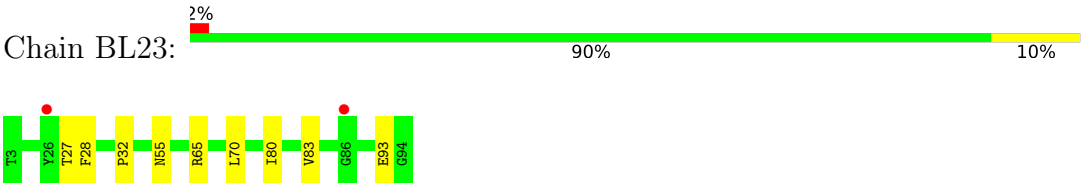
• Molecule 18: 50S ribosomal protein L23

Chain AL23:



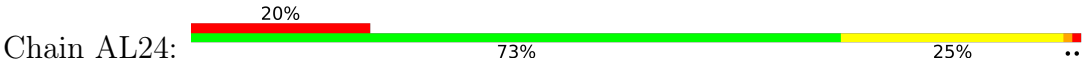
• Molecule 18: 50S ribosomal protein L23

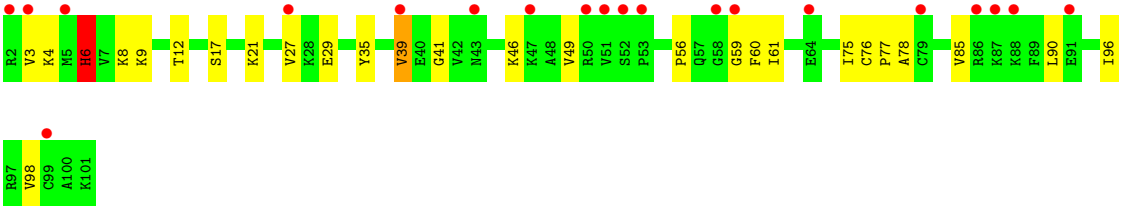
Chain BL23:



• Molecule 19: 50S ribosomal protein L24

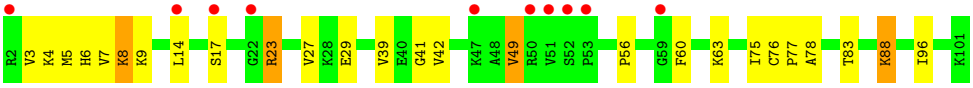
Chain AL24:





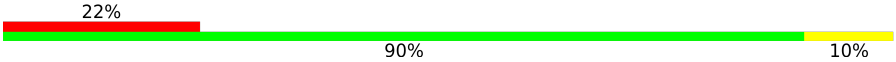
• Molecule 19: 50S ribosomal protein L24

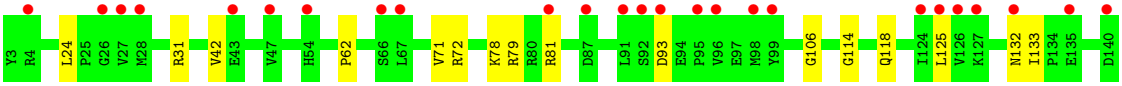
Chain BL24:

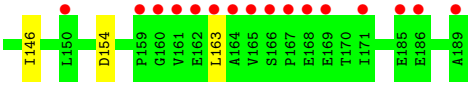


• Molecule 20: 50S ribosomal protein L25

Chain AL25:

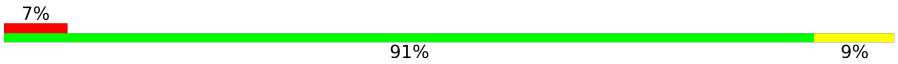






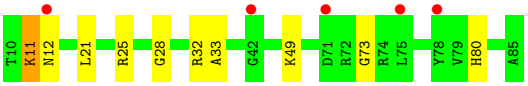
• Molecule 20: 50S ribosomal protein L25

Chain BL25:



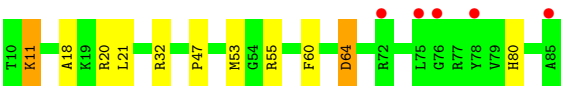
• Molecule 21: 50S ribosomal protein L27

Chain AL27:



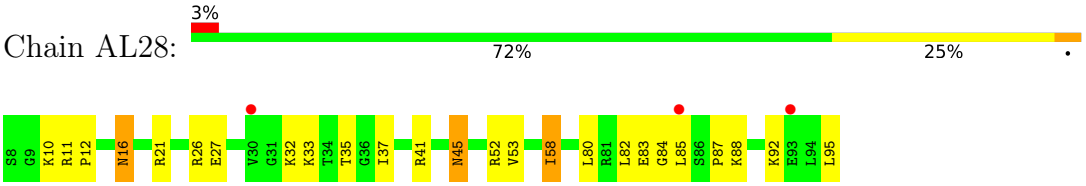
• Molecule 21: 50S ribosomal protein L27

Chain BL27:



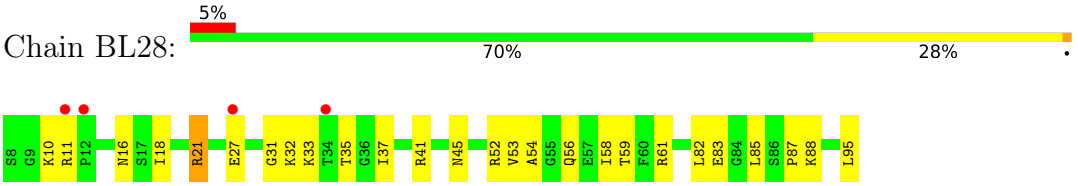
• Molecule 22: 50S ribosomal protein L28

Chain AL28:



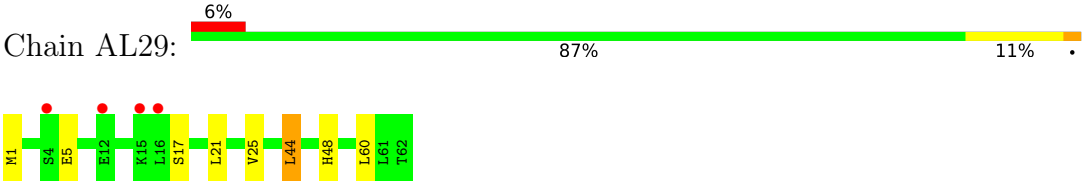
• Molecule 22: 50S ribosomal protein L28

Chain BL28:



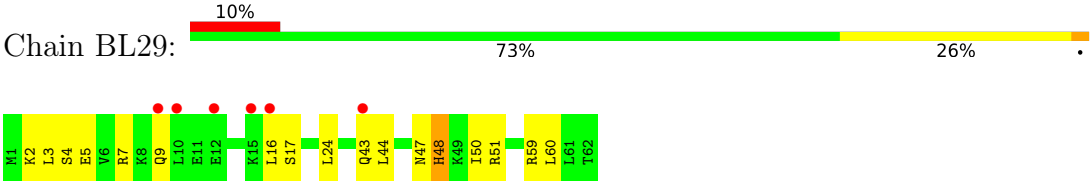
• Molecule 23: 50S ribosomal protein L29

Chain AL29:



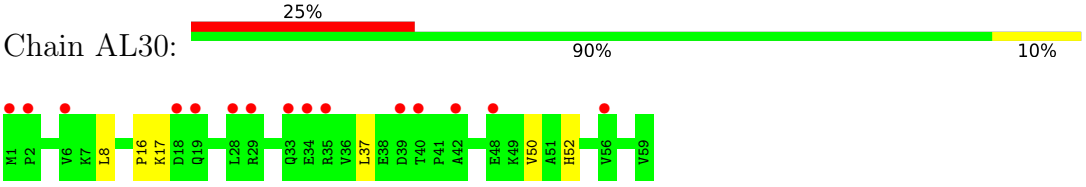
• Molecule 23: 50S ribosomal protein L29

Chain BL29:



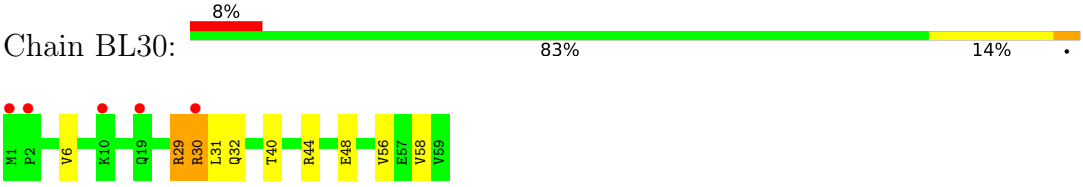
• Molecule 24: 50S ribosomal protein L30

Chain AL30:



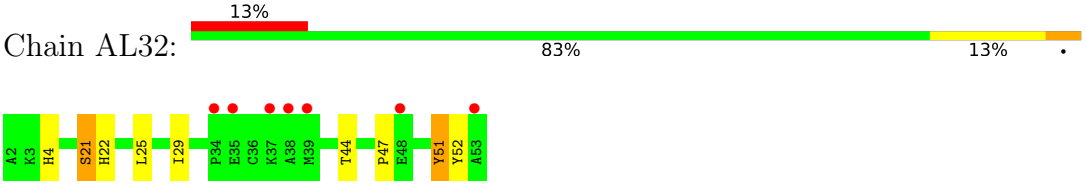
• Molecule 24: 50S ribosomal protein L30

Chain BL30:



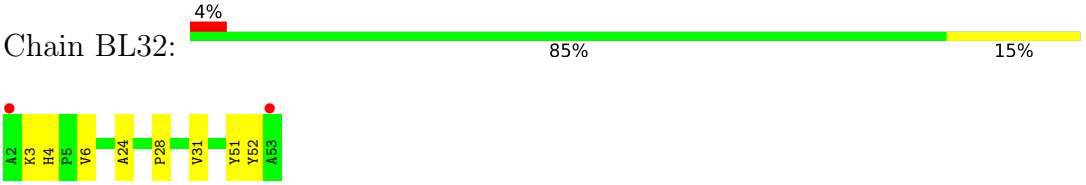
• Molecule 25: 50S ribosomal protein L32

Chain AL32:



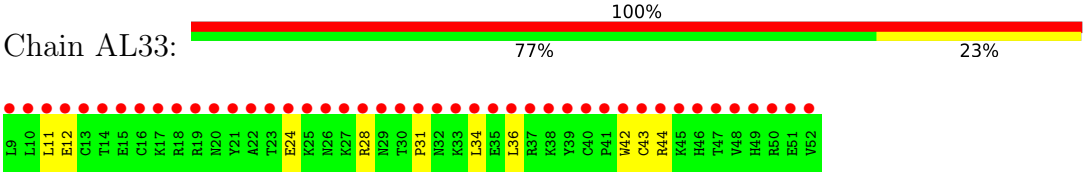
• Molecule 25: 50S ribosomal protein L32

Chain BL32:



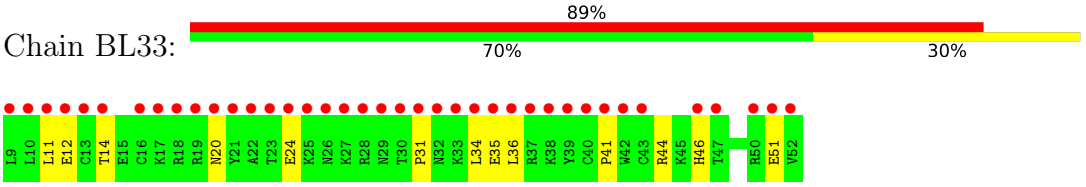
• Molecule 26: 50S ribosomal protein L33

Chain AL33:



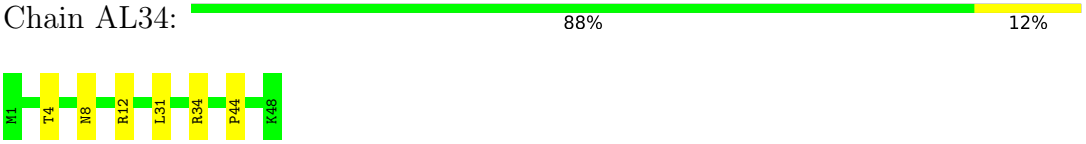
• Molecule 26: 50S ribosomal protein L33

Chain BL33:



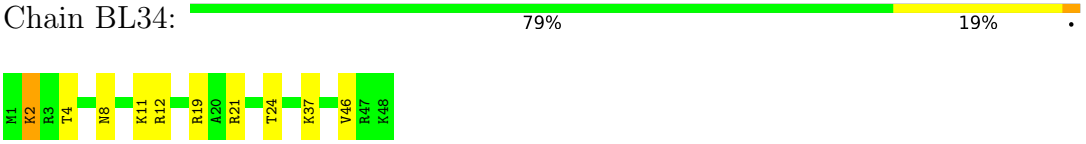
• Molecule 27: 50S ribosomal protein L34

Chain AL34:



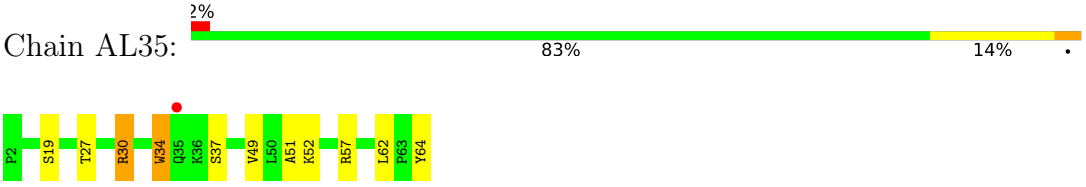
• Molecule 27: 50S ribosomal protein L34

Chain BL34:



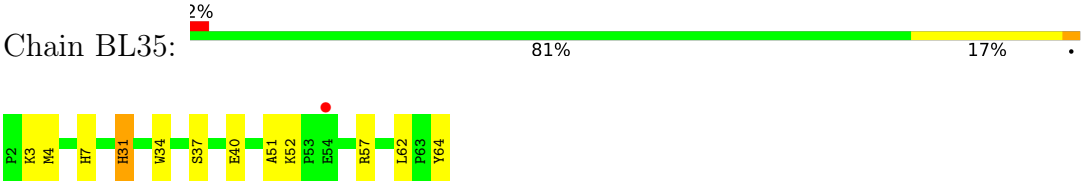
• Molecule 28: 50S ribosomal protein L35

Chain AL35:



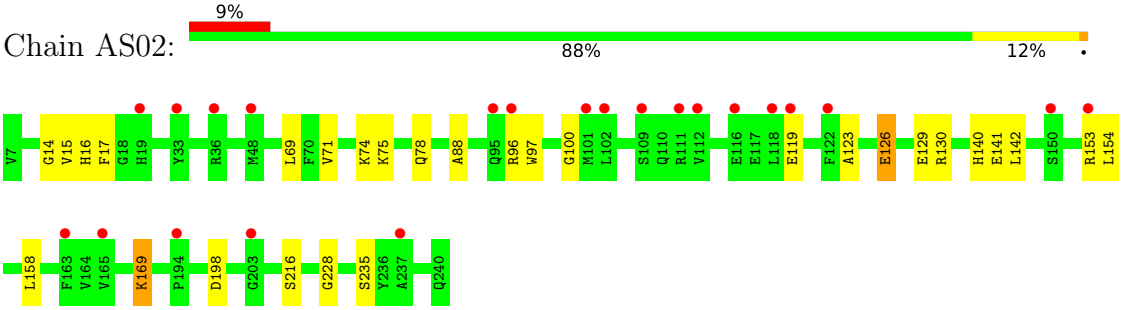
• Molecule 28: 50S ribosomal protein L35

Chain BL35:



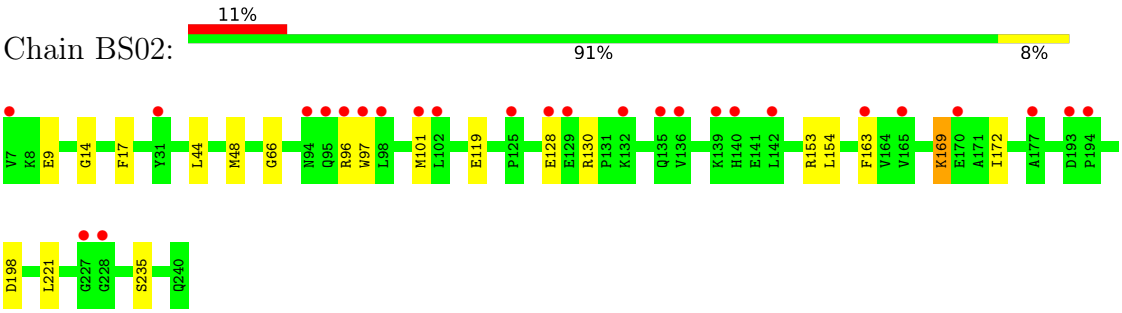
• Molecule 29: 30S ribosomal protein S2

Chain AS02:



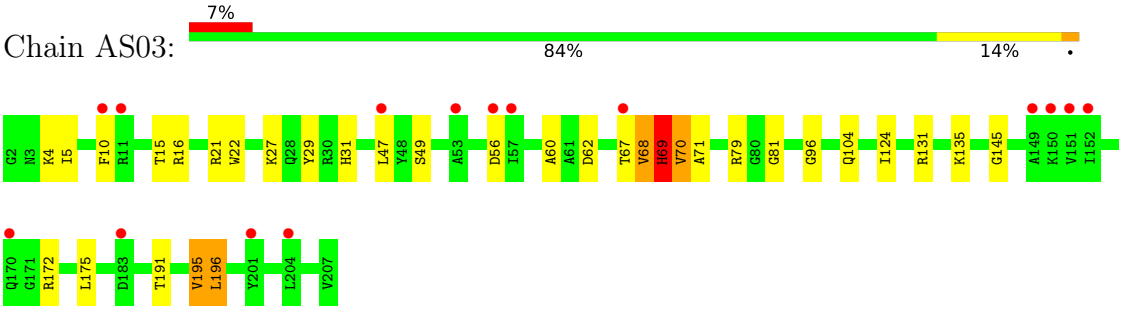
• Molecule 29: 30S ribosomal protein S2

Chain BS02:



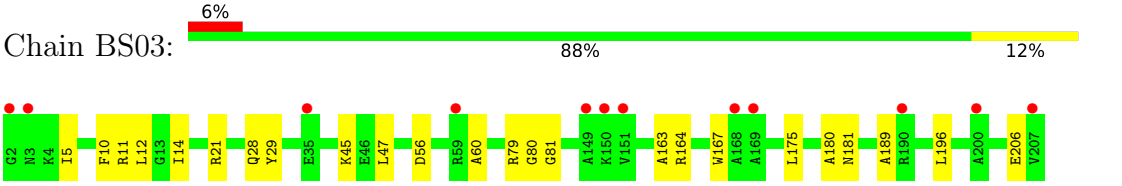
• Molecule 30: 30S ribosomal protein S3

Chain AS03:



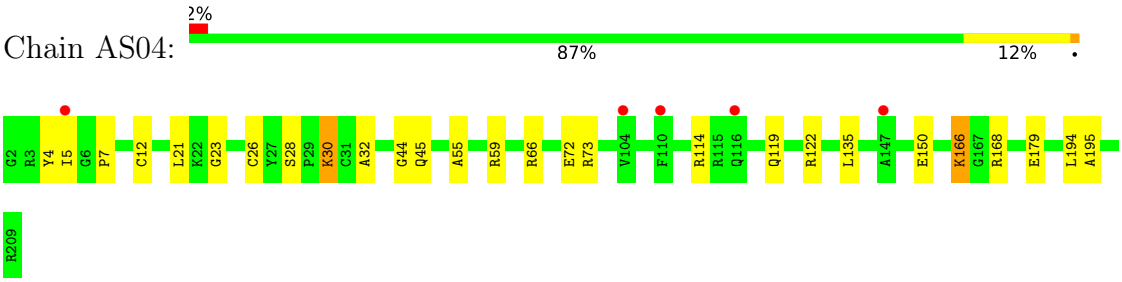
• Molecule 30: 30S ribosomal protein S3

Chain BS03:



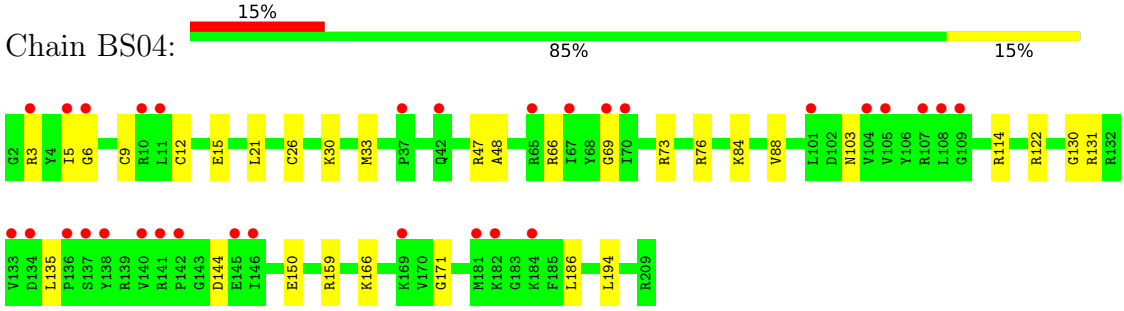
• Molecule 31: 30S ribosomal protein S4

Chain AS04:



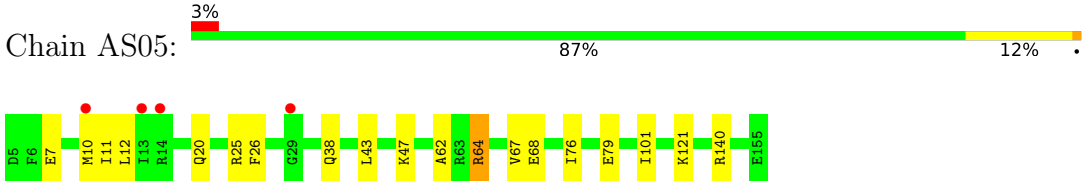
• Molecule 31: 30S ribosomal protein S4

Chain BS04:



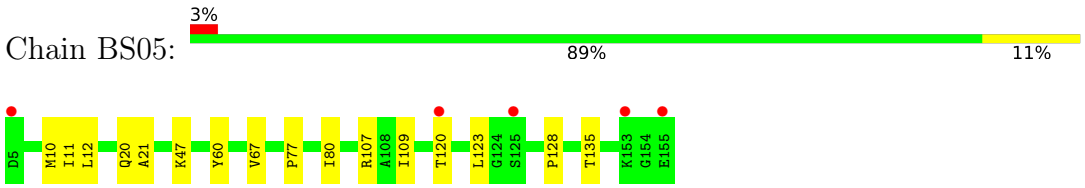
• Molecule 32: 30S ribosomal protein S5

Chain AS05:



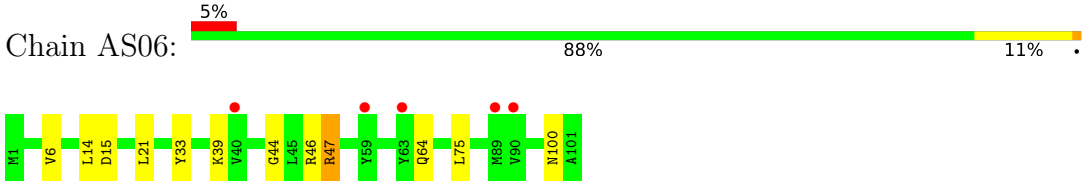
• Molecule 32: 30S ribosomal protein S5

Chain BS05:



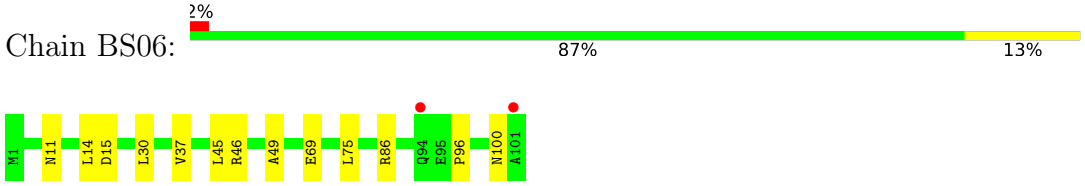
• Molecule 33: 30S ribosomal protein S6

Chain AS06:



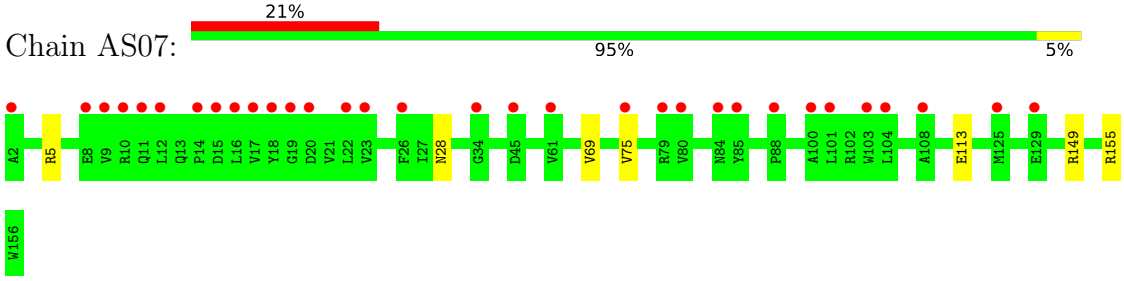
• Molecule 33: 30S ribosomal protein S6

Chain BS06:



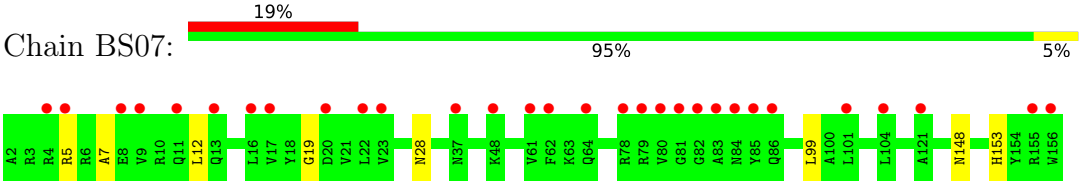
• Molecule 34: 30S ribosomal protein S7

Chain AS07:



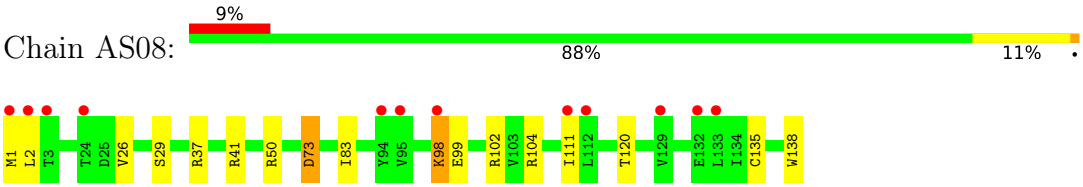
• Molecule 34: 30S ribosomal protein S7

Chain BS07:



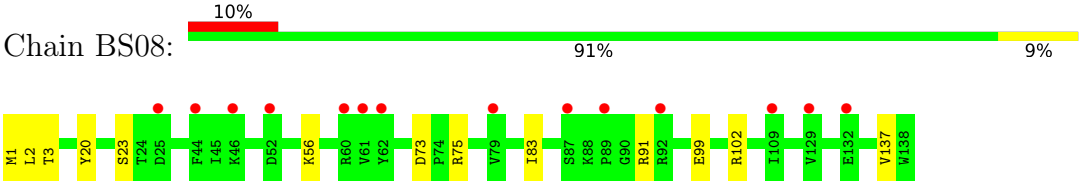
• Molecule 35: 30S ribosomal protein S8

Chain AS08:



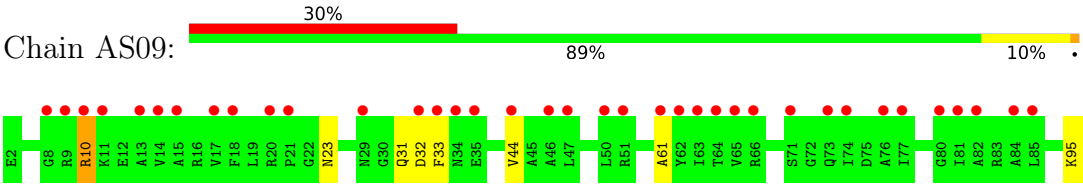
• Molecule 35: 30S ribosomal protein S8

Chain BS08:



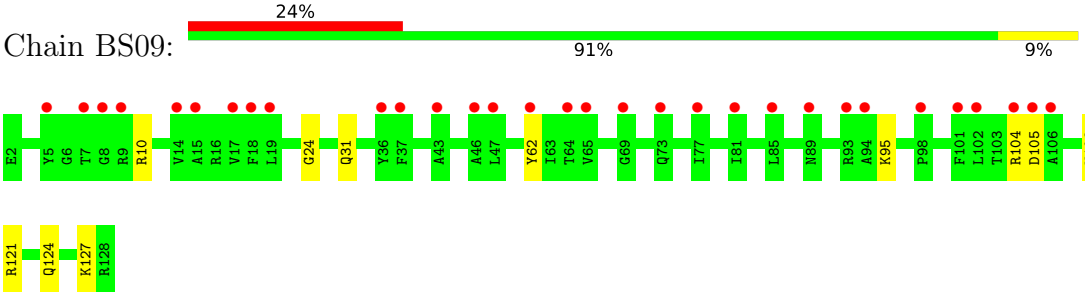
• Molecule 36: 30S ribosomal protein S9

Chain AS09:



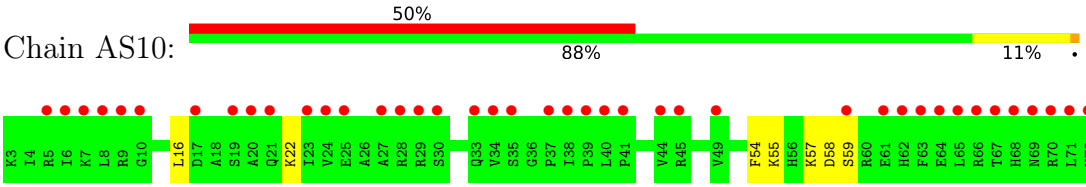
• Molecule 36: 30S ribosomal protein S9

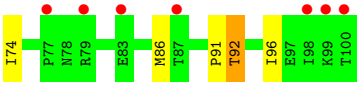
Chain BS09:



• Molecule 37: 30S ribosomal protein S10

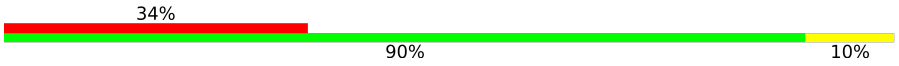
Chain AS10:

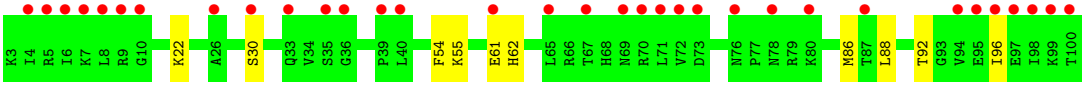




• Molecule 37: 30S ribosomal protein S10

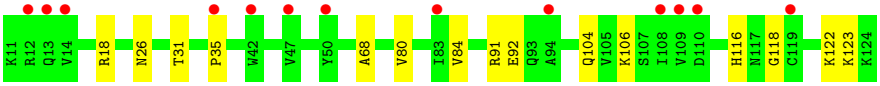
Chain BS10:





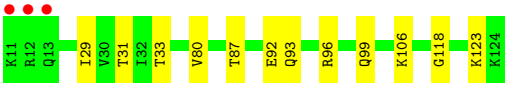
• Molecule 38: 30S ribosomal protein S11

Chain AS11:



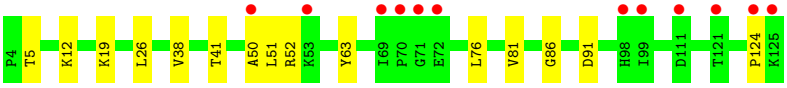
• Molecule 38: 30S ribosomal protein S11

Chain BS11:



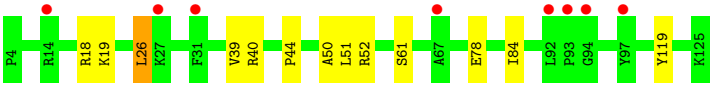
• Molecule 39: 30S ribosomal protein S12

Chain AS12:



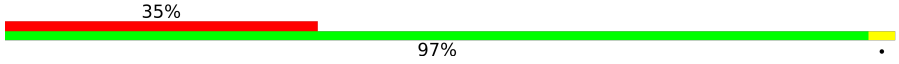
• Molecule 39: 30S ribosomal protein S12

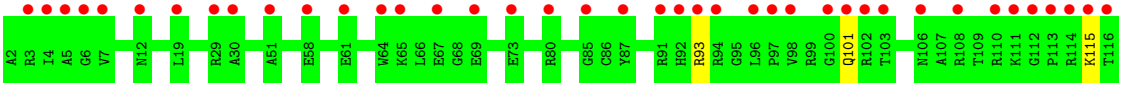
Chain BS12:



• Molecule 40: 30S ribosomal protein S13

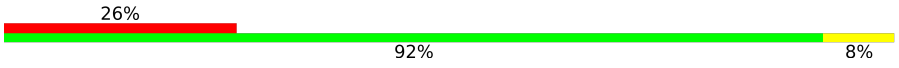
Chain AS13:

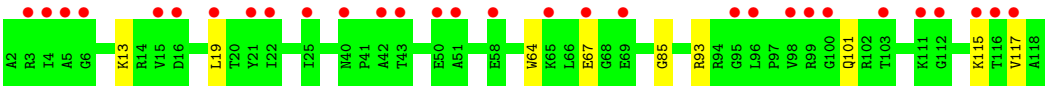




• Molecule 40: 30S ribosomal protein S13

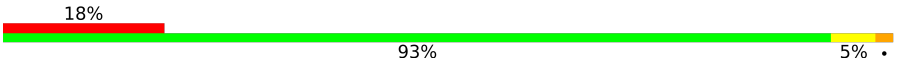
Chain BS13:

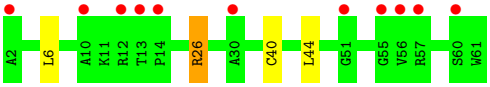




• Molecule 41: 30S ribosomal protein S14

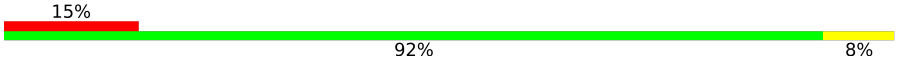
Chain AS14:





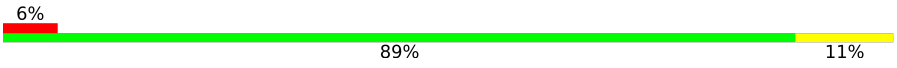
• Molecule 41: 30S ribosomal protein S14

Chain BS14:



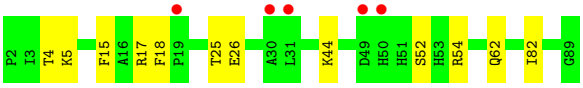
• Molecule 42: 30S ribosomal protein S15

Chain AS15:



• Molecule 42: 30S ribosomal protein S15

Chain BS15:

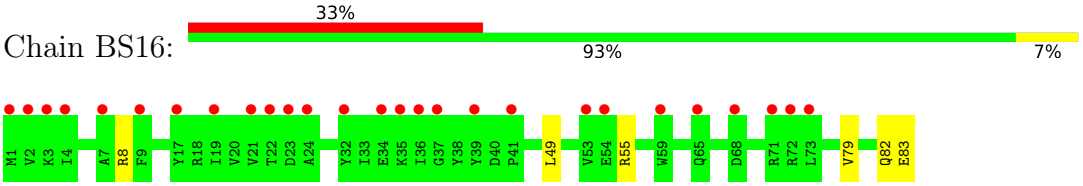


• Molecule 43: 30S ribosomal protein S16

Chain AS16:

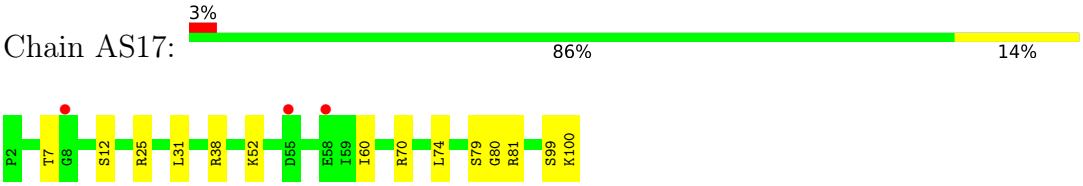
• Molecule 43: 30S ribosomal protein S16

Chain BS16:



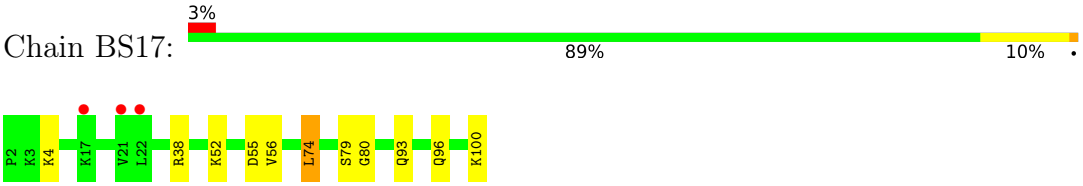
• Molecule 44: 30S ribosomal protein S17

Chain AS17:



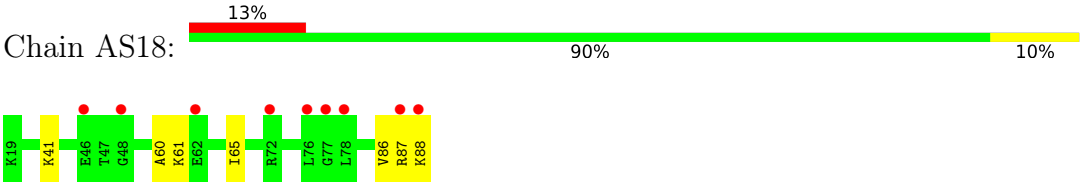
• Molecule 44: 30S ribosomal protein S17

Chain BS17:



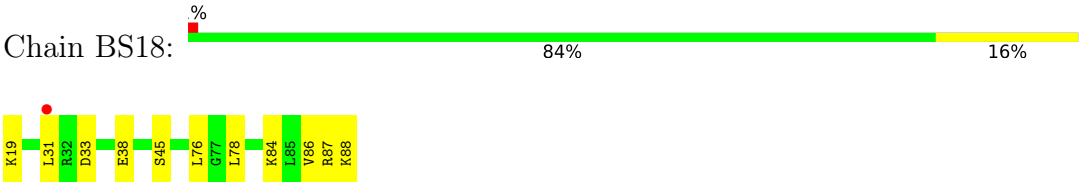
• Molecule 45: 30S ribosomal protein S18

Chain AS18:



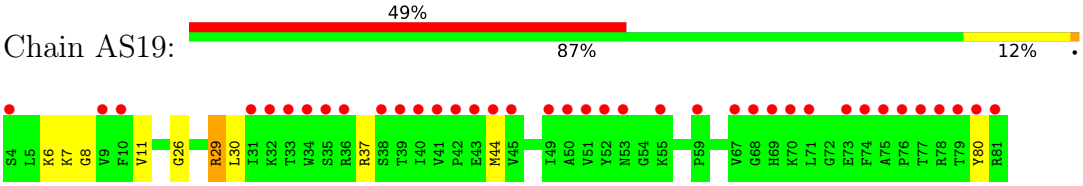
• Molecule 45: 30S ribosomal protein S18

Chain BS18:



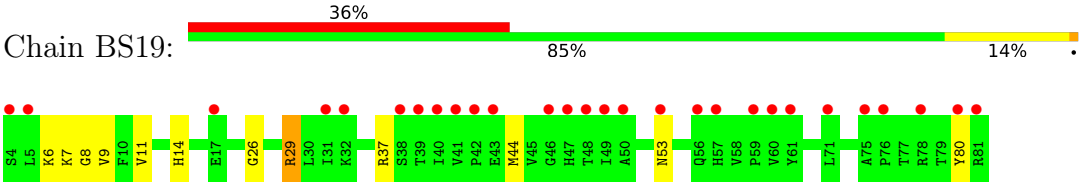
• Molecule 46: 30S ribosomal protein S19

Chain AS19:



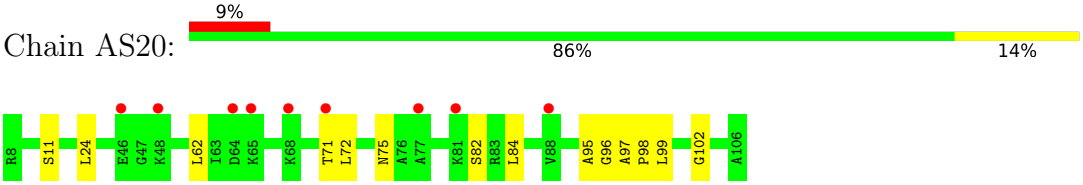
• Molecule 46: 30S ribosomal protein S19

Chain BS19:



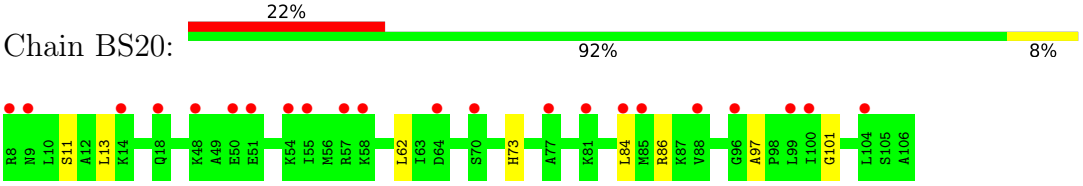
• Molecule 47: 30S ribosomal protein S20

Chain AS20:



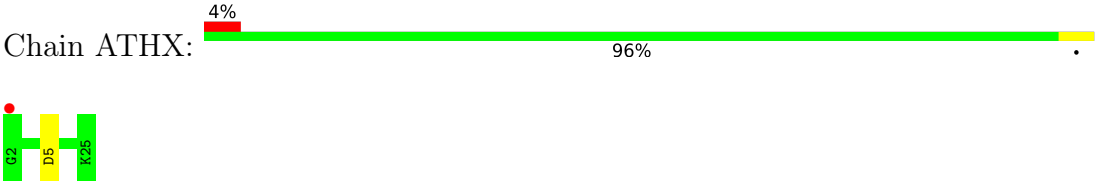
• Molecule 47: 30S ribosomal protein S20

Chain BS20:



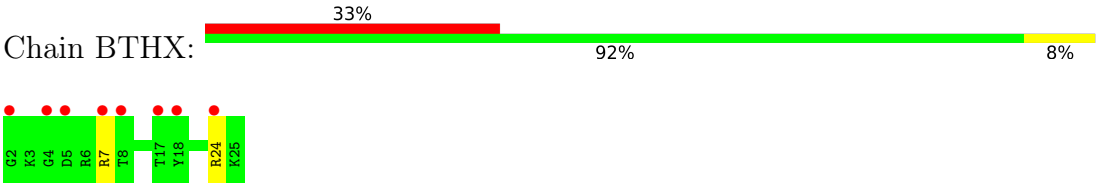
• Molecule 48: 30S ribosomal protein Thx

Chain ATHX:



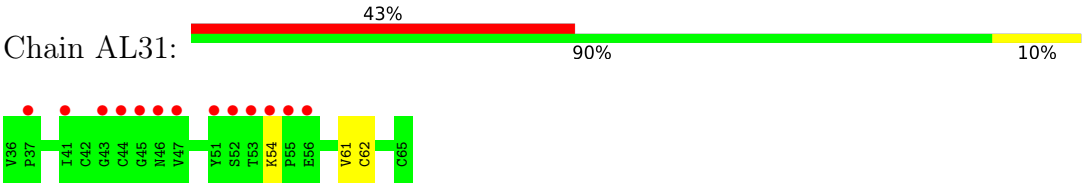
• Molecule 48: 30S ribosomal protein Thx

Chain BTHX:



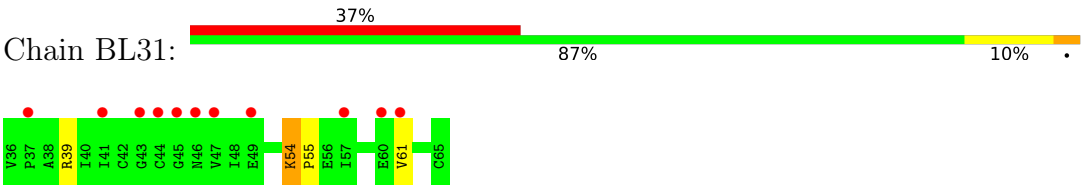
• Molecule 49: 50S ribosomal protein L31

Chain AL31:



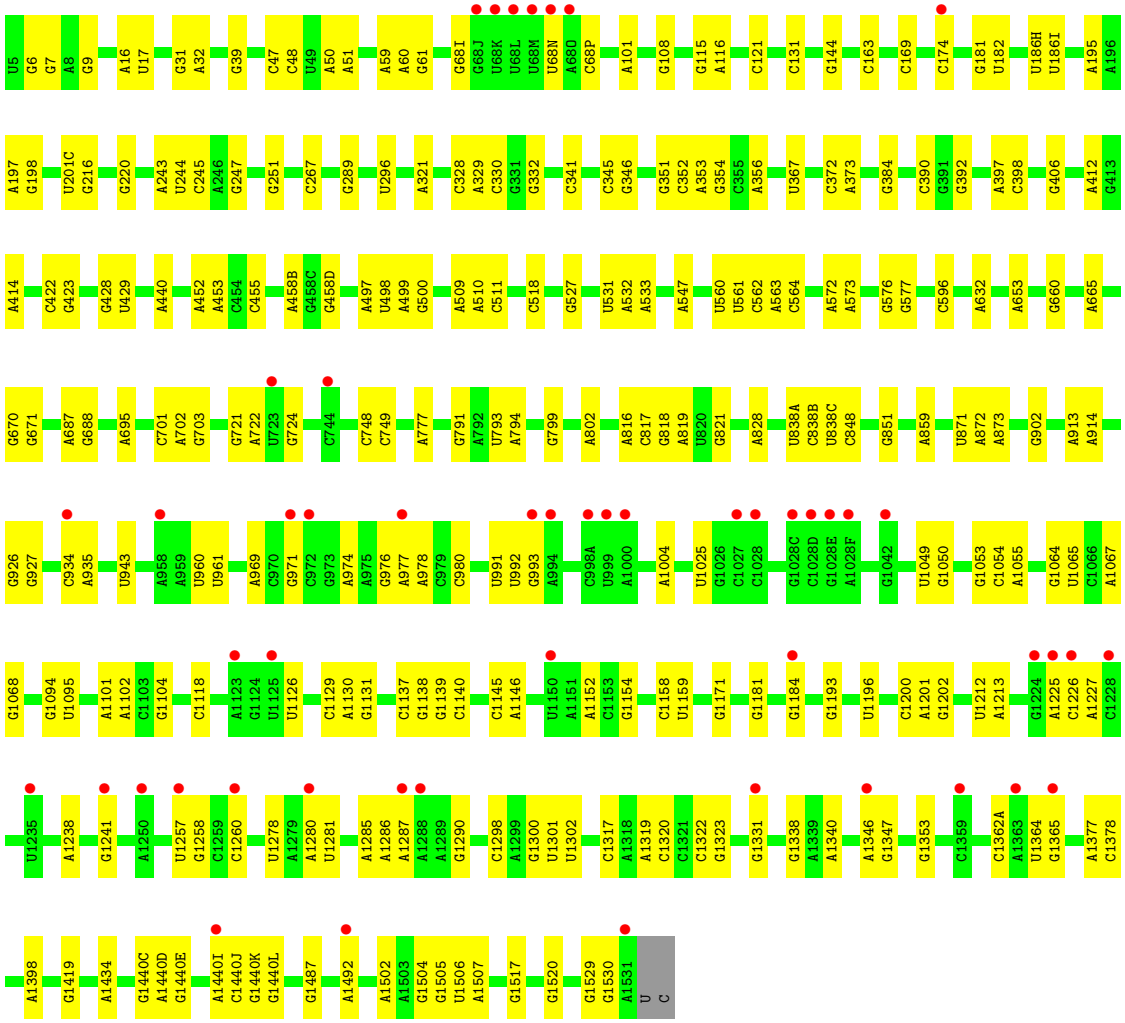
• Molecule 49: 50S ribosomal protein L31

Chain BL31:



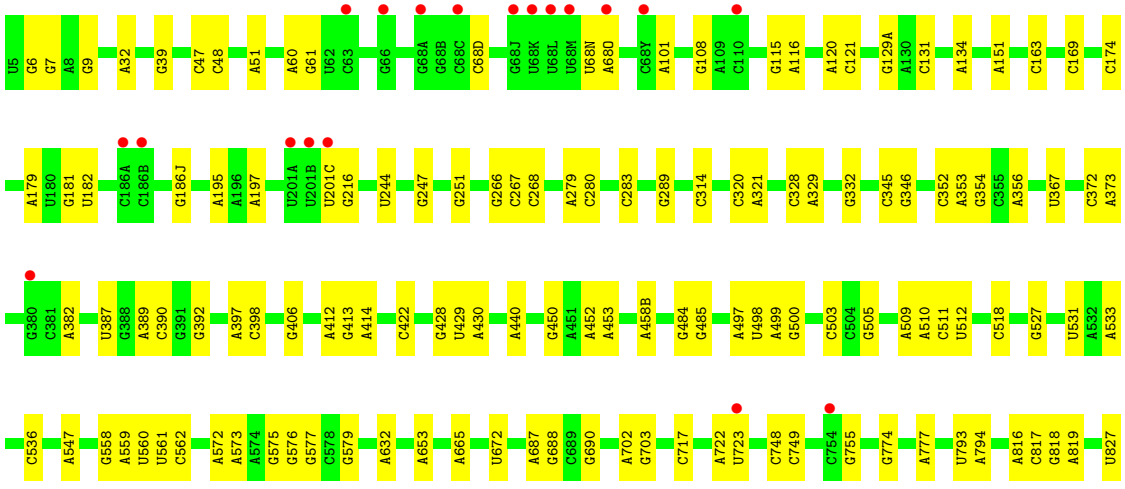
• Molecule 50: 16S ribosomal RNA

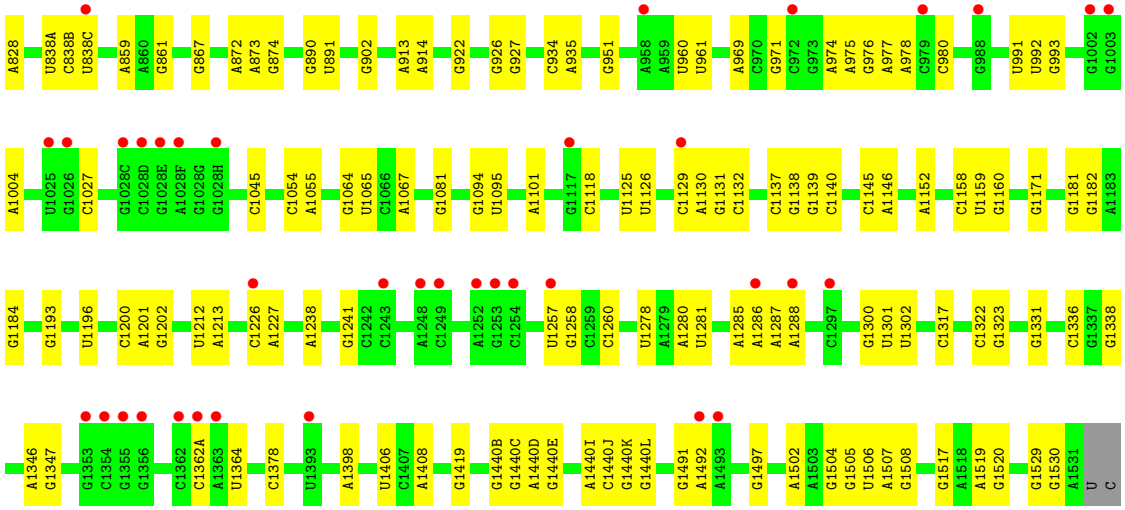
Chain A16S:



• Molecule 50: 16S ribosomal RNA

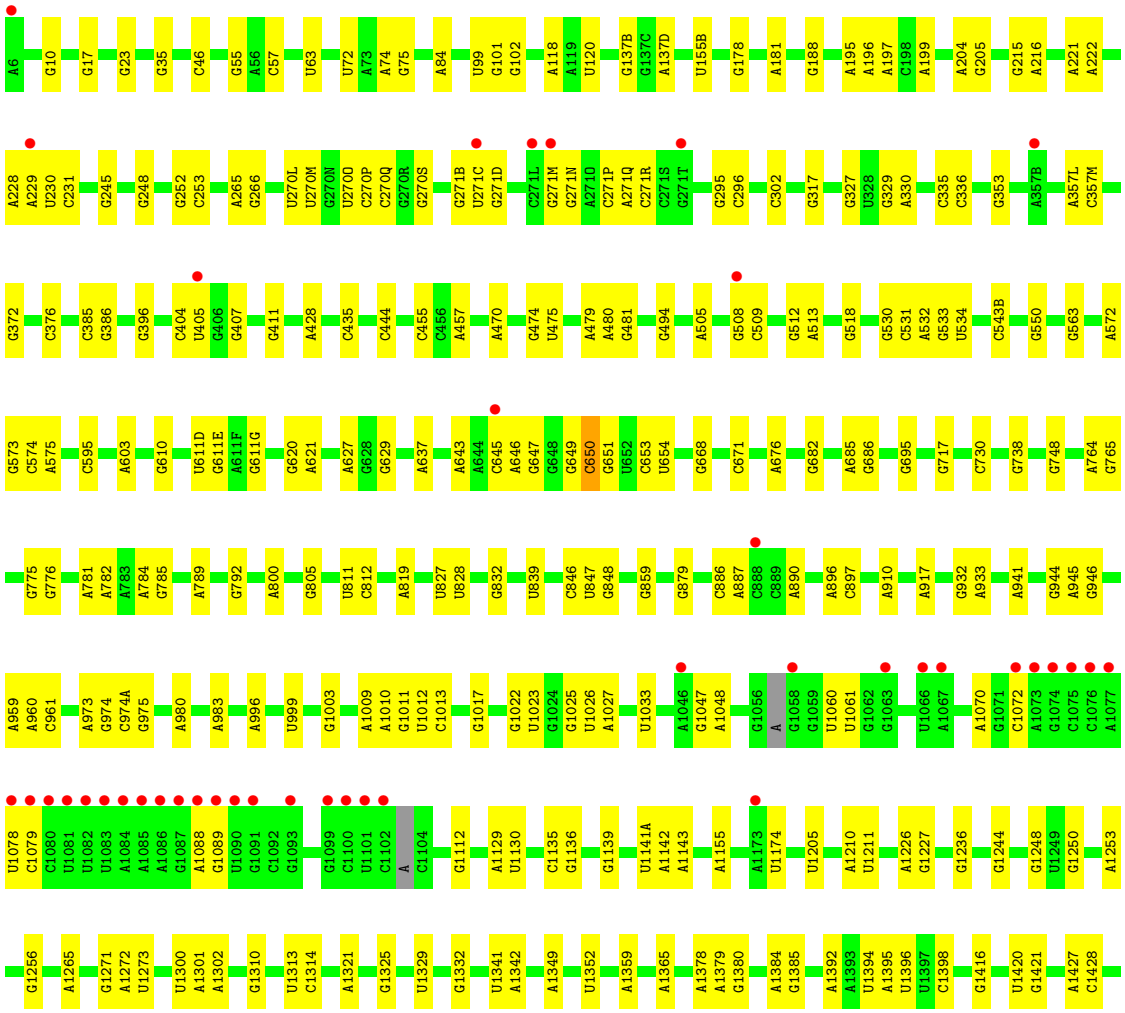
Chain B16S:

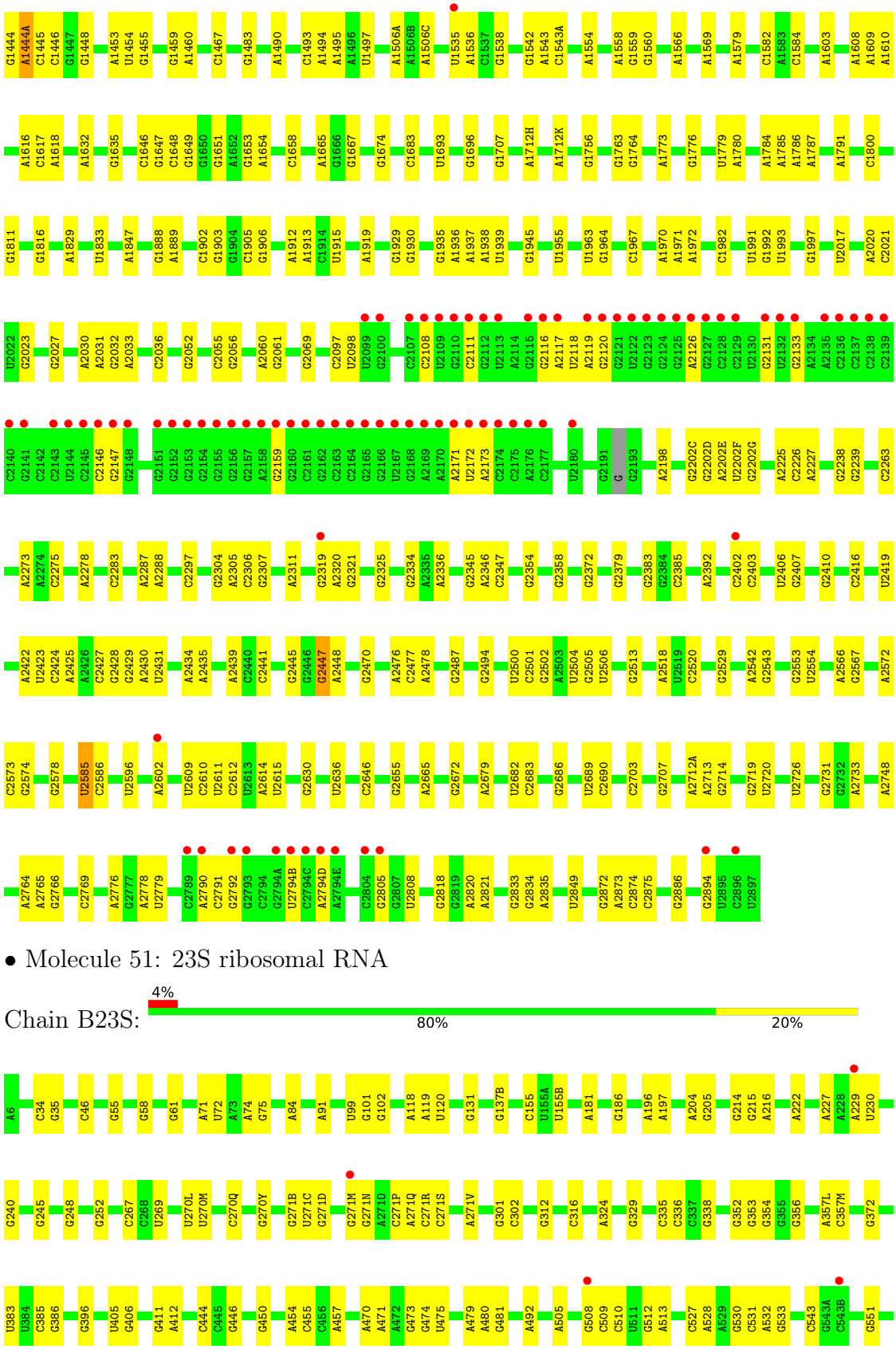




• Molecule 51: 23S ribosomal RNA

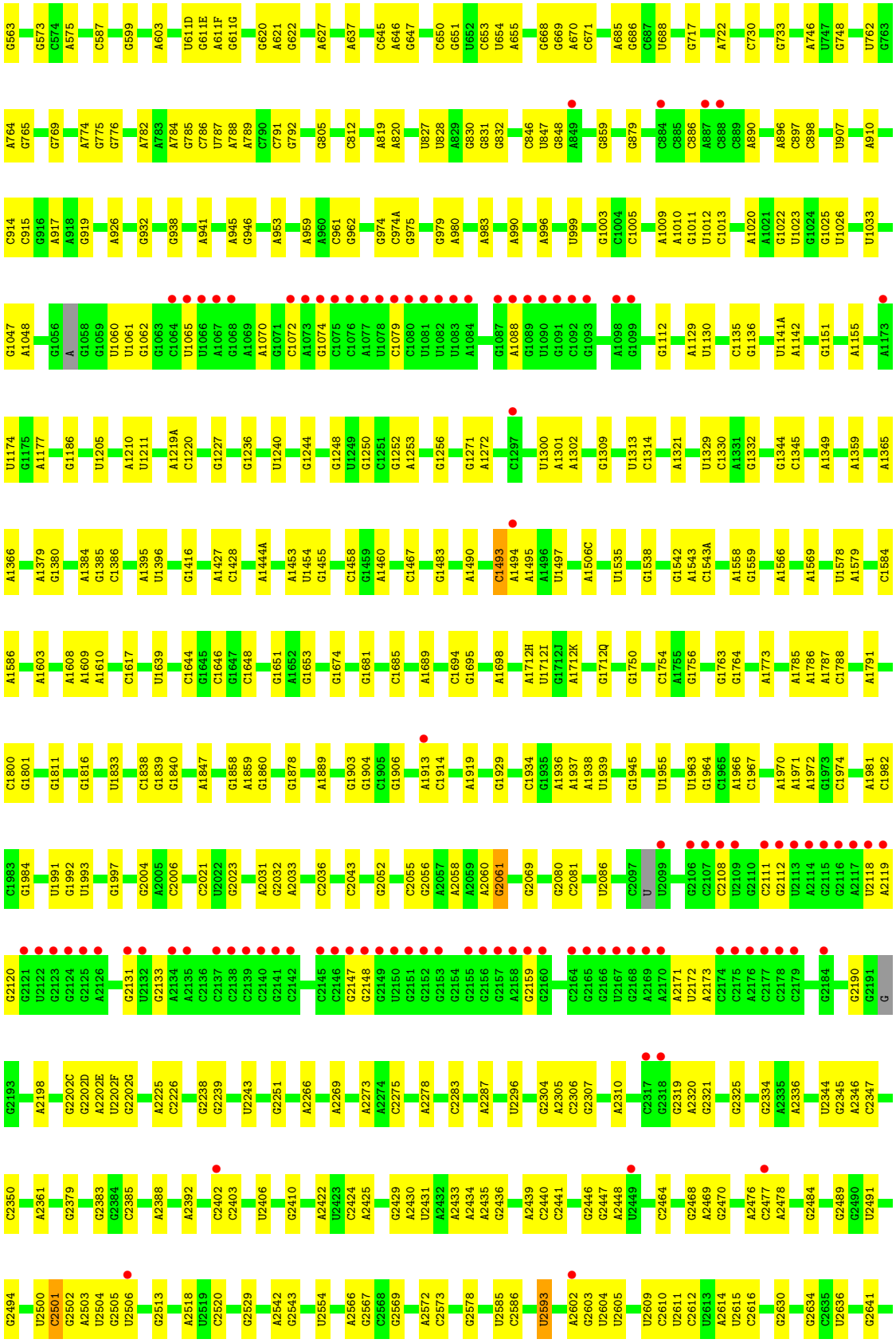
Chain A23S:

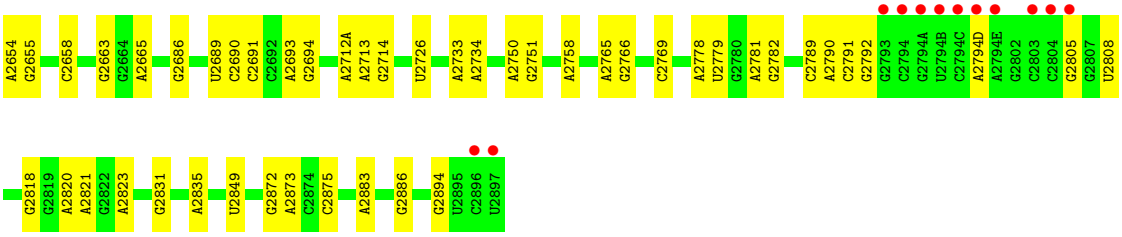




• Molecule 51: 23S ribosomal RNA

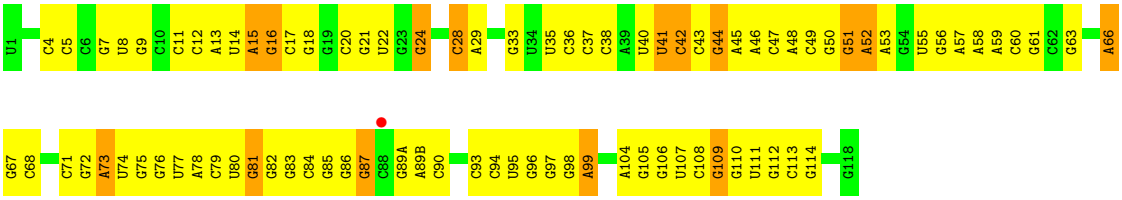
Chain B23S:


G563 C573 C574 A575 C587 G599 A603 U611D G611E A611F G611G G620 A621 G622 A627 A637 C645 A646 G647 C650 G651 U652 C653 U654 A655 G668 G669 A670 C671 A685 G686 C687 U688 G717 A722 C730 G733 A746 U747 G748 U762 G763
A764 G765 G769 A774 G775 G776 A782 A783 A784 G785 C786 U787 A788 A789 C790 C791 G792 G805 C812 A819 A820 U827 U828 A829 G830 G831 G832 C846 U847 G848 A849 G859 G879 C884 C885 C886 A887 C888 C889 A890 A896 C897 C898 U907 A910
C914 C915 G916 A917 A918 G919 A926 G932 G938 A941 A945 G946 A953 A959 A960 C961 G962 G974 C974A G975 G979 A980 A983 A990 A996 U999 G1003 C1004 C1005 A1009 A1010 G1011 U1012 C1013 A1020 A1021 G1022 U1023 G1024 G1025 U1026 U1033
G1047 A1048 G1056 A G1058 G1059 U1060 U1061 G1062 G1063 C1064 U1065 U1066 A1067 G1068 A1069 A1070 G1071 C1072 A1073 G1074 C1075 C1076 A1077 U1078 C1079 C1080 U1081 U1082 U1083 A1084 G1087 A1088 G1089 U1090 G1091 C1092 G1093 A1098 C1099 G1112 A1129 U1130 C1135 G1136 U1141A A1142 G1151 A1155 A1173
U1174 G1175 A1177 G1186 U1205 A1210 U1211 A1219A C1220 G1227 G1236 U1240 G1244 G1248 U1249 G1250 C1251 G1252 A1253 G1256 G1271 A1272 C1297 U1300 A1301 A1302 G1309 U1313 C1314 A1321 U1329 C1330 A1331 G1332 G1344 C1345 A1349 A1359 A1365
A1366 A1379 G1380 A1384 G1385 C1386 A1395 U1396 G1416 A1427 C1428 A1444A A1453 U1454 G1455 C1458 G1459 A1460 C1467 G1483 A1490 C1493 A1494 A1495 A1496 U1497 A1506C U1535 G1538 G1542 A1543 C1543A A1558 G1559 A1566 A1569 U1578 A1579 C1584
A1586 A1603 A1608 A1609 A1610 C1617 U1639 C1644 G1645 C1646 G1647 C1648 G1651 A1652 G1653 G1674 G1681 C1685 A1689 C1694 G1695 A1698 A1712H U1712I G1712J A1712K G1712Q G1750 C1754 A1755 G1756 G1763 G1764 A1773 A1785 A1786 A1787 C1788 A1791
C1800 G1801 G1811 G1816 U1833 C1838 G1839 G1840 A1847 G1858 A1859 G1860 G1878 A1889 G1903 G1904 C1905 G1906 A1913 C1914 A1919 G1929 C1934 G1935 A1936 A1937 A1938 U1939 G1945 U1955 U1963 G1964 C1965 A1966 C1967 A1970 A1971 A1972 G1973 C1974 A1981 C1982
C1983 G1984 U1991 G1992 U1993 G1997 G2004 A2005 C2006 C2021 U2022 G2023 A2031 G2032 A2033 C2036 C2043 G2052 C2055 G2056 A2057 A2058 A2059 A2060 G2061 C2069 G2080 C2081 U2086 C2097 U U2099 G2106 C2107 C2108 U2109 G2110 C2111 G2112 U2113 A2114 G2115 G2116 A2117 U2118 A2119
G2120 G2121 U2122 G2123 G2124 G2125 A2126 G2131 U2132 G2133 A2134 A2135 C2136 C2137 C2138 C2139 C2140 G2141 C2142 C2145 C2146 G2147 G2148 G2149 U2150 G2151 G2152 G2153 G2154 G2155 G2156 G2157 A2158 G2159 G2160 C2164 G2165 G2166 U2167 G2168 A2169 A2170 A2171 U2172 A2173 C2174 C2175 A2176 C2177 C2178 C2179 G2184 G2190 G2191 G
G2193 A2198 G2202C G2202D A2202E U2202F G2202G A2225 C2226 G2238 G2239 U2243 G2251 A2266 A2269 A2273 A2274 C2275 A2278 C2283 A2287 U2296 G2304 A2305 C2306 G2307 A2310 C2317 G2318 G2319 A2320 G2321 G2325 G2334 A2335 A2336 U2344 G2345 A2346 C2347
C2350 A2361 G2379 G2383 G2384 C2385 A2388 A2392 C2402 C2403 U2406 G2410 A2422 U2423 C2424 A2425 G2429 A2430 U2431 A2432 A2433 A2434 A2435 G2436 A2439 C2440 C2441 G2446 G2447 A2448 U2449 C2464 G2468 A2469 G2470 A2476 C2477 A2478 G2484 G2489 G2490 U2491
G2494 U2500 C2501 G2502 A2503 U2504 G2505 U2506 G2513 A2518 U2519 C2520 G2529 A2542 G2543 U2554 A2566 G2567 C2568 G2569 A2572 C2573 G2578 U2585 C2586 U2593 A2602 G2603 U2604 U2605 U2609 C2610 U2611 C2612 U2613 A2614 U2615 C2616 G2630 G2634 C2635 U2636 G2641



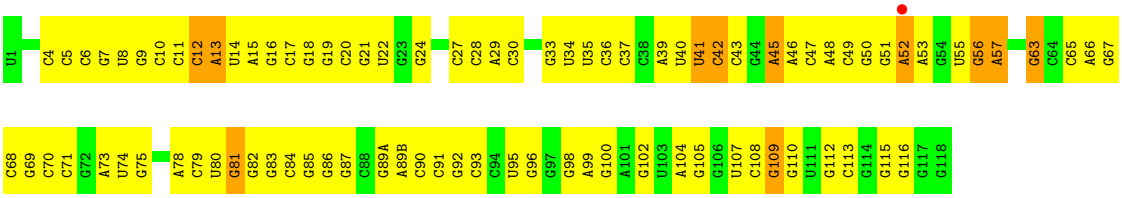
• Molecule 52: 5S ribosomal RNA

Chain A5S:



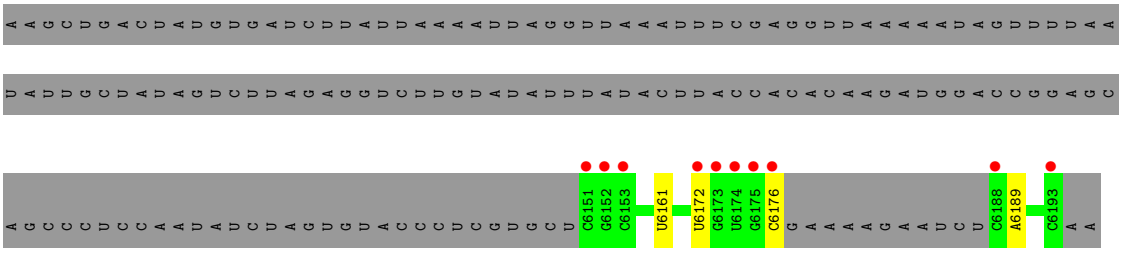
• Molecule 52: 5S ribosomal RNA

Chain B5S:



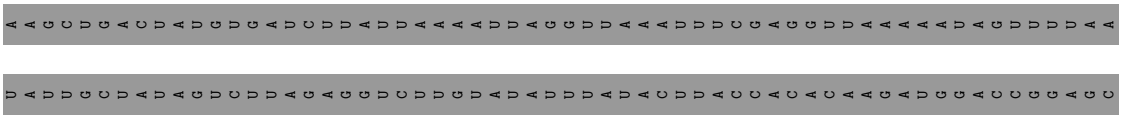
• Molecule 53: IRES RNA

Chain AIRE:



• Molecule 53: IRES RNA

Chain BIRE:



A
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U
C6161
U6161
U6174
G6175
C6176
G
A
A
A
G
A
A
U
C
U
C6188
A6189
C6193
A
A

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.05Å 447.22Å 608.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.00 – 3.80 59.35 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (60.00-3.80) 99.9 (59.35-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 3.77Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.246 , 0.284 0.242 , 0.279	Depositor DCC
R_{free} test set	2000 reflections (0.36%)	wwPDB-VP
Wilson B-factor (Å^2)	119.0	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 93.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	287293	wwPDB-VP
Average B, all atoms (Å^2)	150.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.66% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	AL02	0.33	0/2155	0.56	0/2905
1	BL02	0.40	0/2155	0.60	0/2905
2	AL03	0.31	0/1597	0.52	0/2153
2	BL03	0.33	0/1597	0.56	0/2153
3	AL04	0.31	0/1622	0.53	0/2194
3	BL04	0.32	0/1622	0.54	0/2194
4	AL05	0.22	0/1500	0.43	0/2017
4	BL05	0.23	0/1500	0.44	0/2017
5	AL06	0.25	0/1246	0.46	0/1682
5	BL06	0.33	0/1246	0.51	0/1682
6	AL09	0.29	0/1148	0.51	0/1552
6	BL09	0.30	0/1148	0.53	0/1552
7	AL11	0.22	0/1108	0.41	0/1500
7	BL11	0.25	0/1108	0.43	0/1500
8	AL13	0.37	0/1124	0.56	0/1515
8	BL13	0.32	0/1124	0.51	0/1515
9	AL14	0.29	0/942	0.51	0/1268
9	BL14	0.31	0/942	0.51	0/1268
10	AL15	0.31	0/1131	0.59	0/1504
10	BL15	0.37	0/1131	0.65	0/1504
11	AL16	0.31	0/1085	0.52	0/1449
11	BL16	0.32	0/1085	0.52	0/1449
12	AL17	0.37	0/974	0.57	0/1302
12	BL17	0.32	0/974	0.53	0/1302
13	AL18	0.25	0/779	0.43	0/1036
13	BL18	0.26	0/779	0.44	0/1036
14	AL19	0.27	0/1158	0.49	0/1544
14	BL19	0.27	0/1158	0.48	0/1544
15	AL20	0.32	0/982	0.47	0/1306
15	BL20	0.31	0/982	0.51	0/1306
16	AL21	0.31	0/790	0.52	0/1057
16	BL21	0.35	0/790	0.56	0/1057

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	AL22	0.31	0/902	0.53	0/1209
17	BL22	0.32	0/902	0.51	0/1209
18	AL23	0.28	0/740	0.49	0/993
18	BL23	0.33	0/740	0.49	0/993
19	AL24	0.50	2/789 (0.3%)	1.34	4/1051 (0.4%)
19	BL24	0.34	0/789	0.58	0/1051
20	AL25	0.28	0/1515	0.46	0/2056
20	BL25	0.28	0/1515	0.48	0/2056
21	AL27	0.27	0/613	0.50	0/816
21	BL27	0.27	0/613	0.49	0/816
22	AL28	0.32	0/702	0.59	1/932 (0.1%)
22	BL28	0.34	0/702	0.60	0/932
23	AL29	0.27	0/523	0.49	0/690
23	BL29	0.32	0/523	0.55	0/690
24	AL30	0.24	0/473	0.44	0/634
24	BL30	0.27	0/473	0.47	0/634
25	AL32	0.38	0/419	0.59	0/567
25	BL32	0.41	0/419	0.63	0/567
26	AL33	0.28	0/388	0.52	0/518
26	BL33	0.24	0/388	0.47	0/518
27	AL34	0.35	0/427	0.49	0/561
27	BL34	0.39	0/427	0.54	0/561
28	AL35	0.36	0/516	0.56	0/679
28	BL35	0.43	0/516	0.70	1/679 (0.1%)
29	AS02	0.27	0/1936	0.46	1/2609 (0.0%)
29	BS02	0.26	0/1936	0.45	0/2609
30	AS03	0.89	8/1637 (0.5%)	0.95	13/2205 (0.6%)
30	BS03	0.26	0/1637	0.42	0/2205
31	AS04	0.30	0/1733	0.49	0/2318
31	BS04	0.25	0/1733	0.42	0/2318
32	AS05	0.24	0/1172	0.45	0/1576
32	BS05	0.25	0/1172	0.44	0/1576
33	AS06	0.23	0/856	0.44	0/1154
33	BS06	0.25	0/856	0.45	0/1154
34	AS07	0.25	0/1276	0.42	0/1709
34	BS07	0.26	0/1276	0.42	0/1709
35	AS08	0.23	0/1136	0.45	0/1527
35	BS08	0.24	0/1136	0.44	0/1527
36	AS09	0.25	0/1029	0.41	0/1378
36	BS09	0.21	0/1029	0.40	0/1378
37	AS10	0.28	0/808	0.47	0/1085
37	BS10	0.25	0/808	0.46	0/1085
38	AS11	0.27	0/857	0.48	0/1157

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	BS11	0.28	0/857	0.47	0/1157
39	AS12	0.29	0/973	0.50	0/1301
39	BS12	0.28	0/973	0.48	0/1301
40	AS13	0.27	0/944	0.43	0/1265
40	BS13	0.21	0/944	0.43	0/1265
41	AS14	0.30	0/501	0.45	0/664
41	BS14	0.22	0/501	0.39	0/664
42	AS15	0.39	0/745	0.54	0/992
42	BS15	0.38	0/745	0.52	0/992
43	AS16	0.31	0/717	0.48	0/963
43	BS16	0.25	0/717	0.46	0/963
44	AS17	0.31	0/837	0.48	0/1117
44	BS17	0.30	0/837	0.49	0/1117
45	AS18	0.24	0/579	0.43	0/768
45	BS18	0.25	0/579	0.45	0/768
46	AS19	0.30	0/643	0.46	0/865
46	BS19	0.27	0/643	0.46	0/865
47	AS20	0.26	0/764	0.47	0/1006
47	BS20	0.27	0/764	0.47	0/1006
48	ATHX	0.19	0/213	0.37	0/277
48	BTHX	0.20	0/213	0.40	0/277
49	AL31	0.20	0/229	0.45	0/309
49	BL31	0.20	0/229	0.41	0/309
50	A16S	0.27	0/36194	0.59	0/56493
50	B16S	0.25	0/36193	0.57	0/56490
51	A23S	0.39	2/69356 (0.0%)	0.71	11/108266 (0.0%)
51	B23S	0.39	0/69359	0.74	23/108270 (0.0%)
52	A5S	0.24	0/2853	0.55	0/4451
52	B5S	0.24	0/2853	0.56	0/4451
53	AIRE	0.25	0/748	0.50	0/1160
53	BIRE	0.27	0/748	0.57	0/1160
All	All	0.34	12/312170 (0.0%)	0.64	54/466611 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
10	AL15	0	1
10	BL15	0	1
19	AL24	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
30	AS03	0	2
All	All	0	5

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	A23S	253	C	C4-N4	40.77	1.70	1.33
51	A23S	253	C	N3-C4	19.94	1.48	1.33
30	AS03	69	HIS	C-O	13.83	1.49	1.23
30	AS03	70	VAL	CB-CG1	13.29	1.80	1.52
30	AS03	69	HIS	N-CA	12.82	1.72	1.46

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	A23S	1444(A)	A	P-O3'-C3'	37.85	165.12	119.70
19	AL24	6	HIS	CG-ND1-CE1	-32.52	62.67	108.20
30	AS03	69	HIS	CB-CG-ND1	-19.53	74.38	123.20
19	AL24	6	HIS	CG-CD2-NE2	-17.32	76.28	109.20
30	AS03	69	HIS	N-CA-CB	17.00	141.21	110.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	AL15	51	PHE	Peptide
19	AL24	6	HIS	Sidechain
30	AS03	68	VAL	Mainchain
30	AS03	69	HIS	Sidechain
10	BL15	51	PHE	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AL02	2105	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BL02	2105	0	0	0	0
2	AL03	1564	0	0	0	0
2	BL03	1564	0	0	0	0
3	AL04	1587	0	0	0	0
3	BL04	1587	0	0	0	0
4	AL05	1475	0	0	0	0
4	BL05	1475	0	0	0	0
5	AL06	1223	0	0	0	0
5	BL06	1223	0	0	0	0
6	AL09	1133	0	0	0	0
6	BL09	1133	0	0	0	0
7	AL11	1088	0	0	0	0
7	BL11	1088	0	0	0	0
8	AL13	1097	0	0	0	0
8	BL13	1097	0	0	0	0
9	AL14	932	0	0	0	0
9	BL14	932	0	0	0	0
10	AL15	1114	0	0	0	0
10	BL15	1114	0	0	0	0
11	AL16	1065	0	0	0	0
11	BL16	1065	0	0	0	0
12	AL17	960	0	0	0	0
12	BL17	960	0	0	0	0
13	AL18	771	0	0	0	0
13	BL18	771	0	0	0	0
14	AL19	1144	0	0	0	0
14	BL19	1144	0	0	0	0
15	AL20	964	0	0	0	0
15	BL20	964	0	0	0	0
16	AL21	779	0	0	0	0
16	BL21	779	0	0	0	0
17	AL22	891	0	0	0	0
17	BL22	891	0	0	0	0
18	AL23	726	0	0	0	0
18	BL23	726	0	0	0	0
19	AL24	776	0	0	0	0
19	BL24	776	0	0	0	0
20	AL25	1483	0	0	0	0
20	BL25	1483	0	0	0	0
21	AL27	605	0	0	0	0
21	BL27	605	0	0	0	0
22	AL28	695	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	BL28	695	0	0	0	0
23	AL29	521	0	0	0	0
23	BL29	521	0	0	0	0
24	AL30	468	0	0	0	0
24	BL30	468	0	0	0	0
25	AL32	405	0	0	0	0
25	BL32	405	0	0	0	0
26	AL33	381	0	0	0	0
26	BL33	381	0	0	0	0
27	AL34	419	0	0	0	0
27	BL34	419	0	0	0	0
28	AL35	508	0	0	0	0
28	BL35	508	0	0	0	0
29	AS02	1901	0	0	0	0
29	BS02	1901	0	0	0	0
30	AS03	1613	0	0	0	0
30	BS03	1613	0	0	0	0
31	AS04	1703	0	0	0	0
31	BS04	1703	0	0	0	0
32	AS05	1156	0	0	0	0
32	BS05	1156	0	0	0	0
33	AS06	843	0	0	0	0
33	BS06	843	0	0	0	0
34	AS07	1257	0	0	0	0
34	BS07	1257	0	0	0	0
35	AS08	1116	0	0	0	0
35	BS08	1116	0	0	0	0
36	AS09	1011	0	0	0	0
36	BS09	1011	0	0	0	0
37	AS10	795	0	0	0	0
37	BS10	795	0	0	0	0
38	AS11	843	0	0	0	0
38	BS11	843	0	0	0	0
39	AS12	957	0	0	0	0
39	BS12	957	0	0	0	0
40	AS13	934	0	0	0	0
40	BS13	934	0	0	0	0
41	AS14	492	0	0	0	0
41	BS14	492	0	0	0	0
42	AS15	734	0	0	0	0
42	BS15	734	0	0	0	0
43	AS16	701	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	BS16	701	0	0	0	0
44	AS17	824	0	0	0	0
44	BS17	824	0	0	0	0
45	AS18	574	0	0	0	0
45	BS18	574	0	0	0	0
46	AS19	630	0	0	0	0
46	BS19	630	0	0	0	0
47	AS20	762	0	0	0	0
47	BS20	762	0	0	0	0
48	ATHX	209	0	0	0	0
48	BTHX	209	0	0	0	0
49	AL31	226	0	0	0	0
49	BL31	226	0	0	0	0
50	A16S	32332	0	0	0	0
50	B16S	32331	0	0	0	0
51	A23S	61929	0	0	0	0
51	B23S	61931	0	0	0	0
52	A5S	2551	0	1295	97	0
52	B5S	2551	0	1295	104	0
53	AIRE	672	0	0	0	0
53	BIRE	672	0	0	0	0
54	AS04	1	0	0	0	0
54	AS14	1	0	0	0	0
54	BS04	1	0	0	0	0
54	BS14	1	0	0	0	0
All	All	287293	0	2590	201	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 34.

The worst 5 of 201 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:A5S:51:G:H21	52:A5S:52:A:H62	1.05	0.95
52:B5S:40:U:H3'	52:B5S:41:U:H5"	1.50	0.89
52:A5S:40:U:H3'	52:A5S:41:U:H5"	1.55	0.89
52:B5S:10:C:C2	52:B5S:11:C:H5	1.90	0.88
52:A5S:56:G:H21	52:A5S:59:A:H61	1.21	0.86

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	AL02	269/271 (99%)	197 (73%)	49 (18%)	23 (9%)	1 12
1	BL02	269/271 (99%)	184 (68%)	56 (21%)	29 (11%)	0 8
2	AL03	202/204 (99%)	145 (72%)	41 (20%)	16 (8%)	1 14
2	BL03	202/204 (99%)	140 (69%)	46 (23%)	16 (8%)	1 14
3	AL04	200/202 (99%)	154 (77%)	31 (16%)	15 (8%)	1 15
3	BL04	200/202 (99%)	142 (71%)	41 (20%)	17 (8%)	1 12
4	AL05	179/181 (99%)	134 (75%)	35 (20%)	10 (6%)	2 21
4	BL05	179/181 (99%)	128 (72%)	35 (20%)	16 (9%)	1 12
5	AL06	157/159 (99%)	117 (74%)	35 (22%)	5 (3%)	4 32
5	BL06	157/159 (99%)	119 (76%)	27 (17%)	11 (7%)	1 17
6	AL09	143/145 (99%)	112 (78%)	26 (18%)	5 (4%)	3 31
6	BL09	143/145 (99%)	97 (68%)	37 (26%)	9 (6%)	1 20
7	AL11	145/147 (99%)	100 (69%)	36 (25%)	9 (6%)	1 20
7	BL11	145/147 (99%)	108 (74%)	28 (19%)	9 (6%)	1 20
8	AL13	135/137 (98%)	95 (70%)	23 (17%)	17 (13%)	0 5
8	BL13	135/137 (98%)	90 (67%)	30 (22%)	15 (11%)	0 7
9	AL14	120/122 (98%)	95 (79%)	16 (13%)	9 (8%)	1 15
9	BL14	120/122 (98%)	94 (78%)	15 (12%)	11 (9%)	1 12
10	AL15	144/146 (99%)	76 (53%)	36 (25%)	32 (22%)	0 1
10	BL15	144/146 (99%)	83 (58%)	41 (28%)	20 (14%)	0 4
11	AL16	132/134 (98%)	93 (70%)	28 (21%)	11 (8%)	1 13
11	BL16	132/134 (98%)	99 (75%)	20 (15%)	13 (10%)	0 10
12	AL17	115/117 (98%)	89 (77%)	17 (15%)	9 (8%)	1 15
12	BL17	115/117 (98%)	82 (71%)	27 (24%)	6 (5%)	2 23
13	AL18	96/98 (98%)	66 (69%)	17 (18%)	13 (14%)	0 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
13	BL18	96/98 (98%)	61 (64%)	24 (25%)	11 (12%)	0 7
14	AL19	135/137 (98%)	85 (63%)	32 (24%)	18 (13%)	0 4
14	BL19	135/137 (98%)	88 (65%)	31 (23%)	16 (12%)	0 6
15	AL20	115/117 (98%)	88 (76%)	21 (18%)	6 (5%)	2 23
15	BL20	115/117 (98%)	88 (76%)	22 (19%)	5 (4%)	2 26
16	AL21	99/101 (98%)	70 (71%)	23 (23%)	6 (6%)	1 20
16	BL21	99/101 (98%)	75 (76%)	14 (14%)	10 (10%)	0 9
17	AL22	110/112 (98%)	86 (78%)	19 (17%)	5 (4%)	2 25
17	BL22	110/112 (98%)	81 (74%)	24 (22%)	5 (4%)	2 25
18	AL23	90/92 (98%)	78 (87%)	10 (11%)	2 (2%)	6 39
18	BL23	90/92 (98%)	78 (87%)	10 (11%)	2 (2%)	6 39
19	AL24	98/100 (98%)	62 (63%)	23 (24%)	13 (13%)	0 4
19	BL24	98/100 (98%)	53 (54%)	28 (29%)	17 (17%)	0 3
20	AL25	185/187 (99%)	144 (78%)	34 (18%)	7 (4%)	3 29
20	BL25	185/187 (99%)	142 (77%)	37 (20%)	6 (3%)	4 32
21	AL27	74/76 (97%)	56 (76%)	12 (16%)	6 (8%)	1 14
21	BL27	74/76 (97%)	58 (78%)	12 (16%)	4 (5%)	2 22
22	AL28	86/88 (98%)	60 (70%)	12 (14%)	14 (16%)	0 3
22	BL28	86/88 (98%)	58 (67%)	14 (16%)	14 (16%)	0 3
23	AL29	60/62 (97%)	45 (75%)	12 (20%)	3 (5%)	2 23
23	BL29	60/62 (97%)	44 (73%)	9 (15%)	7 (12%)	0 6
24	AL30	57/59 (97%)	49 (86%)	6 (10%)	2 (4%)	3 31
24	BL30	57/59 (97%)	41 (72%)	13 (23%)	3 (5%)	2 23
25	AL32	50/52 (96%)	36 (72%)	10 (20%)	4 (8%)	1 14
25	BL32	50/52 (96%)	40 (80%)	7 (14%)	3 (6%)	1 20
26	AL33	42/44 (96%)	27 (64%)	12 (29%)	3 (7%)	1 17
26	BL33	42/44 (96%)	26 (62%)	12 (29%)	4 (10%)	0 11
27	AL34	46/48 (96%)	40 (87%)	4 (9%)	2 (4%)	2 26
27	BL34	46/48 (96%)	36 (78%)	7 (15%)	3 (6%)	1 19
28	AL35	61/63 (97%)	36 (59%)	20 (33%)	5 (8%)	1 13
28	BL35	61/63 (97%)	39 (64%)	14 (23%)	8 (13%)	0 5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	AS02	232/234 (99%)	184 (79%)	34 (15%)	14 (6%)	1	20
29	BS02	232/234 (99%)	183 (79%)	44 (19%)	5 (2%)	6	39
30	AS03	204/206 (99%)	159 (78%)	32 (16%)	13 (6%)	1	20
30	BS03	204/206 (99%)	146 (72%)	47 (23%)	11 (5%)	2	22
31	AS04	206/208 (99%)	154 (75%)	40 (19%)	12 (6%)	1	21
31	BS04	206/208 (99%)	153 (74%)	40 (19%)	13 (6%)	1	20
32	AS05	149/151 (99%)	114 (76%)	30 (20%)	5 (3%)	3	31
32	BS05	149/151 (99%)	120 (80%)	23 (15%)	6 (4%)	3	28
33	AS06	99/101 (98%)	80 (81%)	14 (14%)	5 (5%)	2	23
33	BS06	99/101 (98%)	79 (80%)	14 (14%)	6 (6%)	1	20
34	AS07	153/155 (99%)	132 (86%)	19 (12%)	2 (1%)	12	48
34	BS07	153/155 (99%)	128 (84%)	22 (14%)	3 (2%)	7	41
35	AS08	136/138 (99%)	113 (83%)	15 (11%)	8 (6%)	1	21
35	BS08	136/138 (99%)	106 (78%)	24 (18%)	6 (4%)	2	25
36	AS09	125/127 (98%)	94 (75%)	23 (18%)	8 (6%)	1	20
36	BS09	125/127 (98%)	98 (78%)	23 (18%)	4 (3%)	4	32
37	AS10	96/98 (98%)	76 (79%)	16 (17%)	4 (4%)	3	26
37	BS10	96/98 (98%)	73 (76%)	21 (22%)	2 (2%)	7	40
38	AS11	112/114 (98%)	85 (76%)	19 (17%)	8 (7%)	1	17
38	BS11	112/114 (98%)	91 (81%)	18 (16%)	3 (3%)	5	35
39	AS12	120/122 (98%)	90 (75%)	26 (22%)	4 (3%)	4	32
39	BS12	120/122 (98%)	91 (76%)	25 (21%)	4 (3%)	4	32
40	AS13	115/117 (98%)	96 (84%)	17 (15%)	2 (2%)	9	43
40	BS13	115/117 (98%)	93 (81%)	17 (15%)	5 (4%)	2	26
41	AS14	58/60 (97%)	47 (81%)	10 (17%)	1 (2%)	9	43
41	BS14	58/60 (97%)	47 (81%)	9 (16%)	2 (3%)	3	31
42	AS15	86/88 (98%)	69 (80%)	15 (17%)	2 (2%)	6	38
42	BS15	86/88 (98%)	69 (80%)	16 (19%)	1 (1%)	13	50
43	AS16	81/83 (98%)	61 (75%)	15 (18%)	5 (6%)	1	20
43	BS16	81/83 (98%)	63 (78%)	16 (20%)	2 (2%)	5	36
44	AS17	97/99 (98%)	74 (76%)	18 (19%)	5 (5%)	2	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
44	BS17	97/99 (98%)	81 (84%)	11 (11%)	5 (5%)	2 23
45	AS18	68/70 (97%)	48 (71%)	16 (24%)	4 (6%)	1 21
45	BS18	68/70 (97%)	45 (66%)	20 (29%)	3 (4%)	2 25
46	AS19	76/78 (97%)	53 (70%)	18 (24%)	5 (7%)	1 19
46	BS19	76/78 (97%)	50 (66%)	20 (26%)	6 (8%)	1 14
47	AS20	97/99 (98%)	73 (75%)	14 (14%)	10 (10%)	0 9
47	BS20	97/99 (98%)	72 (74%)	21 (22%)	4 (4%)	3 27
48	ATHX	22/24 (92%)	18 (82%)	4 (18%)	0	100 100
48	BTHX	22/24 (92%)	13 (59%)	7 (32%)	2 (9%)	1 12
49	AL31	28/30 (93%)	15 (54%)	11 (39%)	2 (7%)	1 17
49	BL31	28/30 (93%)	20 (71%)	5 (18%)	3 (11%)	0 8
All	All	11410/11606 (98%)	8465 (74%)	2170 (19%)	775 (7%)	1 18

5 of 775 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AL02	26	LYS
1	AL02	33	LEU
1	AL02	34	VAL
1	AL02	154	LYS
1	AL02	239	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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	AL02	213/213 (100%)	185 (87%)	28 (13%)	4 23
1	BL02	213/213 (100%)	177 (83%)	36 (17%)	2 14
2	AL03	165/165 (100%)	137 (83%)	28 (17%)	2 14
2	BL03	165/165 (100%)	131 (79%)	34 (21%)	1 8
3	AL04	161/161 (100%)	150 (93%)	11 (7%)	16 47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	BL04	161/161 (100%)	141 (88%)	20 (12%)	4 24
4	AL05	155/155 (100%)	133 (86%)	22 (14%)	3 21
4	BL05	155/155 (100%)	136 (88%)	19 (12%)	4 24
5	AL06	132/132 (100%)	123 (93%)	9 (7%)	16 47
5	BL06	132/132 (100%)	116 (88%)	16 (12%)	5 25
6	AL09	122/122 (100%)	97 (80%)	25 (20%)	1 8
6	BL09	122/122 (100%)	102 (84%)	20 (16%)	2 15
7	AL11	111/111 (100%)	105 (95%)	6 (5%)	22 53
7	BL11	111/111 (100%)	106 (96%)	5 (4%)	27 57
8	AL13	116/116 (100%)	100 (86%)	16 (14%)	3 22
8	BL13	116/116 (100%)	98 (84%)	18 (16%)	2 17
9	AL14	100/100 (100%)	87 (87%)	13 (13%)	4 23
9	BL14	100/100 (100%)	89 (89%)	11 (11%)	6 29
10	AL15	112/112 (100%)	82 (73%)	30 (27%)	0 3
10	BL15	112/112 (100%)	80 (71%)	32 (29%)	0 2
11	AL16	105/105 (100%)	96 (91%)	9 (9%)	10 40
11	BL16	105/105 (100%)	88 (84%)	17 (16%)	2 15
12	AL17	100/100 (100%)	87 (87%)	13 (13%)	4 23
12	BL17	100/100 (100%)	86 (86%)	14 (14%)	3 21
13	AL18	77/77 (100%)	70 (91%)	7 (9%)	9 36
13	BL18	77/77 (100%)	68 (88%)	9 (12%)	5 27
14	AL19	121/121 (100%)	105 (87%)	16 (13%)	4 22
14	BL19	121/121 (100%)	106 (88%)	15 (12%)	4 24
15	AL20	93/93 (100%)	79 (85%)	14 (15%)	3 18
15	BL20	93/93 (100%)	83 (89%)	10 (11%)	6 30
16	AL21	82/82 (100%)	68 (83%)	14 (17%)	2 14
16	BL21	82/82 (100%)	67 (82%)	15 (18%)	1 11
17	AL22	91/91 (100%)	83 (91%)	8 (9%)	10 38
17	BL22	91/91 (100%)	83 (91%)	8 (9%)	10 38
18	AL23	74/74 (100%)	67 (90%)	7 (10%)	8 34
18	BL23	74/74 (100%)	67 (90%)	7 (10%)	8 34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
19	AL24	84/84 (100%)	69 (82%)	15 (18%)	2 12
19	BL24	84/84 (100%)	71 (84%)	13 (16%)	2 17
20	AL25	162/162 (100%)	150 (93%)	12 (7%)	13 44
20	BL25	162/162 (100%)	151 (93%)	11 (7%)	16 47
21	AL27	61/61 (100%)	56 (92%)	5 (8%)	11 40
21	BL27	61/61 (100%)	52 (85%)	9 (15%)	3 19
22	AL28	73/73 (100%)	60 (82%)	13 (18%)	2 12
22	BL28	73/73 (100%)	60 (82%)	13 (18%)	2 12
23	AL29	58/58 (100%)	52 (90%)	6 (10%)	7 31
23	BL29	58/58 (100%)	47 (81%)	11 (19%)	1 10
24	AL30	51/51 (100%)	47 (92%)	4 (8%)	12 42
24	BL30	51/51 (100%)	42 (82%)	9 (18%)	2 13
25	AL32	45/45 (100%)	38 (84%)	7 (16%)	2 17
25	BL32	45/45 (100%)	40 (89%)	5 (11%)	6 29
26	AL33	43/43 (100%)	36 (84%)	7 (16%)	2 15
26	BL33	43/43 (100%)	34 (79%)	9 (21%)	1 8
27	AL34	41/41 (100%)	37 (90%)	4 (10%)	8 33
27	BL34	41/41 (100%)	33 (80%)	8 (20%)	1 9
28	AL35	53/53 (100%)	45 (85%)	8 (15%)	3 18
28	BL35	53/53 (100%)	49 (92%)	4 (8%)	13 44
29	AS02	202/202 (100%)	186 (92%)	16 (8%)	12 42
29	BS02	202/202 (100%)	186 (92%)	16 (8%)	12 42
30	AS03	160/160 (100%)	140 (88%)	20 (12%)	4 24
30	BS03	160/160 (100%)	147 (92%)	13 (8%)	11 41
31	AS04	180/180 (100%)	163 (91%)	17 (9%)	8 35
31	BS04	180/180 (100%)	162 (90%)	18 (10%)	7 32
32	AS05	116/116 (100%)	101 (87%)	15 (13%)	4 23
32	BS05	116/116 (100%)	106 (91%)	10 (9%)	10 40
33	AS06	90/90 (100%)	82 (91%)	8 (9%)	9 38
33	BS06	90/90 (100%)	83 (92%)	7 (8%)	12 42
34	AS07	126/126 (100%)	121 (96%)	5 (4%)	31 59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
34	BS07	126/126 (100%)	121 (96%)	5 (4%)	31 59
35	AS08	119/119 (100%)	108 (91%)	11 (9%)	9 35
35	BS08	119/119 (100%)	112 (94%)	7 (6%)	19 51
36	AS09	98/98 (100%)	91 (93%)	7 (7%)	14 45
36	BS09	98/98 (100%)	91 (93%)	7 (7%)	14 45
37	AS10	88/88 (100%)	79 (90%)	9 (10%)	7 31
37	BS10	88/88 (100%)	80 (91%)	8 (9%)	9 36
38	AS11	86/86 (100%)	79 (92%)	7 (8%)	11 41
38	BS11	86/86 (100%)	77 (90%)	9 (10%)	7 30
39	AS12	103/103 (100%)	92 (89%)	11 (11%)	6 30
39	BS12	103/103 (100%)	93 (90%)	10 (10%)	8 33
40	AS13	94/94 (100%)	92 (98%)	2 (2%)	53 74
40	BS13	94/94 (100%)	90 (96%)	4 (4%)	29 58
41	AS14	49/49 (100%)	45 (92%)	4 (8%)	11 40
41	BS14	49/49 (100%)	46 (94%)	3 (6%)	18 50
42	AS15	79/79 (100%)	71 (90%)	8 (10%)	7 32
42	BS15	79/79 (100%)	68 (86%)	11 (14%)	3 21
43	AS16	72/72 (100%)	63 (88%)	9 (12%)	4 24
43	BS16	72/72 (100%)	68 (94%)	4 (6%)	21 52
44	AS17	94/94 (100%)	85 (90%)	9 (10%)	8 34
44	BS17	94/94 (100%)	87 (93%)	7 (7%)	13 44
45	AS18	61/61 (100%)	58 (95%)	3 (5%)	25 55
45	BS18	61/61 (100%)	53 (87%)	8 (13%)	4 23
46	AS19	69/69 (100%)	63 (91%)	6 (9%)	10 38
46	BS19	69/69 (100%)	62 (90%)	7 (10%)	7 32
47	AS20	76/76 (100%)	72 (95%)	4 (5%)	22 54
47	BS20	76/76 (100%)	72 (95%)	4 (5%)	22 54
48	ATHX	19/19 (100%)	18 (95%)	1 (5%)	22 54
48	BTHX	19/19 (100%)	19 (100%)	0	100 100
49	AL31	27/27 (100%)	26 (96%)	1 (4%)	34 62
49	BL31	27/27 (100%)	25 (93%)	2 (7%)	13 44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9618/9618 (100%)	8530 (89%)	1088 (11%)	6 28

5 of 1088 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
28	BL35	64	TYR
30	BS03	167	TRP
28	BL35	57	ARG
40	BS13	115	LYS
30	AS03	172	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
50	A16S	1503/1506 (99%)	247 (16%)	21 (1%)
50	B16S	1503/1506 (99%)	249 (16%)	21 (1%)
51	A23S	2872/2879 (99%)	541 (18%)	29 (1%)
51	B23S	2872/2879 (99%)	552 (19%)	26 (0%)
52	A5S	118/119 (99%)	18 (15%)	0
52	B5S	118/119 (99%)	15 (12%)	0
53	AIRE	30/196 (15%)	4 (13%)	0
53	BIRE	30/196 (15%)	4 (13%)	0
All	All	9046/9400 (96%)	1630 (18%)	97 (1%)

5 of 1630 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
50	A16S	6	G
50	A16S	7	G
50	A16S	9	G
50	A16S	16	A
50	A16S	17	U

5 of 97 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
50	B16S	499	A

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Mol	Chain	Res	Type
51	B23S	196	A
50	B16S	560	U
50	B16S	1064	G
51	B23S	474	G

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	AL02	271/271 (100%)	0.09	4 (1%) 73 66	54, 99, 150, 228	0
1	BL02	271/271 (100%)	-0.01	1 (0%) 92 89	42, 88, 128, 197	0
2	AL03	204/204 (100%)	0.39	7 (3%) 45 37	63, 120, 179, 294	0
2	BL03	204/204 (100%)	0.16	6 (2%) 51 42	52, 114, 168, 253	0
3	AL04	202/202 (100%)	0.04	4 (1%) 65 58	60, 113, 184, 265	0
3	BL04	202/202 (100%)	0.03	3 (1%) 73 66	52, 109, 174, 242	0
4	AL05	181/181 (100%)	1.30	54 (29%) 0 0	134, 212, 272, 318	0
4	BL05	181/181 (100%)	1.42	51 (28%) 0 0	149, 227, 281, 309	0
5	AL06	159/159 (100%)	1.68	60 (37%) 0 0	124, 217, 285, 314	0
5	BL06	159/159 (100%)	0.40	9 (5%) 23 19	91, 142, 199, 240	0
6	AL09	145/145 (100%)	1.17	44 (30%) 0 0	82, 185, 244, 324	0
6	BL09	145/145 (100%)	0.75	21 (14%) 2 2	76, 156, 202, 244	0
7	AL11	147/147 (100%)	3.85	118 (80%) 0 0	256, 322, 358, 387	0
7	BL11	147/147 (100%)	4.54	113 (76%) 0 0	225, 321, 363, 388	0
8	AL13	137/137 (100%)	0.32	8 (5%) 23 18	82, 133, 194, 207	0
8	BL13	137/137 (100%)	0.34	6 (4%) 34 29	69, 120, 186, 258	0
9	AL14	122/122 (100%)	0.08	0 100 100	63, 111, 148, 180	0
9	BL14	122/122 (100%)	0.34	3 (2%) 57 49	65, 101, 142, 171	0
10	AL15	146/146 (100%)	0.45	8 (5%) 25 21	63, 138, 225, 281	0
10	BL15	146/146 (100%)	0.55	13 (8%) 9 8	46, 134, 208, 283	0
11	AL16	134/134 (100%)	0.46	10 (7%) 14 11	85, 136, 201, 289	0
11	BL16	134/134 (100%)	0.55	11 (8%) 11 9	77, 126, 219, 300	0
12	AL17	117/117 (100%)	0.52	8 (6%) 17 13	64, 113, 171, 197	0
12	BL17	117/117 (100%)	0.49	2 (1%) 70 62	67, 105, 162, 218	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	AL18	98/98 (100%)	1.15	26 (26%) 0 0	125, 187, 243, 293	0
13	BL18	98/98 (100%)	0.72	17 (17%) 1 1	140, 201, 253, 275	0
14	AL19	137/137 (100%)	0.27	7 (5%) 28 24	78, 132, 216, 266	0
14	BL19	137/137 (100%)	0.15	4 (2%) 51 42	74, 124, 226, 284	0
15	AL20	117/117 (100%)	0.04	2 (1%) 70 62	66, 113, 181, 243	0
15	BL20	117/117 (100%)	-0.17	0 100 100	62, 112, 172, 232	0
16	AL21	101/101 (100%)	0.27	2 (1%) 65 58	86, 140, 206, 307	0
16	BL21	101/101 (100%)	0.18	5 (4%) 28 25	75, 130, 202, 283	0
17	AL22	112/112 (100%)	0.60	4 (3%) 42 35	71, 104, 172, 250	0
17	BL22	112/112 (100%)	0.30	3 (2%) 54 45	57, 95, 152, 210	0
18	AL23	92/92 (100%)	0.13	0 100 100	77, 117, 171, 217	0
18	BL23	92/92 (100%)	0.37	2 (2%) 62 54	62, 97, 139, 182	0
19	AL24	100/100 (100%)	1.14	20 (20%) 1 1	103, 144, 262, 296	0
19	BL24	100/100 (100%)	0.82	10 (10%) 7 6	83, 129, 234, 266	0
20	AL25	187/187 (100%)	0.96	41 (21%) 0 1	119, 190, 253, 309	0
20	BL25	187/187 (100%)	0.35	14 (7%) 14 11	111, 179, 225, 276	0
21	AL27	76/76 (100%)	0.34	5 (6%) 18 14	91, 135, 187, 233	0
21	BL27	76/76 (100%)	0.42	5 (6%) 18 14	88, 132, 198, 248	0
22	AL28	88/88 (100%)	0.35	3 (3%) 45 37	61, 109, 186, 283	0
22	BL28	88/88 (100%)	0.37	4 (4%) 33 28	61, 105, 182, 248	0
23	AL29	62/62 (100%)	0.33	4 (6%) 18 14	99, 137, 237, 255	0
23	BL29	62/62 (100%)	0.28	6 (9%) 7 7	59, 108, 218, 253	0
24	AL30	59/59 (100%)	1.40	15 (25%) 0 0	101, 132, 214, 248	0
24	BL30	59/59 (100%)	0.92	5 (8%) 10 9	78, 131, 207, 286	0
25	AL32	52/52 (100%)	0.51	7 (13%) 3 3	66, 117, 205, 239	0
25	BL32	52/52 (100%)	0.06	2 (3%) 40 33	54, 105, 215, 269	0
26	AL33	44/44 (100%)	9.55	44 (100%) 0 0	140, 241, 282, 301	0
26	BL33	44/44 (100%)	5.13	39 (88%) 0 0	193, 248, 287, 304	0
27	AL34	48/48 (100%)	-0.04	0 100 100	59, 89, 129, 203	0
27	BL34	48/48 (100%)	0.14	0 100 100	41, 71, 113, 175	0
28	AL35	63/63 (100%)	0.21	1 (1%) 72 64	69, 119, 192, 227	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	BL35	63/63 (100%)	0.16	1 (1%) 72 64	71, 114, 188, 225	0
29	AS02	234/234 (100%)	0.56	22 (9%) 8 7	128, 202, 274, 300	0
29	BS02	234/234 (100%)	0.64	26 (11%) 5 5	113, 213, 279, 309	0
30	AS03	206/206 (100%)	0.44	15 (7%) 15 12	124, 200, 264, 308	0
30	BS03	206/206 (100%)	0.34	12 (5%) 23 18	119, 196, 253, 298	0
31	AS04	208/208 (100%)	0.23	5 (2%) 59 50	99, 152, 216, 239	0
31	BS04	208/208 (100%)	0.73	31 (14%) 2 2	128, 204, 275, 307	0
32	AS05	151/151 (100%)	0.11	4 (2%) 56 47	94, 144, 199, 262	0
32	BS05	151/151 (100%)	0.04	5 (3%) 46 38	105, 164, 216, 261	0
33	AS06	101/101 (100%)	0.17	5 (4%) 28 25	122, 172, 234, 258	0
33	BS06	101/101 (100%)	-0.10	2 (1%) 65 58	96, 149, 203, 230	0
34	AS07	155/155 (100%)	0.91	32 (20%) 1 1	154, 214, 272, 300	0
34	BS07	155/155 (100%)	0.95	30 (19%) 1 1	151, 222, 282, 309	0
35	AS08	138/138 (100%)	0.47	12 (8%) 10 8	92, 142, 195, 229	0
35	BS08	138/138 (100%)	0.58	14 (10%) 7 6	95, 168, 215, 256	0
36	AS09	127/127 (100%)	1.61	38 (29%) 0 0	139, 274, 335, 355	0
36	BS09	127/127 (100%)	1.31	31 (24%) 0 0	150, 262, 310, 343	0
37	AS10	98/98 (100%)	2.25	49 (50%) 0 0	138, 260, 344, 356	0
37	BS10	98/98 (100%)	1.61	33 (33%) 0 0	142, 246, 308, 339	0
38	AS11	114/114 (100%)	0.43	13 (11%) 5 5	95, 150, 210, 267	0
38	BS11	114/114 (100%)	0.11	3 (2%) 56 47	85, 138, 193, 251	0
39	AS12	122/122 (100%)	0.72	12 (9%) 7 7	74, 121, 166, 201	0
39	BS12	122/122 (100%)	0.53	8 (6%) 18 14	105, 147, 192, 230	0
40	AS13	117/117 (100%)	1.65	41 (35%) 0 0	152, 259, 315, 352	0
40	BS13	117/117 (100%)	1.11	30 (25%) 0 0	159, 253, 318, 340	0
41	AS14	60/60 (100%)	1.05	11 (18%) 1 1	148, 194, 241, 329	0
41	BS14	60/60 (100%)	1.02	9 (15%) 2 2	144, 196, 242, 301	0
42	AS15	88/88 (100%)	0.32	5 (5%) 23 19	100, 139, 183, 229	0
42	BS15	88/88 (100%)	0.48	5 (5%) 23 19	92, 146, 201, 215	0
43	AS16	83/83 (100%)	0.84	12 (14%) 2 2	104, 137, 187, 233	0
43	BS16	83/83 (100%)	1.44	27 (32%) 0 0	148, 199, 260, 310	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	AS17	99/99 (100%)	0.15	3 (3%) 50 40	92, 125, 166, 223	0
44	BS17	99/99 (100%)	0.36	3 (3%) 50 40	105, 149, 191, 235	0
45	AS18	70/70 (100%)	0.85	9 (12%) 3 4	110, 174, 234, 253	0
45	BS18	70/70 (100%)	0.49	1 (1%) 75 68	100, 150, 195, 247	0
46	AS19	78/78 (100%)	2.27	38 (48%) 0 0	170, 255, 301, 353	0
46	BS19	78/78 (100%)	1.70	28 (35%) 0 0	172, 257, 302, 314	0
47	AS20	99/99 (100%)	0.69	9 (9%) 9 7	106, 149, 228, 256	0
47	BS20	99/99 (100%)	1.18	22 (22%) 0 0	120, 178, 249, 291	0
48	ATHX	24/24 (100%)	0.68	1 (4%) 36 30	153, 263, 279, 301	0
48	BTHX	24/24 (100%)	1.20	8 (33%) 0 0	209, 276, 325, 350	0
49	AL31	30/30 (100%)	1.85	13 (43%) 0 0	206, 272, 323, 351	0
49	BL31	30/30 (100%)	1.81	11 (36%) 0 0	216, 303, 332, 352	0
50	A16S	1504/1506 (99%)	0.19	50 (3%) 46 38	76, 144, 270, 413	0
50	B16S	1504/1506 (99%)	0.23	56 (3%) 41 34	79, 171, 296, 397	0
51	A23S	2876/2879 (99%)	0.23	126 (4%) 34 29	58, 115, 252, 440	0
51	B23S	2876/2879 (99%)	0.14	117 (4%) 37 31	52, 103, 243, 414	0
52	A5S	119/119 (100%)	-0.03	1 (0%) 86 81	122, 178, 230, 282	0
52	B5S	119/119 (100%)	-0.19	1 (0%) 86 81	124, 178, 236, 309	0
53	AIRE	32/196 (16%)	1.84	10 (31%) 0 0	131, 266, 505, 516	0
53	BIRE	32/196 (16%)	0.48	2 (6%) 20 15	145, 222, 413, 466	0
All	All	20668/21006 (98%)	0.49	1913 (9%) 8 7	41, 141, 282, 516	0

The worst 5 of 1913 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	BL11	1	MET	31.2
26	AL33	49	HIS	20.9
26	AL33	13	CYS	20.3
26	AL33	47	THR	17.4
26	AL33	22	ALA	16.8

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	ZN	BS04	301	1/1	0.90	0.23	100,100,100,100	0
54	ZN	AS14	101	1/1	0.95	0.13	120,120,120,120	0
54	ZN	BS14	101	1/1	0.96	0.10	137,137,137,137	0
54	ZN	AS04	301	1/1	0.99	0.24	78,78,78,78	0

6.5 Other polymers (i)

There are no such residues in this entry.