



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2018 – 09:52 pm GMT

PDB ID : 4V8A
Title : The structure of thermorubin in complex with the 70S ribosome from *Thermus thermophilus*.
Authors : Bulkley, D.; Johnson, F.A.; Steitz, T.A.
Deposited on : 2011-12-05
Resolution : 3.20 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

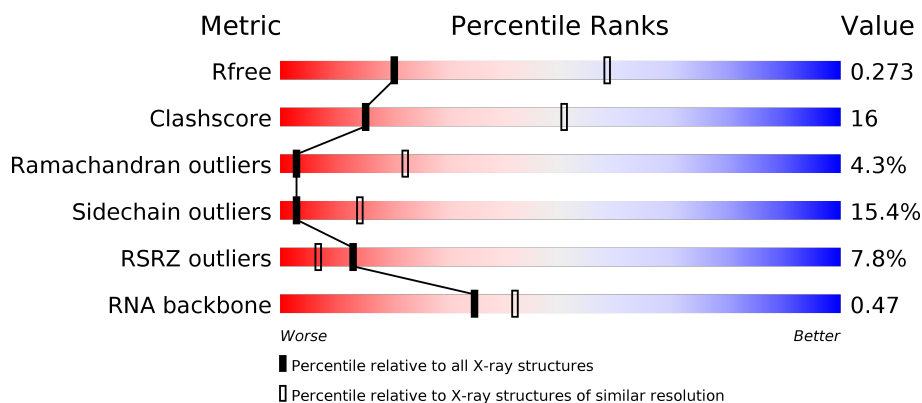
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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









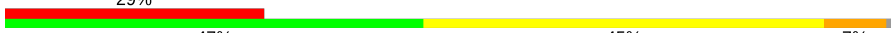







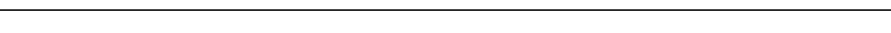




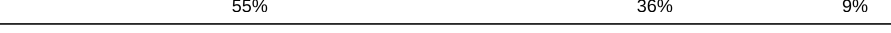





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	111664	1121 (3.22-3.18)
Clashscore	122126	1091 (3.20-3.20)
Ramachandran outliers	120053	1074 (3.20-3.20)
Sidechain outliers	120020	1073 (3.20-3.20)
RSRZ outliers	108989	1083 (3.22-3.18)
RNA backbone	2636	1107 (3.60-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	2915	<div> <div>4%</div> <div>36% 43% 15% . .</div> </div>
1	BA	2915	<div> <div>3%</div> <div>45% 34% 15% . .</div> </div>
2	AB	122	<div> <div>3%</div> <div>27% 52% 16% . .</div> </div>
2	BB	122	<div> <div></div> <div>49% 35% 13% . .</div> </div>




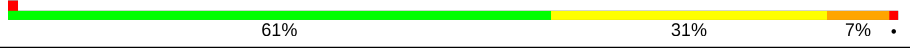
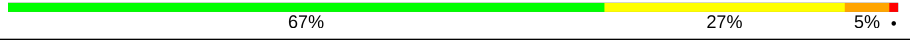





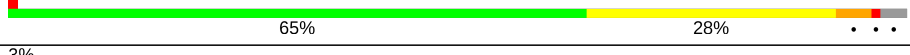

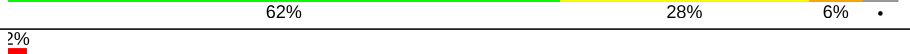


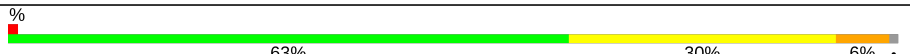









Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	AD	276	
3	BD	276	% 
4	AE	206	
4	BE	206	
5	AF	205	% 
5	BF	205	
6	AG	182	
6	BG	182	4% 
7	AH	180	21% 
7	BH	180	
8	AI	148	14% 
8	BI	148	% 
9	AN	140	% 
9	BN	140	
10	AO	122	
10	BO	122	
11	AP	150	3% 
11	BP	150	
12	AQ	141	% 
12	BQ	141	
13	AR	118	
13	BR	118	
14	AS	112	12% 
14	BS	112	
15	AT	146	% 

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	BT	146	% 
16	AU	118	
16	BU	118	
17	AV	101	% 
17	BV	101	
18	AW	113	
18	BW	113	
19	AX	96	
19	BX	96	
20	AY	110	6% 
20	BY	110	% 
21	AZ	206	3% 
21	BZ	206	
22	A0	85	2% 
22	B0	85	
23	A1	98	2% 
23	B1	98	% 
24	A2	72	% 
24	B2	72	
25	A3	60	8% 
25	B3	60	
26	A4	71	10% 
26	B4	71	8% 
27	A5	60	
27	B5	60	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	A6	54	
28	B6	54	
29	A7	49	
29	B7	49	
30	A8	65	
30	B8	65	
31	CA	1521	
31	DA	1521	
32	CB	256	
32	DB	256	
33	CC	239	
33	DC	239	
34	CD	209	
34	DD	209	
35	CE	162	
35	DE	162	
36	CF	101	
36	DF	101	
37	CG	156	
37	DG	156	
38	CH	138	
38	DH	138	
39	CI	128	
39	DI	128	
40	CJ	105	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
40	DJ	105	
41	CK	129	
41	DK	129	
42	CL	132	
42	DL	132	
43	CM	126	
43	DM	126	
44	CN	61	
44	DN	61	
45	CO	89	
45	DO	89	
46	CP	88	
46	DP	88	
47	CQ	105	
47	DQ	105	
48	CR	88	
48	DR	88	
49	CS	93	
49	DS	93	
50	CT	106	
50	DT	106	
51	CU	27	
51	DU	27	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
52	T8B	AA	3001	-	-	X	-
52	T8B	BA	3001	-	-	X	-

2 Entry composition

There are 53 unique types of molecules in this entry. The entry contains 279316 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 RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	2827	Total	C	N	O	P	0	0	0
			60900	27102	11403	19569	2826			
1	BA	2827	Total	C	N	O	P	0	0	0
			60900	27102	11403	19569	2826			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	272A	G	U	CONFLICT	GB AP008226.1
BA	272A	G	U	CONFLICT	GB AP008226.1

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	120	Total	C	N	O	P	0	0	0
			2574	1146	476	833	119			
2	BB	120	Total	C	N	O	P	0	0	0
			2574	1146	476	833	119			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AB	120	G	A	CONFLICT	GB AP008226.1
BB	120	G	A	CONFLICT	GB AP008226.1

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AD	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			
3	BD	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AE	204	Total	C	N	O	S	0	0	0
			1555	982	297	270	6			
4	BE	204	Total	C	N	O	S	0	0	0
			1555	982	297	270	6			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AF	203	Total	C	N	O	S	0	0	1
			1576	1005	297	272	2			
5	BF	203	Total	C	N	O	S	0	0	1
			1576	1005	297	272	2			

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AG	181	Total	C	N	O	S	0	0	0
			1368	879	242	244	3			
6	BG	181	Total	C	N	O	S	0	0	0
			1368	879	242	244	3			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AH	174	Total	C	N	O	S	0	0	0
			1317	837	243	236	1			
7	BH	174	Total	C	N	O	S	0	0	0
			1317	837	243	236	1			

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AI	145	Total	C	N	O	S	0	0	0
			1046	674	180	191	1			
8	BI	145	Total	C	N	O	S	0	0	0
			1046	674	180	191	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	110	GLU	ASP	CONFLICT	UNP Q5SLQ1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
BI	110	GLU	ASP	CONFLICT	UNP Q5SLQ1

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AN	140	Total	C	N	O	S	0	0	0
			1112	717	207	184	4			
9	BN	140	Total	C	N	O	S	0	0	0
			1112	717	207	184	4			

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AO	122	Total	C	N	O	S	0	0	0
			923	583	168	168	4			
10	BO	122	Total	C	N	O	S	0	0	0
			923	583	168	168	4			

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AP	147	Total	C	N	O	S	0	0	0
			1119	695	227	194	3			
11	BP	147	Total	C	N	O	S	0	0	0
			1119	695	227	194	3			

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
12	BQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
13	BR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	AS	110	Total	C	N	O	0	0	0
			865	544	172	149			
14	BS	110	Total	C	N	O	0	0	0
			865	544	172	149			

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AT	131	Total	C	N	O	S	0	0	0
			1063	666	213	183	1			
15	BT	131	Total	C	N	O	S	0	0	0
			1063	666	213	183	1			

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			
16	BU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AV	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			
17	BV	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AW	112	Total	C	N	O	S	0	0	0
			881	554	172	153	2			
18	BW	112	Total	C	N	O	S	0	0	0
			881	554	172	153	2			

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AX	95	Total	C	N	O	S	0	0	0
			742	483	134	124	1			
19	BX	95	Total	C	N	O	S	0	0	0
			742	483	134	124	1			

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AY	107	Total	C	N	O	S	0	0	0
			785	503	145	131	6			
20	BY	107	Total	C	N	O	S	0	0	0
			785	503	145	131	6			

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AZ	198	Total	C	N	O	S	0	0	0
			1522	972	269	279	2			
21	BZ	198	Total	C	N	O	S	0	0	0
			1522	972	269	279	2			

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	A0	76	Total	C	N	O	S	0	0	0
			594	368	125	100	1			
22	B0	76	Total	C	N	O	S	0	0	0
			594	368	125	100	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	A1	97	Total	C	N	O	S	0	0	0
			745	469	144	131	1			
23	B1	97	Total	C	N	O	S	0	0	0
			745	469	144	131	1			

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	A2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	B2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	A3	59	Total	C	N	O	S	0	0	0
			458	293	87	78				
25	B3	59	Total	C	N	O	S	0	0	0
			458	293	87	78				

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	A4	46	Total	C	N	O	S	0	0	0
			349	223	57	64	5			
26	B4	46	Total	C	N	O	S	0	0	0
			349	223	57	64	5			

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	A5	59	Total	C	N	O	S	0	0	0
			455	286	90	74	5			
27	B5	59	Total	C	N	O	S	0	0	0
			455	286	90	74	5			

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	A6	53	Total	C	N	O	S	0	0	0
			449	278	90	77	4			
28	B6	53	Total	C	N	O	S	0	0	0
			449	278	90	77	4			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	A7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
29	B7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	A8	64	Total	C	N	O	S	0	0	0
			509	326	99	82	2			
30	B8	64	Total	C	N	O	S	0	0	0
			509	326	99	82	2			

- Molecule 31 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	CA	1498	Total	C	N	O	P	0	0	0
			32208	14334	5974	10402	1498			
31	DA	1498	Total	C	N	O	P	0	0	0
			32208	14334	5974	10402	1498			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CA	?	-	U	DELETION	GB AP008226.1
DA	?	-	U	DELETION	GB AP008226.1

- Molecule 32 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	CB	229	Total	C	N	O	S	0	0	0
			1777	1134	318	320	5			
32	DB	229	Total	C	N	O	S	0	0	0
			1777	1134	318	320	5			

- Molecule 33 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	CC	206	Total	C	N	O	S	0	0	0
			1450	906	279	264	1			
33	DC	206	Total	C	N	O	S	0	0	0
			1450	906	279	264	1			

- Molecule 34 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	CD	208	Total	C	N	O	S	0	0	0
			1520	960	283	272	5			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	DD	208	Total	C	N	O	S	0	0	0
			1520	960	283	272	5			

- Molecule 35 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	CE	148	Total	C	N	O	S	0	0	0
			1105	699	204	198	4			
35	DE	148	Total	C	N	O	S	0	0	0
			1105	699	204	198	4			

- Molecule 36 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	CF	100	Total	C	N	O	S	0	0	0
			781	495	137	146	3			
36	DF	100	Total	C	N	O	S	0	0	0
			781	495	137	146	3			

- Molecule 37 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	CG	155	Total	C	N	O	S	0	0	0
			1167	727	224	210	6			
37	DG	155	Total	C	N	O	S	0	0	0
			1167	727	224	210	6			

- Molecule 38 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	CH	138	Total	C	N	O	S	0	0	0
			1045	665	188	190	2			
38	DH	138	Total	C	N	O	S	0	0	0
			1045	665	188	190	2			

- Molecule 39 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
39	CI	125	Total	C	N	O	0	0	0
			852	533	163	156			
39	DI	125	Total	C	N	O	0	0	0
			852	533	163	156			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CI	58	ARG	HIS	CONFLICT	UNP P80374
DI	58	ARG	HIS	CONFLICT	UNP P80374

- Molecule 40 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	CJ	96	Total	C	N	O	0	0	0
			659	408	131	120			
40	DJ	96	Total	C	N	O	0	0	0
			659	408	131	120			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CJ	75	LEU	ILE	CONFLICT	UNP Q5SHN7
DJ	75	LEU	ILE	CONFLICT	UNP Q5SHN7

- Molecule 41 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	CK	114	Total	C	N	O	S	0	0	0
			828	516	155	154	3			
41	DK	114	Total	C	N	O	S	0	0	0
			828	516	155	154	3			

- Molecule 42 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	CL	122	Total	C	N	O	S	0	0	0
			909	570	179	159	1			
42	DL	122	Total	C	N	O	S	0	0	0
			909	570	179	159	1			

- Molecule 43 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	CM	114	Total	C	N	O	S	0	0	0
			801	494	164	142	1			
43	DM	114	Total	C	N	O	S	0	0	0
			801	494	164	142	1			

- Molecule 44 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	CN	60	Total	C	N	O	S	0	0	0
			478	303	99	72	4			
44	DN	60	Total	C	N	O	S	0	0	0
			478	303	99	72	4			

- Molecule 45 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	CO	88	Total	C	N	O	S	0	0	0
			724	453	143	126	2			
45	DO	88	Total	C	N	O	S	0	0	0
			724	453	143	126	2			

- Molecule 46 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	CP	82	Total	C	N	O	S	0	0	0
			651	416	123	111	1			
46	DP	82	Total	C	N	O	S	0	0	0
			651	416	123	111	1			

- Molecule 47 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	CQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
47	DQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 48 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
48	CR	68	Total	C	N	O	0	0	0
			514	329	98	87			
48	DR	68	Total	C	N	O	0	0	0
			514	329	98	87			

- Molecule 49 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	CS	78	Total	C	N	O	S	0	0	0
			544	342	105	95	2			
49	DS	78	Total	C	N	O	S	0	0	0
			544	342	105	95	2			

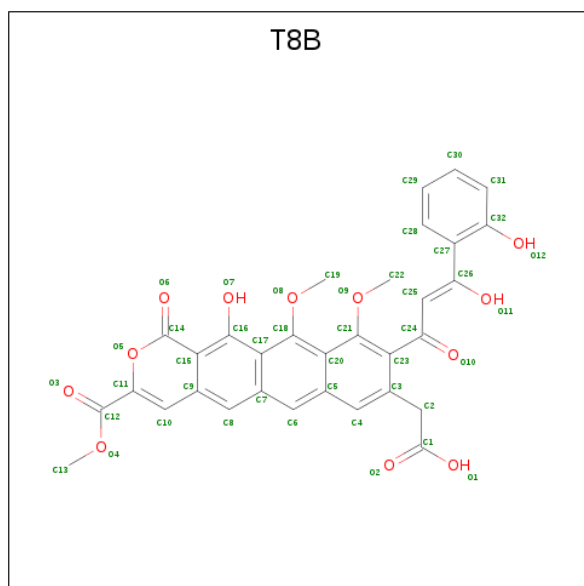
- Molecule 50 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	CT	96	Total	C	N	O	S	0	0	0
			708	435	151	120	2			
50	DT	96	Total	C	N	O	S	0	0	0
			708	435	151	120	2			

- Molecule 51 is a protein called 30S ribosomal protein THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
51	CU	23	Total	C	N	O	0	0	0
			199	122	48	29			
51	DU	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 52 is Thermorubin (three-letter code: T8B) (formula: $C_{32}H_{24}O_{12}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
52	AA	1	Total	C	O	0	0
			44	32	12		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
52	BA	1	Total	C	O	0	0
			44	32	12		

- Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

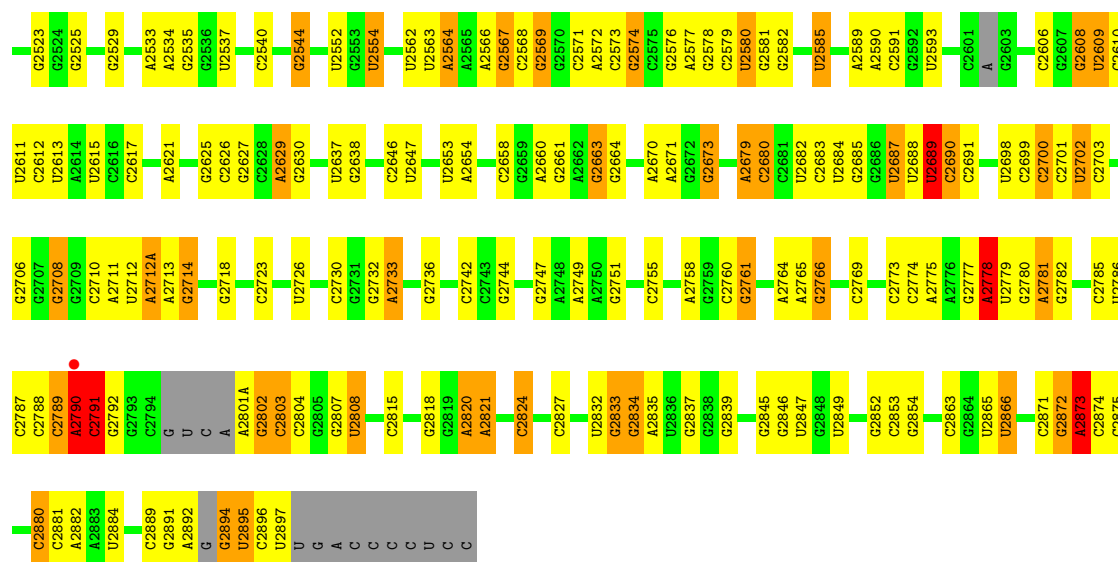
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
53	AA	2	Total	Mg	0	0
			2	2		
53	BA	2	Total	Mg	0	0
			2	2		

U1805	C1710	C1638	A1542	G1478	C1399	G1248	C1179	U	A1045	C975	C902	G836	G769
C1711	U1639	U1638	A1545	G1479	C1403	U1249	C1180	G	A1046	G975A	C903	C837	G770
C1712	C1640	G1480	C1546	G1480	C1404	G1250	G1183	G1107	G1047	C976	C904	C838	
G1720	C1644	U1481	C1547	U1481	U1405	G1252	G1184	C1109	A1048	G977	U905	U839	U773
G1721	G1645	G1482	C1548	G1482	U1406	A1253	C1185	C1109	C1049	A980	G906	C840	A774
U1722	C1646	G1484		G1484	C1407	A1253	C1186	G1110	A1050		U907	A841	G775
A1739	G1647	G1485	A1558	G1485	C1408	G1266	G1187	A1111	G1051		C908	G842	G776
G1740	C1648	A1486	G1559	A1486	C1409	U1267	U1188	U1112	C1052		A909		A777
A1741	G1651	G1487	G1560	G1487	G1410	G1268	A1189	G1113	C	A983	A910	G845	G778
G1742	G1652	U1488		U1488	A1411	G1269	G1190	G1114	G	C985	A911	G848	U779
G1743	A1652	U1489	C1564	U1489	A1412	G1260	G1191	G1115	G	G986	C912	G849	G780
	G1653	A1490	C1565	A1490	G1413	G1261	G1192	C1116	G	G987	U913	A849	A781
G1746	A1654	G1491		G1491			G1193		G	A988	C914	C850	A782
G1753	A1655	G1492	G1568	G1492	G1416	A1265	G1120	G1120	G	G989	C915	A783	A783
C1754	A1656	C1493	A1569	C1493	C1417	U1266	U1198	G1121	U	A990	G916	G854	A784
A1755	C1657	A1494	A1570	A1494	G1418	U1267	U1199	G1122	U	C991	A917	G855	G785
U1833		A1495	A1571	A1495	A1419	G1273	G1200	G1123	U	C992	G918	C856	C786
U1834	C1680	A1496	A1572	A1496	U1420	A1274	U1205	G1124	U	G993	G919	C857	U787
G1835	G1681	U1497		U1497	G1421	A1275	G1206	G1125	G	C994	G920	U858	A788
C1837	C1682		C1575		G1422	G1271	C1202		C	C995	G921	C859	
U1838	C1683	C1500	U1576	G1500	G1423	A1278	C1203	U1130	U	A996	U922	U860	G792
G1839	A1665	C1501	C1577	C1501	G1423		A1204	G1131	U	G997	C923	A861	A793
G1840	G1666	U1503	A1578	U1503	A1427	A1278	U1211	U1133	G	C998	G938	G862	G794
C1844	G1667	C1504	A1580	C1504	G1428	A1278	U1212	G1136	A	U999	G932	A863	C795
G1847	A1668	C1505	G1581	C1505	G1429	U1282	G1211	G1137	A	A1001	G933	C865	C797
A1848	A1669	C1506	C1582	C1506	C1430	G1283	U1212	G1138	C	A1002	A933	A866	G799
G1849	G1670	U1507	A1583	U1507	U1431	A1284	A1213	G1139	C	C1004	G938	U868	A802
G1850	U1671	A1508	C1584	A1508	C1432	G1285	G1215	C1140	G	C1005	U877	C867	U803
	C1672	C1509	A1586	C1509	U1433	A1286	G1216	U1141	C	C1006	A941	A870	A804
G1773	U1673	A1509A	A1587	A1509A	A1434	A1287		U1142	C	C1007	G942	C805	
U1775	G1674		C1588		C1437	U1288	A1220	A1142A	A	C1008	G943	C806	
	G1678	U1514	G1591	U1514	U1438	U1288	C1221	A1143	C	U1009	G945	G874	U807
A1779	C1684	C1516	C1592	C1516	U1439	U1292	C1221A	G1144	C	G946	G947	C876	
G1781	C1685	G1517	G1593	G1517	G1369	C1293	G1222	A1148	C	C1012	G948	U877	C812
C1782	C1686	U1518	G1594	U1518	C1370		G1223		U	C1013	G949	A878	U813
A1783	G1687	G1519		G1519	G1371	C1297		C1153	U	U1014	C949	C879	C814
G1784	U1688	U1520	C1598	U1520	A1372	C1298	A1226	G1154	A	G1015	C950	G880	C815
A1785	U1688	G1523	U1602	G1523	G1374	G1299	G1227	A1155	A	G1016	C951	C881	C816
A1786	A1689	U1524	U1602	U1524	C1375	U1300	G1228	A1156	A	C1017	G952	C882	C817
A1787	A1690	G1525	A1449	G1525	C1376	A1301	G1229	U1159	G	U1019	A953	C883	C818
G1788	C1691	G1526	G1450	G1526	G1377		C1230	U1160	A	A1020	G954	C884	A819
A1789	U1692	G1527		G1527	A1378	A1308	G1231	G1161	G	A1021		C885	A820
C1790	U1693	A1528	G1455	A1528	A1378	G1309	G1232	C1162	U	G1022	U958	C886	A821
A1791	C1694	A1528A	G1459	A1528A	A1379	G1310	G1232	G1161	U		A959	A887	U822
G1792	G1695	G1529	G1460	G1529	G1381	G1312	G1236	U1165	C	G1025	A960	C888	G823
C1793	G1696	C1530	G1461	C1530	G1382	U1313	A1237	C1166	C	U1026	C961	C889	A824
U1794	G1697	G1531	G1461	G1531	C1383	U1314	G1238	U1167	U	A1027	G962	A890	C825
A1889	A1698	C1532	C1462	C1532	A1384	C1315	G1239	G1168	A	A1028	U963	C892	U826
A1890	G1699	G	C1463	G	G1385	C1316	U1240		A		G966	C893	U827
G1891	G1699	U	C1464	U	C1386	U1317	G1243	G1171	U		C967	C894	U828
C1892	A1700	A	C1464	A	C1387	A1317	A1241	A1171	C	G1033	U969	U895	A829
U1798	A1701	C	C1467	C		G1318	G1242	A1173	G	U1033	G968	A896	C967
G1799	G1702		G1470		A1393	G1319	G1243	A1174	C	C1038	C970	C897	G831
A1900	G1703	G1537	A1471	G1537	U1394	C1320	G1244	U1175	U	G1039	C971	C898	G832
G1801	G1704	G1538	A1472	G1538	A1395	U1323	G1245	G1176	C		G1042	A899	U833
A1802	G1705	G1539	A1472	G1539	U1396		A1246	A1177	U		C1043	A900	C834
G1906	U1709	U1636	A1637	U1636			A1247	C1178	C		G974	A901	A835
A1913		G1541		G1541					A1106				

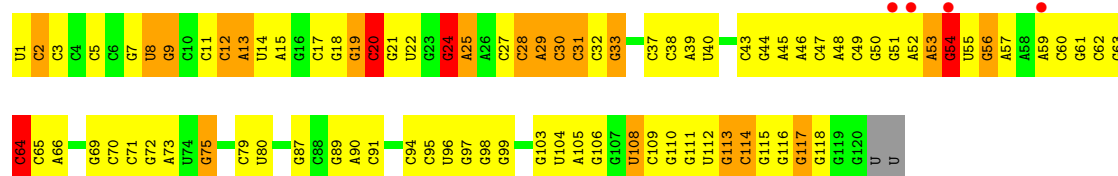




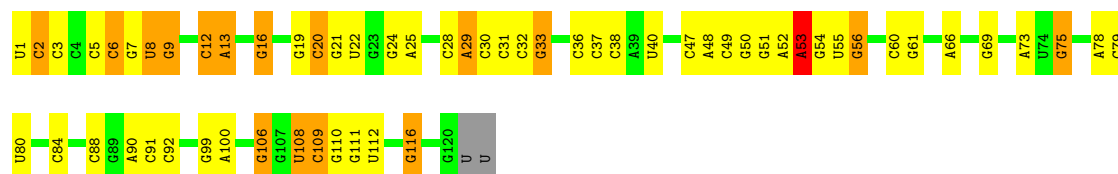
A2439	C2356	C2384	A2057	C1967	A1884	A1791	G1678	C1584	A1494	C1408	G1324	A1241
C2440	U2357	C2285	A2058	G1968	A1885	G1792	U1679	A1586	A1495	A1408	G1325	A1242
C2441	A2360	A2286	A2059	A1969	C1886	C1793	U1680	C1588	A1496	A1413	G1326	G1243
G2445	A2361	A2287	A2060	A1970	C1887	C1794	U1685	C1598	U1497	G1416	G1328	A1247
G2446	G2362	A2288	A2061	A1971	A1888	G1795	C1686	U1602	U1503	G1417	U1329	G1252
G2447	C2363	A2289	G2062	A1972	A1889	C1796	C1687	U1608	C1504	G1418	G1330	G1253
A2448	C2364	C2200	C2063	U1973	A1890	C1797	U1688	U1609	C1505	G1419	A1331	A1254
U2449	G2365	C2201	C2064	G1979	C1895	U1798	U1689	A1608	C1506	U1420	G1332	U1255
A2450	C2370	U2203	G2069	A1981	G1896	C1800	G1696	A1609	A1507	U1421	G1333	G1256
A2451	C2371	C2205	A2071	C1982	G1897	G1801	G1697	A1610	A1508	G1422	G1337	G1257
C2452	U2296	G2206	U2074	C1983	U1898	A1802	A1698	U1613	C1509	G1425	G1338	C1258
C2461	G2375	A2208	U2075	C1990	A1900	A1803	G1699	G1613	A1509B	G1426	G1339	A1262
U2462	A2376	U2218	U2076	U1991	A1901	C1806	U1700	A1614	G1510	G1427	U1340	U1263
C2463	A2377	A2077	A2077	G1992	C1902	A1810	A1701	G1617	U1700	U1514	U1341	U1264
C2464	A2378	G2220	C2078	U1993	G1903	G1811	G1702	U1622	U1515	G1428	G1342	A1265
C2465	G2379	G2221	U2079	G1997	G1906	G1814	C1711	G1622	C1516	G1429	G1343	A1266
C2466	C2380	G2222	U2086	U1998	G1907	U1815	C1712	G1625	U1517	G1430	G1344	U1267
C2467	C2381	G2223	G2087	G1999	C1908	A1816	U1719	G1626	U1518	U1431	A1349	A1268
G2468	G2382	G2224	G2087	G1999	C1908	G1817	U1720	G1633	U1519	G1432	C1350	A1269
A2469	G2383	A2225	G2088	C2007	A1913	G1818	G1721	G1634	G1529	U1433	C1351	C1270
G2470	G2384	G2226	G2089	C2008	C1914	U1819	A1722	G1635	G1530	G1437	U1357	A1272
C2471	C2385	G2227	G2093	C2009	U1915	U1820	U1739	G1636	C1532	A1445	G1358	U1273
G2472	A2310	A2228	U2096	G2012	A1916	U1821	G1740	U1641	G	U1448	A1360	A1274
U2473	A2311	C2229	C2097	A2013	U1917	G1823	A1741	A1642	U	G1449	A1364	A1275
C2474	C2312	G2235	U2098	A2014	A1918	G1824	G1742	G1647	A	U1450	A1365	A1278
C2475	C2313	G2236	U2099	A2015	A1919	G1825	C1743	G1648	C	U1453	A1366	G1279
A2476	C2314	G2237	G2100	A2016	C1920	G1826	U1746	G1649	G1537	U1455	A1367	U1282
C2477	C2315	G2238	G2101	U2016	G1925	U1827	G1756	G1650	G1538	G1455	G1368	G1283
A2478	C2316	G2239	U2102	U2016	U1926	U1828	U1757	G1651	U1540	G1459	C1370	A1286
G2479	C2317	U2102	C2103	U2028	U1927	G1829	G1758	G1652	U1541	U1461	G1371	G1289
G2480	C2318	C2104	C2104	G2029	A1928	A1833	U1759	A1651	A1545	C1467	A1372	C1290
U2481	A2319	G2105	C2105	A2030	A1936	G1834	A1760	A1652	C1547	U1471	U1378	C1291
G2482	A2320	G2106	G2106	A2031	A1937	G1835	C1761	G1653	C1548	U1475	A1379	U1292
U2483	G2325	G2166	G2167	G2023	G1930	U1836	U1762	A1654	U1542	G1476	U1380	U1293
G2489	C2326	U2167	C2107	G2024	U1931	G1837	G1763	A1655	A1558	G1479	G1386	U1294
G2490	C2327	G2168	C2108	U2028	U1932	C1838	G1764	C1656	G1559	U1481	U1394	C1295
A2410	C2328	A2169	U2109	U2029	G1935	G1839	U1772	C1657	A1566	G1482	A1395	G1306
A2411	A2328	A2170	G2110	G2029	A1936	C1837	G1773	G1658	U1571	U1486	A1307	A1307
G2412	G2329	A2171	C2111	A2031	A1937	G1838	A1773	A1665	A1567	A1487	A1308	A1308
G2413	G2330	U2172	G2112	A2031	A1937	G1839	C1774	G1666	G1568	G1478	G1309	G1309
U2492	G2331	A2173	U2113	G2032	A1938	G1840	U1779	G1667	A1569	G1480	G1310	G1310
U2493	G2331	C2174	U2114	A2033	U1938	G1841	U1780	A1668	A1570	U1481	G1311	G1311
A2418	A2334	C2175	G2115	U2034	G1948	C1843	U1781	A1669	U1571	G1475	G1312	U1312
U2419	A2335	A2176	G2116	U2035	G1949	G1846	C1782	A1670	A1577	C1476	U1405	U1313
C2420	A2336	C2177	U2117	G2036	G1950	A1847	U1783	C1671	A1577	A1477	U1406	C1314
G2421	G2337	C2178	A2118	G2037	U1951	A1848	A1784	A1672	C1577	G1479	G1407	
U2422	U2338	C2179	U2119	G2038	A1952	A1849	A1785	G1673	U1578	G1483	G1401	G1309
C2423	C2343	U2180	G2120	G2038	A1953	A1854	A1786	A1674	A1579	G1488	G1402	G1310
A2424	A2344	G2181	G2121	A2042	U1954	A1855	A1787	G1675	A1580	G1489	G1403	G1311
A2425	G2346	G2182	U2122	C2043	U1955	G1858	A1788	A1676	A1581	A1490	G1404	G1312
G2428	C2347	C2183	G2123	C2043	U1956	A1859	U1789	A1677	A1582	U1486	U1405	U1313
G2429	U2348	G2184	G2124	C2050	U1957	A1860	C1782	A1678	C1582	A1487	U1406	C1314
A2430	G2349	C2185	G2125	A2051	G1958	A1876	A1783	G1679	A1583	A1488	G1407	
G2431	G2350	G2186	G2126	G2052	G1959	A1877	A1784	A1674	A1584	G1489	G1401	G1309
A2434	C2351	G2187	G2127	G2053	U1960	A1878	A1785	G1674	A1585	A1490	G1402	G1310
A2435	U2351	C2188	C2128	A2054	U1961	A1879	A1786	A1675	A1586	A1491	G1403	G1311
U2438	G2355	G2189	C2129	C2055	G1963	A1882	A1786	A1676	A1587	A1492	U1404	U1312
C2501	G2501	G2190	U2130	G2056	U1964	A1883	U1790	A1677	A1588	A1493	U1405	U1313
G2502	G2502	G2191	U2131	G2057	U1965	A1884	U1791	A1678	A1589	A1494	U1406	C1314
A2503	C2503	G2192	U2132	G2058	U1966	A1885	U1792	A1679	A1590	A1495	U1407	
G2504	U2504	G2193	G2133	A2059	U1967	A1886	U1793	A1680	A1591	A1496	U1408	
G2505	G2505	G2194	G2134	A2060	U1968	A1887	U1794	A1681	A1592	A1497	U1409	
U2506	U2506	G2195	G2135	A2061	U1969	A1888	U1795	A1682	A1593	A1498	U1410	
G2515	G2515	G2196	G2136	A2062	U1970	A1889	U1796	A1683	A1594	A1499	U1411	
C2516	C2516	G2197	G2137	A2063	U1971	A1890	U1797	A1684	A1595	A1500	U1412	
G2517	G2517	G2198	G2138	C2064	U1972	A1891	U1798	A1685	A1596	A1501	U1413	
A2518	U2518	G2199	G2139	U2065	U1973	A1892	U1799	A1686	A1597	A1502	U1414	
C2520	C2520	G2200	G2140	G2066	U1974	A1893	U1800	A1687	A1598	A1503	U1415	
			G2141	C1982	U1975	A1894	U1801	A1688	A1599	A1504	U1416	
			C2142	C1983	U1976	A1895	U1802	A1689	A1600	A1505	U1417	
			G2143	C1984	U1977	A1896	A1803	A1690	A1601	A1506	U1418	
			U2144	U1978	U1978	A1897	A1804	A1691	A1602	A1507	U1419	
			C2145	U1979	U1979	A1898	A1805	A1692	A1603	A1508	U1420	
			C2146	U1980	U1980	A1899	A1806	A1693	A1604	A1509	U1421	
			G2147	U1981	U1981	A1900	A1807	A1694	A1605	A1510	U1422	
			U2148	U1982	U1982	A1901	A1808	A1695	A1606	A1511	U1423	
			G2149	U1983	U1983	A1902	A1809	A1696	A1607	A1512	U1424	
			G2150	U1984	U1984	A1903	A1810	A1697	A1608	A1513	U1425	
			U2151	U1985	U1985	A1904	A1811	A1698	A1609	A1514	U1426	
			G2152	U1986	U1986	A1905	A1812	A1699	A1610	A1515	U1427	
			G2153	U1987	U1987	A1906	A1813	A1700	A1611	A1516	U1428	
			G2154	U1988	U1988	A1907	A1814	A1701	A1612	A1517	U1429	
			U2155	U1989	U1989	A1908	A1815	A1702	A1613	A1518	U1430	
			G2156	U1990	U1990	A1909	A1816	A1703	A1614	A1519	U1431	
			U2157	U1991	U1991	A1910	A1817	A1704	A1615	A1520	U1432	
			A2158	U1992	U1992	A1911	A1818	A1705	A1616	A1521	U1433	
			G2159	U1993	U1993	A1912	A1819	A1706	A1617	A1522	U1434	
			G2160	U1994	U1994	A1913	A1820	A1707	A1618	A1523	U1435	
			C2161	U1995	U1995	A1914	A1821	A1708	A1619	A1524	U1436	
			G2162	U1996	U1996	A1915	A1822	A1709	A1620	A1525	U1437	
			U2163	U1997	U1997	A1916	A1823	A1710	A1621	A1526	U1438	
			G2164	U1998	U1998	A1917	A1824	A1711	A1622	A1527	U1439	
			C2165	U1999	U1999	A1918	A1825	A1712	A1623	A1528	U1440	
			G2166	U2000	U2000	A1919	A1826	A1713	A1624	A1529	U1441	
			U2167	U2001	U2001	A1920	A1827	A1714	A1625	A1530	U1442	
			G2168	U2002	U2002	A1921	A1828	A1715	A1626	A1531	U1443	
			A2169	U2003	U2003	A1922	A1829	A1716	A1627	A1532	U1444	
			U2170	U2004	U2004	A1923	A1830	A1717	A1628	A1533	U1445	
			G2171	U2005	U2005	A1924	A1831	A1718	A1629	A1534	U1446	
			U2172	U2006	U2006	A1925	A1832	A1719	A1630	A1535	U1447	
			A2173	U2007	U2007	A1926	A1833	A1720	A1631	A1536	U1448	
			C2174	U2008	U2008	A1927	A1834	A1721	A1632	A1537	U1449	
			G2175	U2009	U2009	A1928	A1835	A1722	A1633	A1538	U1450	
			A2176	U2010	U2010	A1929	A1836	A1723	A1634	A1539	U1451	
			C2177	U2011	U2011	A1930	A1837	A1724	A1635	A1540	U1452	
			U2178	U2012	U2012	A193						



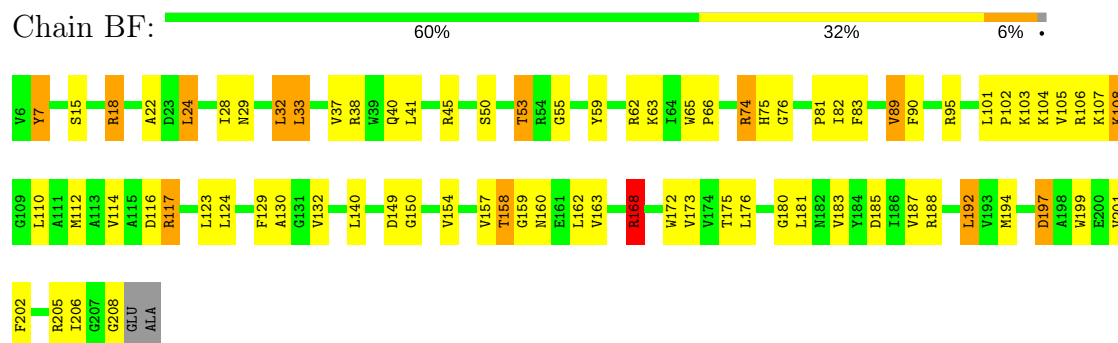
• Molecule 2: 5S ribosomal RNA

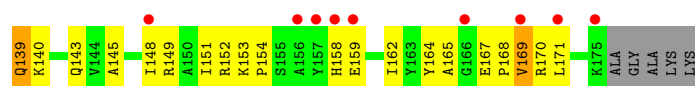


• Molecule 2: 5S ribosomal RNA

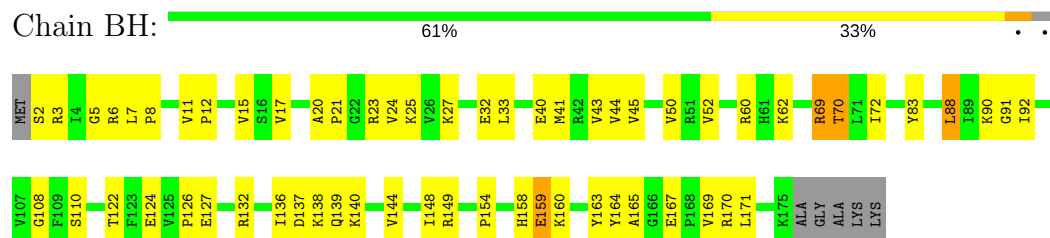


- Molecule 5: 50S ribosomal protein L4

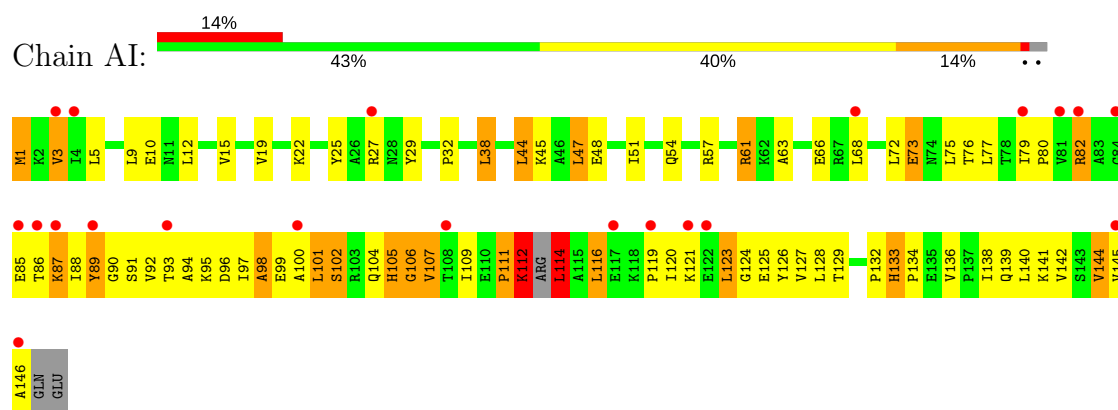




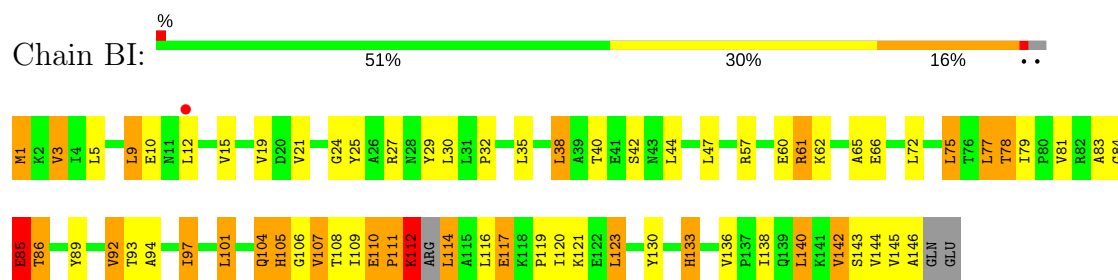
• Molecule 7: 50S ribosomal protein L6



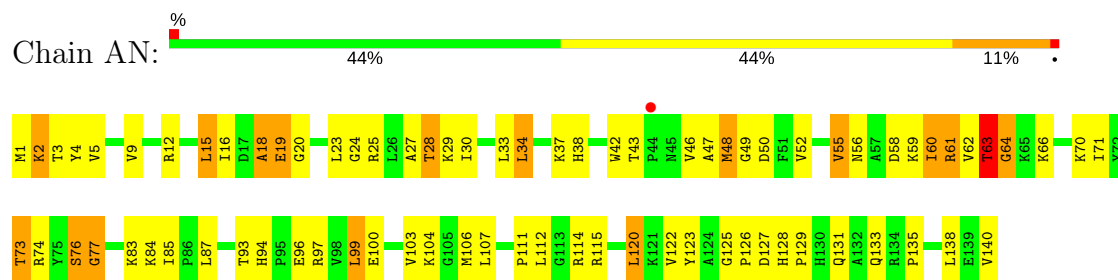
• Molecule 8: 50S ribosomal protein L9



• Molecule 8: 50S ribosomal protein L9

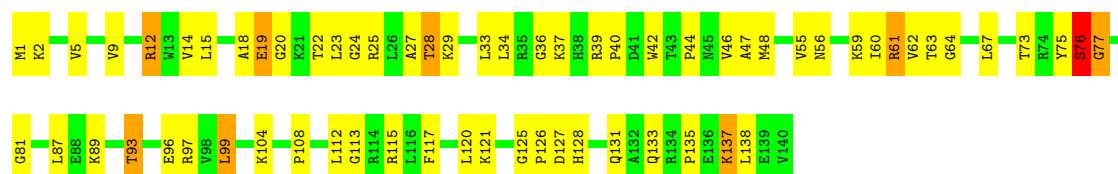


• Molecule 9: 50S ribosomal protein L13

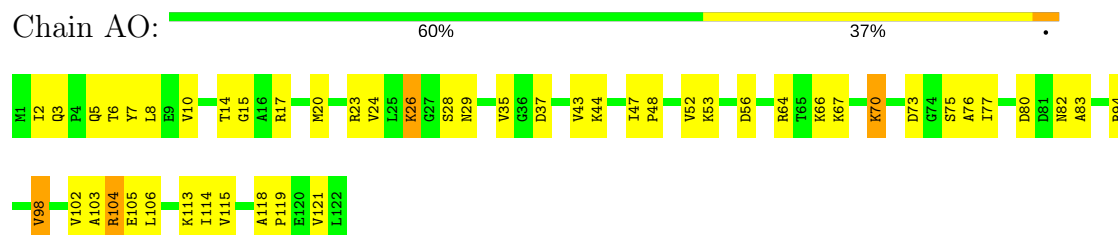


• Molecule 9: 50S ribosomal protein L13

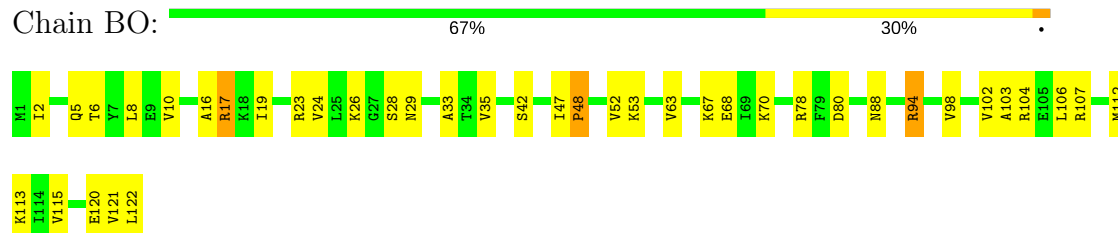




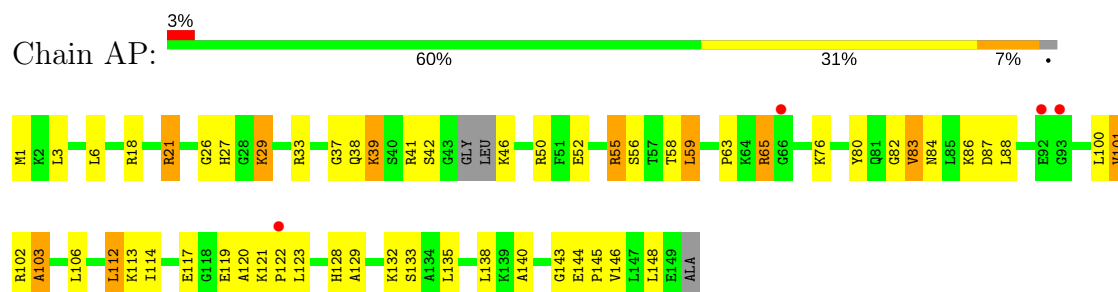
- Molecule 10: 50S ribosomal protein L14



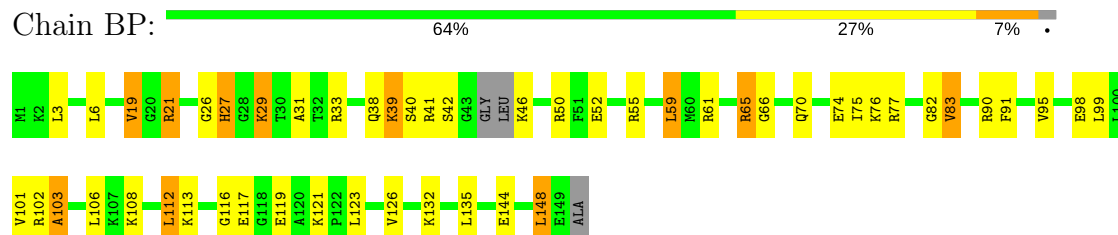
- Molecule 10: 50S ribosomal protein L14



- Molecule 11: 50S ribosomal protein L15



- Molecule 11: 50S ribosomal protein L15

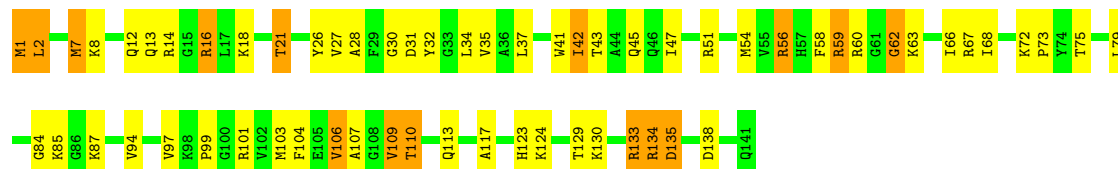


- Molecule 12: 50S ribosomal protein L16

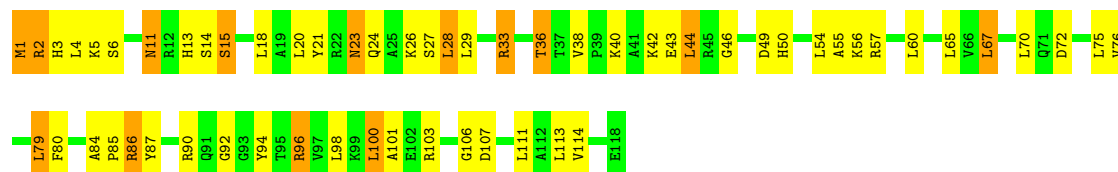




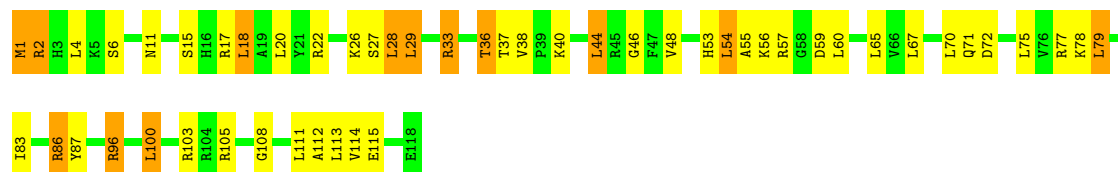
• Molecule 12: 50S ribosomal protein L16



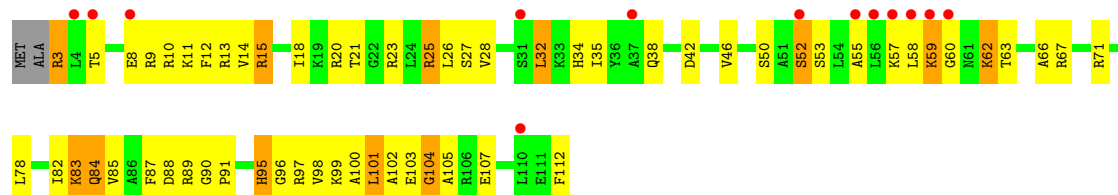
• Molecule 13: 50S ribosomal protein L17



• Molecule 13: 50S ribosomal protein L17

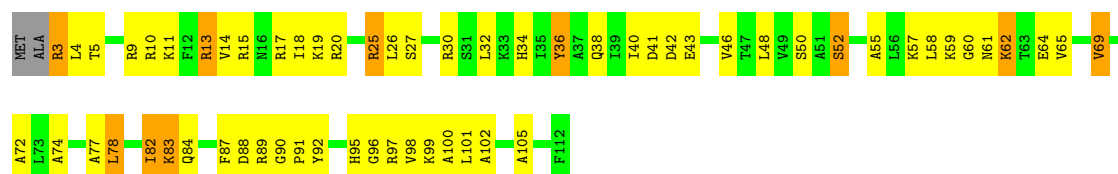


• Molecule 14: 50S ribosomal protein L18

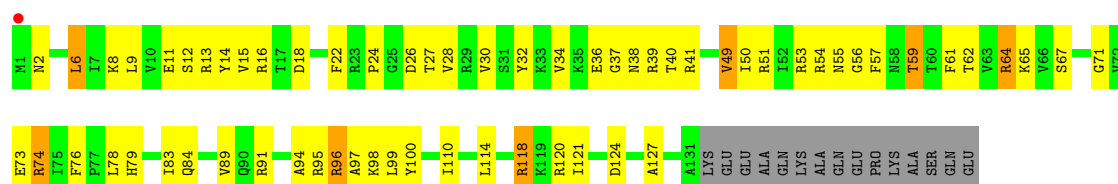


• Molecule 14: 50S ribosomal protein L18

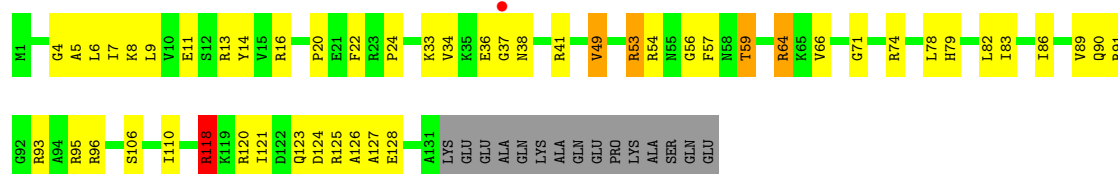




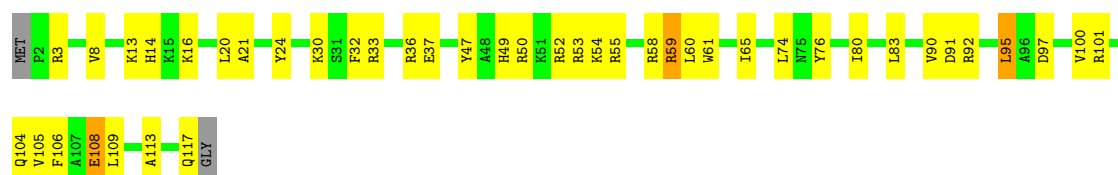
• Molecule 15: 50S ribosomal protein L19



• Molecule 15: 50S ribosomal protein L19



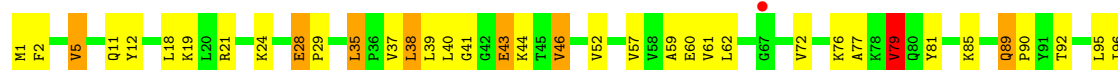
• Molecule 16: 50S ribosomal protein L20



• Molecule 16: 50S ribosomal protein L20



• Molecule 17: 50S ribosomal protein L21





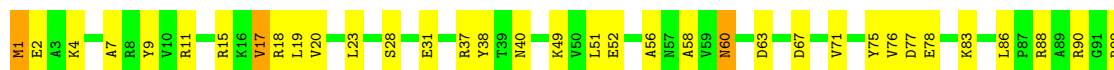
- Molecule 17: 50S ribosomal protein L21

Chain BV: 67% 27% 5% •



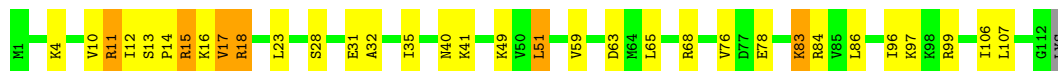
- Molecule 18: 50S ribosomal protein L22

Chain AW: 60% 34% 5% •



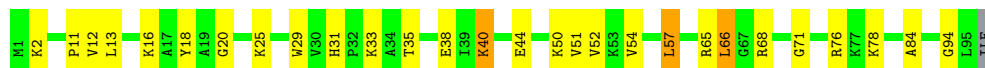
- Molecule 18: 50S ribosomal protein L22

Chain BW: 70% 24% 5% •



- Molecule 19: 50S ribosomal protein L23

Chain AX: 70% 26% 5% •



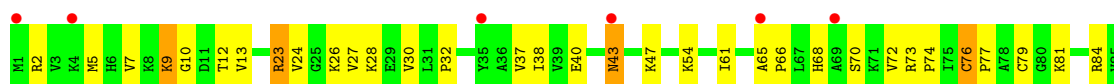
- Molecule 19: 50S ribosomal protein L23

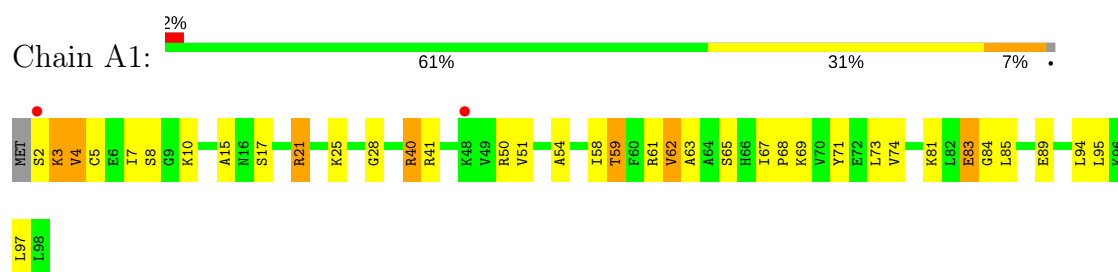
Chain BX: 64% 30% 5% •



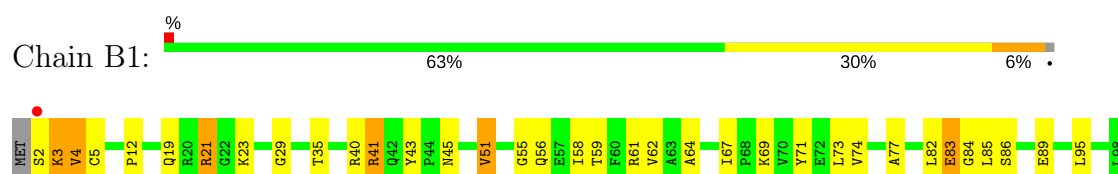
- Molecule 20: 50S ribosomal protein L24

Chain AY: 6% 55% 37% 5% •

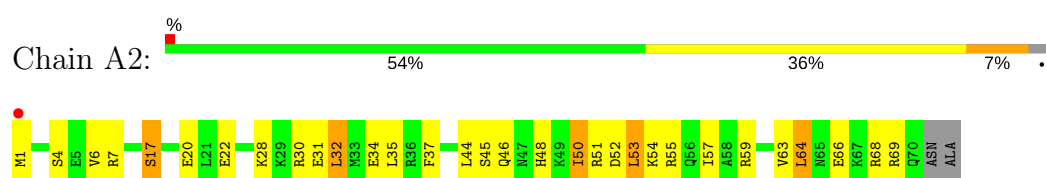




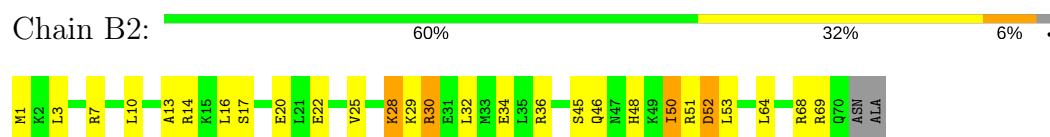
- Molecule 23: 50S ribosomal protein L28



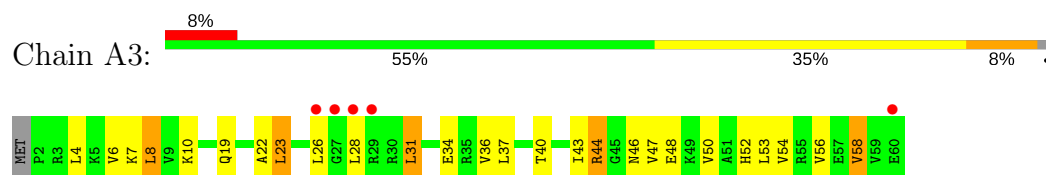
- Molecule 24: 50S ribosomal protein L29



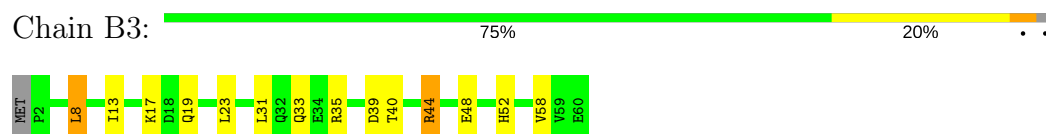
- Molecule 24: 50S ribosomal protein L29



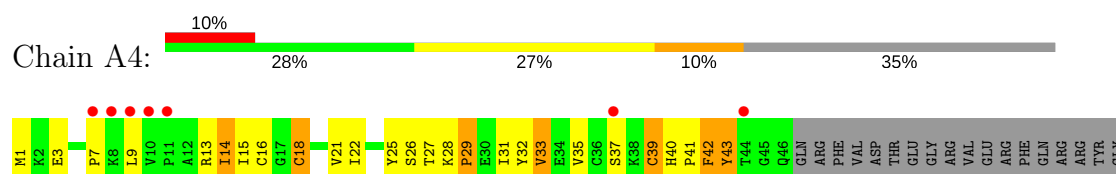
- Molecule 25: 50S ribosomal protein L30



- Molecule 25: 50S ribosomal protein L30

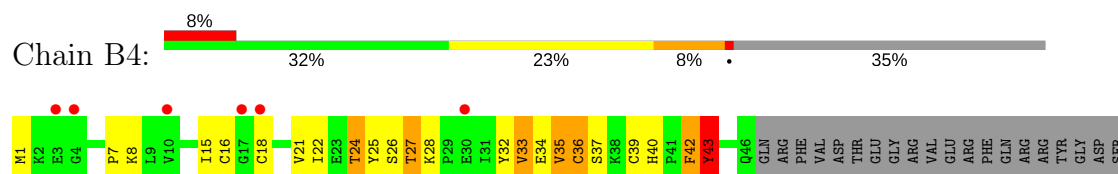


- Molecule 26: 50S ribosomal protein L31



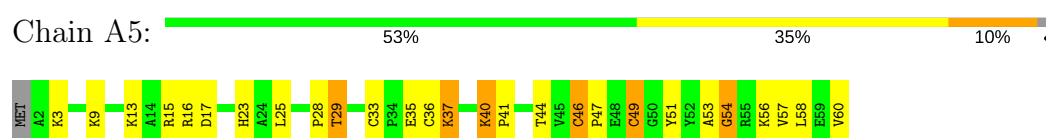
ASP
SER
TYR
ARG
LYS
GLY
ARG

- Molecule 26: 50S ribosomal protein L31

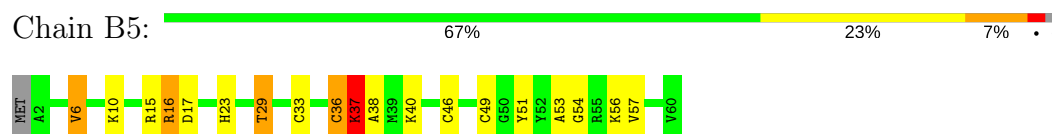


TYR
ARG
LYS
GLY
ARG

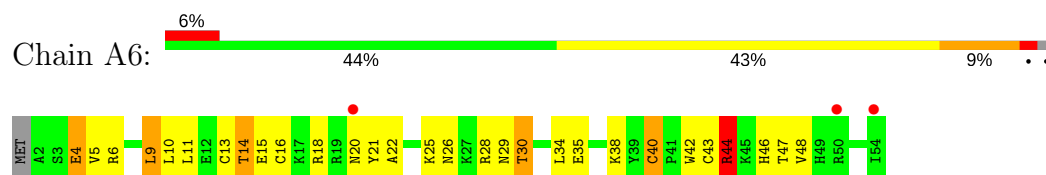
- Molecule 27: 50S ribosomal protein L32



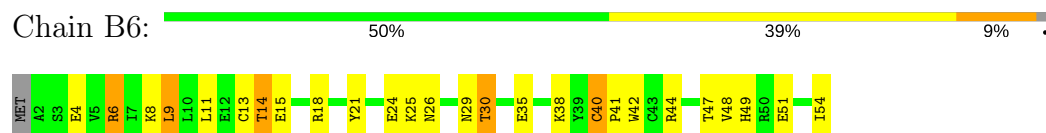
- Molecule 27: 50S ribosomal protein L32



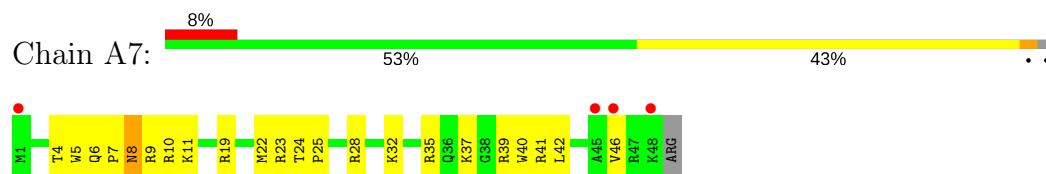
- Molecule 28: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L33

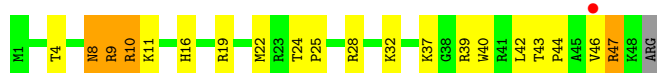


- Molecule 29: 50S ribosomal protein L34



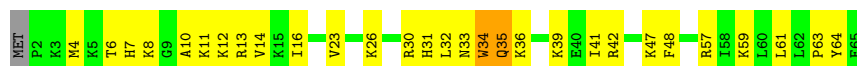
- Molecule 29: 50S ribosomal protein L34





- Molecule 30: 50S ribosomal protein L35

Chain A8: 54% 42%



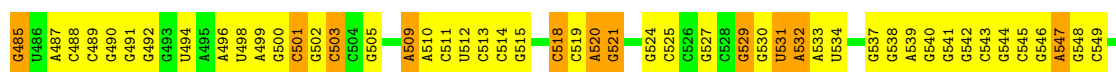
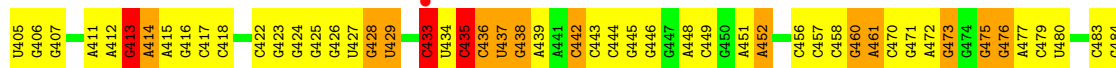
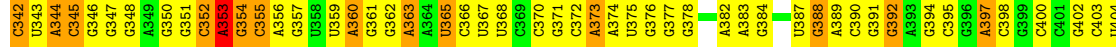
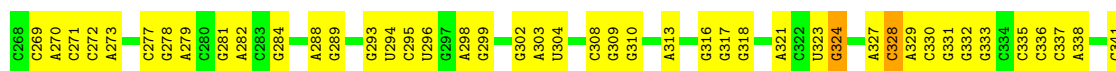
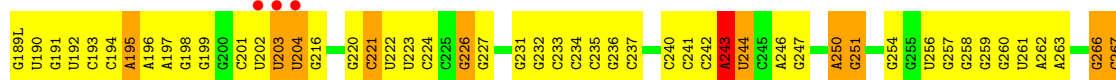
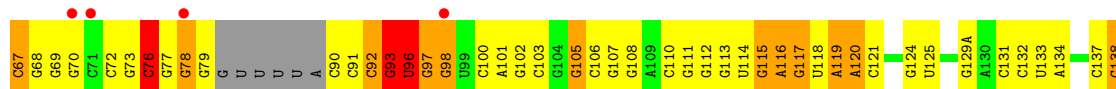
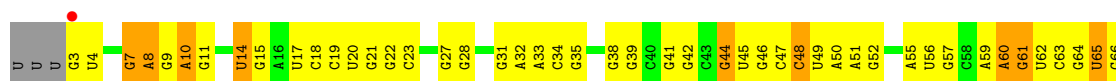
- Molecule 30: 50S ribosomal protein L35

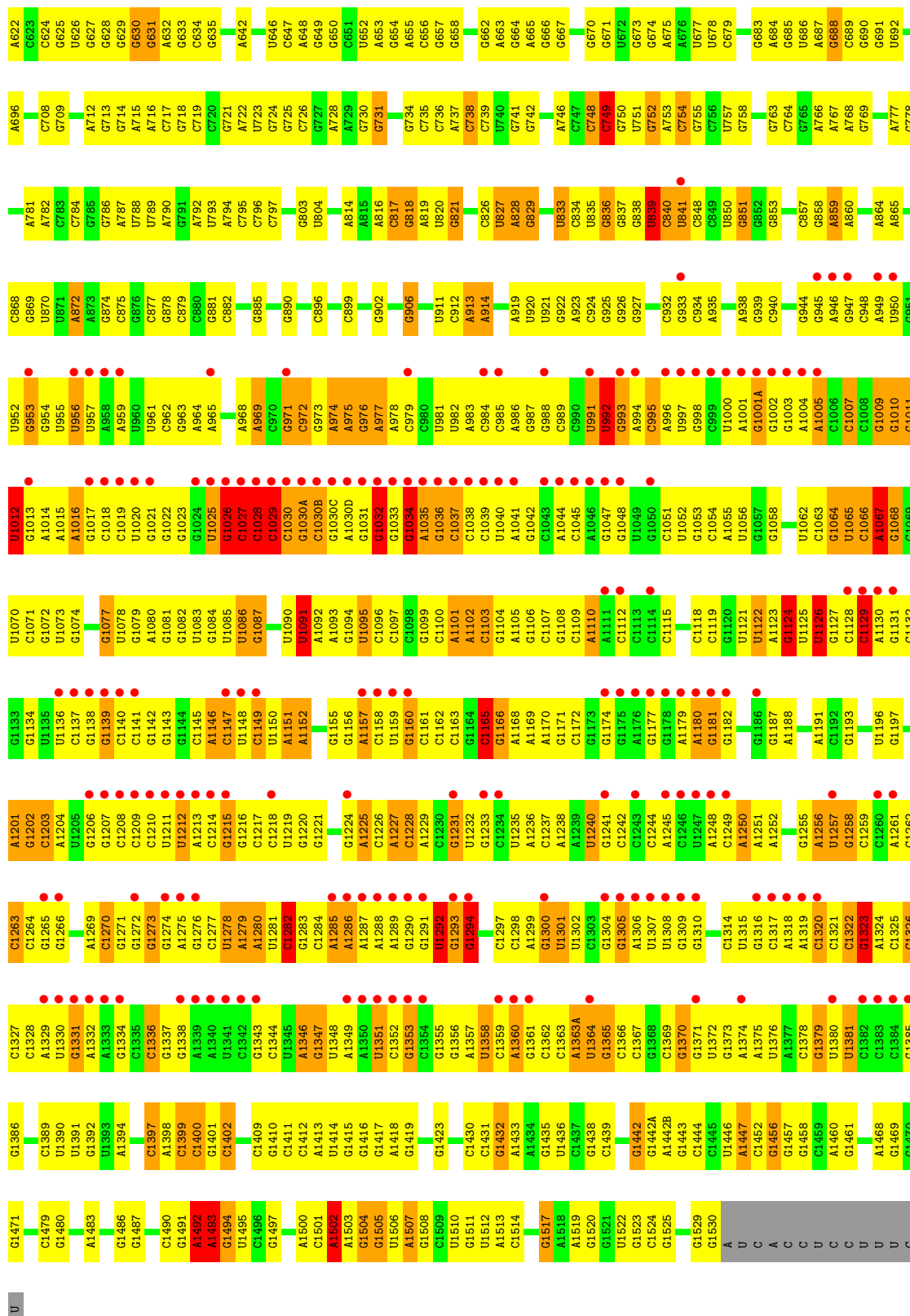
Chain B8: 66% 29%



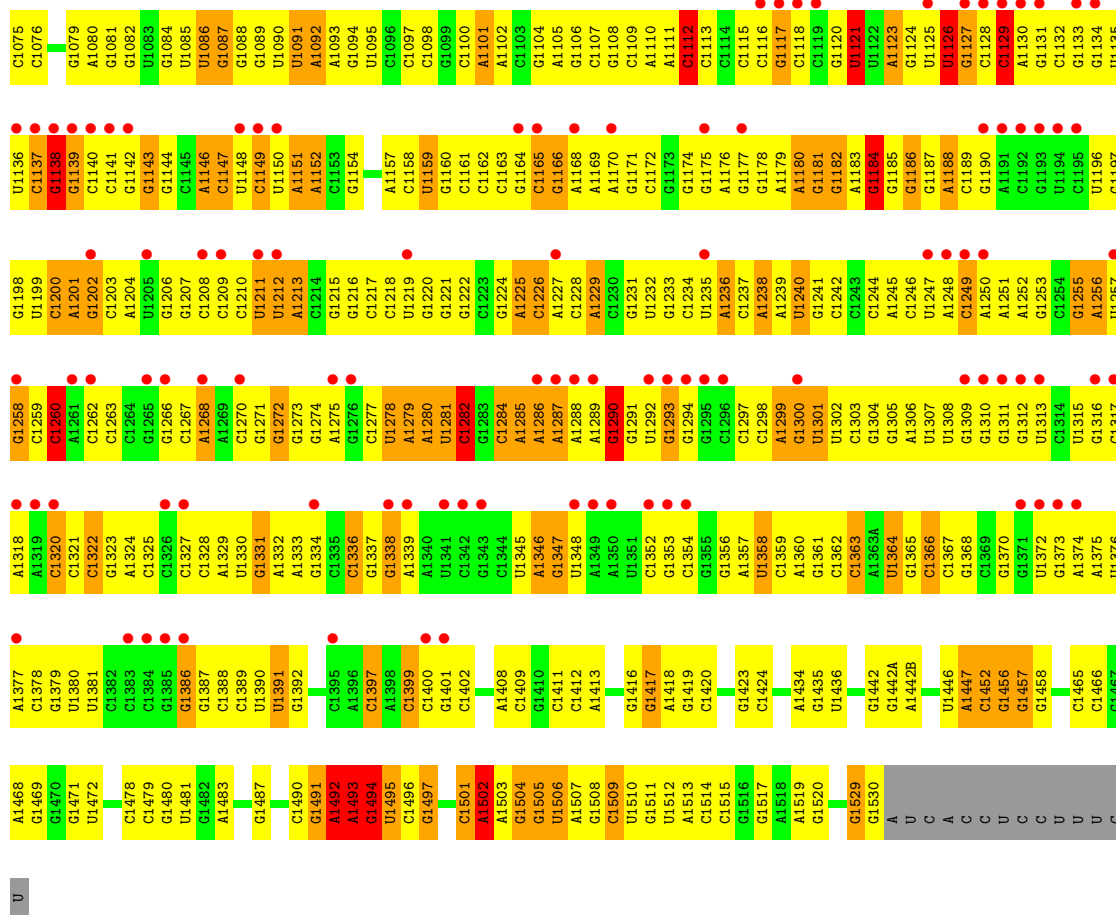
- Molecule 31: 16S ribosomal RNA

Chain CA: 12% 29% 53% 14%

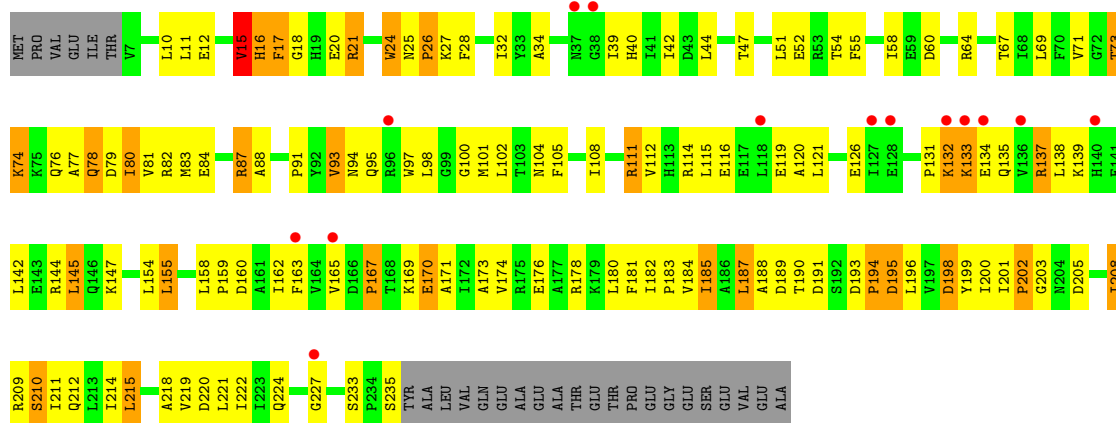




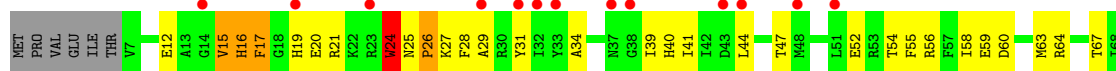


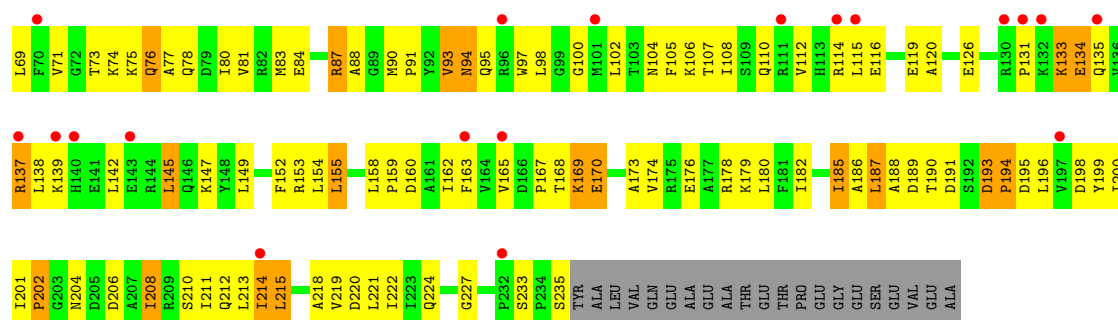


• Molecule 32: 30S ribosomal protein S2

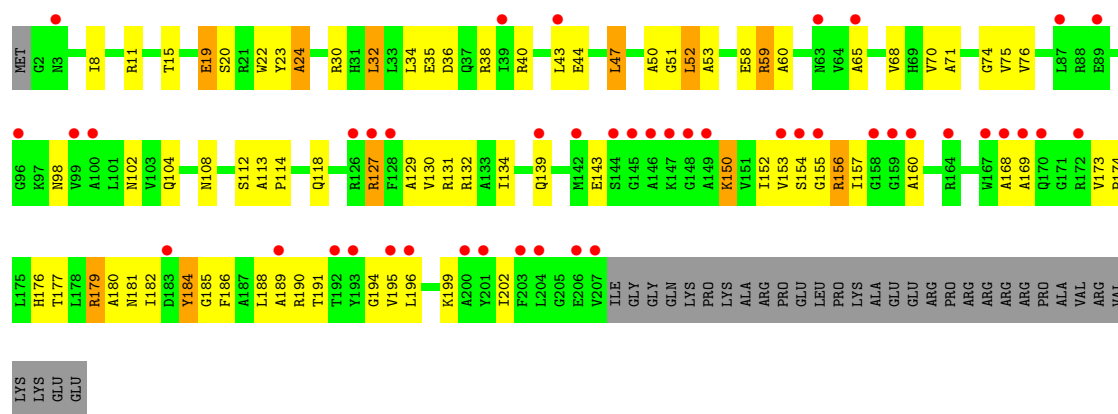


• Molecule 32: 30S ribosomal protein S2

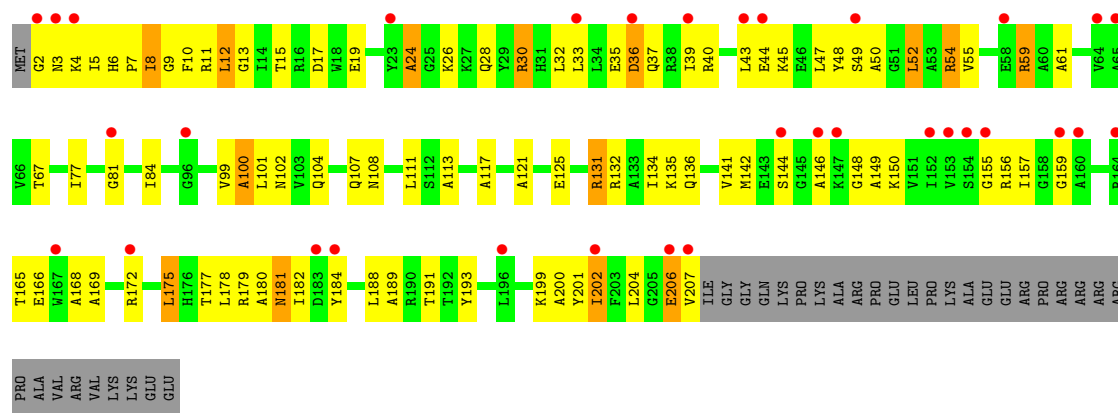




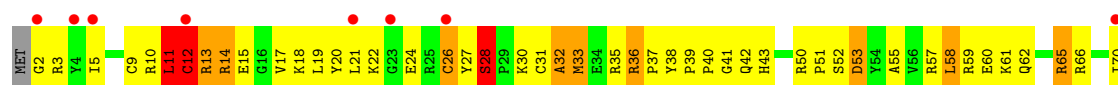
• Molecule 33: 30S ribosomal protein S3

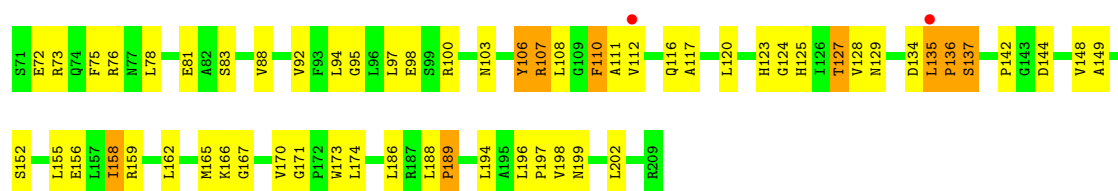


• Molecule 33: 30S ribosomal protein S3

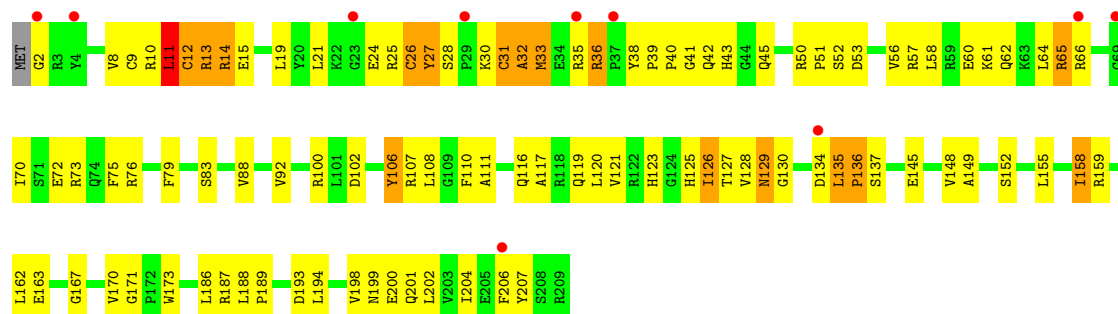


• Molecule 34: 30S ribosomal protein S4

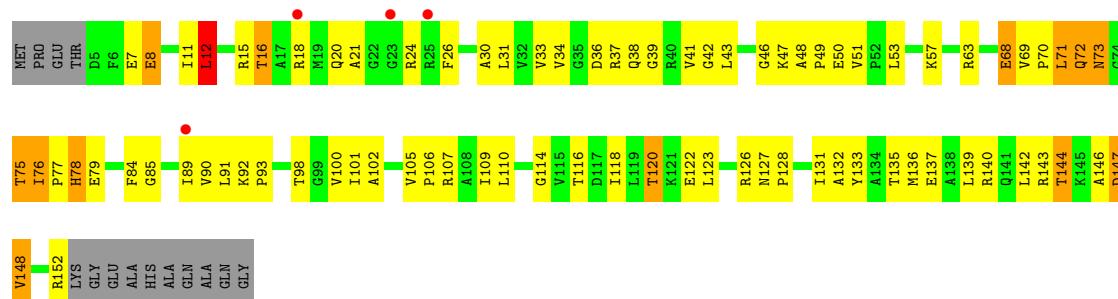
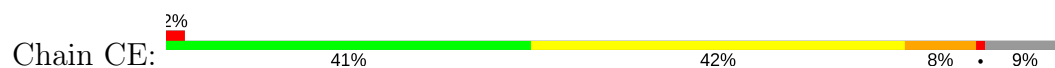




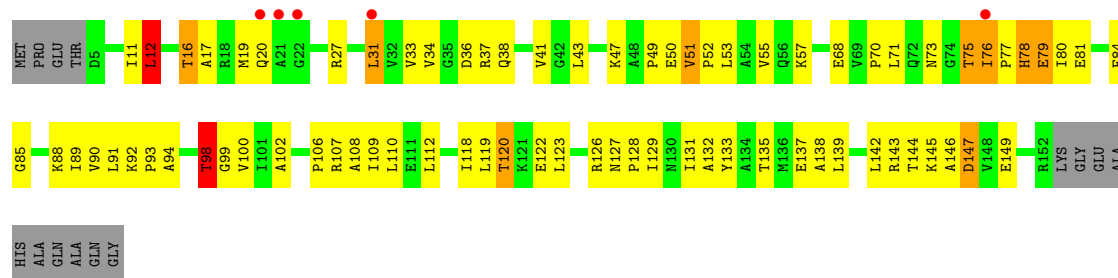
• Molecule 34: 30S ribosomal protein S4



• Molecule 35: 30S ribosomal protein S5

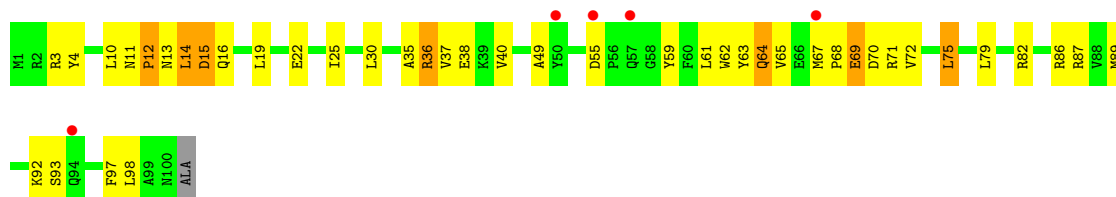


• Molecule 35: 30S ribosomal protein S5

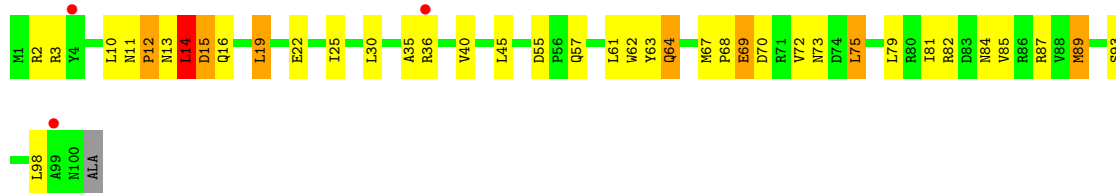


• Molecule 36: 30S ribosomal protein S6

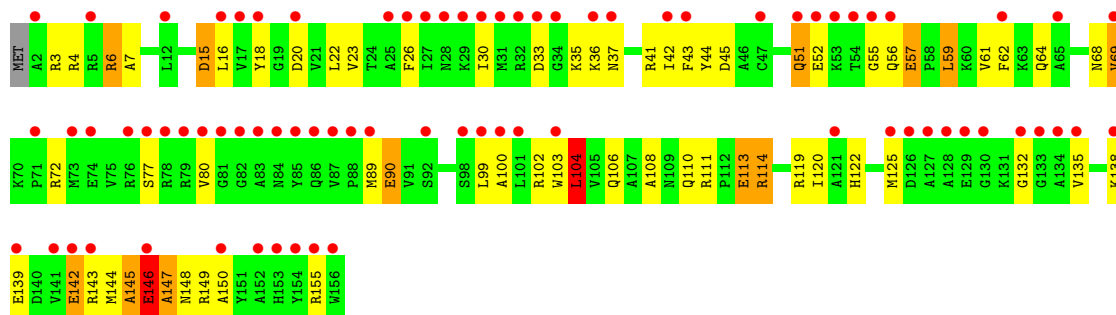




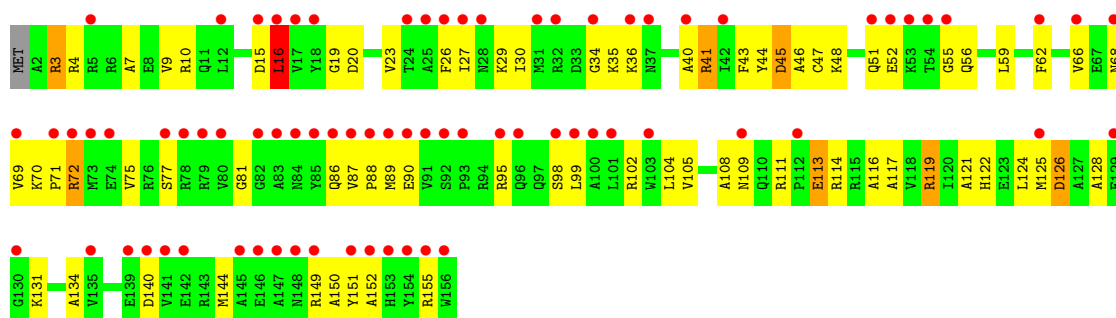
• Molecule 36: 30S ribosomal protein S6



• Molecule 37: 30S ribosomal protein S7

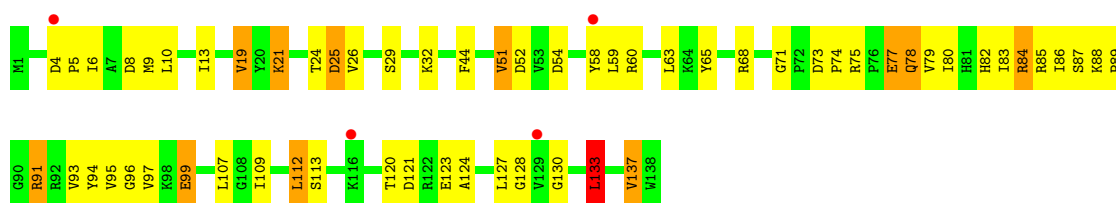


• Molecule 37: 30S ribosomal protein S7

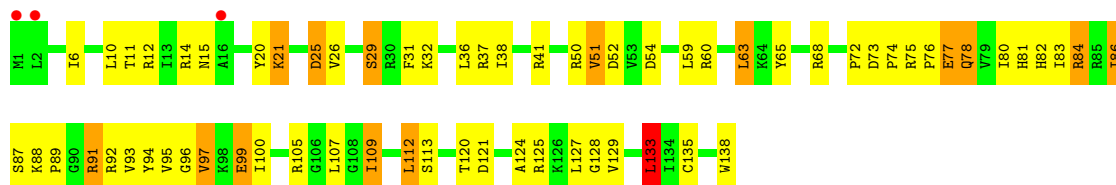


• Molecule 38: 30S ribosomal protein S8

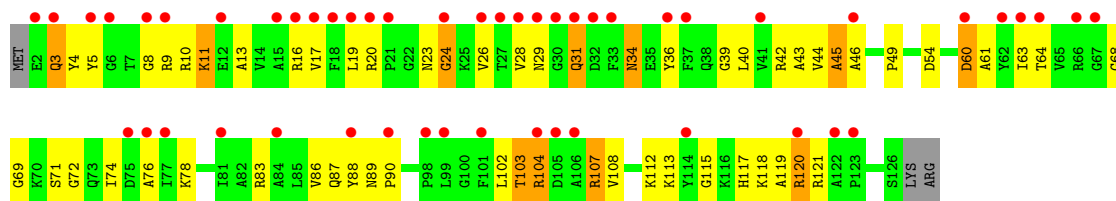
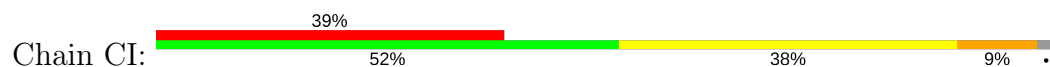




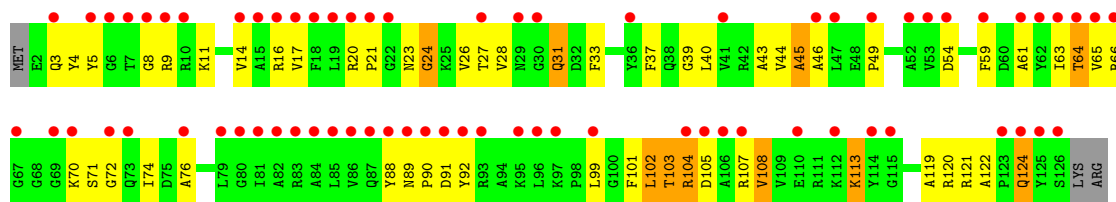
• Molecule 38: 30S ribosomal protein S8



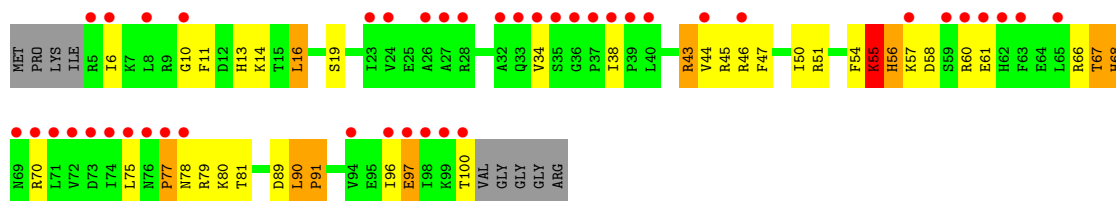
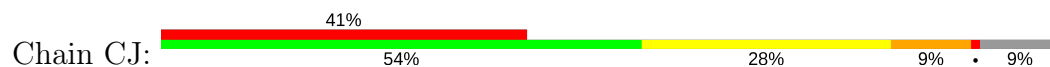
• Molecule 39: 30S ribosomal protein S9



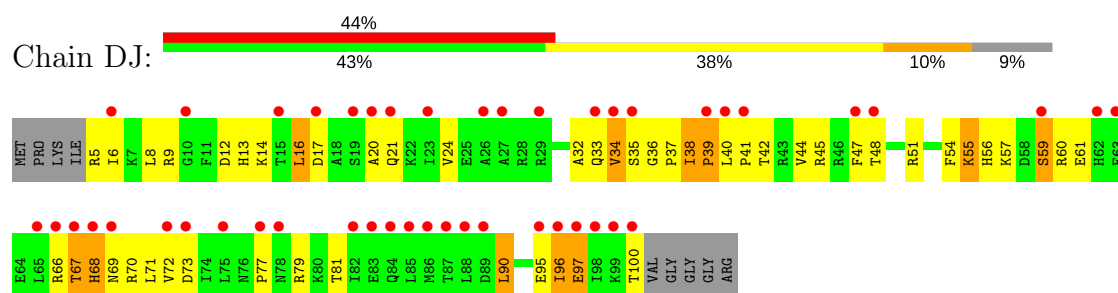
• Molecule 39: 30S ribosomal protein S9



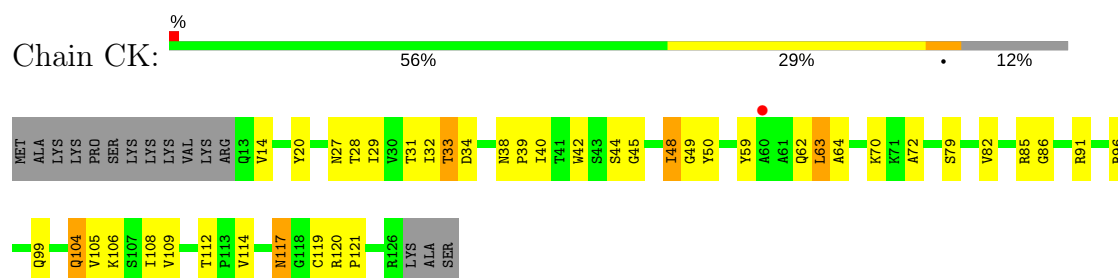
• Molecule 40: 30S ribosomal protein S10



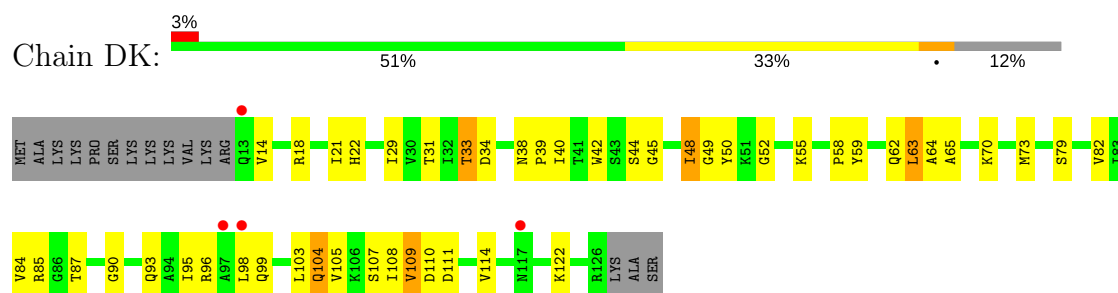
• Molecule 40: 30S ribosomal protein S10



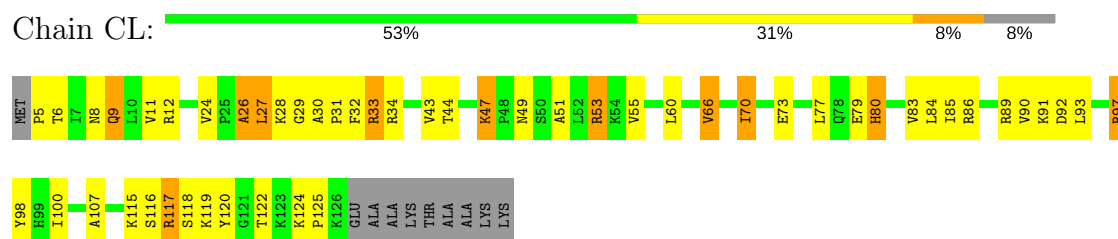
- Molecule 41: 30S ribosomal protein S11



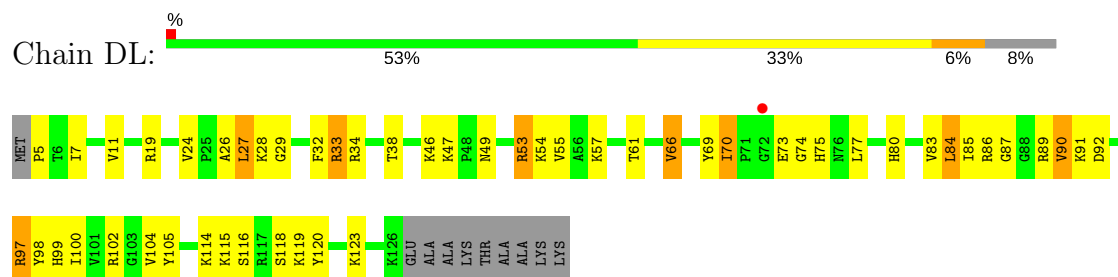
- Molecule 41: 30S ribosomal protein S11



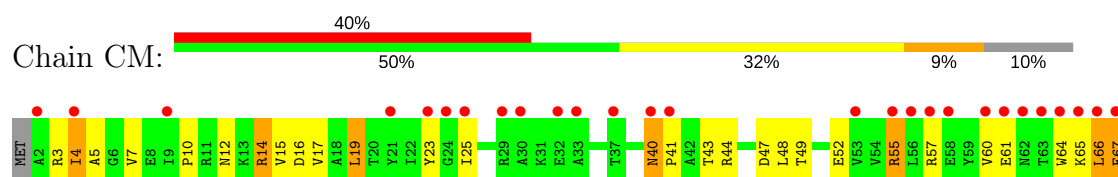
- Molecule 42: 30S ribosomal protein S12



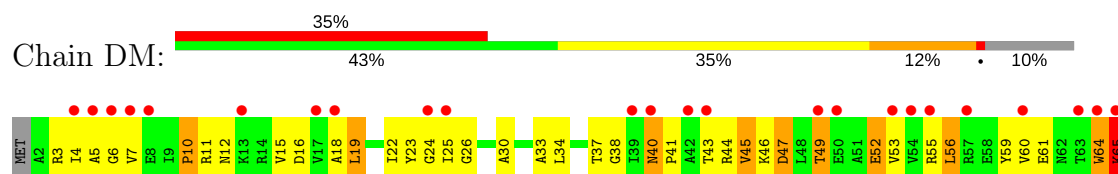
- Molecule 42: 30S ribosomal protein S12



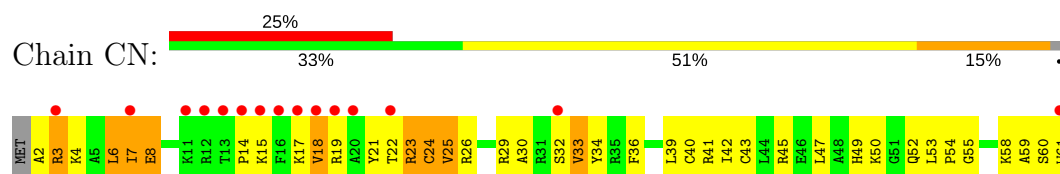
- Molecule 43: 30S ribosomal protein S13



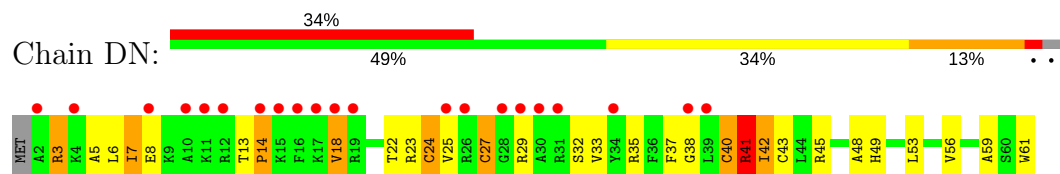
- Molecule 43: 30S ribosomal protein S13



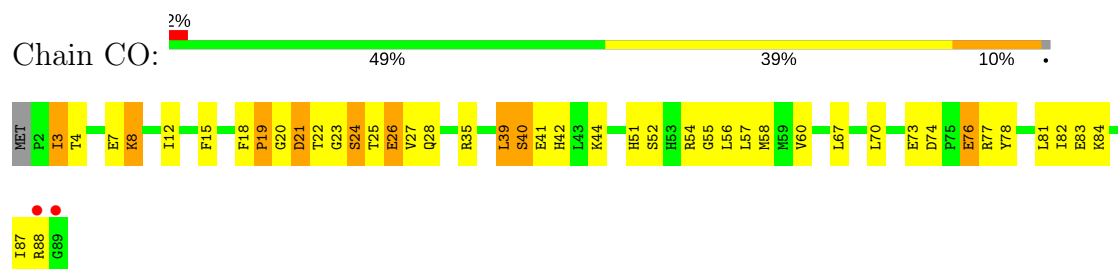
- Molecule 44: 30S ribosomal protein S14



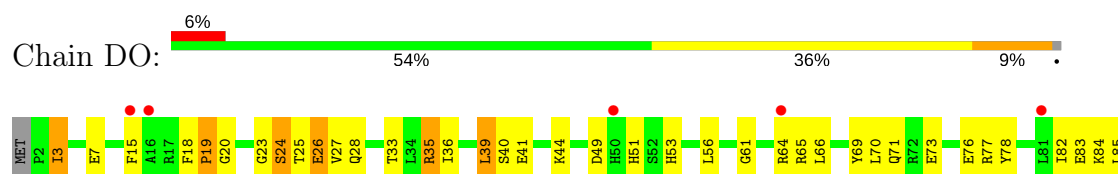
- Molecule 44: 30S ribosomal protein S14



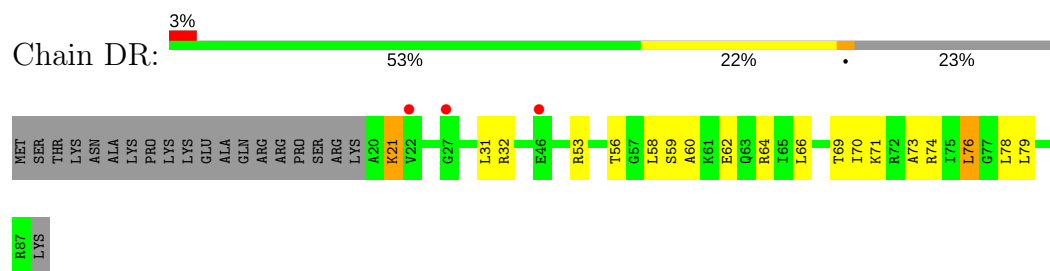
- Molecule 45: 30S ribosomal protein S15



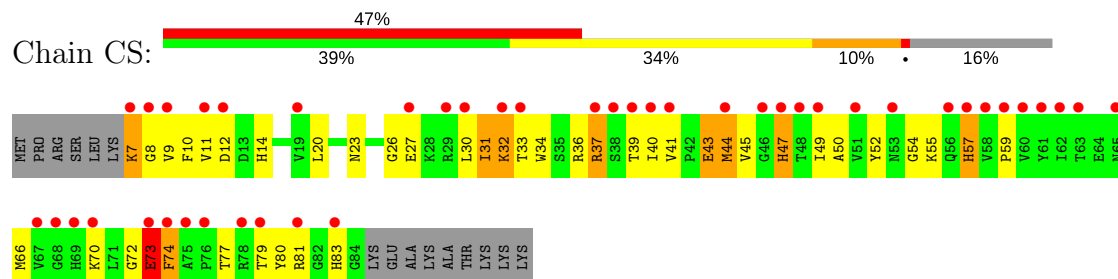
- Molecule 45: 30S ribosomal protein S15



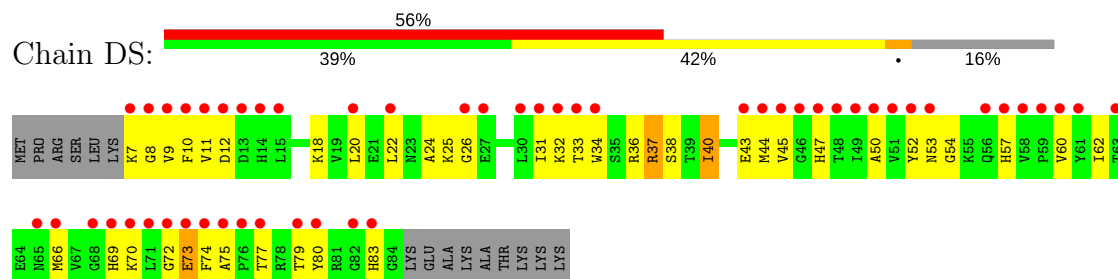
• Molecule 48: 30S ribosomal protein S18



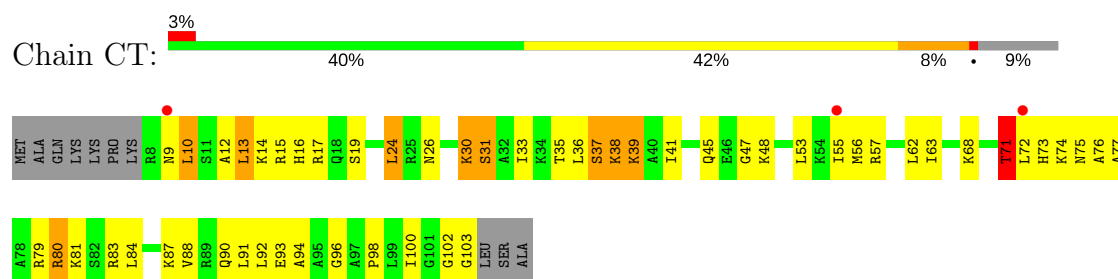
• Molecule 49: 30S ribosomal protein S19



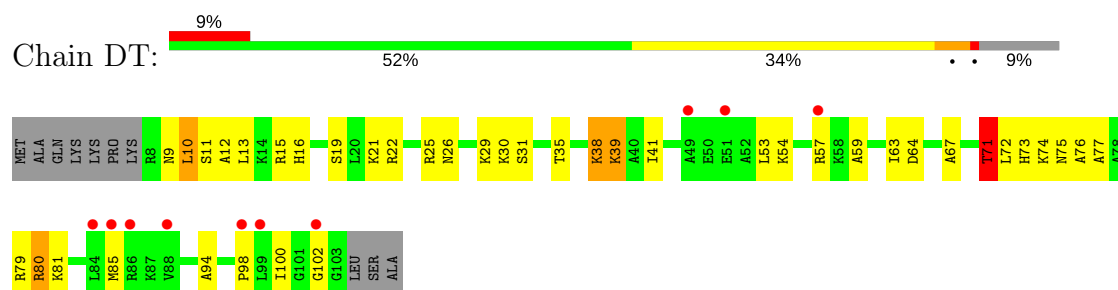
• Molecule 49: 30S ribosomal protein S19



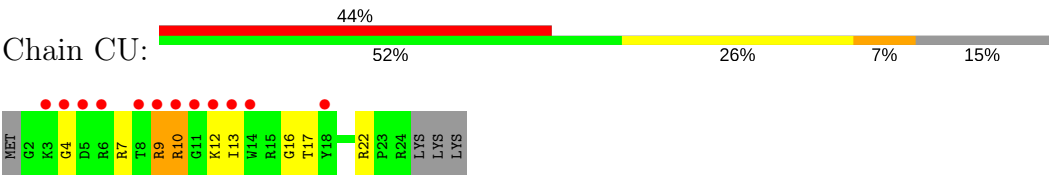
• Molecule 50: 30S ribosomal protein S20



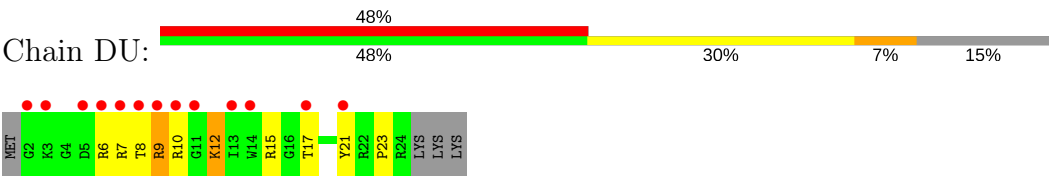
• Molecule 50: 30S ribosomal protein S20



● Molecule 51: 30S ribosomal protein THX



● Molecule 51: 30S ribosomal protein THX



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.37Å 445.46Å 619.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.29 – 3.20 49.43 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.29-3.20) 99.7 (49.43-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.91Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.228 , 0.273 0.228 , 0.273	Depositor DCC
R_{free} test set	63228 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	75.4	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 70.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	279316	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: MG, T8B

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	AA	0.82	17/68203 (0.0%)	1.30	624/106459 (0.6%)
1	BA	1.20	70/68203 (0.1%)	1.37	800/106459 (0.8%)
2	AB	0.94	0/2879	1.25	21/4492 (0.5%)
2	BB	0.88	0/2879	1.26	21/4492 (0.5%)
3	AD	0.54	0/2186	0.75	2/2944 (0.1%)
3	BD	0.67	0/2186	0.81	4/2944 (0.1%)
4	AE	0.55	0/1588	0.76	0/2145
4	BE	0.72	0/1588	0.83	1/2145 (0.0%)
5	AF	0.51	0/1609	0.70	0/2177
5	BF	0.73	0/1609	0.77	0/2177
6	AG	0.61	0/1393	0.66	0/1892
6	BG	0.46	0/1393	0.64	0/1892
7	AH	0.58	0/1343	0.68	1/1820 (0.1%)
7	BH	0.59	0/1343	0.70	0/1820
8	AI	0.63	1/1061 (0.1%)	0.78	0/1451
8	BI	0.50	0/1061	0.74	0/1451
9	AN	0.52	0/1139	0.72	0/1538
9	BN	0.74	0/1139	0.78	0/1538
10	AO	0.50	0/933	0.72	1/1257 (0.1%)
10	BO	0.67	0/933	0.74	0/1257
11	AP	0.50	0/1135	0.75	1/1510 (0.1%)
11	BP	0.64	0/1135	0.81	2/1510 (0.1%)
12	AQ	0.53	0/1143	0.74	0/1527
12	BQ	0.64	0/1143	0.74	0/1527
13	AR	0.51	0/982	0.74	0/1312
13	BR	0.69	0/982	0.82	1/1312 (0.1%)
14	AS	0.64	0/875	0.79	0/1168
14	BS	0.53	0/875	0.79	1/1168 (0.1%)
15	AT	0.52	0/1077	0.73	0/1444
15	BT	0.61	0/1077	0.79	1/1444 (0.1%)
16	AU	0.56	0/977	0.69	0/1301
16	BU	0.88	1/977 (0.1%)	0.81	1/1301 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AV	0.58	0/782	0.67	0/1049
17	BV	0.70	0/782	0.77	0/1049
18	AW	0.56	0/891	0.75	0/1197
18	BW	0.82	0/891	0.80	0/1197
19	AX	0.55	0/756	0.77	1/1016 (0.1%)
19	BX	0.66	0/756	0.76	1/1016 (0.1%)
20	AY	0.50	0/798	0.77	0/1073
20	BY	0.61	0/798	0.80	1/1073 (0.1%)
21	AZ	0.57	0/1555	0.68	0/2118
21	BZ	0.49	0/1555	0.71	0/2118
22	A0	0.50	0/602	0.69	0/804
22	B0	0.66	0/602	0.77	0/804
23	A1	0.51	0/752	0.72	0/1003
23	B1	0.62	0/752	0.76	0/1003
24	A2	0.59	0/590	0.68	0/781
24	B2	0.60	0/590	0.74	0/781
25	A3	0.45	0/463	0.69	0/623
25	B3	0.65	0/463	0.74	0/623
26	A4	0.65	0/358	0.74	0/487
26	B4	0.56	0/358	0.74	1/487 (0.2%)
27	A5	0.67	1/469 (0.2%)	0.83	2/634 (0.3%)
27	B5	0.79	0/469	0.88	0/634
28	A6	0.59	0/456	0.70	0/609
28	B6	0.68	0/456	0.74	0/609
29	A7	0.57	0/426	0.75	0/561
29	B7	0.78	0/426	0.84	0/561
30	A8	0.50	0/516	0.73	0/679
30	B8	0.70	0/516	0.82	0/679
31	CA	0.80	10/36054 (0.0%)	1.18	176/56272 (0.3%)
31	DA	0.77	7/36054 (0.0%)	1.19	211/56272 (0.4%)
32	CB	0.51	0/1811	0.69	0/2452
32	DB	0.56	0/1811	0.69	0/2452
33	CC	0.56	0/1474	0.65	0/2003
33	DC	0.58	0/1474	0.65	0/2003
34	CD	0.53	0/1550	0.72	3/2106 (0.1%)
34	DD	0.84	2/1550 (0.1%)	0.78	4/2106 (0.2%)
35	CE	0.49	0/1121	0.70	1/1517 (0.1%)
35	DE	0.52	0/1121	0.72	1/1517 (0.1%)
36	CF	0.49	0/794	0.64	0/1082
36	DF	0.49	0/794	0.67	1/1082 (0.1%)
37	CG	0.57	0/1186	0.65	0/1603
37	DG	0.56	0/1186	0.62	0/1603
38	CH	0.44	0/1065	0.67	0/1445

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DH	0.44	0/1065	0.64	0/1445
39	CI	0.62	0/867	0.71	0/1180
39	DI	0.62	0/867	0.69	0/1180
40	CJ	0.60	0/672	0.74	1/919 (0.1%)
40	DJ	0.60	0/672	0.70	1/919 (0.1%)
41	CK	0.47	0/843	0.71	0/1144
41	DK	0.47	0/843	0.67	0/1144
42	CL	0.44	0/925	0.67	0/1251
42	DL	0.46	0/925	0.69	0/1251
43	CM	0.67	0/811	0.72	0/1103
43	DM	0.63	0/811	0.73	1/1103 (0.1%)
44	CN	0.60	0/487	0.68	0/649
44	DN	0.59	0/487	0.74	0/649
45	CO	0.49	0/735	0.64	0/981
45	DO	0.47	0/735	0.61	0/981
46	CP	0.51	0/667	0.70	0/905
46	DP	0.43	0/667	0.65	0/905
47	CQ	0.46	0/836	0.68	0/1117
47	DQ	0.47	0/836	0.66	0/1117
48	CR	0.43	0/519	0.64	0/699
48	DR	0.50	0/519	0.67	0/699
49	CS	0.69	0/558	0.88	1/759 (0.1%)
49	DS	0.76	1/558 (0.2%)	0.87	3/759 (0.4%)
50	CT	0.47	0/710	0.72	0/940
50	DT	0.42	0/710	0.68	0/940
51	CU	0.64	0/203	0.67	0/266
51	DU	0.59	0/203	0.70	0/266
All	All	0.86	110/303650 (0.0%)	1.16	1892/454928 (0.4%)

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
26	A4	0	1
34	CD	0	1
34	DD	0	1
42	CL	0	1
42	DL	0	1
All	All	0	5

The worst 5 of 110 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	DD	12	CYS	CB-SG	19.94	2.16	1.82
34	DD	26	CYS	CB-SG	15.79	2.09	1.82
31	DA	1492	A	C6-N6	-12.21	1.24	1.33
31	CA	1492	A	C2-N3	12.12	1.44	1.33
31	CA	1493	A	N9-C4	-11.96	1.30	1.37

The worst 5 of 1892 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	DA	1492	A	C6-N1-C2	-28.45	101.53	118.60
31	DA	1492	A	C5-C6-N1	26.41	130.90	117.70
31	CA	1492	A	C8-N9-C4	-21.05	97.38	105.80
1	BA	1332	G	C2-N3-C4	-19.65	102.08	111.90
1	BA	1332	G	N3-C4-C5	17.99	137.59	128.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	A4	42	PHE	Peptide
34	CD	11	LEU	Peptide
42	CL	26	ALA	Peptide
34	DD	11	LEU	Peptide
42	DL	26	ALA	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	AA	60900	0	30712	1406	0
1	BA	60900	0	30712	1060	0
2	AB	2574	0	1306	87	0
2	BB	2574	0	1306	35	0
3	AD	2136	0	2218	77	0
3	BD	2136	0	2218	81	0
4	AE	1555	0	1607	81	0
4	BE	1555	0	1607	54	0
5	AF	1576	0	1616	57	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	BF	1576	0	1616	59	0
6	AG	1368	0	1324	70	0
6	BG	1368	0	1324	61	0
7	AH	1317	0	1376	66	0
7	BH	1317	0	1376	33	0
8	AI	1046	0	1067	55	2
8	BI	1046	0	1067	47	0
9	AN	1112	0	1180	60	0
9	BN	1112	0	1180	34	0
10	AO	923	0	981	28	0
10	BO	923	0	981	23	0
11	AP	1119	0	1186	38	0
11	BP	1119	0	1186	40	0
12	AQ	1122	0	1179	43	0
12	BQ	1122	0	1179	47	0
13	AR	968	0	1033	43	0
13	BR	968	0	1033	33	0
14	AS	865	0	905	62	0
14	BS	865	0	905	54	0
15	AT	1063	0	1103	48	0
15	BT	1063	0	1103	37	0
16	AU	959	0	1019	31	0
16	BU	959	0	1019	20	0
17	AV	771	0	830	22	0
17	BV	771	0	830	15	0
18	AW	881	0	935	25	0
18	BW	881	0	935	24	0
19	AX	742	0	799	22	0
19	BX	742	0	799	23	0
20	AY	785	0	832	36	0
20	BY	785	0	832	30	0
21	AZ	1522	0	1511	56	0
21	BZ	1522	0	1511	47	0
22	A0	594	0	604	27	0
22	B0	594	0	604	21	0
23	A1	745	0	804	26	0
23	B1	745	0	804	26	0
24	A2	588	0	643	31	0
24	B2	588	0	643	18	0
25	A3	458	0	503	22	0
25	B3	458	0	503	6	0
26	A4	349	0	340	22	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	B4	349	0	340	16	0
27	A5	455	0	476	25	0
27	B5	455	0	476	18	0
28	A6	449	0	464	19	0
28	B6	449	0	466	17	0
29	A7	418	0	467	18	0
29	B7	418	0	467	14	0
30	A8	509	0	565	23	0
30	B8	509	0	565	20	0
31	CA	32208	0	16256	921	2
31	DA	32208	0	16254	923	0
32	CB	1777	0	1747	100	0
32	DB	1777	0	1747	95	0
33	CC	1450	0	1314	45	0
33	DC	1450	0	1314	58	0
34	CD	1520	0	1407	73	0
34	DD	1520	0	1406	85	0
35	CE	1105	0	1130	48	0
35	DE	1105	0	1130	54	0
36	CF	781	0	741	25	0
36	DF	781	0	741	29	0
37	CG	1167	0	1108	39	0
37	DG	1167	0	1108	46	0
38	CH	1045	0	1033	45	0
38	DH	1045	0	1033	53	0
39	CI	852	0	742	43	0
39	DI	852	0	742	52	0
40	CJ	659	0	552	31	0
40	DJ	659	0	552	37	0
41	CK	828	0	822	24	0
41	DK	828	0	822	32	0
42	CL	909	0	927	43	0
42	DL	909	0	927	38	0
43	CM	801	0	743	33	0
43	DM	801	0	743	37	0
44	CN	478	0	498	33	0
44	DN	478	0	497	30	0
45	CO	724	0	749	32	0
45	DO	724	0	749	27	0
46	CP	651	0	638	33	0
46	DP	651	0	638	28	0
47	CQ	823	0	891	33	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	DQ	823	0	891	22	0
48	CR	514	0	530	19	0
48	DR	514	0	530	17	0
49	CS	544	0	457	21	0
49	DS	544	0	457	26	0
50	CT	708	0	764	37	0
50	DT	708	0	764	26	0
51	CU	199	0	208	8	0
51	DU	199	0	208	6	0
52	AA	44	0	20	31	0
52	BA	44	0	20	23	0
53	AA	2	0	0	0	0
53	BA	2	0	0	0	0
All	All	279316	0	185722	7170	2

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 16.

The worst 5 of 7170 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:AA:3001:T8B:C13	31:DA:1492:A:H5''	1.47	1.41
34:DD:26:CYS:SG	34:DD:26:CYS:CB	2.09	1.41
34:DD:12:CYS:SG	34:DD:12:CYS:CB	2.16	1.34
52:AA:3001:T8B:C22	52:AA:3001:T8B:H13	1.58	1.33
52:BA:3001:T8B:H13	52:BA:3001:T8B:C22	1.58	1.32

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AI:89:TYR:O	31:CA:357:G:O2'[2_654]	2.11	0.09
8:AI:91:SER:OG	31:CA:368:U:OP2[2_654]	2.12	0.08

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	
3	AD	273/276 (99%)	240 (88%)	27 (10%)	6 (2%)	7	39
3	BD	273/276 (99%)	246 (90%)	23 (8%)	4 (2%)	11	49
4	AE	202/206 (98%)	177 (88%)	18 (9%)	7 (4%)	4	27
4	BE	202/206 (98%)	174 (86%)	21 (10%)	7 (4%)	4	27
5	AF	198/205 (97%)	168 (85%)	25 (13%)	5 (2%)	6	36
5	BF	198/205 (97%)	170 (86%)	21 (11%)	7 (4%)	4	27
6	AG	179/182 (98%)	136 (76%)	33 (18%)	10 (6%)	2	15
6	BG	179/182 (98%)	135 (75%)	30 (17%)	14 (8%)	1	7
7	AH	172/180 (96%)	143 (83%)	21 (12%)	8 (5%)	2	19
7	BH	172/180 (96%)	144 (84%)	22 (13%)	6 (4%)	4	27
8	AI	143/148 (97%)	103 (72%)	28 (20%)	12 (8%)	1	5
8	BI	143/148 (97%)	109 (76%)	24 (17%)	10 (7%)	1	8
9	AN	138/140 (99%)	113 (82%)	16 (12%)	9 (6%)	1	11
9	BN	138/140 (99%)	119 (86%)	13 (9%)	6 (4%)	3	22
10	AO	120/122 (98%)	108 (90%)	8 (7%)	4 (3%)	4	28
10	BO	120/122 (98%)	109 (91%)	7 (6%)	4 (3%)	4	28
11	AP	143/150 (95%)	117 (82%)	18 (13%)	8 (6%)	2	15
11	BP	143/150 (95%)	126 (88%)	12 (8%)	5 (4%)	4	27
12	AQ	139/141 (99%)	126 (91%)	9 (6%)	4 (3%)	5	32
12	BQ	139/141 (99%)	126 (91%)	9 (6%)	4 (3%)	5	32
13	AR	116/118 (98%)	95 (82%)	16 (14%)	5 (4%)	3	22
13	BR	116/118 (98%)	108 (93%)	7 (6%)	1 (1%)	19	60
14	AS	108/112 (96%)	84 (78%)	21 (19%)	3 (3%)	5	33
14	BS	108/112 (96%)	93 (86%)	12 (11%)	3 (3%)	5	33
15	AT	129/146 (88%)	109 (84%)	16 (12%)	4 (3%)	4	30

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	BT	129/146 (88%)	116 (90%)	12 (9%)	1 (1%)	21	62
16	AU	114/118 (97%)	104 (91%)	10 (9%)	0	100	100
16	BU	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
17	AV	99/101 (98%)	89 (90%)	8 (8%)	2 (2%)	8	42
17	BV	99/101 (98%)	89 (90%)	9 (9%)	1 (1%)	17	58
18	AW	110/113 (97%)	101 (92%)	8 (7%)	1 (1%)	19	60
18	BW	110/113 (97%)	104 (94%)	6 (6%)	0	100	100
19	AX	93/96 (97%)	82 (88%)	9 (10%)	2 (2%)	7	39
19	BX	93/96 (97%)	82 (88%)	9 (10%)	2 (2%)	7	39
20	AY	105/110 (96%)	90 (86%)	10 (10%)	5 (5%)	2	19
20	BY	105/110 (96%)	88 (84%)	13 (12%)	4 (4%)	3	24
21	AZ	196/206 (95%)	153 (78%)	32 (16%)	11 (6%)	2	15
21	BZ	196/206 (95%)	158 (81%)	31 (16%)	7 (4%)	4	26
22	A0	74/85 (87%)	67 (90%)	6 (8%)	1 (1%)	12	50
22	B0	74/85 (87%)	67 (90%)	6 (8%)	1 (1%)	12	50
23	A1	95/98 (97%)	88 (93%)	5 (5%)	2 (2%)	8	40
23	B1	95/98 (97%)	86 (90%)	6 (6%)	3 (3%)	4	29
24	A2	68/72 (94%)	59 (87%)	8 (12%)	1 (2%)	11	49
24	B2	68/72 (94%)	63 (93%)	5 (7%)	0	100	100
25	A3	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
25	B3	57/60 (95%)	54 (95%)	2 (4%)	1 (2%)	9	45
26	A4	44/71 (62%)	30 (68%)	10 (23%)	4 (9%)	1	4
26	B4	44/71 (62%)	30 (68%)	10 (23%)	4 (9%)	1	4
27	A5	57/60 (95%)	50 (88%)	6 (10%)	1 (2%)	9	45
27	B5	57/60 (95%)	49 (86%)	6 (10%)	2 (4%)	4	27
28	A6	51/54 (94%)	46 (90%)	4 (8%)	1 (2%)	8	42
28	B6	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
29	A7	46/49 (94%)	41 (89%)	4 (9%)	1 (2%)	7	39
29	B7	46/49 (94%)	42 (91%)	3 (6%)	1 (2%)	7	39
30	A8	62/65 (95%)	48 (77%)	13 (21%)	1 (2%)	11	47
30	B8	62/65 (95%)	57 (92%)	5 (8%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	CB	227/256 (89%)	171 (75%)	36 (16%)	20 (9%)	1	4
32	DB	227/256 (89%)	173 (76%)	39 (17%)	15 (7%)	1	10
33	CC	204/239 (85%)	163 (80%)	30 (15%)	11 (5%)	2	16
33	DC	204/239 (85%)	144 (71%)	42 (21%)	18 (9%)	1	4
34	CD	206/209 (99%)	154 (75%)	40 (19%)	12 (6%)	2	14
34	DD	206/209 (99%)	152 (74%)	47 (23%)	7 (3%)	4	27
35	CE	146/162 (90%)	112 (77%)	23 (16%)	11 (8%)	1	7
35	DE	146/162 (90%)	116 (80%)	25 (17%)	5 (3%)	4	27
36	CF	98/101 (97%)	87 (89%)	8 (8%)	3 (3%)	4	30
36	DF	98/101 (97%)	85 (87%)	9 (9%)	4 (4%)	3	23
37	CG	153/156 (98%)	127 (83%)	16 (10%)	10 (6%)	1	11
37	DG	153/156 (98%)	129 (84%)	18 (12%)	6 (4%)	3	24
38	CH	136/138 (99%)	116 (85%)	18 (13%)	2 (2%)	11	49
38	DH	136/138 (99%)	118 (87%)	13 (10%)	5 (4%)	4	25
39	CI	123/128 (96%)	93 (76%)	20 (16%)	10 (8%)	1	6
39	DI	123/128 (96%)	94 (76%)	21 (17%)	8 (6%)	1	11
40	CJ	94/105 (90%)	66 (70%)	19 (20%)	9 (10%)	1	4
40	DJ	94/105 (90%)	74 (79%)	14 (15%)	6 (6%)	1	11
41	CK	112/129 (87%)	96 (86%)	12 (11%)	4 (4%)	4	26
41	DK	112/129 (87%)	90 (80%)	19 (17%)	3 (3%)	5	34
42	CL	120/132 (91%)	98 (82%)	17 (14%)	5 (4%)	3	23
42	DL	120/132 (91%)	100 (83%)	15 (12%)	5 (4%)	3	23
43	CM	112/126 (89%)	84 (75%)	18 (16%)	10 (9%)	1	4
43	DM	112/126 (89%)	80 (71%)	20 (18%)	12 (11%)	0	3
44	CN	58/61 (95%)	43 (74%)	10 (17%)	5 (9%)	1	5
44	DN	58/61 (95%)	48 (83%)	7 (12%)	3 (5%)	2	17
45	CO	86/89 (97%)	71 (83%)	12 (14%)	3 (4%)	4	27
45	DO	86/89 (97%)	68 (79%)	16 (19%)	2 (2%)	7	38
46	CP	80/88 (91%)	50 (62%)	23 (29%)	7 (9%)	1	4
46	DP	80/88 (91%)	52 (65%)	25 (31%)	3 (4%)	3	24
47	CQ	97/105 (92%)	84 (87%)	8 (8%)	5 (5%)	2	17

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	DQ	97/105 (92%)	81 (84%)	13 (13%)	3 (3%)	4	30
48	CR	66/88 (75%)	55 (83%)	10 (15%)	1 (2%)	11	49
48	DR	66/88 (75%)	60 (91%)	6 (9%)	0	100	100
49	CS	76/93 (82%)	48 (63%)	17 (22%)	11 (14%)	0	1
49	DS	76/93 (82%)	54 (71%)	17 (22%)	5 (7%)	1	10
50	CT	94/106 (89%)	73 (78%)	13 (14%)	8 (8%)	1	5
50	DT	94/106 (89%)	72 (77%)	15 (16%)	7 (7%)	1	8
51	CU	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
51	DU	21/27 (78%)	16 (76%)	3 (14%)	2 (10%)	1	4
All	All	11280/12044 (94%)	9338 (83%)	1460 (13%)	482 (4%)	3	22

5 of 482 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AD	239	ARG
3	AD	275	LYS
5	AF	60	SER
6	AG	14	GLU
6	AG	78	SER

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	
3	AD	215/218 (99%)	185 (86%)	30 (14%)	4	18
3	BD	215/218 (99%)	189 (88%)	26 (12%)	5	24
4	AE	163/166 (98%)	139 (85%)	24 (15%)	3	16
4	BE	163/166 (98%)	134 (82%)	29 (18%)	2	10
5	AF	158/162 (98%)	133 (84%)	25 (16%)	3	13
5	BF	158/162 (98%)	138 (87%)	20 (13%)	5	22
6	AG	128/156 (82%)	110 (86%)	18 (14%)	4	17

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	BG	128/156 (82%)	114 (89%)	14 (11%)	7	29
7	AH	141/148 (95%)	125 (89%)	16 (11%)	6	28
7	BH	141/148 (95%)	124 (88%)	17 (12%)	5	24
8	AI	102/124 (82%)	76 (74%)	26 (26%)	0	2
8	BI	102/124 (82%)	76 (74%)	26 (26%)	0	2
9	AN	117/119 (98%)	94 (80%)	23 (20%)	1	8
9	BN	117/119 (98%)	91 (78%)	26 (22%)	1	5
10	AO	98/100 (98%)	89 (91%)	9 (9%)	10	36
10	BO	98/100 (98%)	89 (91%)	9 (9%)	10	36
11	AP	113/116 (97%)	96 (85%)	17 (15%)	3	15
11	BP	113/116 (97%)	97 (86%)	16 (14%)	3	17
12	AQ	111/111 (100%)	94 (85%)	17 (15%)	3	15
12	BQ	111/111 (100%)	94 (85%)	17 (15%)	3	15
13	AR	101/101 (100%)	80 (79%)	21 (21%)	1	6
13	BR	101/101 (100%)	79 (78%)	22 (22%)	1	5
14	AS	84/88 (96%)	67 (80%)	17 (20%)	1	7
14	BS	84/88 (96%)	72 (86%)	12 (14%)	3	17
15	AT	110/127 (87%)	99 (90%)	11 (10%)	8	33
15	BT	110/127 (87%)	100 (91%)	10 (9%)	10	37
16	AU	93/94 (99%)	83 (89%)	10 (11%)	7	29
16	BU	93/94 (99%)	77 (83%)	16 (17%)	2	11
17	AV	80/82 (98%)	63 (79%)	17 (21%)	1	6
17	BV	80/82 (98%)	63 (79%)	17 (21%)	1	6
18	AW	89/92 (97%)	75 (84%)	14 (16%)	3	13
18	BW	89/92 (97%)	78 (88%)	11 (12%)	5	23
19	AX	75/78 (96%)	67 (89%)	8 (11%)	7	30
19	BX	75/78 (96%)	66 (88%)	9 (12%)	5	25
20	AY	80/91 (88%)	70 (88%)	10 (12%)	5	23
20	BY	80/91 (88%)	72 (90%)	8 (10%)	8	33
21	AZ	159/179 (89%)	139 (87%)	20 (13%)	5	23
21	BZ	159/179 (89%)	137 (86%)	22 (14%)	4	18

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	A0	59/67 (88%)	52 (88%)	7 (12%)	6	25
22	B0	59/67 (88%)	52 (88%)	7 (12%)	6	25
23	A1	78/83 (94%)	68 (87%)	10 (13%)	5	22
23	B1	78/83 (94%)	70 (90%)	8 (10%)	8	32
24	A2	65/67 (97%)	56 (86%)	9 (14%)	4	18
24	B2	65/67 (97%)	57 (88%)	8 (12%)	5	24
25	A3	49/52 (94%)	43 (88%)	6 (12%)	5	24
25	B3	49/52 (94%)	43 (88%)	6 (12%)	5	24
26	A4	39/63 (62%)	32 (82%)	7 (18%)	2	10
26	B4	39/63 (62%)	30 (77%)	9 (23%)	1	4
27	A5	50/52 (96%)	43 (86%)	7 (14%)	4	18
27	B5	50/52 (96%)	43 (86%)	7 (14%)	4	18
28	A6	50/52 (96%)	40 (80%)	10 (20%)	1	7
28	B6	50/52 (96%)	41 (82%)	9 (18%)	2	10
29	A7	41/42 (98%)	35 (85%)	6 (15%)	3	16
29	B7	41/42 (98%)	32 (78%)	9 (22%)	1	5
30	A8	52/55 (94%)	45 (86%)	7 (14%)	4	19
30	B8	52/55 (94%)	47 (90%)	5 (10%)	9	34
32	CB	177/220 (80%)	141 (80%)	36 (20%)	1	7
32	DB	177/220 (80%)	142 (80%)	35 (20%)	1	8
33	CC	114/188 (61%)	95 (83%)	19 (17%)	2	11
33	DC	114/188 (61%)	96 (84%)	18 (16%)	3	13
34	CD	139/181 (77%)	117 (84%)	22 (16%)	3	13
34	DD	139/181 (77%)	120 (86%)	19 (14%)	4	19
35	CE	108/123 (88%)	86 (80%)	22 (20%)	1	7
35	DE	108/123 (88%)	88 (82%)	20 (18%)	2	9
36	CF	77/90 (86%)	65 (84%)	12 (16%)	3	13
36	DF	77/90 (86%)	65 (84%)	12 (16%)	3	13
37	CG	104/127 (82%)	86 (83%)	18 (17%)	2	11
37	DG	104/127 (82%)	88 (85%)	16 (15%)	3	14
38	CH	103/119 (87%)	85 (82%)	18 (18%)	2	11

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	DH	103/119 (87%)	84 (82%)	19 (18%)	2	9
39	CI	62/99 (63%)	53 (86%)	9 (14%)	3	16
39	DI	62/99 (63%)	54 (87%)	8 (13%)	5	21
40	CJ	52/92 (56%)	42 (81%)	10 (19%)	1	9
40	DJ	52/92 (56%)	41 (79%)	11 (21%)	1	6
41	CK	81/99 (82%)	69 (85%)	12 (15%)	3	16
41	DK	81/99 (82%)	71 (88%)	10 (12%)	5	24
42	CL	92/109 (84%)	81 (88%)	11 (12%)	5	25
42	DL	92/109 (84%)	83 (90%)	9 (10%)	9	34
43	CM	63/101 (62%)	49 (78%)	14 (22%)	1	5
43	DM	63/101 (62%)	49 (78%)	14 (22%)	1	5
44	CN	46/50 (92%)	35 (76%)	11 (24%)	1	3
44	DN	46/50 (92%)	33 (72%)	13 (28%)	0	1
45	CO	77/80 (96%)	65 (84%)	12 (16%)	3	13
45	DO	77/80 (96%)	66 (86%)	11 (14%)	3	17
46	CP	63/74 (85%)	49 (78%)	14 (22%)	1	5
46	DP	63/74 (85%)	53 (84%)	10 (16%)	3	13
47	CQ	94/97 (97%)	90 (96%)	4 (4%)	32	68
47	DQ	94/97 (97%)	84 (89%)	10 (11%)	7	30
48	CR	49/77 (64%)	44 (90%)	5 (10%)	8	32
48	DR	49/77 (64%)	46 (94%)	3 (6%)	20	58
49	CS	42/80 (52%)	25 (60%)	17 (40%)	0	0
49	DS	42/80 (52%)	36 (86%)	6 (14%)	3	17
50	CT	65/82 (79%)	53 (82%)	12 (18%)	2	9
50	DT	65/82 (79%)	57 (88%)	8 (12%)	5	24
51	CU	18/22 (82%)	16 (89%)	2 (11%)	7	28
51	DU	18/22 (82%)	14 (78%)	4 (22%)	1	5
All	All	8652/9990 (87%)	7319 (85%)	1333 (15%)	3	14

5 of 1333 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	BR	6	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	B2	34	GLU
40	DJ	72	VAL
13	BR	96	ARG
17	BV	85	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 63 such sidechains are listed below:

Mol	Chain	Res	Type
13	BR	13	HIS
35	CE	78	HIS
43	DM	106	ASN
19	BX	31	HIS
30	B8	35	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	2819/2915 (96%)	581 (20%)	59 (2%)
1	BA	2819/2915 (96%)	586 (20%)	60 (2%)
2	AB	119/122 (97%)	25 (21%)	0
2	BB	119/122 (97%)	21 (17%)	0
31	CA	1496/1521 (98%)	339 (22%)	31 (2%)
31	DA	1496/1521 (98%)	341 (22%)	27 (1%)
All	All	8868/9116 (97%)	1893 (21%)	177 (1%)

5 of 1893 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	10	G
1	AA	14	A
1	AA	15	G
1	AA	34	C
1	AA	45	C

5 of 177 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	BA	1047	G
1	BA	1819	A
31	DA	560	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	BA	1106	A
1	BA	1301	A

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
52	T8B	AA	3001	53	40,48,48	1.00	2 (5%)	50,71,71	1.31	8 (16%)
52	T8B	BA	3001	53	40,48,48	1.00	2 (5%)	50,71,71	1.31	8 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	T8B	AA	3001	53	-	0/22/26/26	0/5/5/5
52	T8B	BA	3001	53	-	0/22/26/26	0/5/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	AA	3001	T8B	C25-C24	2.28	1.50	1.43
52	BA	3001	T8B	C25-C24	2.29	1.50	1.43
52	BA	3001	T8B	O11-C26	2.97	1.38	1.32
52	AA	3001	T8B	O11-C26	2.98	1.38	1.32

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	BA	3001	T8B	C21-C23-C24	-3.82	120.19	125.11
52	AA	3001	T8B	C21-C23-C24	-3.81	120.21	125.11
52	AA	3001	T8B	C2-C3-C4	-2.69	118.75	122.08
52	BA	3001	T8B	C2-C3-C4	-2.69	118.76	122.08
52	BA	3001	T8B	O4-C12-C11	-2.20	108.73	112.42

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	AA	3001	T8B	31	0
52	BA	3001	T8B	23	0

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, 95th 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	AA	2827/2915 (96%)	0.03	117 (4%) 37 24	46, 70, 113, 128	0
1	BA	2827/2915 (96%)	0.08	73 (2%) 56 41	27, 56, 110, 126	0
2	AB	120/122 (98%)	0.03	4 (3%) 46 30	68, 95, 108, 111	0
2	BB	120/122 (98%)	-0.24	0 100 100	46, 80, 95, 103	0
3	AD	275/276 (99%)	-0.15	0 100 100	45, 67, 83, 103	0
3	BD	275/276 (99%)	-0.16	2 (0%) 87 81	36, 59, 78, 103	0
4	AE	204/206 (99%)	-0.10	1 (0%) 90 86	47, 72, 87, 98	0
4	BE	204/206 (99%)	-0.18	0 100 100	33, 60, 81, 96	0
5	AF	203/205 (99%)	-0.34	2 (0%) 82 73	44, 77, 95, 112	0
5	BF	203/205 (99%)	-0.23	0 100 100	27, 64, 90, 110	0
6	AG	181/182 (99%)	1.35	52 (28%) 0 0	89, 106, 114, 116	0
6	BG	181/182 (99%)	0.10	8 (4%) 34 21	81, 101, 110, 118	0
7	AH	174/180 (96%)	0.91	37 (21%) 1 0	80, 93, 101, 108	0
7	BH	174/180 (96%)	-0.16	0 100 100	63, 78, 91, 98	0
8	AI	145/148 (97%)	0.59	21 (14%) 2 1	72, 104, 116, 123	0
8	BI	145/148 (97%)	-0.10	1 (0%) 87 81	68, 90, 98, 100	0
9	AN	140/140 (100%)	-0.08	1 (0%) 87 81	59, 73, 90, 94	0
9	BN	140/140 (100%)	-0.19	0 100 100	38, 57, 82, 85	0
10	AO	122/122 (100%)	-0.33	0 100 100	56, 73, 85, 91	0
10	BO	122/122 (100%)	-0.22	0 100 100	43, 64, 82, 89	0
11	AP	147/150 (98%)	-0.01	4 (2%) 54 40	47, 81, 96, 105	0
11	BP	147/150 (98%)	-0.17	0 100 100	28, 68, 91, 100	0
12	AQ	141/141 (100%)	-0.04	1 (0%) 87 81	60, 78, 91, 97	0
12	BQ	141/141 (100%)	-0.09	0 100 100	44, 65, 78, 88	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AR	118/118 (100%)	-0.18	0 100 100	47, 66, 78, 88	0
13	BR	118/118 (100%)	-0.19	0 100 100	35, 53, 69, 86	0
14	AS	110/112 (98%)	0.53	13 (11%) 4 2	74, 91, 102, 109	0
14	BS	110/112 (98%)	-0.13	0 100 100	58, 79, 93, 100	0
15	AT	131/146 (89%)	-0.22	1 (0%) 86 78	66, 76, 99, 109	0
15	BT	131/146 (89%)	-0.27	1 (0%) 86 78	55, 68, 91, 102	0
16	AU	116/118 (98%)	-0.05	0 100 100	53, 70, 84, 89	0
16	BU	116/118 (98%)	-0.15	0 100 100	34, 50, 70, 84	0
17	AV	101/101 (100%)	-0.19	1 (0%) 82 73	48, 79, 93, 103	0
17	BV	101/101 (100%)	-0.31	0 100 100	31, 61, 81, 95	0
18	AW	112/113 (99%)	-0.24	0 100 100	50, 59, 80, 104	0
18	BW	112/113 (99%)	-0.31	0 100 100	36, 45, 75, 106	0
19	AX	95/96 (98%)	-0.08	0 100 100	54, 71, 89, 93	0
19	BX	95/96 (98%)	-0.17	0 100 100	33, 59, 83, 91	0
20	AY	107/110 (97%)	0.15	7 (6%) 19 10	71, 81, 94, 105	0
20	BY	107/110 (97%)	-0.24	1 (0%) 84 76	56, 71, 89, 103	0
21	AZ	198/206 (96%)	0.01	7 (3%) 44 28	80, 92, 103, 108	0
21	BZ	198/206 (96%)	-0.35	0 100 100	64, 82, 97, 103	0
22	A0	76/85 (89%)	0.24	2 (2%) 56 41	59, 74, 84, 89	0
22	B0	76/85 (89%)	-0.24	0 100 100	46, 60, 74, 82	0
23	A1	97/98 (98%)	0.12	2 (2%) 63 49	54, 71, 94, 99	0
23	B1	97/98 (98%)	-0.08	1 (1%) 82 73	42, 65, 91, 95	0
24	A2	70/72 (97%)	-0.05	1 (1%) 75 63	65, 81, 92, 101	0
24	B2	70/72 (97%)	-0.13	0 100 100	52, 70, 85, 102	0
25	A3	59/60 (98%)	0.46	5 (8%) 11 6	63, 74, 92, 101	0
25	B3	59/60 (98%)	-0.16	0 100 100	43, 56, 84, 94	0
26	A4	46/71 (64%)	0.54	7 (15%) 2 1	101, 109, 113, 119	0
26	B4	46/71 (64%)	0.26	6 (13%) 3 2	98, 107, 113, 118	0
27	A5	59/60 (98%)	-0.35	0 100 100	46, 64, 78, 91	0
27	B5	59/60 (98%)	-0.19	0 100 100	28, 52, 71, 89	0
28	A6	53/54 (98%)	0.14	3 (5%) 24 13	62, 77, 87, 89	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	B6	53/54 (98%)	-0.10	0 100 100	52, 66, 77, 85	0
29	A7	48/49 (97%)	0.14	4 (8%) 11 6	43, 54, 79, 99	0
29	B7	48/49 (97%)	-0.00	1 (2%) 63 49	29, 44, 73, 89	0
30	A8	64/65 (98%)	0.13	0 100 100	60, 68, 76, 85	0
30	B8	64/65 (98%)	0.13	0 100 100	45, 56, 65, 79	0
31	CA	1498/1521 (98%)	0.57	190 (12%) 3 2	59, 99, 120, 126	0
31	DA	1498/1521 (98%)	0.52	180 (12%) 4 2	65, 99, 120, 128	0
32	CB	229/256 (89%)	0.12	14 (6%) 21 11	93, 103, 111, 117	0
32	DB	229/256 (89%)	0.65	32 (13%) 2 2	95, 105, 112, 115	0
33	CC	206/239 (86%)	1.00	45 (21%) 0 0	92, 106, 112, 115	0
33	DC	206/239 (86%)	0.87	33 (16%) 1 1	97, 108, 115, 120	0
34	CD	208/209 (99%)	0.03	10 (4%) 30 18	85, 98, 108, 114	0
34	DD	208/209 (99%)	0.02	10 (4%) 30 18	87, 97, 107, 123	0
35	CE	148/162 (91%)	-0.14	4 (2%) 54 40	74, 93, 103, 110	0
35	DE	148/162 (91%)	0.10	5 (3%) 45 30	84, 96, 104, 110	0
36	CF	100/101 (99%)	-0.07	5 (5%) 29 16	80, 92, 101, 107	0
36	DF	100/101 (99%)	-0.14	3 (3%) 50 35	84, 93, 103, 110	0
37	CG	155/156 (99%)	2.14	77 (49%) 0 0	99, 109, 115, 120	0
37	DG	155/156 (99%)	2.07	75 (48%) 0 0	97, 109, 115, 119	0
38	CH	138/138 (100%)	0.05	4 (2%) 51 37	82, 94, 101, 104	0
38	DH	138/138 (100%)	-0.09	3 (2%) 62 48	86, 96, 102, 106	0
39	CI	125/128 (97%)	1.89	50 (40%) 0 0	97, 111, 117, 120	0
39	DI	125/128 (97%)	2.77	71 (56%) 0 0	100, 112, 118, 120	0
40	CJ	96/105 (91%)	2.13	43 (44%) 0 0	100, 109, 115, 117	0
40	DJ	96/105 (91%)	1.91	46 (47%) 0 0	97, 110, 115, 119	0
41	CK	114/129 (88%)	-0.12	1 (0%) 84 76	72, 93, 101, 105	0
41	DK	114/129 (88%)	0.22	4 (3%) 44 28	75, 95, 103, 107	0
42	CL	122/132 (92%)	-0.23	0 100 100	72, 85, 96, 100	0
42	DL	122/132 (92%)	-0.15	1 (0%) 86 78	77, 87, 96, 105	0
43	CM	114/126 (90%)	2.13	51 (44%) 0 0	102, 111, 118, 126	0
43	DM	114/126 (90%)	1.76	44 (38%) 0 0	101, 109, 115, 117	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	CN	60/61 (98%)	1.19	15 (25%) 0 0	99, 108, 116, 118	0
44	DN	60/61 (98%)	1.59	21 (35%) 0 0	103, 111, 116, 122	0
45	CO	88/89 (98%)	0.02	2 (2%) 60 47	72, 91, 101, 107	0
45	DO	88/89 (98%)	0.18	5 (5%) 24 13	81, 93, 103, 107	0
46	CP	82/88 (93%)	0.62	6 (7%) 15 8	88, 96, 106, 112	0
46	DP	82/88 (93%)	0.43	3 (3%) 41 27	86, 94, 103, 111	0
47	CQ	99/105 (94%)	0.04	2 (2%) 65 51	78, 90, 98, 102	0
47	DQ	99/105 (94%)	0.17	3 (3%) 50 35	79, 92, 100, 103	0
48	CR	68/88 (77%)	0.15	9 (13%) 3 2	80, 91, 102, 103	0
48	DR	68/88 (77%)	0.21	3 (4%) 34 21	85, 93, 104, 106	0
49	CS	78/93 (83%)	2.61	44 (56%) 0 0	107, 111, 117, 123	0
49	DS	78/93 (83%)	2.84	52 (66%) 0 0	91, 112, 117, 119	0
50	CT	96/106 (90%)	0.18	3 (3%) 49 33	84, 93, 99, 102	0
50	DT	96/106 (90%)	0.69	10 (10%) 6 4	82, 92, 100, 101	0
51	CU	23/27 (85%)	2.89	12 (52%) 0 0	106, 112, 117, 119	0
51	DU	23/27 (85%)	2.65	13 (56%) 0 0	104, 109, 112, 113	0
All	All	20372/21160 (96%)	0.26	1591 (7%) 13 7	27, 84, 115, 128	0

The worst 5 of 1591 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
39	CI	30	GLY	12.5
49	CS	40	ILE	12.5
43	CM	85	GLY	12.2
31	CA	1353	G	11.0
31	CA	1286	A	10.7

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 carbohydrates 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, 95th 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(\AA^2)	Q<0.9
53	MG	BA	3002	1/1	0.85	0.15	30,30,30,30	0
52	T8B	AA	3001	44/44	0.85	0.28	20,20,20,20	0
52	T8B	BA	3001	44/44	0.89	0.34	20,20,20,20	0
53	MG	BA	3003	1/1	0.94	0.16	30,30,30,30	0
53	MG	AA	3002	1/1	0.95	0.20	30,30,30,30	0
53	MG	AA	3003	1/1	0.98	0.17	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.