



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 29, 2026 – 12:05 PM UTC

PDB ID : 4WT8 / pdb\_00004wt8  
Title : Crystal Structure of bactobolin A bound to 70S ribosome-tRNA complex  
Authors : Amunts, A.; Fiedorczuk, K.; Ramakrishnan, V.  
Deposited on : 2014-10-29  
Resolution : 3.40 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](mailto: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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

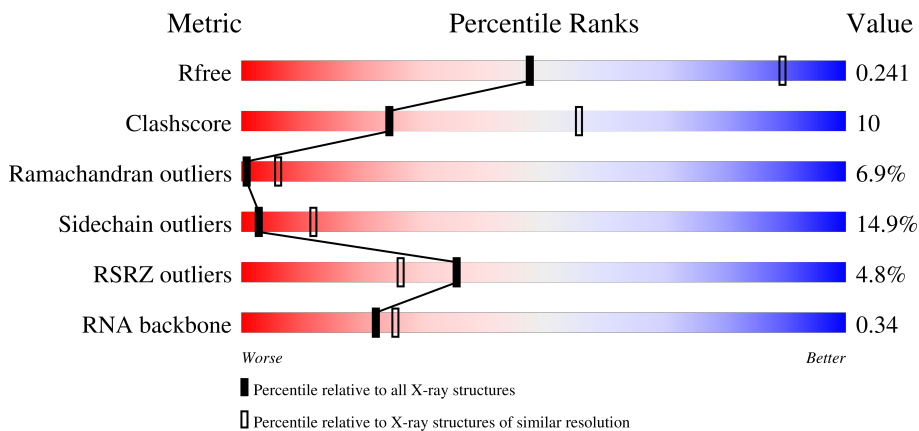
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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))
$R_{free}$	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)
RNA backbone	3983	1157 (3.80-3.00)

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

Mol	Chain	Length	Quality of chain
1	A2	9	
2	AA	234	
2	BA	234	
3	AC	238	

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Mol	Chain	Length	Quality of chain
4	AD	208	
4	BD	208	
5	AE	150	
5	BE	150	
6	AF	101	
6	BF	101	
7	AG	155	
7	BG	155	
8	AH	138	
8	BH	138	
9	AI	127	
9	BI	127	
10	AJ	98	
10	BJ	98	
11	AK	119	
11	BK	119	
12	AL	124	
12	BL	124	
13	AM	124	
13	BM	124	
14	AN	60	
14	BN	60	
15	AO	88	
15	BO	88	
16	AP	83	

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Mol	Chain	Length	Quality of chain
16	BP	83	5% 63% 34% .
17	AR	99	% 74% 25% .
17	BR	99	3% 67% 29% ..
18	AS	70	% 60% 31% 7% .
18	BS	70	% 61% 30% 6% .
19	AT	78	12% 44% 47% 8% .
19	BT	78	18% 42% 42% 14% .
20	AU	99	12% 65% 27% 6% .
20	BU	99	15% 63% 31% 6% .
21	AW	24	8% 75% 25%
21	BW	24	38% 58% 38% .
22	Ab	1504	% 55% 33% 10% .
22	Bb	1504	% 57% 32% 10% .
23	B2	10	20% 20% 50% 30%
24	BC	206	7% 70% 25% 5%
25	C2	76	11% 53% 32% 14% .
25	C3	76	4% 42% 46% 12%
25	D3	76	39% 36% 24% .
26	C4	77	% 32% 34% 27% 6%
27	CA	206	14% 75% 15% . 8%
28	CB	271	% 58% 29% 10% .
28	DB	271	2% 55% 30% 11% .
29	CC	204	5% 54% 34% 10% .
29	DC	204	5% 47% 36% 15% .
30	CD	207	% 57% 33% 9% .



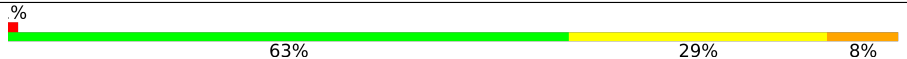
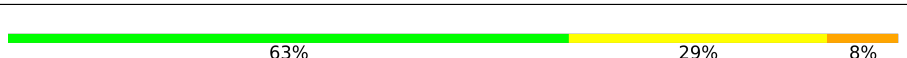
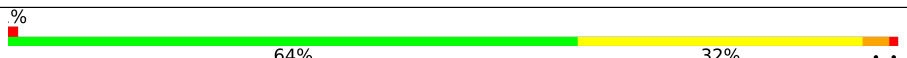
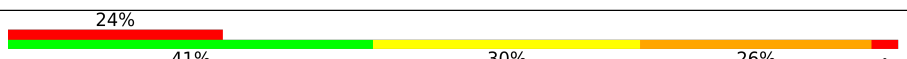
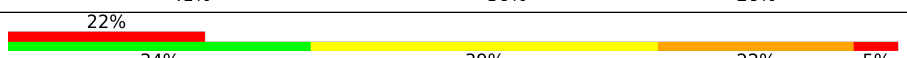
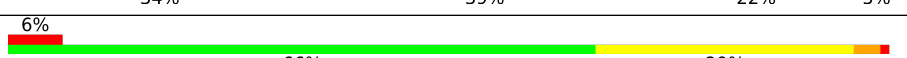
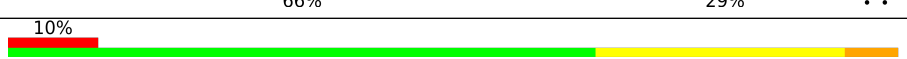

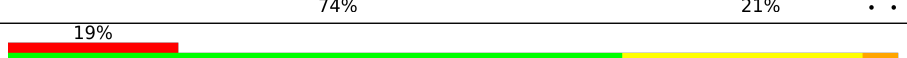







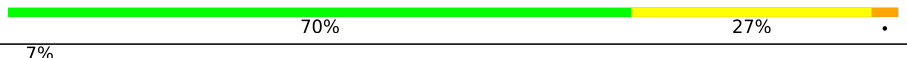
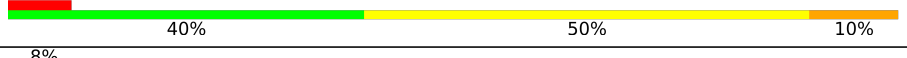

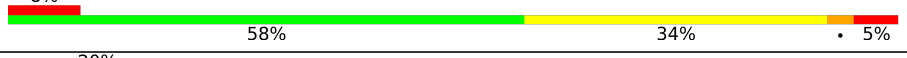
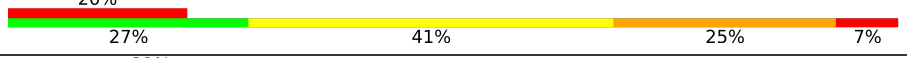
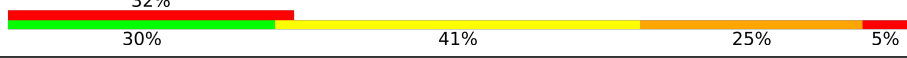

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Mol	Chain	Length	Quality of chain
30	DD	207	3% 60% 28% 12%
31	CE	181	7% 54% 35% 10%
31	DE	181	11% 58% 30% 9%
32	CF	159	12% 58% 30% 9%
32	DF	159	9% 53% 31% 12%
33	CI	145	4% 59% 34% 7%
33	DI	145	4% 61% 30% 8%
34	CJ	130	100%
34	DJ	130	95% 5%
35	CM	138	5% 61% 24% 13%
35	DM	138	7% 57% 30% 11%
36	CN	122	2% 61% 32% 7%
36	DN	122	68% 25% 7%
37	CO	146	11% 36% 34% 21% 8%
37	DO	146	14% 38% 25% 29% 8%
38	CP	141	6% 70% 25% 6%
38	DP	141	6% 60% 35% 5%
39	CQ	117	6% 55% 40% 5%
39	DQ	117	4% 55% 37% 7%
40	CR	98	13% 57% 32% 8%
40	DR	98	37% 47% 37% 14%
41	CS	137	9% 42% 34% 19% 5%
41	DS	137	8% 42% 35% 16% 7%
42	CT	117	3% 56% 33% 9%
42	DT	117	3% 57% 33% 9%

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Mol	Chain	Length	Quality of chain
43	CU	101	
43	DU	101	
44	CW	113	
45	CX	92	
45	DX	92	
46	CY	100	
46	DY	100	
47	CZ	176	
47	DZ	176	
48	Ca	84	
48	Da	84	
49	CH	93	
49	DH	93	
50	CK	71	
50	DK	71	
51	CL	59	
51	DL	59	
52	C5	30	
52	D5	30	
53	C6	59	
53	D6	59	
54	C7	44	
54	D7	44	
55	C8	48	
55	D8	48	

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Mol	Chain	Length	Quality of chain
56	C9	63	
56	D9	63	
57	C0	36	
57	D0	36	
58	C1	2899	
58	D1	2899	
59	Cs	119	
59	Ds	119	
60	D2	20	
61	D4	76	
62	DA	206	
63	DW	113	
64	DV	55	

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
66	3V6	D1	3001	-	-	X	-
67	MG	D1	3002	-	-	X	-

## 2 Entry composition [i](#)

There are 67 unique types of molecules in this entry. The entry contains 295910 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 mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A2	9	173	76	29	59	9	0	0	0

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	AA	234	1901	1213	341	342	5	0	0	0
2	BA	234	1901	1213	341	342	5	0	0	0

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	AC	206	1612	1016	314	281	1	0	0	0

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	AD	208	1703	1066	339	291	7	0	0	0
4	BD	208	1703	1066	339	291	7	0	0	0

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	AE	150	1147	724	217	202	4	0	0	0
5	BE	150	1147	724	217	202	4	0	0	0

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
6	BF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
7	BG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
8	BH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O	0	0	0
			1011	639	198	174			
9	BI	127	Total	C	N	O	0	0	0
			1011	639	198	174			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	58	ARG	HIS	conflict	UNP P80374

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	98	Total	C	N	O	S	0	0	0
			795	499	156	139	1			
10	BJ	98	Total	C	N	O	S	0	0	0
			795	499	156	139	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
11	BK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	124	Total	C	N	O	S	0	0	0
			971	611	195	164	1			
12	BL	124	Total	C	N	O	S	0	0	0
			971	611	195	164	1			

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	124	Total	C	N	O	S	0	0	0
			988	611	205	170	2			
13	BM	124	Total	C	N	O	S	0	0	0
			988	611	205	170	2			

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
14	BN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
15	BO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	83	Total	C	N	O	S	0	0	0
			701	443	139	118	1			
16	BP	83	Total	C	N	O	S	0	0	0
			701	443	139	118	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AR	99	Total	C	N	O	S	0	0	0
			824	528	151	143	2			
17	BR	99	Total	C	N	O	S	0	0	0
			824	528	151	143	2			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AS	70	Total	C	N	O	0	0	0
			574	367	112	95			
18	BS	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AT	78	Total	C	N	O	S	0	0	0
			630	403	114	111	2			
19	BT	78	Total	C	N	O	S	0	0	0
			630	403	114	111	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AU	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			
20	BU	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 21 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AW	24	Total	C	N	O	0	0	0
			209	128	50	31			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
21	BW	24	209	128	50	31	0	0	0

- Molecule 22 is a RNA chain called RNA (1504-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
22	Ab	1504	32329	14390	5992	10444	1503	0	0	0
22	Bb	1504	32329	14390	5992	10444	1503	0	0	0

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
23	B2	10	194	86	34	64	10	0	0	0

- Molecule 24 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
24	BC	206	1613	1016	314	282	1	0	0	0

- Molecule 25 is a RNA chain called A site tNA, E site tNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
25	C2	75	1597	713	285	525	74	0	0	0
25	C3	76	1619	723	290	531	75	0	0	0
25	D3	76	1619	723	290	531	75	0	0	0

- Molecule 26 is a RNA chain called P site trNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
26	C4	77	1640	732	297	535	76	0	0	0

- Molecule 27 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
27	CA	190	1156	706	220	230	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CA	106	ALA	GLY	conflict	UNP Q5SLP7

- Molecule 28 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
28	CB	271	2105	1329	416	357	3	0	0	0
28	DB	271	2105	1329	416	357	3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
29	CC	204	1564	988	299	271	6	0	0	0
29	DC	204	1564	988	299	271	6	0	0	0

- Molecule 30 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
30	CD	207	1624	1035	303	283	3	0	0	0
30	DD	207	1624	1035	303	283	3	0	0	0

- Molecule 31 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
31	CE	181	1474	942	268	260	4	0	0	0
31	DE	181	1474	942	268	260	4	0	0	0

- Molecule 32 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	CF	159	Total	C	N	O	S	0	0	0
			1223	773	228	221	1			
32	DF	159	Total	C	N	O	S	0	0	0
			1223	773	228	221	1			

- Molecule 33 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	CI	145	Total	C	N	O	S	0	0	0
			1132	723	200	208	1			
33	DI	145	Total	C	N	O	S	0	0	0
			1132	723	200	208	1			

- Molecule 34 is a protein called ribosomal L10 protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
34	CJ	130	Total	C	N	O	0	0	0
			651	390	130	131			
34	DJ	130	Total	C	N	O	0	0	0
			651	390	130	131			

- Molecule 35 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	CM	138	Total	C	N	O	S	0	0	0
			1105	712	206	183	4			
35	DM	138	Total	C	N	O	S	0	0	0
			1105	712	206	183	4			

- Molecule 36 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	CN	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
36	DN	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 37 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	CO	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
37	DO	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	CP	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
38	DP	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 39 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
39	CQ	117	Total	C	N	O	0	0	0
			960	599	202	159			
39	DQ	117	Total	C	N	O	0	0	0
			960	599	202	159			

- Molecule 40 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	CR	98	Total	C	N	O	0	0	0
			771	486	154	131			
40	DR	98	Total	C	N	O	0	0	0
			771	486	154	131			

- Molecule 41 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	CS	137	Total	C	N	O	S	0	0	0
			1142	710	234	197	1			
41	DS	137	Total	C	N	O	S	0	0	0
			1142	710	234	197	1			

- Molecule 42 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	CT	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			
42	DT	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CT	32	ALA	PHE	conflict	UNP P60491
DT	32	ALA	PHE	conflict	UNP P60491

- Molecule 43 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	CU	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
43	DU	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 44 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	CW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			

- Molecule 45 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
45	CX	92	Total	C	N	O	0	0	0
			726	471	131	124			
45	DX	92	Total	C	N	O	0	0	0
			726	471	131	124			

- Molecule 46 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	CY	100	Total	C	N	O	S	0	0	0
			776	500	148	124	4			
46	DY	100	Total	C	N	O	S	0	0	0
			776	500	148	124	4			

- Molecule 47 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	CZ	176	Total	C	N	O	S	0	0	0
			1404	897	252	253	2			
47	DZ	176	Total	C	N	O	S	0	0	0
			1404	897	252	253	2			

- Molecule 48 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	Ca	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			
48	Da	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

- Molecule 49 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	CH	93	Total	C	N	O	S	0	0	0
			734	460	147	126	1			
49	DH	93	Total	C	N	O	S	0	0	0
			734	460	147	126	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DH	81	ARG	LYS	conflict	UNP P60494

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	CK	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			
50	DK	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			

- Molecule 51 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	CL	59	Total	C	N	O	S	0	0	0
			468	298	90	79	1			
51	DL	59	Total	C	N	O	S	0	0	0
			468	298	90	79	1			

- Molecule 52 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	C5	30	Total	C	N	O	S	0	0	0
			226	142	36	44	4			
52	D5	30	Total	C	N	O	S	0	0	0
			226	142	36	44	4			

- Molecule 53 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	C6	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
53	D6	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 54 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	C7	44	Total	C	N	O	S	0	0	0
			381	235	77	65	4			
54	D7	44	Total	C	N	O	S	0	0	0
			381	235	77	65	4			

- Molecule 55 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	C8	48	Total	C	N	O	S	0	0	0
			419	257	104	56	2			
55	D8	48	Total	C	N	O	S	0	0	0
			419	257	104	56	2			

- Molecule 56 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	C9	63	Total	C	N	O	S	0	0	0
			508	326	101	79	2			
56	D9	63	Total	C	N	O	S	0	0	0
			508	326	101	79	2			

- Molecule 57 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	C0	36	Total	C	N	O	S	0	0	0
			299	183	67	46	3			
57	D0	36	Total	C	N	O	S	0	0	0
			299	183	67	46	3			

- Molecule 58 is a RNA chain called 23S rRNA (2899-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
58	C1	2807	60459	26907	11311	19435	2806	0	0	0
58	D1	2807	60459	26907	11311	19435	2806	0	0	0

- Molecule 59 is a RNA chain called 5S rRNA (119-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
59	Cs	119	2551	1136	471	826	118	0	0	0
59	Ds	119	2551	1136	471	826	118	0	0	0

- Molecule 60 is a RNA chain called tRNA (5'-D(\*AP\*UP\*CP\*CP\*CP\*CP\*GP\*UP\*GP\*UP\*CP\*CP\*UP\*UP\*GP\*GP\*UP\*UP\*CP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
60	D2	20	416	186	65	146	19	0	0	0

- Molecule 61 is a RNA chain called tRNA (76-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
61	D4	76	1623	723	294	530	76	0	0	0

- Molecule 62 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
62	DA	190	1155	705	220	230	0	0	0

- Molecule 63 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
63	DW	113	896	563	176	155	2	0	0	0

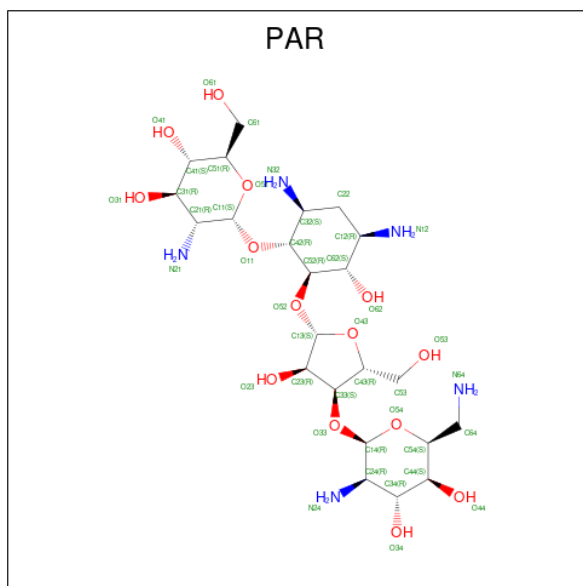
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DW	113	ALA	-	expression tag	UNP Q5SHP3

- Molecule 64 is a RNA chain called DNA (55-MER).

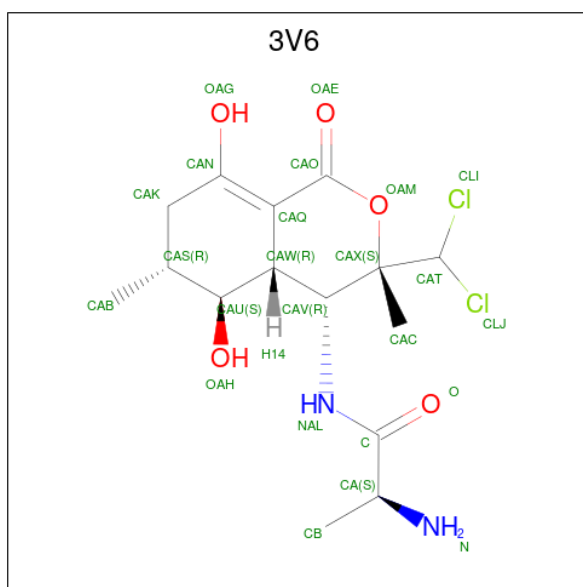
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
64	DV	55	1167	527	220	379	41	0	0	0

- Molecule 65 is PAROMOMYCIN (CCD ID: PAR) (formula:  $C_{23}H_{45}N_5O_{14}$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
65	Ab	1	42	23	5	14	0	0
65	Bb	1	42	23	5	14	0	0

- Molecule 66 is Bactobolin A (CCD ID: 3V6) (formula:  $C_{15}H_{22}Cl_2N_2O_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
66	C1	1	Total	C	Cl	N	O	0	0
			24	15	2	2	5		
66	D1	1	Total	C	Cl	N	O	0	0
			24	15	2	2	5		

- Molecule 67 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

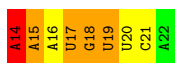
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
67	C1	1	Total	Mg	0	0
			1	1		
67	D1	1	Total	Mg	0	0
			1	1		

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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: mRNA

Chain A2: 



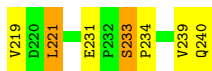
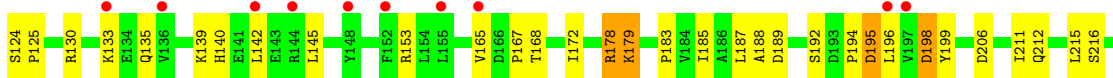
- Molecule 2: 30S ribosomal protein S2

Chain AA: 



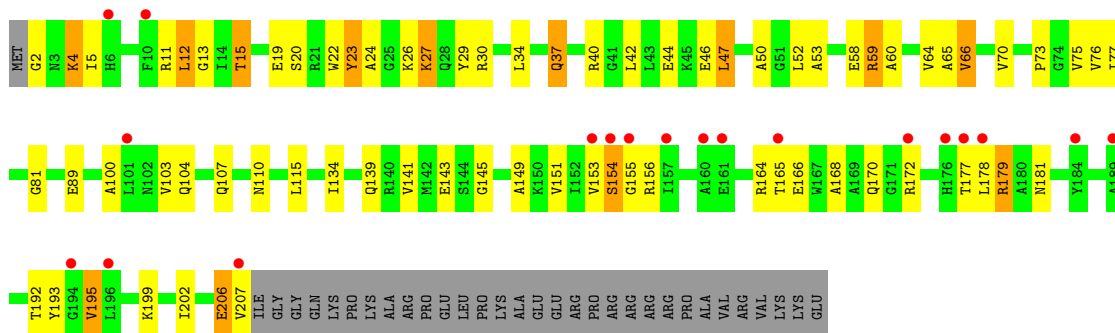
- Molecule 2: 30S ribosomal protein S2

Chain BA: 

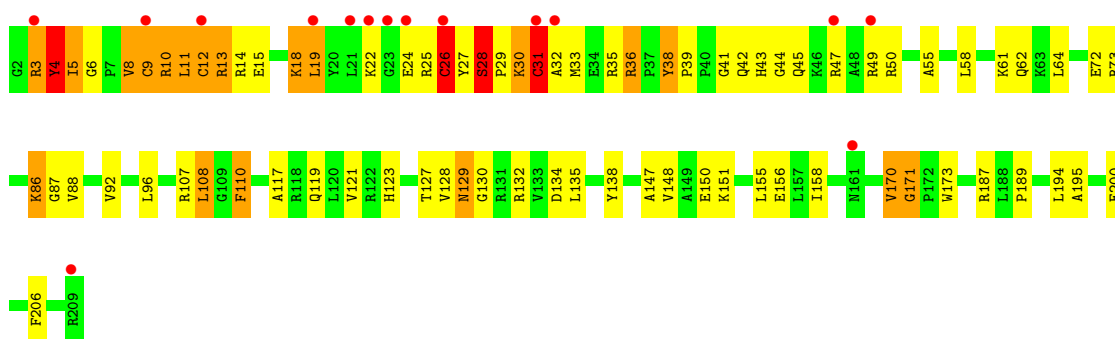


- Molecule 3: 30S ribosomal protein S3

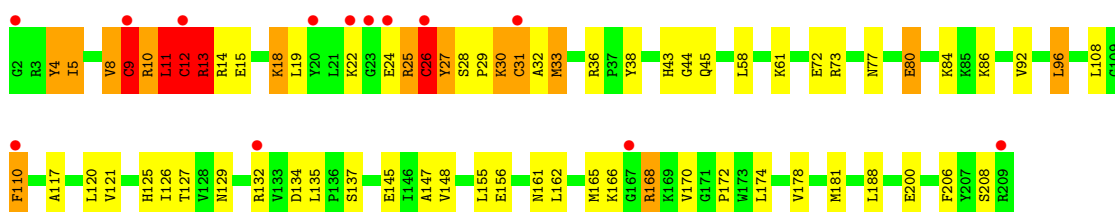
Chain AC: 



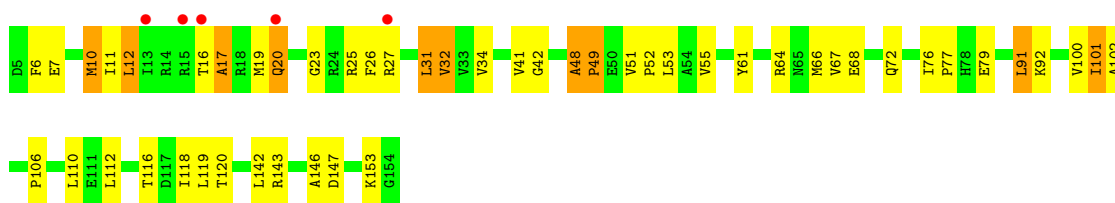
• Molecule 4: 30S ribosomal protein S4



• Molecule 4: 30S ribosomal protein S4

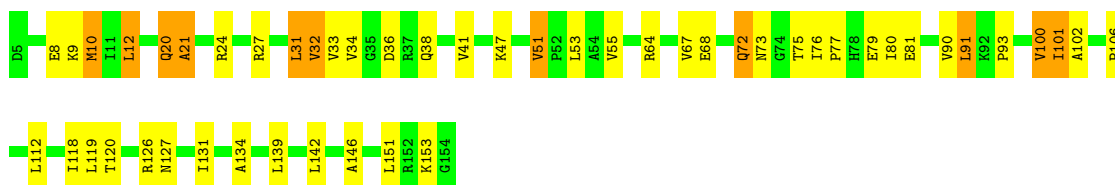


• Molecule 5: 30S ribosomal protein S5

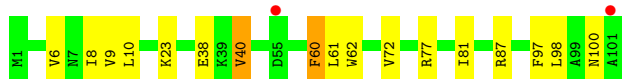
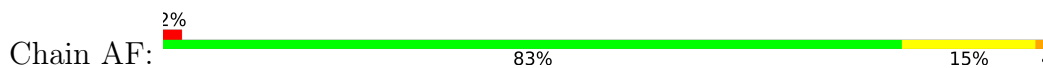


• Molecule 5: 30S ribosomal protein S5

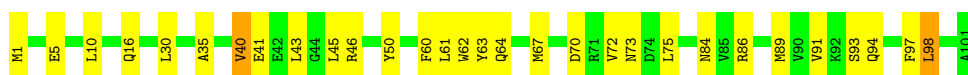




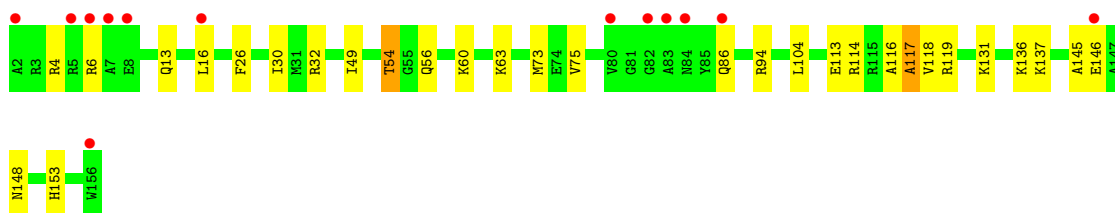
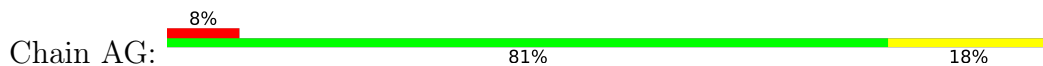
- Molecule 6: 30S ribosomal protein S6



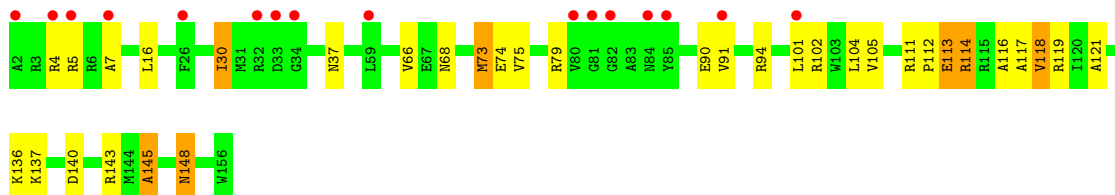
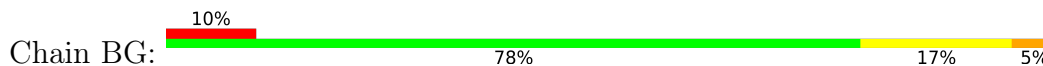
- Molecule 6: 30S ribosomal protein S6



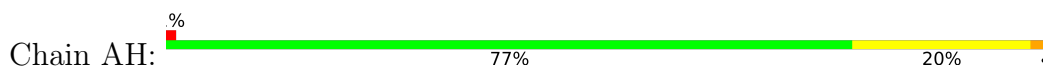
- Molecule 7: 30S ribosomal protein S7



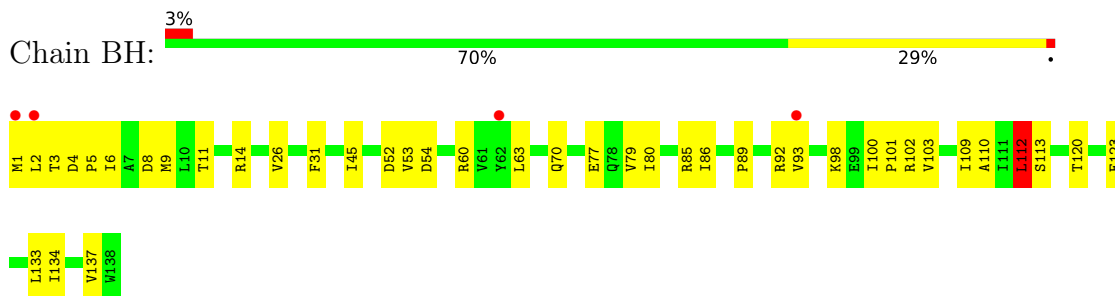
- Molecule 7: 30S ribosomal protein S7



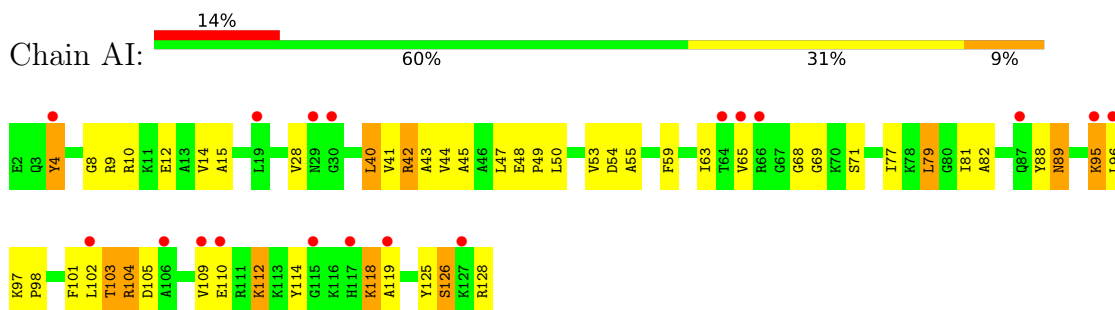
- Molecule 8: 30S ribosomal protein S8



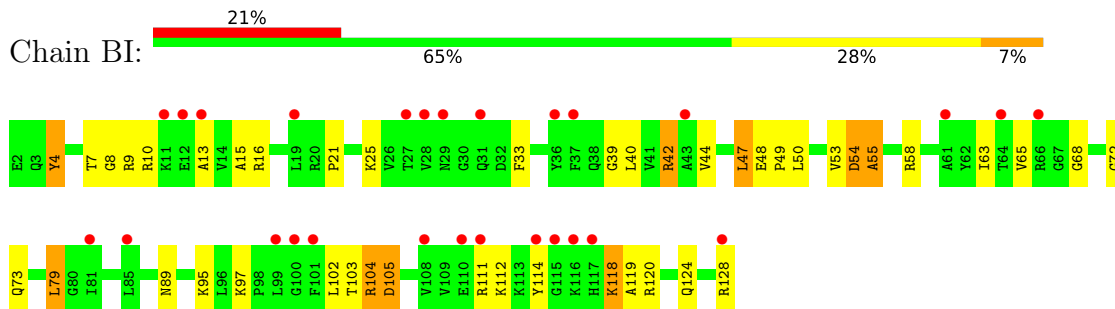
- Molecule 8: 30S ribosomal protein S8



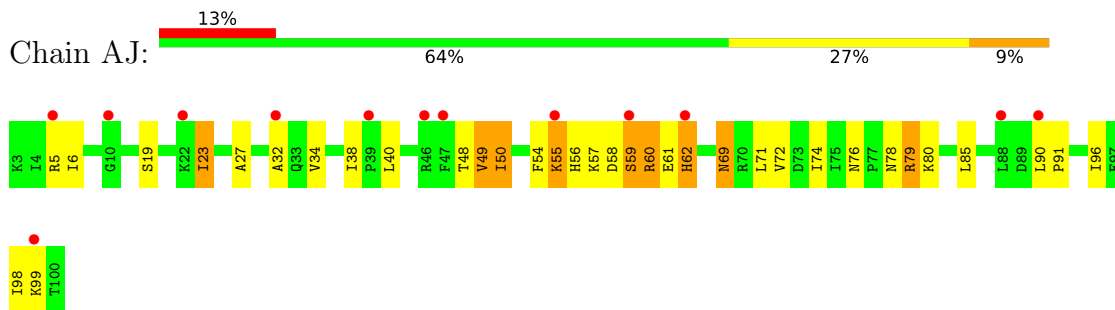
- Molecule 9: 30S ribosomal protein S9



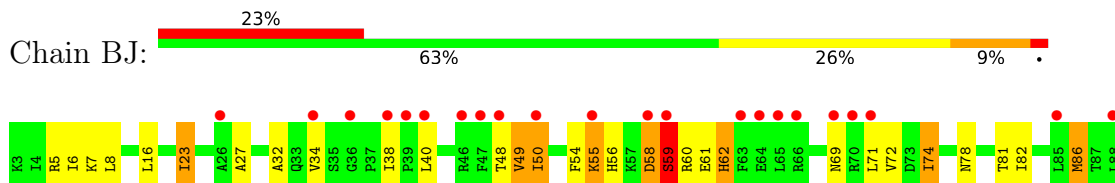
- Molecule 9: 30S ribosomal protein S9

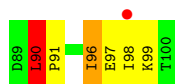


- Molecule 10: 30S ribosomal protein S10

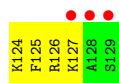


- Molecule 10: 30S ribosomal protein S10

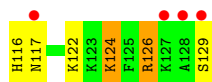
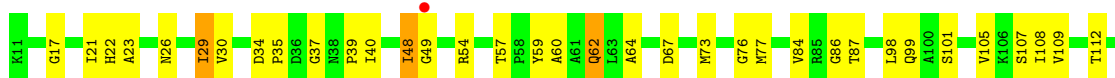




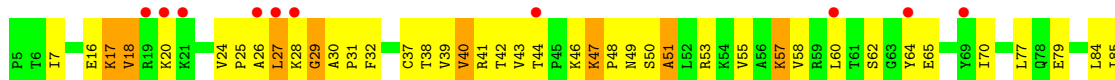
- Molecule 11: 30S ribosomal protein S11



- Molecule 11: 30S ribosomal protein S11



- Molecule 12: 30S ribosomal protein S12

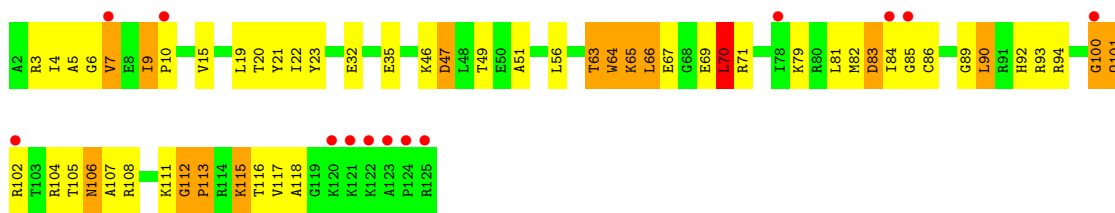


- Molecule 12: 30S ribosomal protein S12

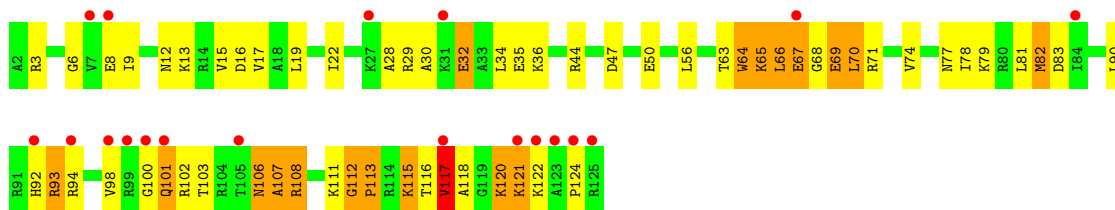


- Molecule 13: 30S ribosomal protein S13

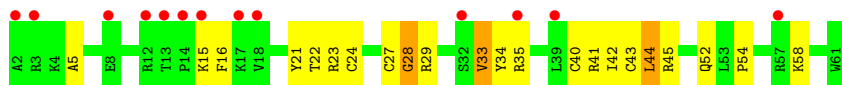




- Molecule 13: 30S ribosomal protein S13



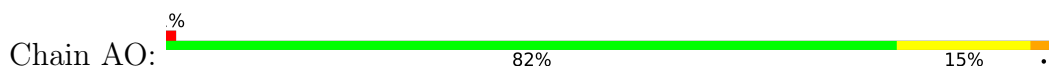
- Molecule 14: 30S ribosomal protein S14 type Z



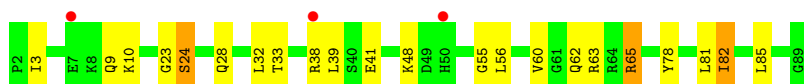
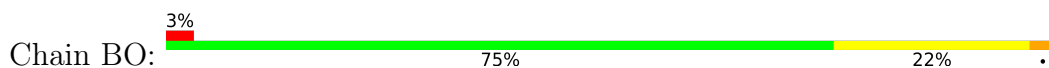
- Molecule 14: 30S ribosomal protein S14 type Z



- Molecule 15: 30S ribosomal protein S15

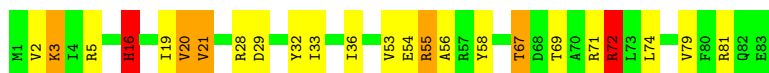


- Molecule 15: 30S ribosomal protein S15



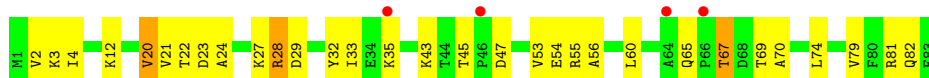
- Molecule 16: 30S ribosomal protein S16

Chain AP:  71% 20% 6%




• Molecule 16: 30S ribosomal protein S16

Chain BP:  5% 63% 34%



• Molecule 17: 30S ribosomal protein S17

Chain AR:  74% 25%



• Molecule 17: 30S ribosomal protein S17

Chain BR:  3% 67% 29%



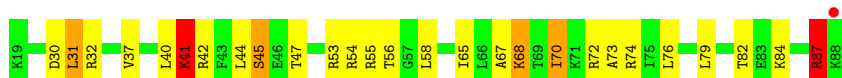
• Molecule 18: 30S ribosomal protein S18

Chain AS:  60% 31% 7%



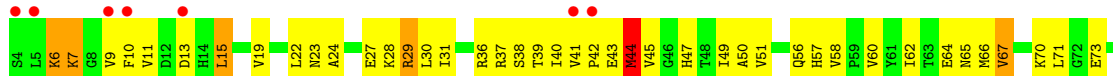
• Molecule 18: 30S ribosomal protein S18

Chain BS:  61% 30% 6%



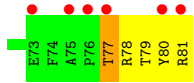
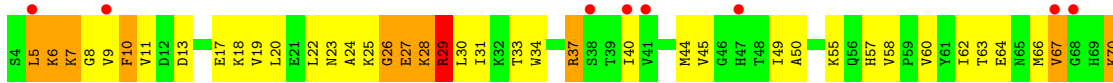
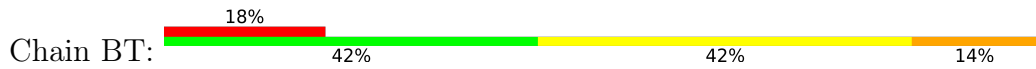
• Molecule 19: 30S ribosomal protein S19

Chain AT:  12% 44% 47% 8%

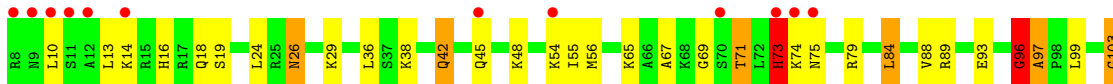




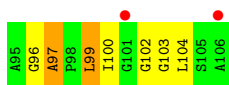
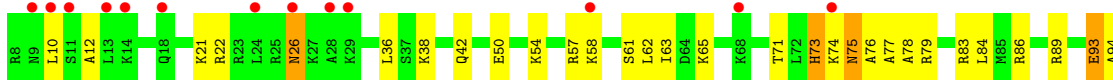
- Molecule 19: 30S ribosomal protein S19



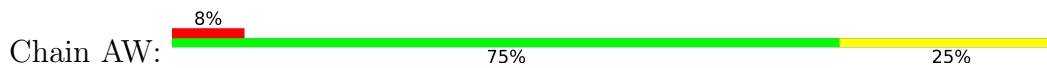
- Molecule 20: 30S ribosomal protein S20



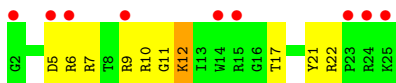
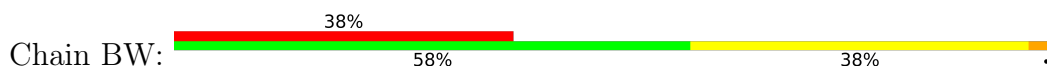
- Molecule 20: 30S ribosomal protein S20



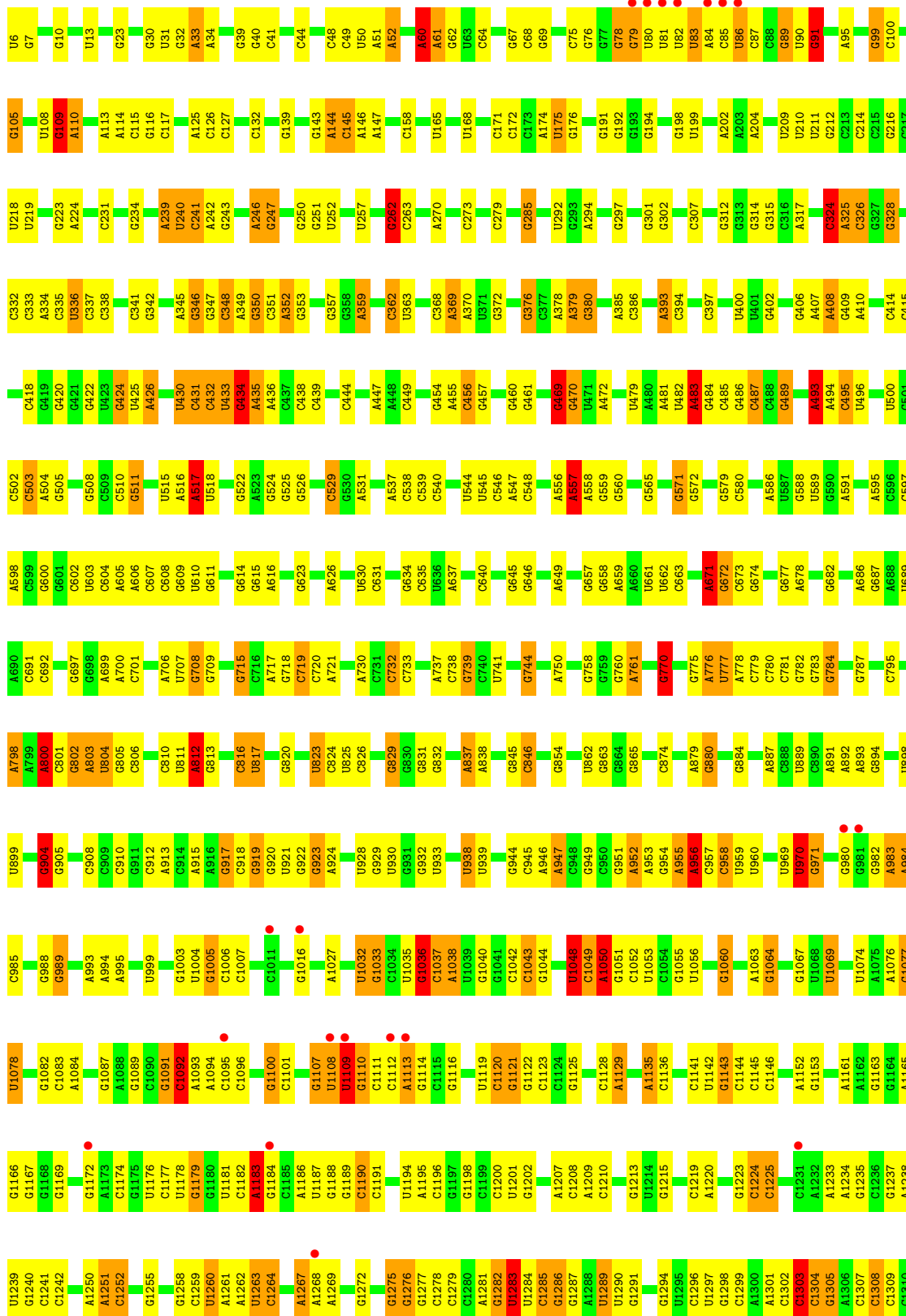
- Molecule 21: 30S ribosomal protein Thx

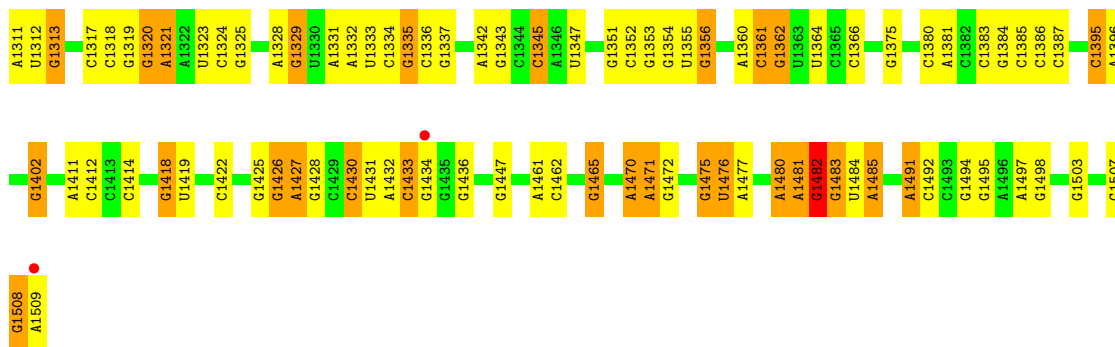


- Molecule 21: 30S ribosomal protein Thx

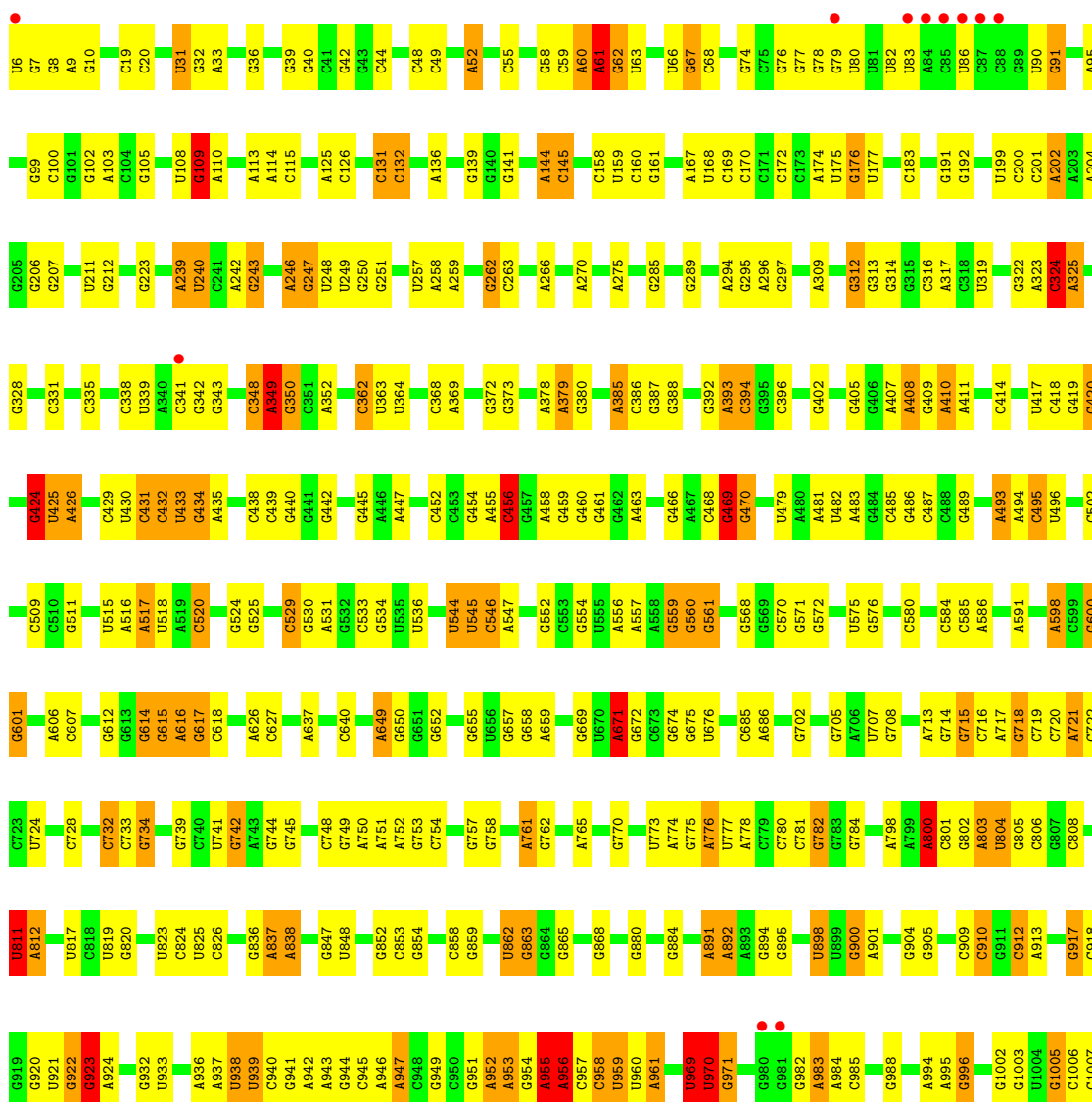


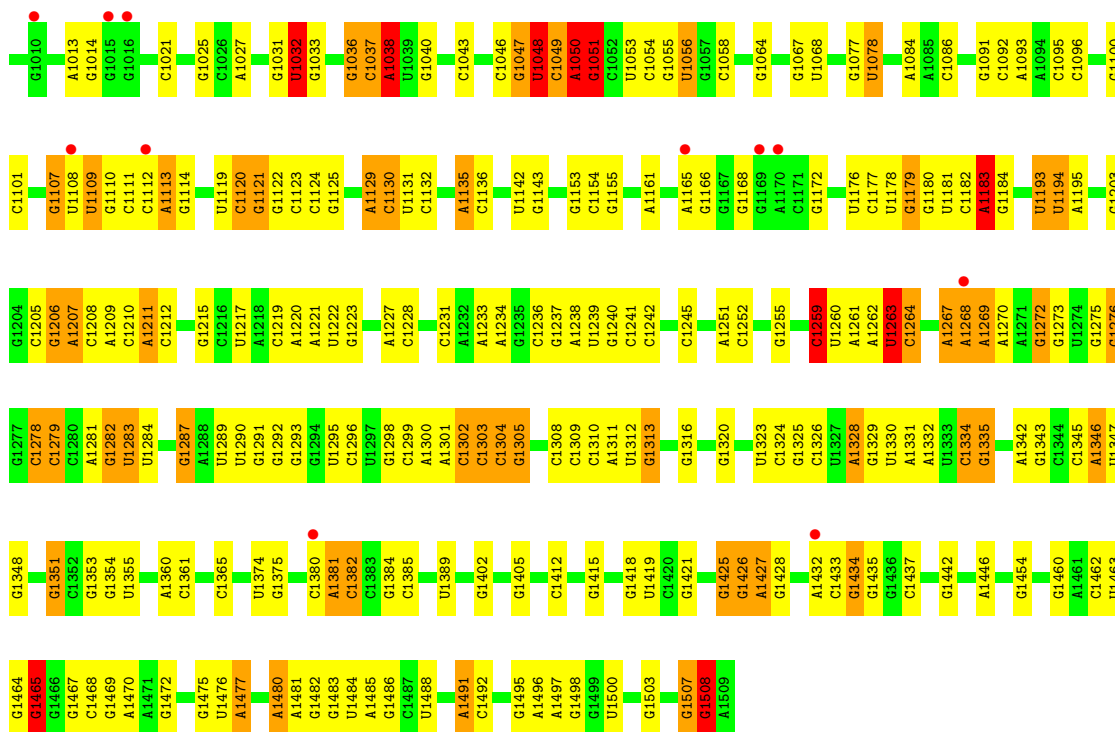
● Molecule 22: RNA (1504-MER)



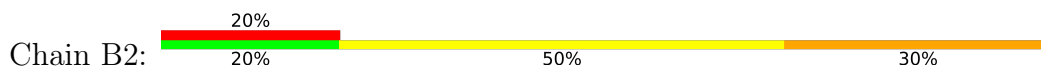


• Molecule 22: RNA (1504-MER)

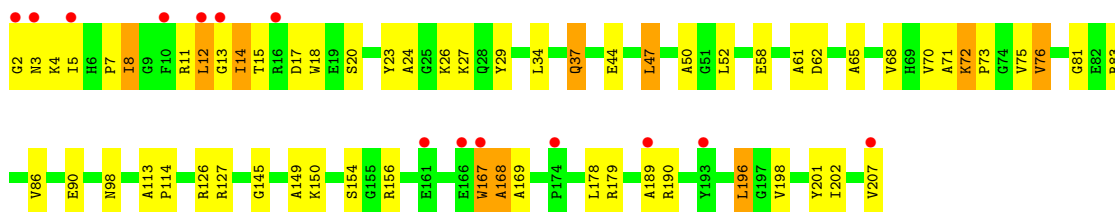




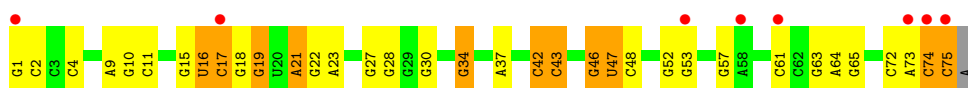
• Molecule 23: mRNA



• Molecule 24: 30S ribosomal protein S3

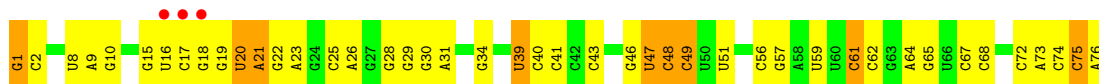


• Molecule 25: A site tNA, E site tNA

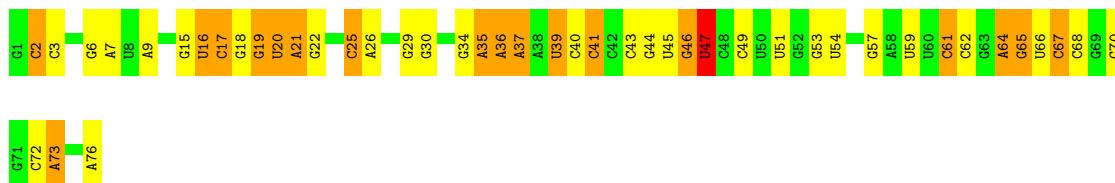


• Molecule 25: A site tNA, E site tNA

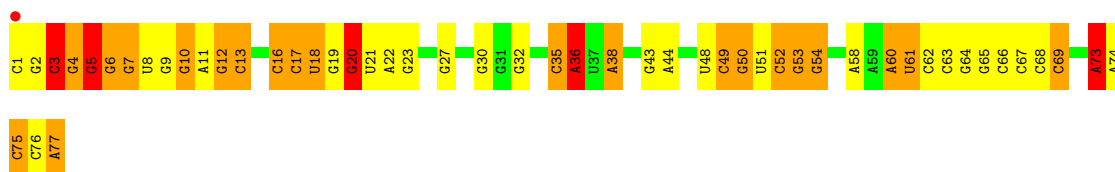




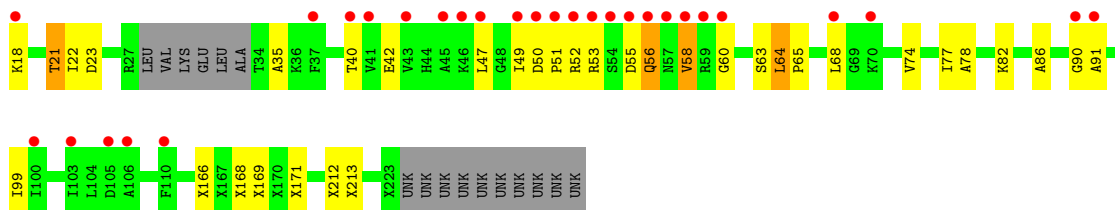
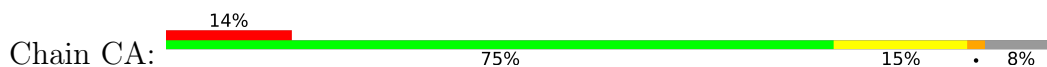
• Molecule 25: A site tNA, E site tNA



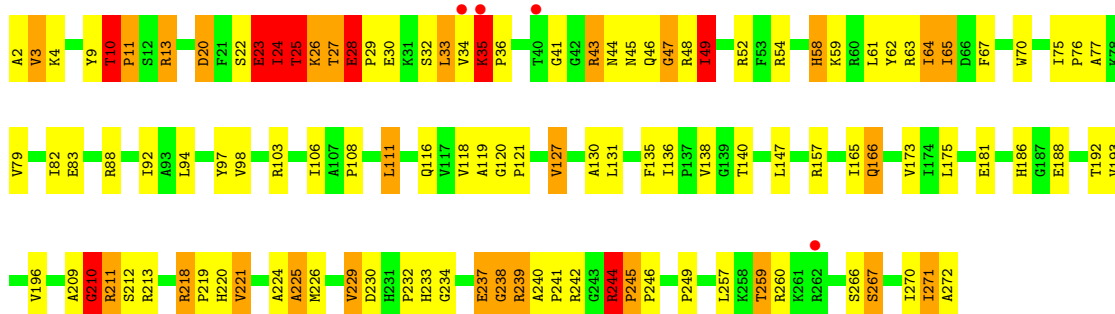
• Molecule 26: P site trNA



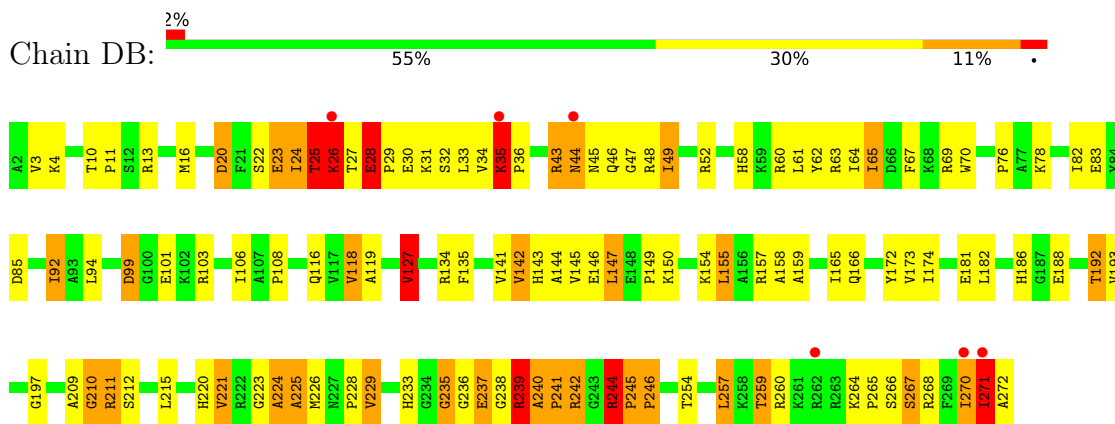
• Molecule 27: 50S ribosomal protein L1



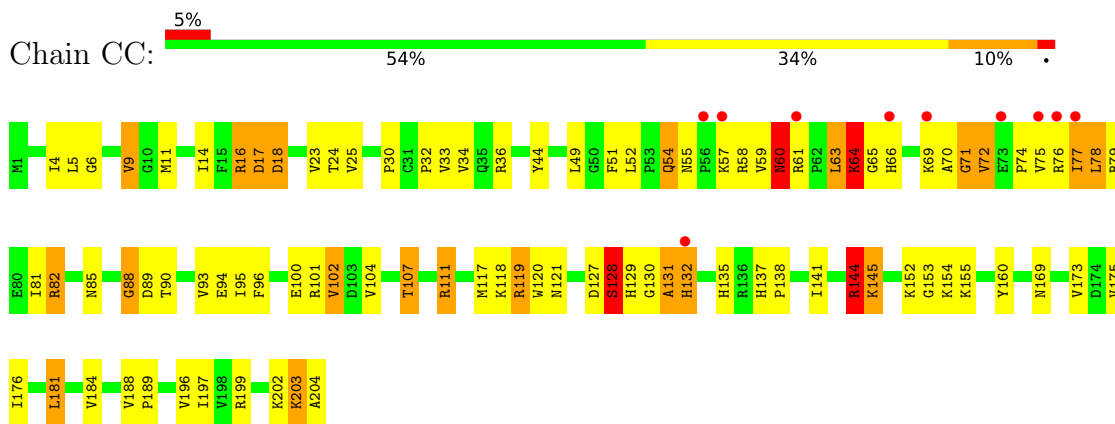
• Molecule 28: 50S ribosomal protein L2



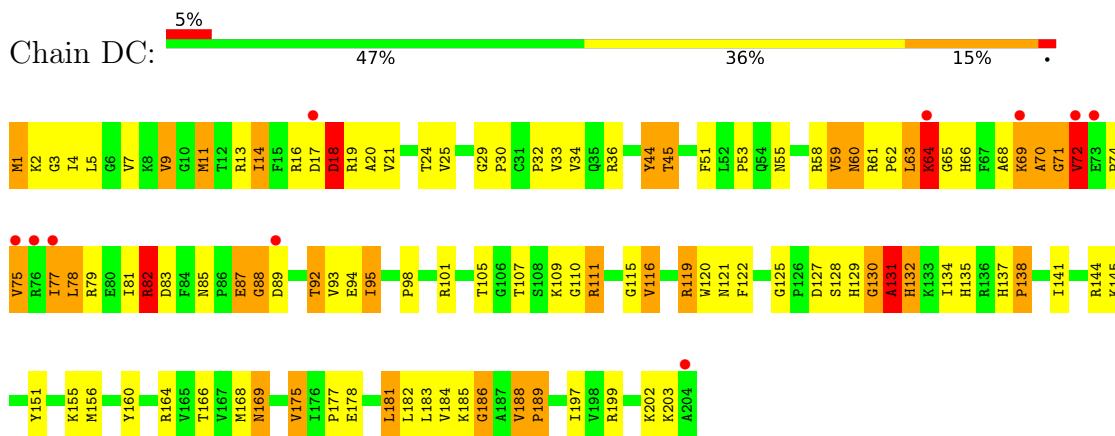
• Molecule 28: 50S ribosomal protein L2



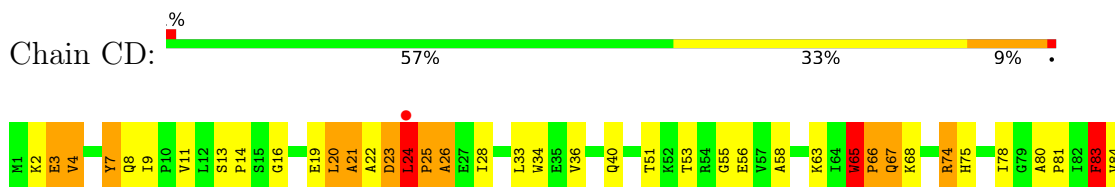
• Molecule 29: 50S ribosomal protein L3



• Molecule 29: 50S ribosomal protein L3

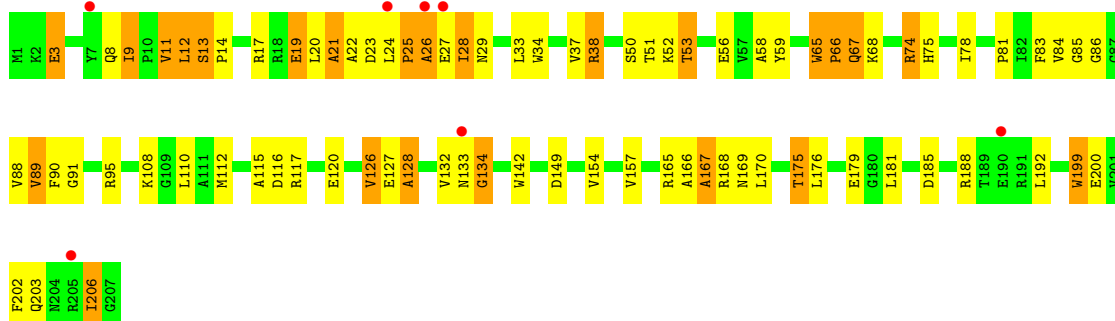


• Molecule 30: 50S ribosomal protein L4

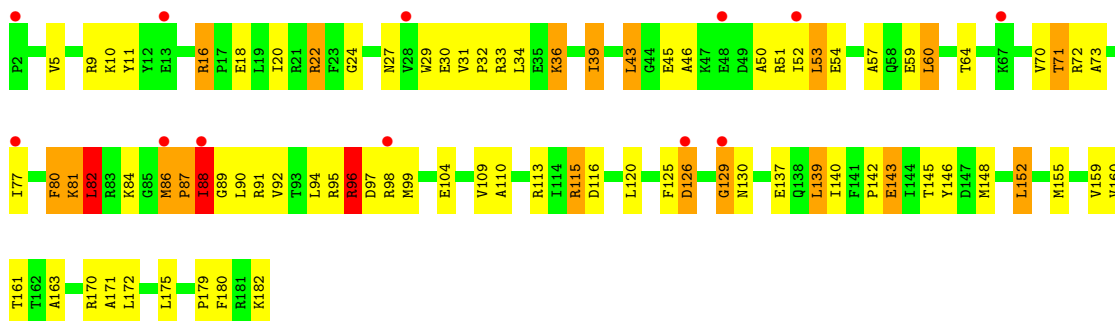




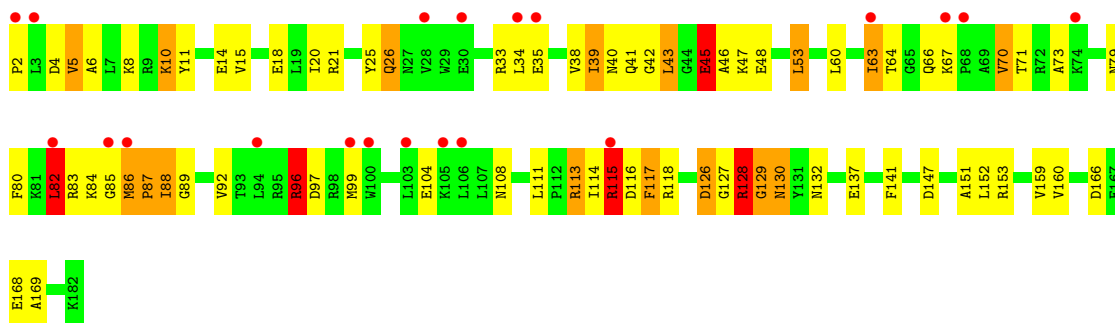
- Molecule 30: 50S ribosomal protein L4



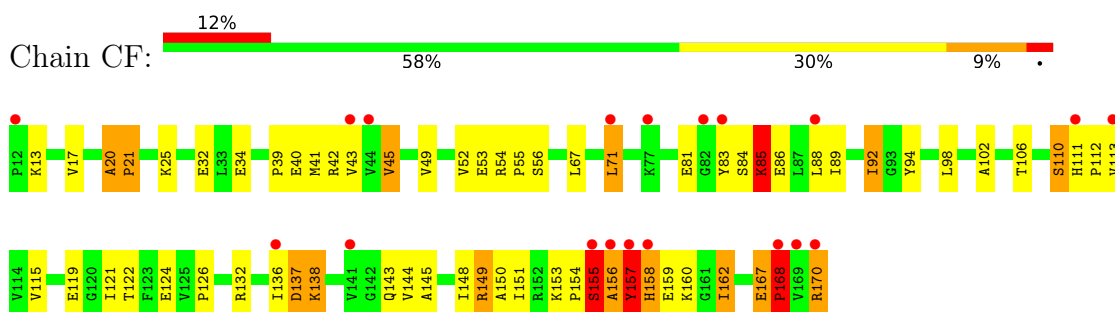
- Molecule 31: 50S ribosomal protein L5



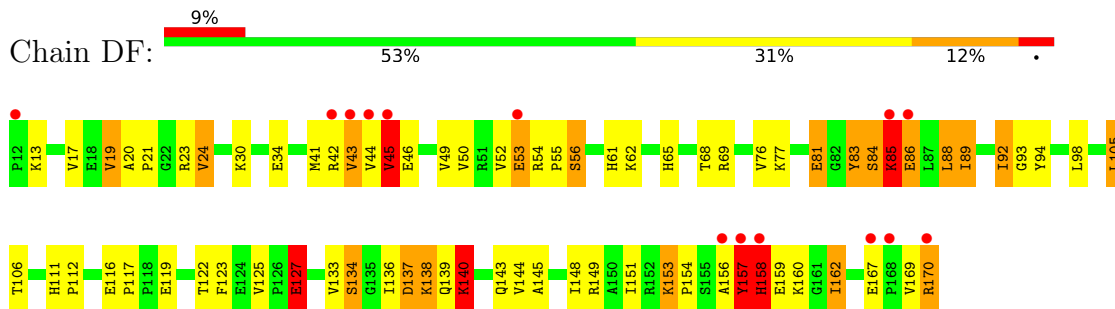
- Molecule 31: 50S ribosomal protein L5



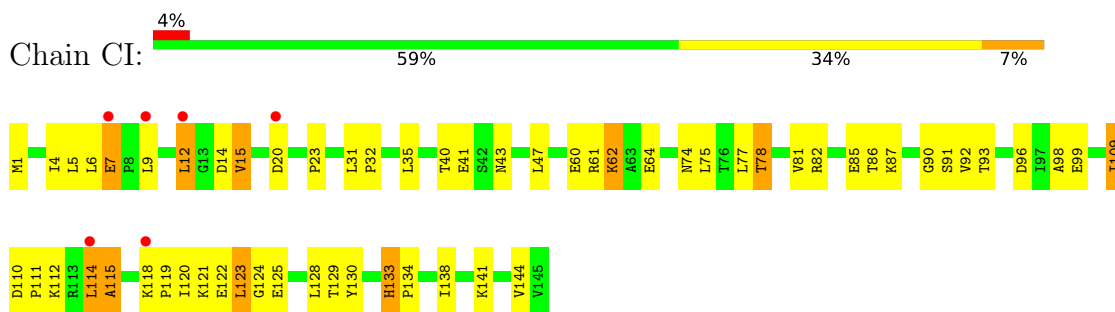
- Molecule 32: 50S ribosomal protein L6



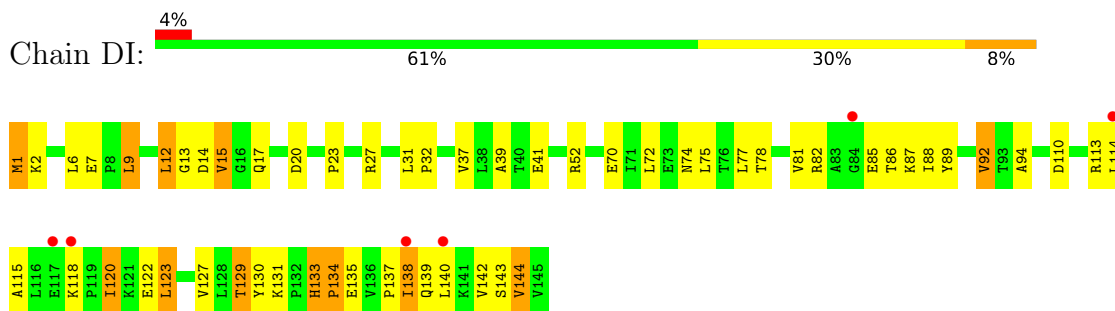
- Molecule 32: 50S ribosomal protein L6



- Molecule 33: 50S ribosomal protein L9



- Molecule 33: 50S ribosomal protein L9



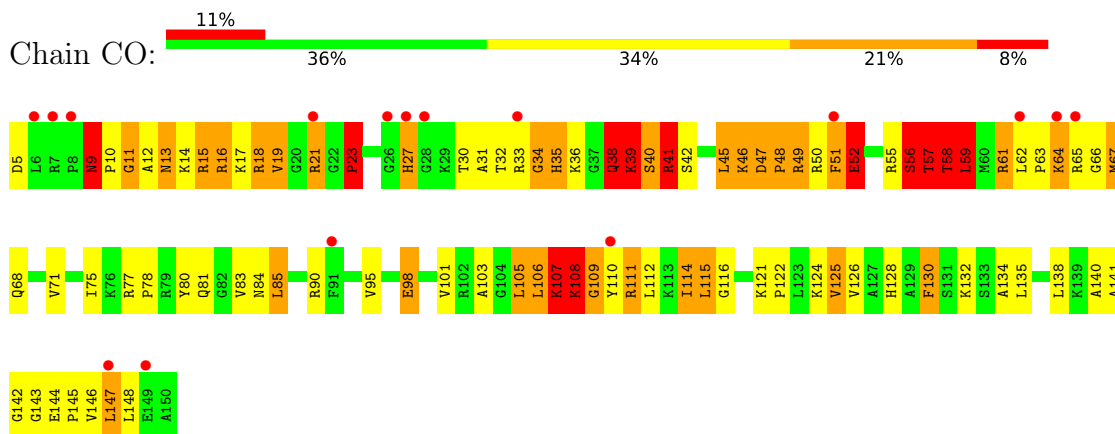
- Molecule 34: ribosomal L10 protein



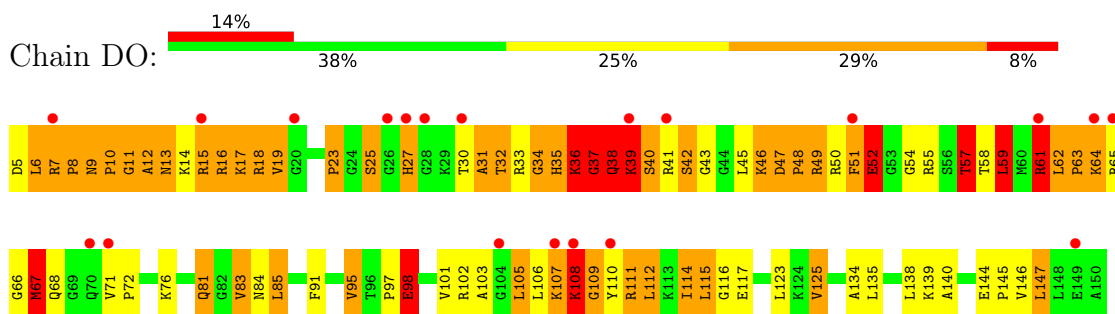
There are no outlier residues recorded for this chain.

- Molecule 34: ribosomal L10 protein

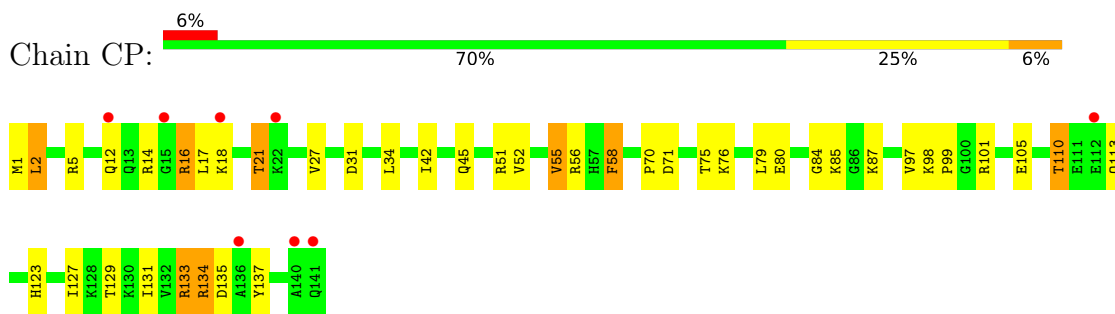




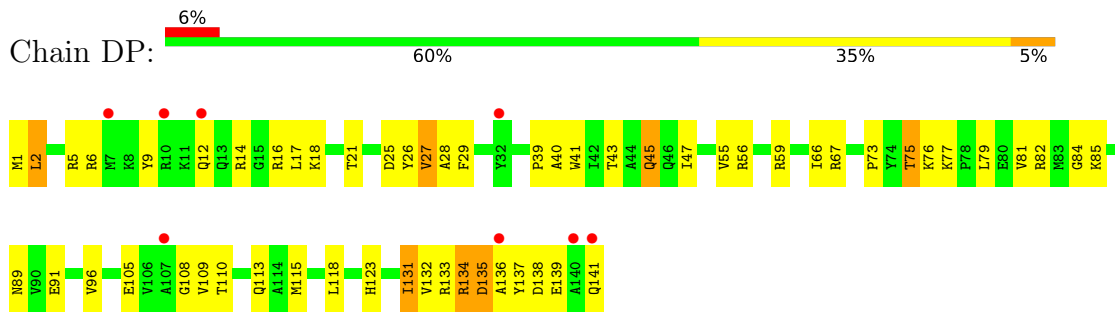
• Molecule 37: 50S ribosomal protein L15



• Molecule 38: 50S ribosomal protein L16



• Molecule 38: 50S ribosomal protein L16

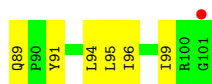


• Molecule 39: 50S ribosomal protein L17





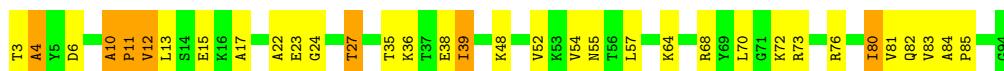




- Molecule 44: 50S ribosomal protein L22



- Molecule 45: 50S ribosomal protein L23



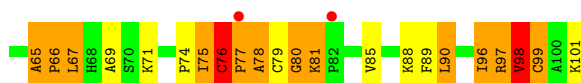
- Molecule 45: 50S ribosomal protein L23



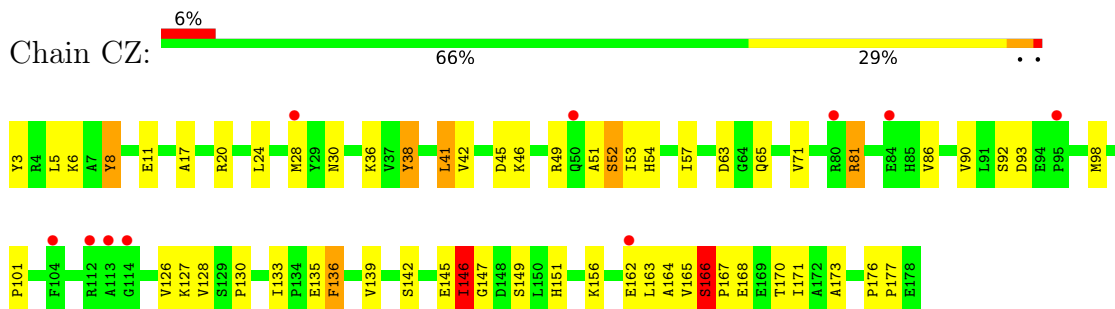
- Molecule 46: 50S ribosomal protein L24



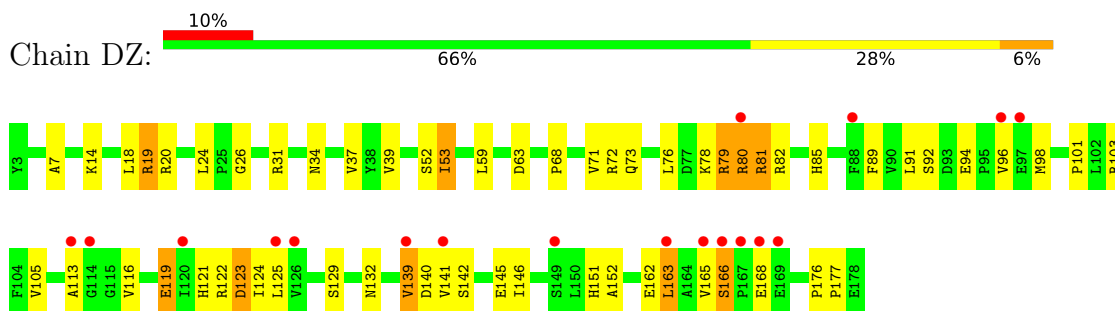
- Molecule 46: 50S ribosomal protein L24



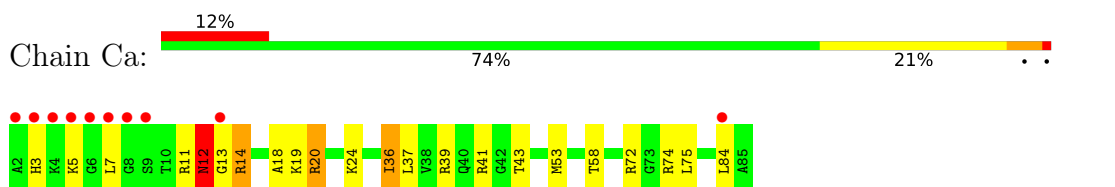
- Molecule 47: 50S ribosomal protein L25



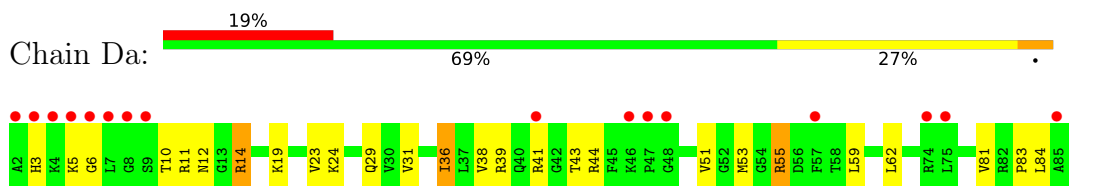
- Molecule 47: 50S ribosomal protein L25



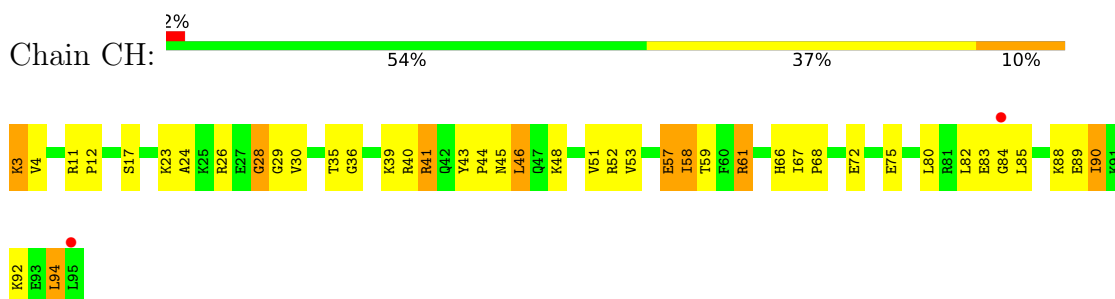
- Molecule 48: 50S ribosomal protein L27



- Molecule 48: 50S ribosomal protein L27

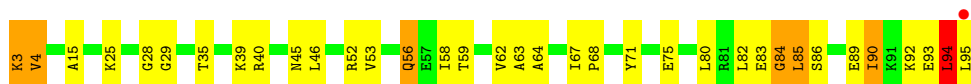


- Molecule 49: 50S ribosomal protein L28



- Molecule 49: 50S ribosomal protein L28

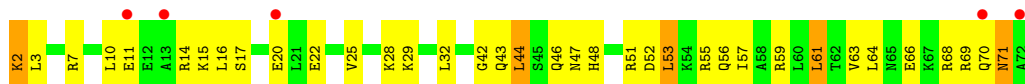




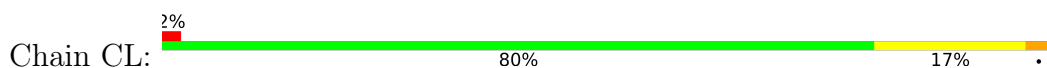
- Molecule 50: 50S ribosomal protein L29



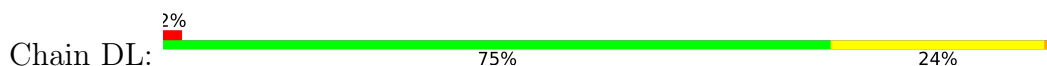
- Molecule 50: 50S ribosomal protein L29



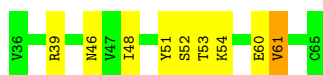
- Molecule 51: 50S ribosomal protein L30



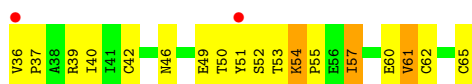
- Molecule 51: 50S ribosomal protein L30



- Molecule 52: 50S ribosomal protein L31



- Molecule 52: 50S ribosomal protein L31



- Molecule 53: 50S ribosomal protein L32



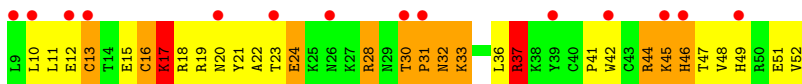
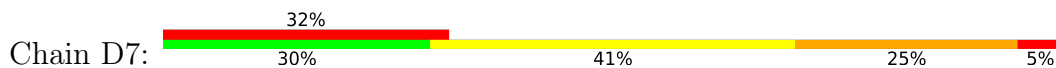
- Molecule 53: 50S ribosomal protein L32



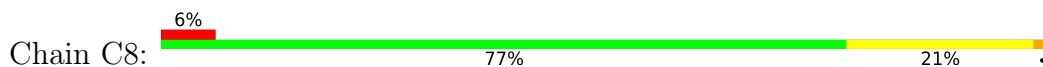
- Molecule 54: 50S ribosomal protein L33



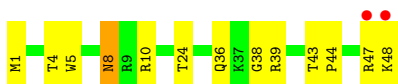
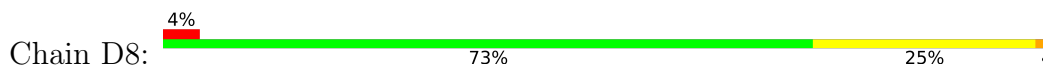
- Molecule 54: 50S ribosomal protein L33



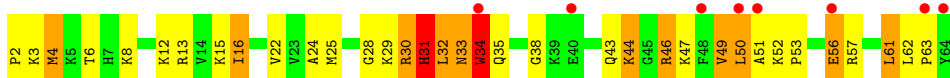
- Molecule 55: 50S ribosomal protein L34



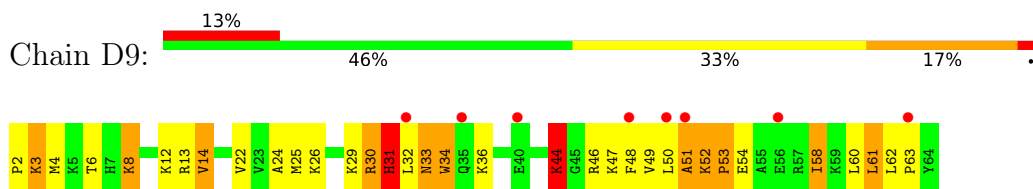
- Molecule 55: 50S ribosomal protein L34



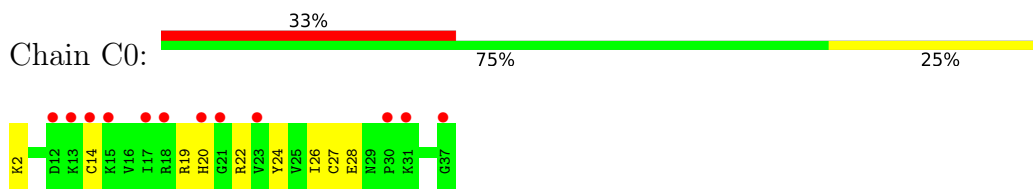
- Molecule 56: 50S ribosomal protein L35



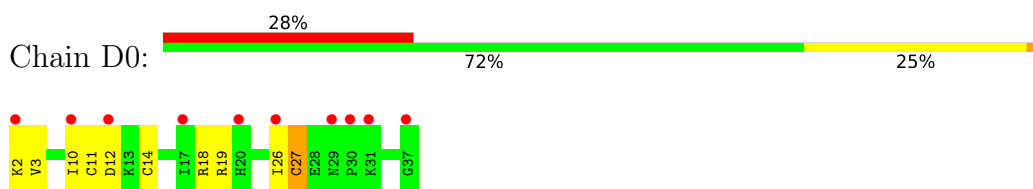
• Molecule 56: 50S ribosomal protein L35



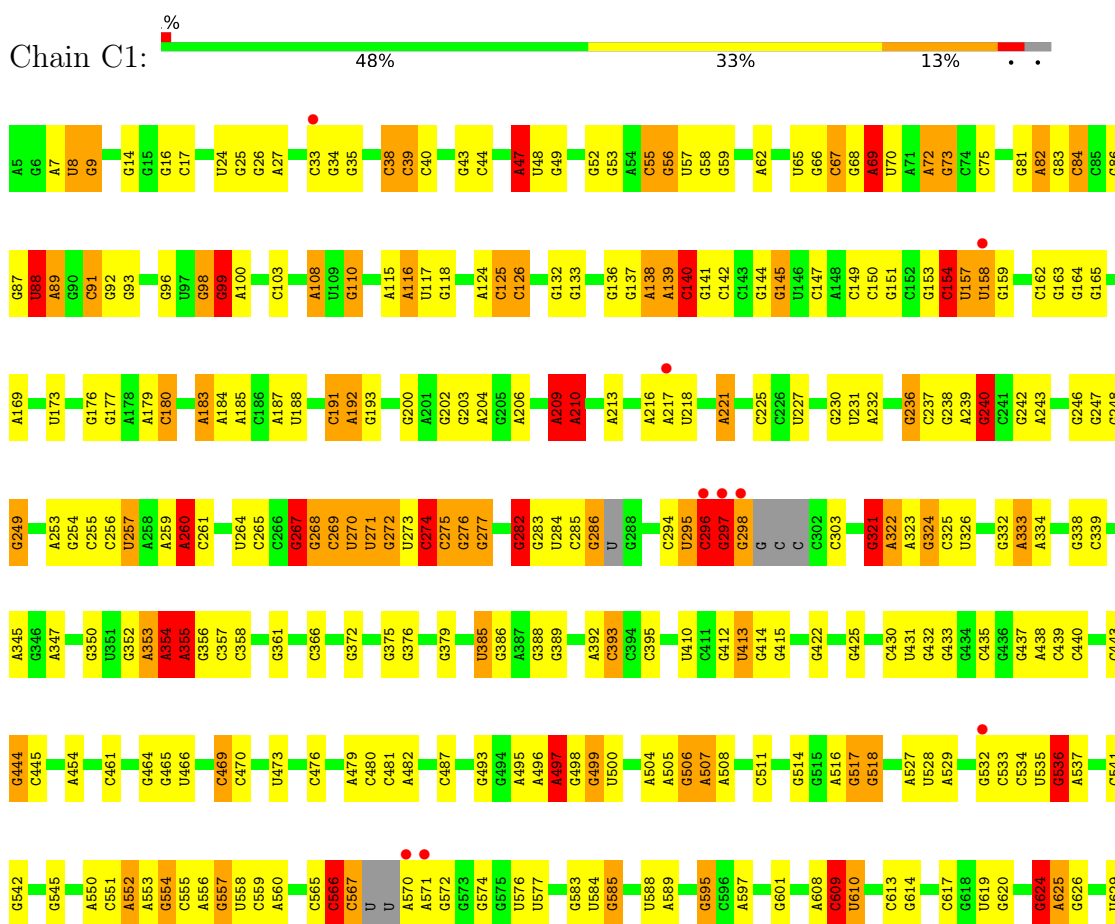
• Molecule 57: 50S ribosomal protein L36



• Molecule 57: 50S ribosomal protein L36

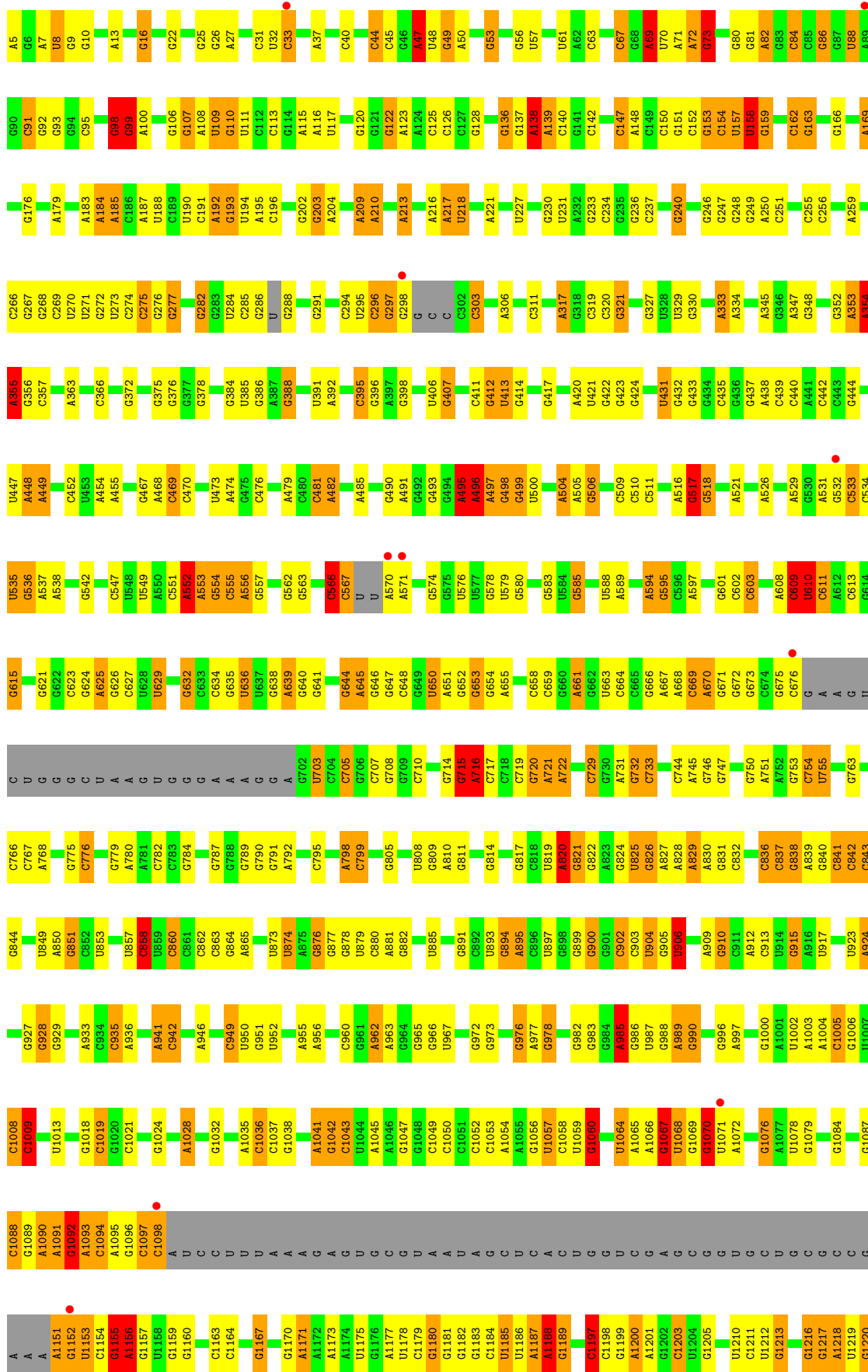


• Molecule 58: 23S rRNA (2899-MER)

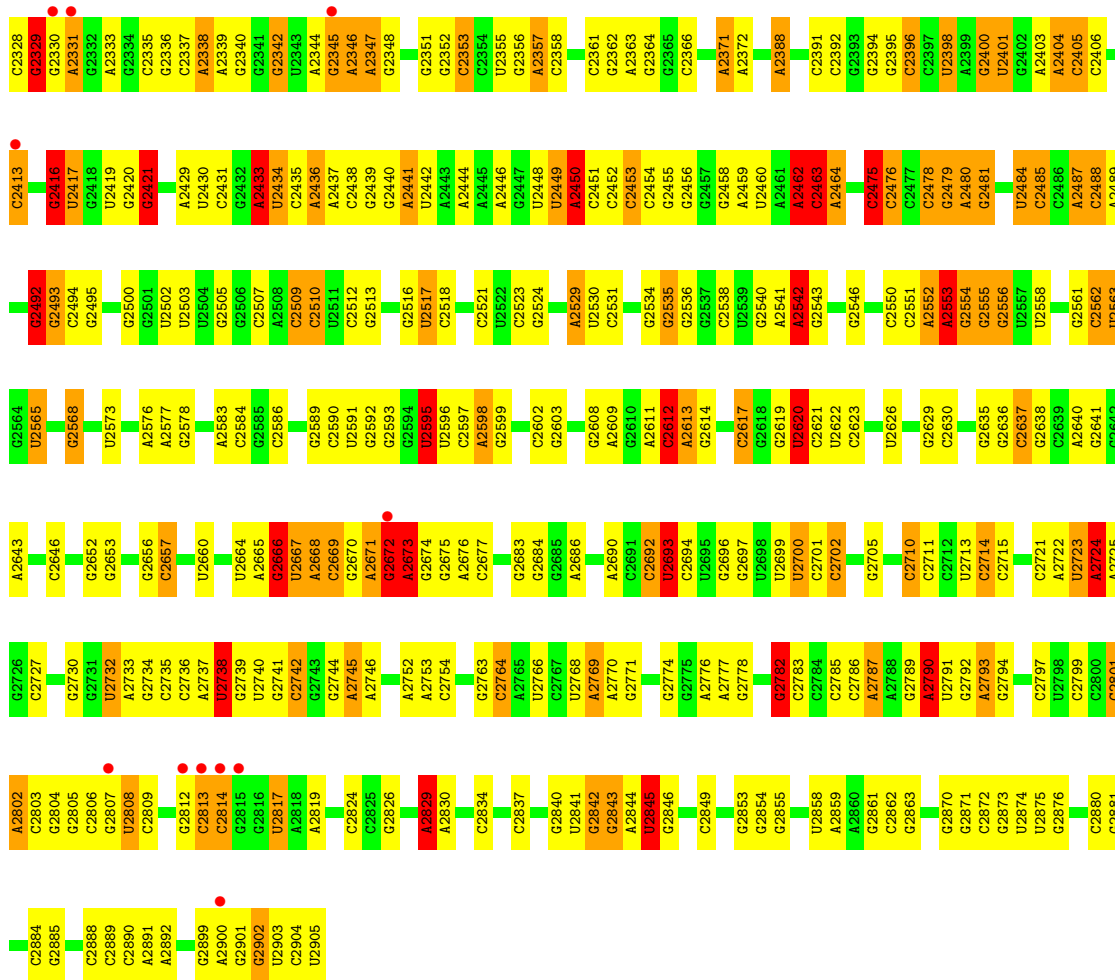




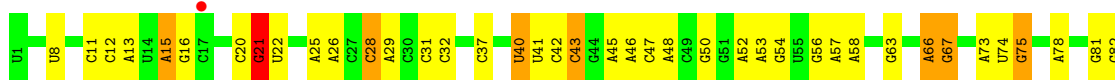




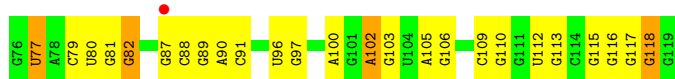
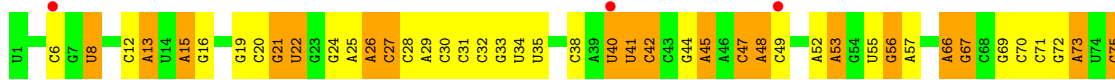
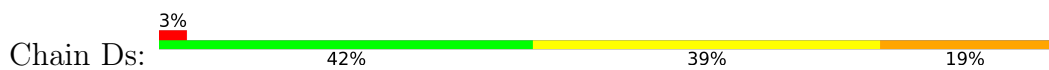
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G2267	C2185	G2104	G2030	G1950	C1873	C1801	C1703	A1625	C1546	G1474	G1393	A1312	C1223
G2268	G2186	G2107	G2031	G1951	C1874	G1802	C1704	G1627	U1547	G1475	A1394	A1313	C1224
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C2273	C2198	U2113	U2043	U1881	G1880	U1810	U1719	C1632	G1403	G1486	A1323	A1319	U1232
C2274	C2199	G2114	A2054	U1882	U1881	A1810	G1720	C1633	A1555	G1487	A1233	A1320	U1233
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A2299	G2226	U2143	G2073	G1989	C1907	G1843	A1746	C1662	A	G1515	G1434	C1351	C1265
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C2314	G2243	C2161	C2088	C2009	G1925	A1860	G1775	A1683	G1605	G1533	C1453	C1378	U1294
C2315	G2244	C2162	U2089	G2010	C1926	G1861	G1776	A1684	G1606	U1534	G1459	G1378	G1295
C2316	G2245	C2163	G2090	G2011	G1927	U1885	G1777	C1884	U1685	A1535	U1460	A1381	G1298
C2317	G2246	G2168	G2091	C2011	G1927	C1862	A1778	U1686	U1685	A1536	U1461	A1382	U1299
C2318	G2249	G2169	A2092	U2012	U1933	U1863	A1779	C1886	A1612	G1537	C1462	G1382	A1298
C2319	G2250	G2169	G2093	G2013	A1934	U1864	G1780	C1886	A1613	G1538	C1463	G1383	A1299
C2320	C2251	G2170	G2093	U2014	C1935	G1865	G1780	G1691	A1614	G1539	C1464	G1384	U1300
C2321	U2097	G2178	U2097	C2017	U1936	C1867	G1783	G1692	A1615	A1540	U1465	U1385	U1300
C2322	A2098	A2178	A2098	G2018	U1937	C1868	C1784	G1693	A1616	A1541	U1466	G1389	G1301
C2323	G2254	G2179	G2254	G2018	U1938	C1869	A1785	C1694	C1621	U1542	G1468	G1389	G1301
C2324	G2255	G2180	G2257	C2027	U1938	G1870	A1792	A1698	U1622	C1543	G1468	G1390	G1309



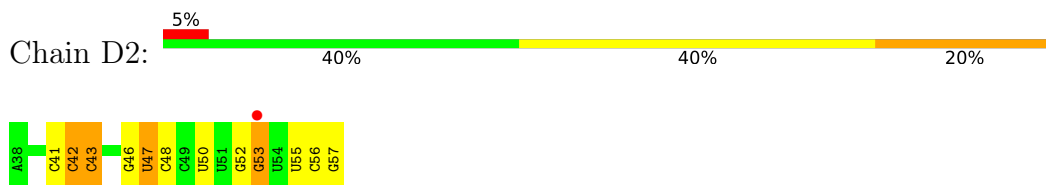
• Molecule 59: 5S rRNA (119-MER)



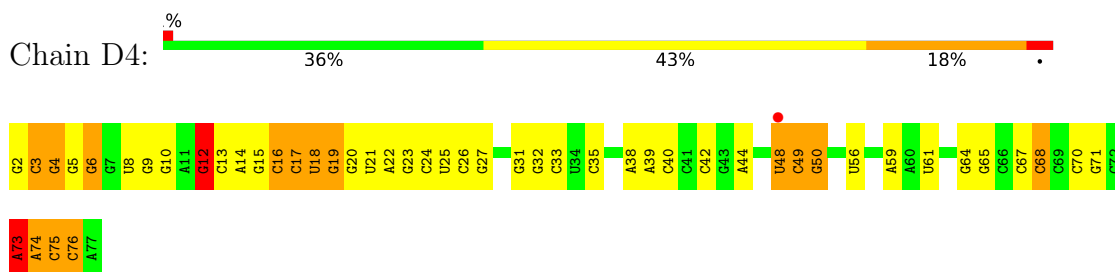
• Molecule 59: 5S rRNA (119-MER)



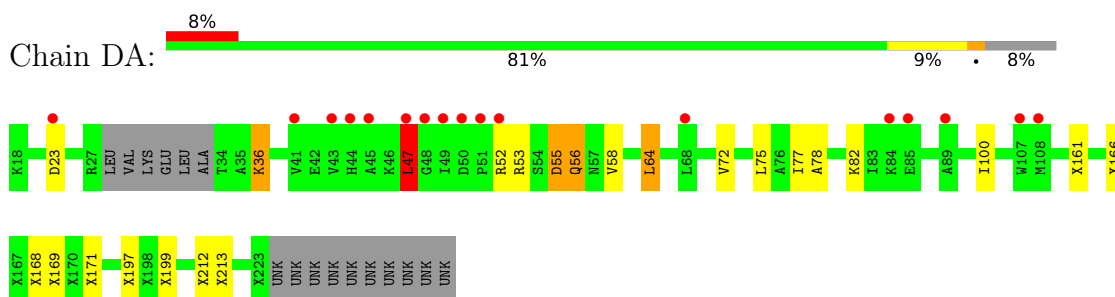
- Molecule 60: tRNA (5'-D(\*AP\*UP\*CP\*CP\*CP\*CP\*GP\*UP\*GP\*UP\*CP\*CP\*UP\*UP\*GP\*GP\*UP\*UP\*CP\*G)-3')



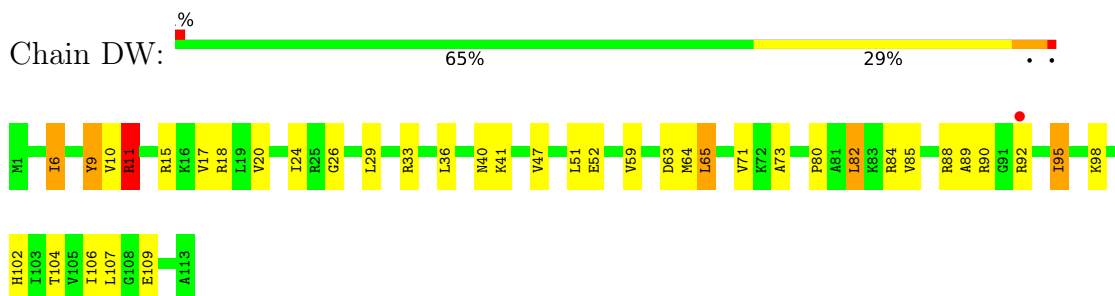
- Molecule 61: tRNA (76-MER)



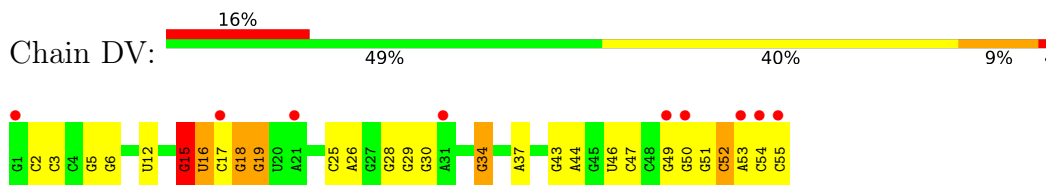
- Molecule 62: 50S ribosomal protein L1



- Molecule 63: 50S ribosomal protein L22



- Molecule 64: DNA (55-MER)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	214.21Å 457.45Å 639.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.91 – 3.40 49.91 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.5 (49.91-3.40) 98.5 (49.91-3.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.28	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.46 (at 3.40Å)	Xtrriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.204 , 0.241 0.208 , 0.241	Depositor DCC
$R_{free}$ test set	42005 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	74.2	Xtrriage
Anisotropy	0.256	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 68.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	295910	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.91% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: PAR, 3V6, MG

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	A2	0.48	0/192	1.08	1/297 (0.3%)
2	AA	0.73	0/1936	0.99	7/2609 (0.3%)
2	BA	0.71	0/1936	0.92	0/2609
3	AC	0.89	0/1636	1.05	2/2205 (0.1%)
4	AD	0.90	4/1733 (0.2%)	1.12	13/2318 (0.6%)
4	BD	0.95	11/1733 (0.6%)	1.19	16/2318 (0.7%)
5	AE	0.80	0/1163	1.04	5/1564 (0.3%)
5	BE	0.73	0/1163	0.98	3/1564 (0.2%)
6	AF	0.73	0/856	0.97	2/1154 (0.2%)
6	BF	0.80	0/856	1.00	1/1154 (0.1%)
7	AG	0.71	0/1276	0.99	3/1709 (0.2%)
7	BG	0.78	0/1276	1.03	3/1709 (0.2%)
8	AH	0.74	0/1136	0.99	3/1527 (0.2%)
8	BH	0.72	0/1136	0.98	3/1527 (0.2%)
9	AI	0.80	0/1029	1.03	1/1378 (0.1%)
9	BI	0.78	0/1029	1.00	3/1378 (0.2%)
10	AJ	0.86	0/808	1.03	2/1085 (0.2%)
10	BJ	0.92	1/808 (0.1%)	1.00	0/1085
11	AK	0.83	0/900	1.12	5/1213 (0.4%)
11	BK	0.78	0/900	1.06	1/1213 (0.1%)
12	AL	0.90	0/987	1.17	7/1320 (0.5%)
12	BL	0.92	1/987 (0.1%)	1.13	4/1320 (0.3%)
13	AM	0.82	0/999	1.16	8/1336 (0.6%)
13	BM	0.87	0/999	1.13	5/1336 (0.4%)
14	AN	0.81	0/501	1.06	1/664 (0.2%)
14	BN	0.92	1/501 (0.2%)	1.10	1/664 (0.2%)
15	AO	0.71	0/745	0.90	0/992
15	BO	0.73	0/745	1.04	0/992
16	AP	0.79	0/717	1.01	3/963 (0.3%)
16	BP	0.79	0/717	1.01	1/963 (0.1%)
17	AR	0.75	0/837	1.03	0/1117
17	BR	0.67	0/837	0.94	0/1117

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
18	AS	0.74	0/579	0.92	1/768 (0.1%)
18	BS	0.76	0/579	1.01	0/768
19	AT	0.85	0/643	1.04	0/865
19	BT	0.81	0/643	1.01	0/865
20	AU	0.77	0/765	1.06	1/1007 (0.1%)
20	BU	0.71	0/765	1.06	3/1007 (0.3%)
21	AW	0.83	0/213	1.04	1/277 (0.4%)
21	BW	0.87	0/213	1.08	0/277
22	Ab	0.52	1/36190 (0.0%)	0.98	180/56486 (0.3%)
22	Bb	0.52	1/36190 (0.0%)	0.97	148/56486 (0.3%)
23	B2	0.44	0/216	1.03	1/334 (0.3%)
24	BC	0.79	0/1637	0.97	3/2205 (0.1%)
25	C2	0.44	0/1784	0.79	0/2780
25	C3	0.47	0/1809	0.92	4/2819 (0.1%)
25	D3	0.46	0/1809	0.88	2/2819 (0.1%)
26	C4	0.52	0/1832	1.05	15/2855 (0.5%)
27	CA	0.90	0/646	1.00	2/869 (0.2%)
28	CB	0.98	4/2155 (0.2%)	1.21	10/2905 (0.3%)
28	DB	1.09	4/2155 (0.2%)	1.32	16/2905 (0.6%)
29	CC	1.01	5/1597 (0.3%)	1.20	8/2153 (0.4%)
29	DC	1.03	3/1597 (0.2%)	1.24	9/2153 (0.4%)
30	CD	0.90	0/1659	1.19	8/2244 (0.4%)
30	DD	0.94	0/1659	1.25	9/2244 (0.4%)
31	CE	0.82	0/1499	1.08	7/2016 (0.3%)
31	DE	0.83	0/1499	1.03	3/2016 (0.1%)
32	CF	0.87	0/1246	1.12	8/1682 (0.5%)
32	DF	0.97	1/1246 (0.1%)	1.24	9/1682 (0.5%)
33	CI	0.88	0/1147	1.07	2/1551 (0.1%)
33	DI	0.87	2/1147 (0.2%)	1.04	2/1551 (0.1%)
35	CM	0.85	0/1132	1.09	5/1525 (0.3%)
35	DM	0.88	0/1132	1.12	4/1525 (0.3%)
36	CN	0.84	0/943	1.09	3/1269 (0.2%)
36	DN	0.90	0/943	1.15	3/1269 (0.2%)
37	CO	1.12	4/1131 (0.4%)	1.46	17/1504 (1.1%)
37	DO	1.22	8/1131 (0.7%)	1.52	16/1504 (1.1%)
38	CP	0.83	1/1143 (0.1%)	1.02	1/1527 (0.1%)
38	DP	0.89	0/1143	1.14	4/1527 (0.3%)
39	CQ	0.94	1/974 (0.1%)	1.18	2/1302 (0.2%)
39	DQ	1.07	2/974 (0.2%)	1.29	4/1302 (0.3%)
40	CR	0.92	0/779	1.10	3/1036 (0.3%)
40	DR	1.03	0/779	1.18	2/1036 (0.2%)
41	CS	0.94	0/1156	1.31	8/1542 (0.5%)
41	DS	1.03	1/1156 (0.1%)	1.40	15/1542 (1.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
42	CT	0.85	0/975	1.12	2/1297 (0.2%)
42	DT	1.00	0/975	1.23	4/1297 (0.3%)
43	CU	0.85	0/790	1.13	2/1057 (0.2%)
43	DU	0.91	1/790 (0.1%)	1.22	4/1057 (0.4%)
44	CW	0.96	1/907 (0.1%)	1.11	3/1216 (0.2%)
45	CX	0.88	0/740	1.12	1/993 (0.1%)
45	DX	0.90	0/740	1.21	3/993 (0.3%)
46	CY	1.14	0/789	1.38	10/1051 (1.0%)
46	DY	1.16	2/789 (0.3%)	1.44	12/1051 (1.1%)
47	CZ	0.74	1/1436 (0.1%)	1.02	3/1949 (0.2%)
47	DZ	0.77	0/1436	1.02	7/1949 (0.4%)
48	Ca	0.85	0/671	1.06	2/892 (0.2%)
48	Da	0.95	1/671 (0.1%)	1.18	3/892 (0.3%)
49	CH	0.91	0/741	1.22	2/984 (0.2%)
49	DH	0.85	0/741	1.10	3/984 (0.3%)
50	CK	0.74	0/600	1.03	1/793 (0.1%)
50	DK	0.79	0/600	1.10	1/793 (0.1%)
51	CL	0.74	0/473	1.08	0/634
51	DL	0.87	1/473 (0.2%)	1.10	0/634
52	C5	0.86	0/229	1.13	0/309
52	D5	0.90	0/229	1.17	3/309 (1.0%)
53	C6	0.99	1/473 (0.2%)	1.22	5/639 (0.8%)
53	D6	0.92	0/473	1.22	2/639 (0.3%)
54	C7	1.26	1/387 (0.3%)	1.26	2/515 (0.4%)
54	D7	1.10	0/387	1.22	4/515 (0.8%)
55	C8	0.96	0/427	1.20	0/561
55	D8	1.05	0/427	1.16	0/561
56	C9	1.02	1/516 (0.2%)	1.42	7/679 (1.0%)
56	D9	1.03	1/516 (0.2%)	1.30	3/679 (0.4%)
57	C0	0.86	0/302	0.88	0/397
57	D0	0.92	0/302	0.98	1/397 (0.3%)
58	C1	0.55	2/67709 (0.0%)	1.07	518/105690 (0.5%)
58	D1	0.58	6/67709 (0.0%)	1.11	628/105690 (0.6%)
59	Cs	0.50	0/2853	0.99	17/4451 (0.4%)
59	Ds	0.54	0/2853	1.04	20/4451 (0.4%)
60	D2	0.46	0/459	0.86	0/712
61	D4	0.52	0/1813	1.02	10/2825 (0.4%)
62	DA	0.90	0/645	1.00	1/867 (0.1%)
63	DW	0.94	0/907	1.11	1/1216 (0.1%)
64	DV	0.44	0/1269	0.80	1/1956 (0.1%)
All	All	0.66	75/318931 (0.0%)	1.07	1929/476973 (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
2	AA	0	1
3	AC	0	1
12	AL	0	1
13	AM	0	1
13	BM	0	1
14	BN	0	1
18	BS	0	1
19	AT	0	1
20	AU	0	1
22	Ab	1	0
22	Bb	1	0
25	C3	1	0
25	D3	1	0
28	CB	0	4
28	DB	0	3
29	DC	0	2
30	CD	0	1
31	CE	0	2
32	DF	0	1
33	CI	0	1
34	DJ	0	1
37	CO	0	6
37	DO	0	6
39	DQ	0	1
41	CS	0	1
41	DS	0	3
42	CT	0	1
42	DT	0	1
46	CY	0	1
46	DY	0	2
47	DZ	0	1
48	Da	0	1
53	C6	0	1
54	C7	0	1
54	D7	0	1
56	D9	0	1
58	C1	20	0
58	D1	21	0
All	All	45	52

The worst 5 of 75 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	DB	220	HIS	C-O	8.89	1.34	1.24
41	DS	79	HIS	CA-C	8.53	1.62	1.52
4	AD	12	CYS	CA-CB	8.31	1.67	1.53
29	DC	127	ASP	CA-C	7.92	1.63	1.52
37	DO	40	SER	N-CA	7.32	1.55	1.46

The worst 5 of 1929 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	D1	2013	G	C2'-C3'-O3'	17.75	136.13	109.50
58	C1	1345	U	C2'-C3'-O3'	16.55	134.33	109.50
22	Bb	1476	U	C2'-C3'-O3'	16.34	134.01	109.50
58	C1	2013	G	C2'-C3'-O3'	15.74	133.11	109.50
58	D1	1740	C	C2'-C3'-O3'	15.50	136.95	113.70

5 of 45 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	Ab	408	A	C1'
22	Bb	408	A	C1'
25	C3	47	U	C1'
58	C1	98	G	C1'
58	C1	715	G	C4',C3',C1'

5 of 52 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AA	23	ARG	Peptide
3	AC	26	LYS	Peptide
12	AL	91	LYS	Peptide
13	AM	69	GLU	Peptide
19	AT	28	LYS	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	A2	173	0	85	17	0
2	AA	1901	0	1951	38	0
2	BA	1901	0	1951	37	0
3	AC	1612	0	1677	41	0
4	AD	1703	0	1763	56	0
4	BD	1703	0	1763	50	0
5	AE	1147	0	1207	35	0
5	BE	1147	0	1207	24	0
6	AF	843	0	857	7	0
6	BF	843	0	857	18	0
7	AG	1257	0	1296	9	0
7	BG	1257	0	1296	20	0
8	AH	1116	0	1177	15	0
8	BH	1116	0	1177	22	0
9	AI	1011	0	1043	39	0
9	BI	1011	0	1043	33	0
10	AJ	795	0	840	27	0
10	BJ	795	0	840	23	0
11	AK	885	0	904	15	0
11	BK	885	0	904	26	0
12	AL	971	0	1057	28	0
12	BL	971	0	1057	23	0
13	AM	988	0	1059	43	0
13	BM	988	0	1059	33	0
14	AN	492	0	529	23	0
14	BN	492	0	529	16	0
15	AO	734	0	771	9	0
15	BO	734	0	771	13	0
16	AP	701	0	720	16	0
16	BP	701	0	720	20	0
17	AR	824	0	891	15	0
17	BR	824	0	891	22	0
18	AS	574	0	644	17	0
18	BS	574	0	644	17	0
19	AT	630	0	652	28	0
19	BT	630	0	652	36	0
20	AU	763	0	861	27	0
20	BU	763	0	861	17	0
21	AW	209	0	221	2	0
21	BW	209	0	221	9	0
22	Ab	32329	0	16318	341	0
22	Bb	32329	0	16318	330	1
23	B2	194	0	95	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	BC	1613	0	1677	34	0
25	C2	1597	0	811	23	0
25	C3	1619	0	822	28	0
25	D3	1619	0	822	46	0
26	C4	1640	0	837	57	0
27	CA	1156	0	755	15	0
28	CB	2105	0	2182	99	0
28	DB	2105	0	2182	100	0
29	CC	1564	0	1629	61	0
29	DC	1564	0	1629	85	0
30	CD	1624	0	1677	64	0
30	DD	1624	0	1677	52	0
31	CE	1474	0	1535	52	0
31	DE	1474	0	1535	57	0
32	CF	1223	0	1282	27	0
32	DF	1223	0	1282	51	0
33	CI	1132	0	1218	25	1
33	DI	1132	0	1218	29	0
34	CJ	651	0	155	0	0
34	DJ	651	0	155	4	0
35	CM	1105	0	1180	38	0
35	DM	1105	0	1180	38	0
36	CN	933	0	996	24	0
36	DN	933	0	996	25	0
37	CO	1114	0	1187	91	0
37	DO	1114	0	1187	111	0
38	CP	1122	0	1179	28	0
38	DP	1122	0	1179	39	0
39	CQ	960	0	1021	33	0
39	DQ	960	0	1021	37	0
40	CR	771	0	832	35	0
40	DR	771	0	832	31	0
41	CS	1142	0	1202	85	0
41	DS	1142	0	1202	89	0
42	CT	958	0	1018	48	0
42	DT	958	0	1018	48	0
43	CU	779	0	852	47	0
43	DU	779	0	852	46	0
44	CW	896	0	953	25	0
45	CX	726	0	778	19	0
45	DX	726	0	778	21	0
46	CY	776	0	870	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	DY	776	0	868	61	0
47	CZ	1404	0	1432	38	0
47	DZ	1404	0	1432	26	0
48	Ca	662	0	688	13	0
48	Da	662	0	688	12	0
49	CH	734	0	808	17	0
49	DH	734	0	808	20	0
50	CK	598	0	653	12	0
50	DK	598	0	653	17	0
51	CL	468	0	523	9	0
51	DL	468	0	523	8	0
52	C5	226	0	229	2	0
52	D5	226	0	229	11	0
53	C6	459	0	478	14	0
53	D6	459	0	477	16	0
54	C7	381	0	390	18	0
54	D7	381	0	390	22	0
55	C8	419	0	467	8	0
55	D8	419	0	467	5	0
56	C9	508	0	576	38	0
56	D9	508	0	576	37	0
57	C0	299	0	326	4	0
57	D0	299	0	324	5	0
58	C1	60459	0	30486	643	0
58	D1	60459	0	30488	738	0
59	Cs	2551	0	1295	19	0
59	Ds	2551	0	1295	28	0
60	D2	416	0	215	8	0
61	D4	1623	0	825	47	0
62	DA	1155	0	757	14	0
63	DW	896	0	956	20	0
64	DV	1167	0	624	18	0
65	Ab	42	0	45	4	0
65	Bb	42	0	45	3	0
66	C1	24	0	20	5	0
66	D1	24	0	21	11	0
67	C1	1	0	0	0	0
67	D1	1	0	0	2	0
All	All	295910	0	199849	4856	1

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 10.

The worst 5 of 4856 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)
61:D4:2:G:C2	61:D4:73:A:N3	1.85	1.31
58:C1:1331:A:O2'	58:C1:1333:U:OP2	1.54	1.25
58:D1:927:G:O2'	64:DV:19:G:C6	1.93	1.22
58:C1:2492:G:O2'	58:C1:2493:G:OP2	1.60	1.17
29:DC:132:HIS:ND1	58:D1:1704:C:OP1	1.79	1.16

All (1) 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)
22:Bb:364:U:OP1	33:Cl:91:SER:OG[4_455]	2.14	0.06

## 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	
2	AA	232/234 (99%)	174 (75%)	47 (20%)	11 (5%)	2	12
2	BA	232/234 (99%)	180 (78%)	41 (18%)	11 (5%)	2	12
3	AC	204/238 (86%)	145 (71%)	42 (21%)	17 (8%)	0	4
4	AD	206/208 (99%)	161 (78%)	33 (16%)	12 (6%)	1	8
4	BD	206/208 (99%)	168 (82%)	27 (13%)	11 (5%)	1	10
5	AE	148/150 (99%)	130 (88%)	15 (10%)	3 (2%)	6	25
5	BE	148/150 (99%)	130 (88%)	14 (10%)	4 (3%)	4	20
6	AF	99/101 (98%)	92 (93%)	5 (5%)	2 (2%)	6	25
6	BF	99/101 (98%)	89 (90%)	9 (9%)	1 (1%)	12	40
7	AG	153/155 (99%)	124 (81%)	26 (17%)	3 (2%)	6	25
7	BG	153/155 (99%)	135 (88%)	17 (11%)	1 (1%)	18	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	AH	136/138 (99%)	110 (81%)	24 (18%)	2 (2%)	8	30
8	BH	136/138 (99%)	116 (85%)	19 (14%)	1 (1%)	18	47
9	AI	125/127 (98%)	97 (78%)	23 (18%)	5 (4%)	2	15
9	BI	125/127 (98%)	98 (78%)	22 (18%)	5 (4%)	2	15
10	AJ	96/98 (98%)	79 (82%)	13 (14%)	4 (4%)	2	14
10	BJ	96/98 (98%)	76 (79%)	15 (16%)	5 (5%)	1	10
11	AK	117/119 (98%)	102 (87%)	14 (12%)	1 (1%)	14	42
11	BK	117/119 (98%)	93 (80%)	20 (17%)	4 (3%)	3	17
12	AL	122/124 (98%)	92 (75%)	20 (16%)	10 (8%)	0	4
12	BL	122/124 (98%)	94 (77%)	16 (13%)	12 (10%)	0	3
13	AM	122/124 (98%)	83 (68%)	26 (21%)	13 (11%)	0	2
13	BM	122/124 (98%)	83 (68%)	26 (21%)	13 (11%)	0	2
14	AN	58/60 (97%)	43 (74%)	12 (21%)	3 (5%)	1	10
14	BN	58/60 (97%)	41 (71%)	14 (24%)	3 (5%)	1	10
15	AO	86/88 (98%)	73 (85%)	9 (10%)	4 (5%)	2	12
15	BO	86/88 (98%)	72 (84%)	13 (15%)	1 (1%)	10	35
16	AP	81/83 (98%)	63 (78%)	15 (18%)	3 (4%)	2	16
16	BP	81/83 (98%)	67 (83%)	14 (17%)	0	100	100
17	AR	97/99 (98%)	89 (92%)	5 (5%)	3 (3%)	3	18
17	BR	97/99 (98%)	84 (87%)	10 (10%)	3 (3%)	3	18
18	AS	68/70 (97%)	57 (84%)	5 (7%)	6 (9%)	0	3
18	BS	68/70 (97%)	54 (79%)	10 (15%)	4 (6%)	1	8
19	AT	76/78 (97%)	61 (80%)	7 (9%)	8 (10%)	0	2
19	BT	76/78 (97%)	55 (72%)	13 (17%)	8 (10%)	0	2
20	AU	97/99 (98%)	77 (79%)	14 (14%)	6 (6%)	1	7
20	BU	97/99 (98%)	75 (77%)	19 (20%)	3 (3%)	3	18
21	AW	22/24 (92%)	19 (86%)	2 (9%)	1 (4%)	2	12
21	BW	22/24 (92%)	17 (77%)	3 (14%)	2 (9%)	0	3
24	BC	204/206 (99%)	153 (75%)	41 (20%)	10 (5%)	1	11
27	CA	83/206 (40%)	56 (68%)	22 (26%)	5 (6%)	1	7
28	CB	269/271 (99%)	210 (78%)	39 (14%)	20 (7%)	1	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	DB	269/271 (99%)	209 (78%)	38 (14%)	22 (8%)	0	4
29	CC	202/204 (99%)	143 (71%)	43 (21%)	16 (8%)	1	4
29	DC	202/204 (99%)	145 (72%)	32 (16%)	25 (12%)	0	1
30	CD	205/207 (99%)	162 (79%)	30 (15%)	13 (6%)	1	7
30	DD	205/207 (99%)	166 (81%)	24 (12%)	15 (7%)	1	5
31	CE	179/181 (99%)	132 (74%)	32 (18%)	15 (8%)	0	4
31	DE	179/181 (99%)	139 (78%)	28 (16%)	12 (7%)	1	6
32	CF	157/159 (99%)	112 (71%)	25 (16%)	20 (13%)	0	1
32	DF	157/159 (99%)	113 (72%)	26 (17%)	18 (12%)	0	2
33	CI	143/145 (99%)	112 (78%)	22 (15%)	9 (6%)	1	7
33	DI	143/145 (99%)	104 (73%)	29 (20%)	10 (7%)	1	6
35	CM	136/138 (99%)	103 (76%)	24 (18%)	9 (7%)	1	6
35	DM	136/138 (99%)	96 (71%)	30 (22%)	10 (7%)	1	5
36	CN	120/122 (98%)	106 (88%)	10 (8%)	4 (3%)	3	17
36	DN	120/122 (98%)	110 (92%)	8 (7%)	2 (2%)	7	28
37	CO	144/146 (99%)	84 (58%)	29 (20%)	31 (22%)	0	0
37	DO	144/146 (99%)	86 (60%)	26 (18%)	32 (22%)	0	0
38	CP	139/141 (99%)	118 (85%)	17 (12%)	4 (3%)	3	19
38	DP	139/141 (99%)	117 (84%)	17 (12%)	5 (4%)	2	16
39	CQ	115/117 (98%)	93 (81%)	14 (12%)	8 (7%)	1	6
39	DQ	115/117 (98%)	98 (85%)	11 (10%)	6 (5%)	1	10
40	CR	96/98 (98%)	62 (65%)	23 (24%)	11 (12%)	0	2
40	DR	96/98 (98%)	66 (69%)	15 (16%)	15 (16%)	0	0
41	CS	135/137 (98%)	92 (68%)	24 (18%)	19 (14%)	0	0
41	DS	135/137 (98%)	89 (66%)	28 (21%)	18 (13%)	0	1
42	CT	115/117 (98%)	103 (90%)	10 (9%)	2 (2%)	7	28
42	DT	115/117 (98%)	93 (81%)	15 (13%)	7 (6%)	1	7
43	CU	99/101 (98%)	75 (76%)	11 (11%)	13 (13%)	0	1
43	DU	99/101 (98%)	72 (73%)	13 (13%)	14 (14%)	0	0
44	CW	111/113 (98%)	92 (83%)	12 (11%)	7 (6%)	1	7
45	CX	90/92 (98%)	77 (86%)	7 (8%)	6 (7%)	1	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	DX	90/92 (98%)	79 (88%)	9 (10%)	2 (2%)	5	24
46	CY	98/100 (98%)	60 (61%)	17 (17%)	21 (21%)	0	0
46	DY	98/100 (98%)	60 (61%)	18 (18%)	20 (20%)	0	0
47	CZ	174/176 (99%)	121 (70%)	42 (24%)	11 (6%)	1	7
47	DZ	174/176 (99%)	136 (78%)	28 (16%)	10 (6%)	1	9
48	Ca	82/84 (98%)	72 (88%)	9 (11%)	1 (1%)	10	35
48	Da	82/84 (98%)	74 (90%)	7 (8%)	1 (1%)	10	35
49	CH	91/93 (98%)	73 (80%)	10 (11%)	8 (9%)	0	3
49	DH	91/93 (98%)	73 (80%)	12 (13%)	6 (7%)	1	6
50	CK	69/71 (97%)	50 (72%)	12 (17%)	7 (10%)	0	3
50	DK	69/71 (97%)	54 (78%)	11 (16%)	4 (6%)	1	8
51	CL	57/59 (97%)	51 (90%)	5 (9%)	1 (2%)	6	26
51	DL	57/59 (97%)	52 (91%)	3 (5%)	2 (4%)	3	16
52	C5	28/30 (93%)	20 (71%)	5 (18%)	3 (11%)	0	2
52	D5	28/30 (93%)	18 (64%)	7 (25%)	3 (11%)	0	2
53	C6	57/59 (97%)	48 (84%)	5 (9%)	4 (7%)	1	6
53	D6	57/59 (97%)	46 (81%)	7 (12%)	4 (7%)	1	6
54	C7	40/44 (91%)	22 (55%)	9 (22%)	9 (22%)	0	0
54	D7	40/44 (91%)	21 (52%)	8 (20%)	11 (28%)	0	0
55	C8	46/48 (96%)	42 (91%)	4 (9%)	0	100	100
55	D8	46/48 (96%)	45 (98%)	1 (2%)	0	100	100
56	C9	61/63 (97%)	47 (77%)	11 (18%)	3 (5%)	1	11
56	D9	61/63 (97%)	41 (67%)	15 (25%)	5 (8%)	0	4
57	C0	34/36 (94%)	32 (94%)	2 (6%)	0	100	100
57	D0	34/36 (94%)	32 (94%)	2 (6%)	0	100	100
62	DA	83/206 (40%)	52 (63%)	28 (34%)	3 (4%)	2	16
63	DW	111/113 (98%)	94 (85%)	11 (10%)	6 (5%)	1	10
All	All	11440/11918 (96%)	8901 (78%)	1752 (15%)	787 (7%)	1	6

5 of 787 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AA	83	MET

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Mol	Chain	Res	Type
2	AA	165	VAL
3	AC	4	LYS
3	AC	12	LEU
3	AC	47	LEU

### 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
2	AA	202/202 (100%)	180 (89%)	22 (11%)	6 22
2	BA	202/202 (100%)	182 (90%)	20 (10%)	7 26
3	AC	160/187 (86%)	144 (90%)	16 (10%)	7 26
4	AD	180/180 (100%)	160 (89%)	20 (11%)	6 21
4	BD	180/180 (100%)	161 (89%)	19 (11%)	6 23
5	AE	115/115 (100%)	103 (90%)	12 (10%)	7 24
5	BE	115/115 (100%)	99 (86%)	16 (14%)	3 14
6	AF	90/90 (100%)	85 (94%)	5 (6%)	19 46
6	BF	90/90 (100%)	85 (94%)	5 (6%)	19 46
7	AG	126/126 (100%)	111 (88%)	15 (12%)	5 19
7	BG	126/126 (100%)	114 (90%)	12 (10%)	8 29
8	AH	119/119 (100%)	108 (91%)	11 (9%)	8 29
8	BH	119/119 (100%)	106 (89%)	13 (11%)	6 22
9	AI	98/98 (100%)	83 (85%)	15 (15%)	3 10
9	BI	98/98 (100%)	89 (91%)	9 (9%)	8 29
10	AJ	88/88 (100%)	77 (88%)	11 (12%)	4 18
10	BJ	88/88 (100%)	76 (86%)	12 (14%)	3 15
11	AK	90/90 (100%)	80 (89%)	10 (11%)	6 21
11	BK	90/90 (100%)	82 (91%)	8 (9%)	9 31
12	AL	104/104 (100%)	87 (84%)	17 (16%)	2 10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	BL	104/104 (100%)	87 (84%)	17 (16%)	2	10
13	AM	99/99 (100%)	84 (85%)	15 (15%)	3	10
13	BM	99/99 (100%)	81 (82%)	18 (18%)	2	7
14	AN	49/49 (100%)	46 (94%)	3 (6%)	17	43
14	BN	49/49 (100%)	45 (92%)	4 (8%)	10	35
15	AO	79/79 (100%)	76 (96%)	3 (4%)	29	54
15	BO	79/79 (100%)	74 (94%)	5 (6%)	16	42
16	AP	72/72 (100%)	65 (90%)	7 (10%)	8	28
16	BP	72/72 (100%)	61 (85%)	11 (15%)	3	10
17	AR	94/94 (100%)	90 (96%)	4 (4%)	26	51
17	BR	94/94 (100%)	84 (89%)	10 (11%)	6	23
18	AS	61/61 (100%)	54 (88%)	7 (12%)	5	20
18	BS	61/61 (100%)	52 (85%)	9 (15%)	3	12
19	AT	69/69 (100%)	54 (78%)	15 (22%)	1	3
19	BT	69/69 (100%)	54 (78%)	15 (22%)	1	3
20	AU	76/76 (100%)	67 (88%)	9 (12%)	5	20
20	BU	76/76 (100%)	63 (83%)	13 (17%)	2	9
21	AW	19/19 (100%)	18 (95%)	1 (5%)	20	47
21	BW	19/19 (100%)	17 (90%)	2 (10%)	6	23
24	BC	160/160 (100%)	142 (89%)	18 (11%)	5	21
27	CA	61/74 (82%)	53 (87%)	8 (13%)	4	16
28	CB	213/213 (100%)	176 (83%)	37 (17%)	2	8
28	DB	213/213 (100%)	174 (82%)	39 (18%)	2	7
29	CC	165/165 (100%)	133 (81%)	32 (19%)	1	5
29	DC	165/165 (100%)	137 (83%)	28 (17%)	2	9
30	CD	165/165 (100%)	140 (85%)	25 (15%)	3	10
30	DD	165/165 (100%)	139 (84%)	26 (16%)	2	10
31	CE	155/155 (100%)	135 (87%)	20 (13%)	4	16
31	DE	155/155 (100%)	125 (81%)	30 (19%)	1	5
32	CF	132/132 (100%)	113 (86%)	19 (14%)	3	13
32	DF	132/132 (100%)	105 (80%)	27 (20%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	CI	122/122 (100%)	102 (84%)	20 (16%)	2	10
33	DI	122/122 (100%)	103 (84%)	19 (16%)	2	10
35	CM	117/117 (100%)	93 (80%)	24 (20%)	1	4
35	DM	117/117 (100%)	93 (80%)	24 (20%)	1	4
36	CN	100/100 (100%)	81 (81%)	19 (19%)	1	6
36	DN	100/100 (100%)	86 (86%)	14 (14%)	3	13
37	CO	112/112 (100%)	81 (72%)	31 (28%)	0	1
37	DO	112/112 (100%)	84 (75%)	28 (25%)	0	1
38	CP	111/111 (100%)	97 (87%)	14 (13%)	4	18
38	DP	111/111 (100%)	96 (86%)	15 (14%)	4	15
39	CQ	100/100 (100%)	81 (81%)	19 (19%)	1	6
39	DQ	100/100 (100%)	83 (83%)	17 (17%)	2	9
40	CR	77/77 (100%)	63 (82%)	14 (18%)	2	7
40	DR	77/77 (100%)	58 (75%)	19 (25%)	1	2
41	CS	120/120 (100%)	92 (77%)	28 (23%)	1	2
41	DS	120/120 (100%)	98 (82%)	22 (18%)	2	7
42	CT	92/92 (100%)	76 (83%)	16 (17%)	2	8
42	DT	92/92 (100%)	80 (87%)	12 (13%)	4	16
43	CU	82/82 (100%)	61 (74%)	21 (26%)	0	1
43	DU	82/82 (100%)	65 (79%)	17 (21%)	1	4
44	CW	91/92 (99%)	79 (87%)	12 (13%)	4	16
45	CX	74/74 (100%)	60 (81%)	14 (19%)	1	6
45	DX	74/74 (100%)	60 (81%)	14 (19%)	1	6
46	CY	84/84 (100%)	65 (77%)	19 (23%)	1	3
46	DY	84/84 (100%)	65 (77%)	19 (23%)	1	3
47	CZ	155/155 (100%)	142 (92%)	13 (8%)	10	34
47	DZ	155/155 (100%)	134 (86%)	21 (14%)	4	15
48	Ca	66/66 (100%)	57 (86%)	9 (14%)	3	15
48	Da	66/66 (100%)	57 (86%)	9 (14%)	3	15
49	CH	78/78 (100%)	57 (73%)	21 (27%)	0	1
49	DH	78/78 (100%)	64 (82%)	14 (18%)	2	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	CK	66/66 (100%)	55 (83%)	11 (17%)	2	9
50	DK	66/66 (100%)	53 (80%)	13 (20%)	1	5
51	CL	51/51 (100%)	48 (94%)	3 (6%)	18	44
51	DL	51/51 (100%)	48 (94%)	3 (6%)	18	44
52	C5	27/27 (100%)	23 (85%)	4 (15%)	3	12
52	D5	27/27 (100%)	24 (89%)	3 (11%)	6	21
53	C6	51/51 (100%)	44 (86%)	7 (14%)	3	14
53	D6	51/51 (100%)	42 (82%)	9 (18%)	2	8
54	C7	43/43 (100%)	33 (77%)	10 (23%)	1	2
54	D7	43/43 (100%)	35 (81%)	8 (19%)	1	6
55	C8	41/41 (100%)	36 (88%)	5 (12%)	5	19
55	D8	41/41 (100%)	32 (78%)	9 (22%)	1	3
56	C9	53/53 (100%)	40 (76%)	13 (24%)	1	2
56	D9	53/53 (100%)	42 (79%)	11 (21%)	1	4
57	C0	33/33 (100%)	30 (91%)	3 (9%)	9	30
57	D0	33/33 (100%)	29 (88%)	4 (12%)	5	19
62	DA	61/74 (82%)	54 (88%)	7 (12%)	5	20
63	DW	91/91 (100%)	82 (90%)	9 (10%)	7	26
All	All	9654/9708 (99%)	8219 (85%)	1435 (15%)	3	12

5 of 1435 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
55	C8	24	THR
36	DN	10	VAL
28	DB	20	ASP
55	C8	15	THR
30	DD	170	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 233 such sidechains are listed below:

Mol	Chain	Res	Type
39	CQ	3	HIS
50	DK	65	ASN
47	CZ	121	HIS

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Mol	Chain	Res	Type
49	DH	45	ASN
39	DQ	71	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A2	8/9 (88%)	4 (50%)	2 (25%)
22	Ab	1503/1504 (99%)	333 (22%)	0
22	Bb	1503/1504 (99%)	345 (22%)	0
23	B2	7/10 (70%)	4 (57%)	1 (14%)
25	C2	74/76 (97%)	25 (33%)	4 (5%)
25	C3	75/76 (98%)	19 (25%)	1 (1%)
25	D3	75/76 (98%)	31 (41%)	3 (4%)
26	C4	76/77 (98%)	36 (47%)	4 (5%)
58	C1	2802/2899 (96%)	818 (29%)	155 (5%)
58	D1	2802/2899 (96%)	829 (29%)	149 (5%)
59	Cs	118/119 (99%)	35 (29%)	0
59	Ds	118/119 (99%)	40 (33%)	0
60	D2	19/20 (95%)	8 (42%)	1 (5%)
61	D4	75/76 (98%)	23 (30%)	5 (6%)
64	DV	41/55 (74%)	14 (34%)	1 (2%)
All	All	9296/9519 (97%)	2564 (27%)	326 (3%)

5 of 2564 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A2	15	A
1	A2	17	U
1	A2	18	G
1	A2	19	U
22	Ab	10	G

5 of 326 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
58	D1	1254	A
58	D1	2193	U
58	D1	1423	A
58	D1	1740	C
58	D1	2458	G

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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
65	PAR	Ab	1601	-	44,45,45	1.42	5 (11%)	63,67,67	1.87	14 (22%)
66	3V6	D1	3001	67	22,25,25	2.29	8 (36%)	24,39,39	2.97	9 (37%)
66	3V6	C1	3001	67	22,25,25	2.03	8 (36%)	24,39,39	2.03	8 (33%)
65	PAR	Bb	1601	-	44,45,45	1.53	7 (15%)	63,67,67	2.19	19 (30%)

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
65	PAR	Ab	1601	-	-	6/18/94/94	2/4/4/4
66	3V6	D1	3001	67	-	3/12/53/53	0/2/2/2
66	3V6	C1	3001	67	-	1/12/53/53	0/2/2/2
65	PAR	Bb	1601	-	-	9/18/94/94	0/4/4/4

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
65	Bb	1601	PAR	C41-C51	5.90	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	D1	3001	3V6	CAK-CAN	-5.55	1.42	1.49
65	Ab	1601	PAR	C34-C24	-5.17	1.47	1.53
66	C1	3001	3V6	CAK-CAS	4.33	1.64	1.53
66	D1	3001	3V6	CAS-CAU	4.00	1.59	1.53

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
65	Ab	1601	PAR	O52-C13-O43	-8.88	102.30	111.37
66	D1	3001	3V6	OAM-CAO-OAE	8.12	127.88	117.56
65	Bb	1601	PAR	O54-C54-C64	-7.95	90.80	106.07
65	Bb	1601	PAR	O52-C13-O43	-5.65	105.59	111.37
66	D1	3001	3V6	OAG-CAN-CAQ	-5.59	114.56	123.15

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
65	Ab	1601	PAR	C23-C13-O52-C52
65	Ab	1601	PAR	O43-C13-O52-C52
65	Bb	1601	PAR	C21-C11-O11-C42
66	C1	3001	3V6	NAL-C-CA-CB
66	D1	3001	3V6	O-C-CA-CB

All (2) ring outliers are listed below:

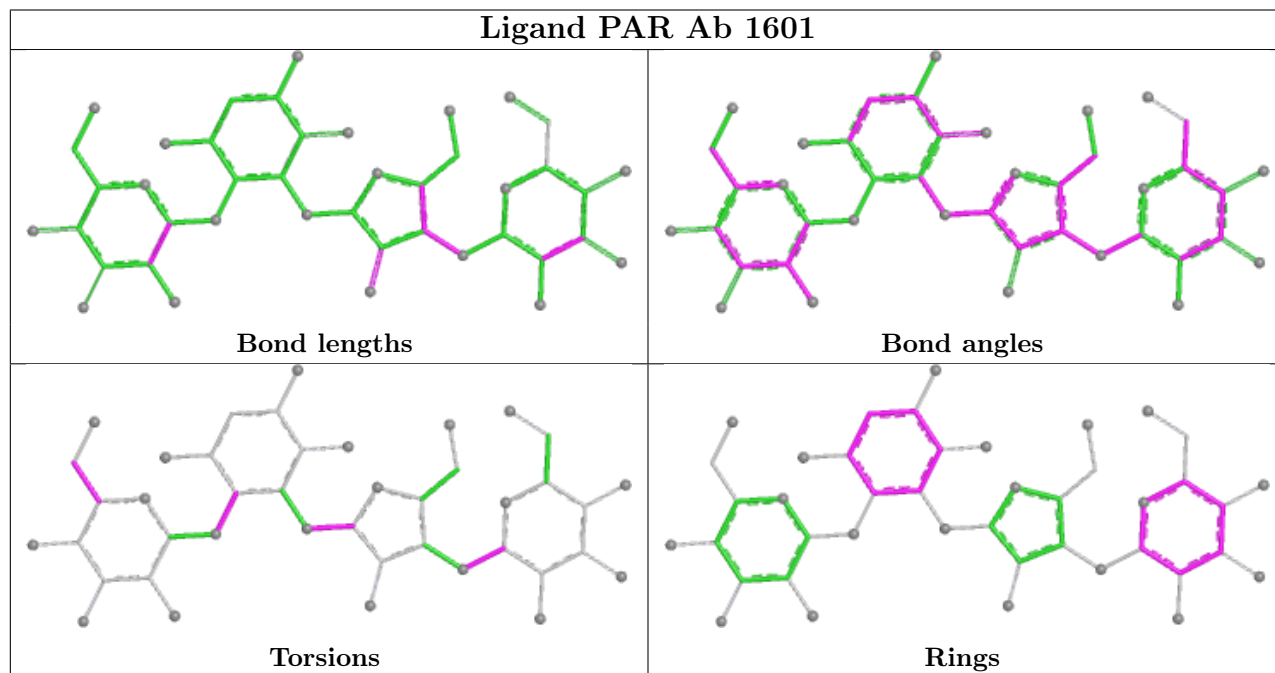
Mol	Chain	Res	Type	Atoms
65	Ab	1601	PAR	C14-C24-C34-C44-C54-O54
65	Ab	1601	PAR	C12-C22-C32-C42-C52-C62

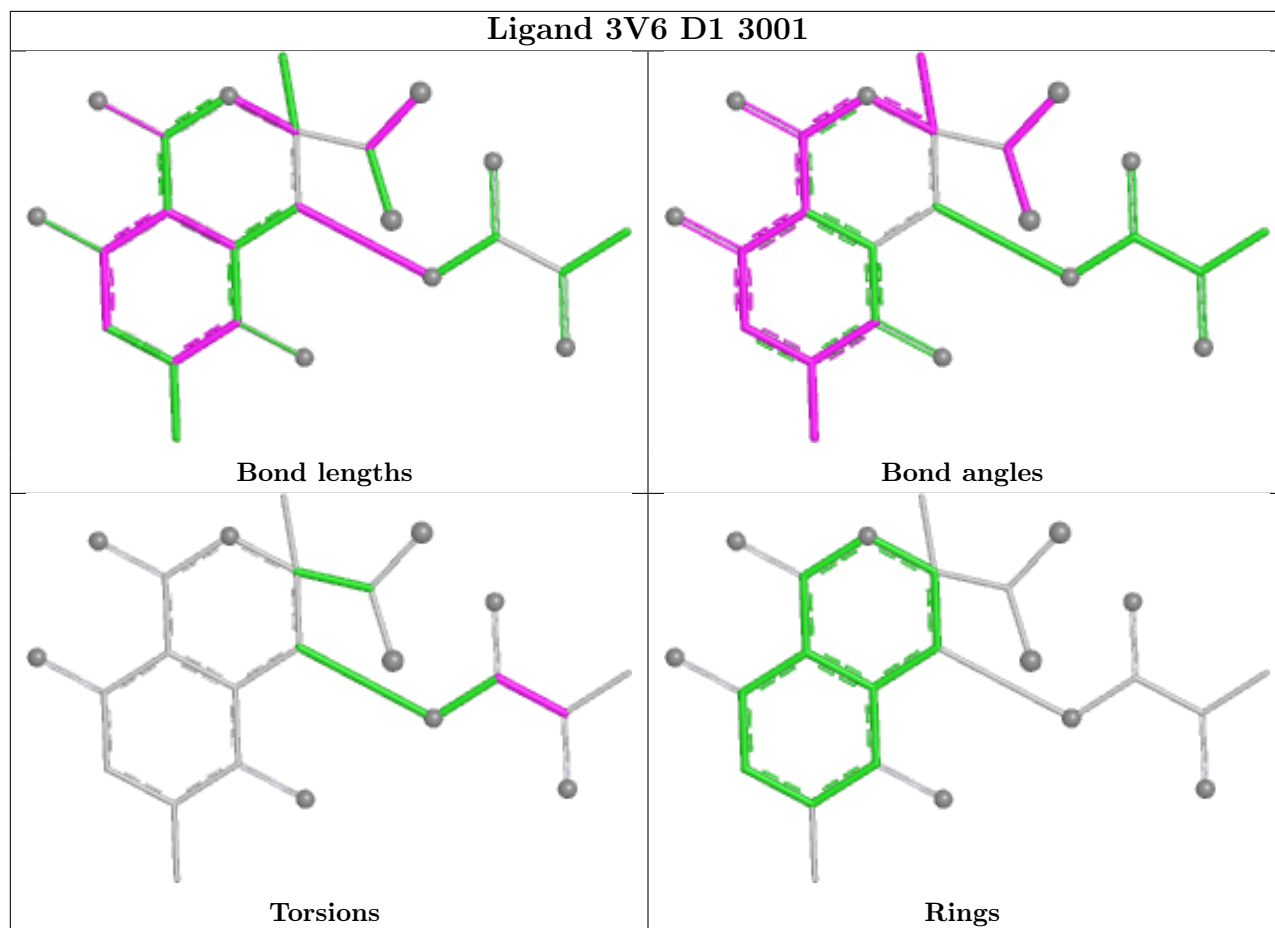
4 monomers are involved in 23 short contacts:

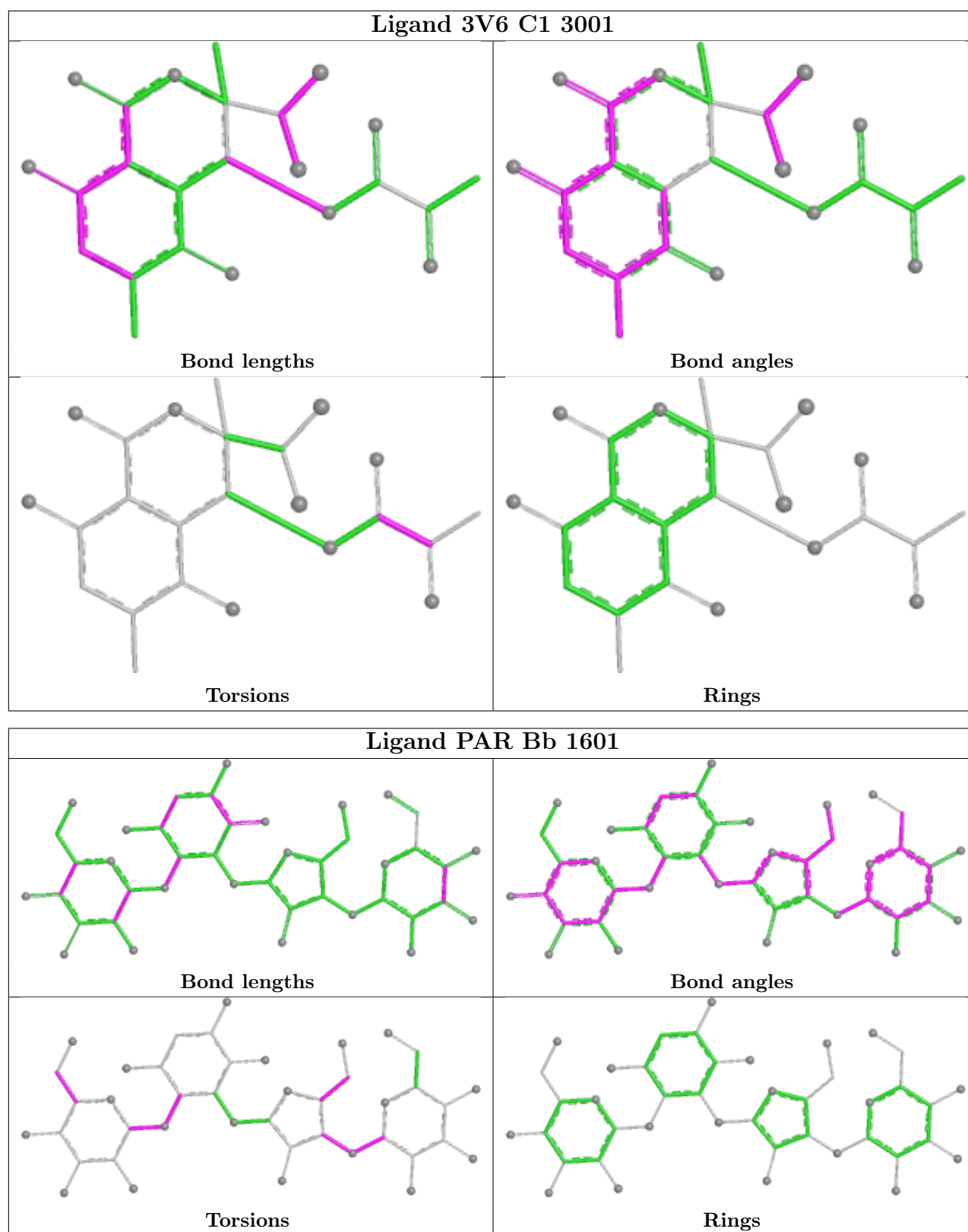
Mol	Chain	Res	Type	Clashes	Symm-Clashes
65	Ab	1601	PAR	4	0
66	D1	3001	3V6	11	0
66	C1	3001	3V6	5	0
65	Bb	1601	PAR	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
62	DA	2
27	CA	2
54	D7	1
54	C7	1
58	D1	1
58	C1	1

The worst 5 of 8 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	DA	110:PHE	C	119:UNK	N	14.86
1	CA	110:PHE	C	119:UNK	N	12.87
1	CA	136:UNK	C	139:UNK	N	8.88
1	D7	46:HIS	C	47:THR	N	7.64
1	C7	46:HIS	C	47:THR	N	7.62

## 6 Fit of model and data i

### 6.1 Protein, DNA and RNA chains i

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A2	9/9 (100%)	0.48	0 <span style="border: 2px solid blue; padding: 2px;">100</span> <span style="border: 2px solid blue; padding: 2px;">100</span>	50, 89, 110, 114	0
2	AA	234/234 (100%)	0.53	6 (2%) <span style="border: 1px solid gray; padding: 2px;">57</span> <span style="border: 1px solid gray; padding: 2px;">42</span>	78, 124, 168, 197	0
2	BA	234/234 (100%)	0.75	12 (5%) <span style="border: 1px solid red; padding: 2px;">33</span> <span style="border: 1px solid red; padding: 2px;">25</span>	80, 130, 179, 209	0
3	AC	206/238 (86%)	0.69	19 (9%) <span style="border: 1px solid red; padding: 2px;">14</span> <span style="border: 1px solid red; padding: 2px;">14</span>	65, 108, 148, 173	0
4	AD	208/208 (100%)	0.54	15 (7%) <span style="border: 1px solid red; padding: 2px;">21</span> <span style="border: 1px solid red; padding: 2px;">18</span>	51, 86, 123, 147	0
4	BD	208/208 (100%)	0.42	13 (6%) <span style="border: 1px solid red; padding: 2px;">26</span> <span style="border: 1px solid red; padding: 2px;">20</span>	48, 78, 117, 144	0
5	AE	150/150 (100%)	0.27	5 (3%) <span style="border: 1px solid gray; padding: 2px;">49</span> <span style="border: 1px solid gray; padding: 2px;">36</span>	66, 91, 124, 144	0
5	BE	150/150 (100%)	0.05	0 <span style="border: 2px solid blue; padding: 2px;">100</span> <span style="border: 2px solid blue; padding: 2px;">100</span>	57, 83, 122, 141	0
6	AF	101/101 (100%)	-0.09	2 (1%) <span style="border: 1px solid gray; padding: 2px;">65</span> <span style="border: 1px solid gray; padding: 2px;">49</span>	55, 85, 109, 170	0
6	BF	101/101 (100%)	0.18	0 <span style="border: 2px solid blue; padding: 2px;">100</span> <span style="border: 2px solid blue; padding: 2px;">100</span>	52, 96, 130, 158	0
7	AG	155/155 (100%)	0.24	13 (8%) <span style="border: 1px solid red; padding: 2px;">17</span> <span style="border: 1px solid red; padding: 2px;">15</span>	58, 86, 125, 181	0
7	BG	155/155 (100%)	0.82	16 (10%) <span style="border: 1px solid red; padding: 2px;">12</span> <span style="border: 1px solid red; padding: 2px;">12</span>	78, 112, 154, 184	0
8	AH	138/138 (100%)	0.29	2 (1%) <span style="border: 1px solid gray; padding: 2px;">73</span> <span style="border: 1px solid gray; padding: 2px;">59</span>	60, 90, 117, 184	0
8	BH	138/138 (100%)	0.46	4 (2%) <span style="border: 1px solid gray; padding: 2px;">53</span> <span style="border: 1px solid gray; padding: 2px;">39</span>	63, 95, 123, 145	0
9	AI	127/127 (100%)	0.99	18 (14%) <span style="border: 1px solid red; padding: 2px;">6</span> <span style="border: 1px solid red; padding: 2px;">8</span>	62, 108, 150, 175	0
9	BI	127/127 (100%)	1.20	27 (21%) <span style="border: 1px solid red; padding: 2px;">2</span> <span style="border: 1px solid red; padding: 2px;">4</span>	77, 131, 179, 215	0
10	AJ	98/98 (100%)	1.12	13 (13%) <span style="border: 1px solid red; padding: 2px;">7</span> <span style="border: 1px solid red; padding: 2px;">8</span>	77, 121, 176, 188	0
10	BJ	98/98 (100%)	1.31	23 (23%) <span style="border: 1px solid red; padding: 2px;">2</span> <span style="border: 1px solid red; padding: 2px;">3</span>	65, 134, 173, 202	0
11	AK	119/119 (100%)	0.20	5 (4%) <span style="border: 1px solid gray; padding: 2px;">40</span> <span style="border: 1px solid gray; padding: 2px;">29</span>	39, 76, 110, 158	0
11	BK	119/119 (100%)	0.47	5 (4%) <span style="border: 1px solid gray; padding: 2px;">40</span> <span style="border: 1px solid gray; padding: 2px;">29</span>	47, 94, 141, 193	0
12	AL	124/124 (100%)	0.62	11 (8%) <span style="border: 1px solid red; padding: 2px;">15</span> <span style="border: 1px solid red; padding: 2px;">14</span>	49, 82, 125, 180	0
12	BL	124/124 (100%)	0.21	9 (7%) <span style="border: 1px solid red; padding: 2px;">21</span> <span style="border: 1px solid red; padding: 2px;">18</span>	41, 60, 104, 158	0
13	AM	124/124 (100%)	0.71	13 (10%) <span style="border: 1px solid red; padding: 2px;">11</span> <span style="border: 1px solid red; padding: 2px;">12</span>	66, 98, 144, 197	0
13	BM	124/124 (100%)	1.10	19 (15%) <span style="border: 1px solid red; padding: 2px;">5</span> <span style="border: 1px solid red; padding: 2px;">7</span>	66, 113, 164, 204	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
14	AN	60/60 (100%)	1.26	13 (21%) 2 4	65, 103, 130, 142	0
14	BN	60/60 (100%)	1.13	8 (13%) 7 8	59, 94, 119, 134	0
15	AO	88/88 (100%)	0.16	1 (1%) 78 65	46, 76, 112, 123	0
15	BO	88/88 (100%)	0.57	3 (3%) 48 35	55, 94, 120, 132	0
16	AP	83/83 (100%)	0.34	0 100 100	52, 73, 101, 136	0
16	BP	83/83 (100%)	0.72	4 (4%) 35 26	59, 89, 135, 152	0
17	AR	99/99 (100%)	0.30	1 (1%) 79 66	59, 80, 108, 115	0
17	BR	99/99 (100%)	0.62	3 (3%) 52 39	65, 94, 126, 135	0
18	AS	70/70 (100%)	0.08	1 (1%) 73 59	56, 88, 119, 156	0
18	BS	70/70 (100%)	0.41	1 (1%) 73 59	66, 94, 142, 180	0
19	AT	78/78 (100%)	0.78	9 (11%) 9 10	67, 110, 164, 180	0
19	BT	78/78 (100%)	1.25	14 (17%) 3 5	79, 118, 161, 184	0
20	AU	99/99 (100%)	0.76	12 (12%) 8 9	62, 86, 125, 146	0
20	BU	99/99 (100%)	1.00	15 (15%) 5 7	64, 107, 146, 154	0
21	AW	24/24 (100%)	1.10	2 (8%) 17 15	63, 80, 112, 138	0
21	BW	24/24 (100%)	2.01	9 (37%) 1 1	64, 91, 132, 163	0
22	Ab	1504/1504 (100%)	-0.24	22 (1%) 72 57	30, 75, 154, 300	0
22	Bb	1504/1504 (100%)	-0.13	22 (1%) 72 57	31, 81, 165, 318	0
23	B2	10/10 (100%)	0.98	2 (20%) 3 4	60, 107, 138, 172	0
24	BC	206/206 (100%)	0.58	14 (6%) 23 19	64, 105, 149, 169	0
25	C2	75/76 (98%)	1.08	8 (10%) 11 11	99, 250, 345, 377	0
25	C3	76/76 (100%)	0.14	3 (3%) 43 31	60, 130, 198, 227	0
25	D3	76/76 (100%)	0.16	0 100 100	59, 147, 212, 228	0
26	C4	77/77 (100%)	-0.29	1 (1%) 75 61	44, 79, 132, 159	0
27	CA	87/206 (42%)	1.59	29 (33%) 1 1	98, 186, 221, 241	0
28	CB	271/271 (100%)	-0.10	4 (1%) 72 57	23, 48, 83, 150	0
28	DB	271/271 (100%)	0.04	6 (2%) 62 47	20, 52, 86, 158	0
29	CC	204/204 (100%)	0.28	10 (4%) 35 26	31, 68, 123, 150	0
29	DC	204/204 (100%)	0.16	10 (4%) 35 26	24, 61, 124, 169	0
30	CD	207/207 (100%)	-0.02	3 (1%) 73 59	29, 64, 133, 194	0
30	DD	207/207 (100%)	0.05	7 (3%) 48 35	20, 65, 146, 223	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
31	CE	181/181 (100%)	0.51	12 (6%) 24 19	59, 92, 137, 213	0
31	DE	181/181 (100%)	0.99	20 (11%) 10 11	76, 117, 154, 198	0
32	CF	159/159 (100%)	0.93	19 (11%) 9 10	82, 134, 175, 219	0
32	DF	159/159 (100%)	0.52	14 (8%) 15 14	45, 85, 126, 178	0
33	CI	145/145 (100%)	0.27	6 (4%) 41 29	40, 88, 128, 150	0
33	DI	145/145 (100%)	0.53	6 (4%) 41 29	60, 108, 139, 165	0
34	CJ	0/130	-	-	-	-
34	DJ	0/130	-	-	-	-
35	CM	138/138 (100%)	0.43	7 (5%) 33 25	47, 78, 118, 130	0
35	DM	138/138 (100%)	0.48	9 (6%) 25 20	36, 73, 121, 151	0
36	CN	122/122 (100%)	0.14	2 (1%) 70 56	35, 66, 89, 111	0
36	DN	122/122 (100%)	-0.32	0 100 100	27, 51, 75, 107	0
37	CO	146/146 (100%)	0.69	16 (10%) 10 11	34, 77, 127, 168	0
37	DO	146/146 (100%)	0.89	20 (13%) 6 8	31, 87, 123, 165	0
38	CP	141/141 (100%)	0.43	8 (5%) 29 22	44, 75, 111, 192	0
38	DP	141/141 (100%)	0.50	8 (5%) 29 22	42, 71, 106, 219	0
39	CQ	117/117 (100%)	0.23	7 (5%) 27 21	38, 63, 94, 127	0
39	DQ	117/117 (100%)	0.23	5 (4%) 40 29	27, 61, 99, 130	0
40	CR	98/98 (100%)	0.79	13 (13%) 7 8	47, 89, 130, 176	0
40	DR	98/98 (100%)	1.76	36 (36%) 1 1	68, 113, 143, 163	0
41	CS	137/137 (100%)	0.68	13 (9%) 14 13	45, 79, 142, 200	0
41	DS	137/137 (100%)	0.50	11 (8%) 18 16	43, 71, 148, 192	0
42	CT	117/117 (100%)	0.21	4 (3%) 48 35	37, 66, 116, 138	0
42	DT	117/117 (100%)	0.25	3 (2%) 57 42	31, 68, 111, 153	0
43	CU	101/101 (100%)	0.17	1 (0%) 79 66	35, 92, 122, 134	0
43	DU	101/101 (100%)	0.43	4 (3%) 42 30	26, 86, 123, 196	0
44	CW	113/113 (100%)	0.00	1 (0%) 81 68	38, 54, 90, 182	0
45	CX	92/92 (100%)	0.25	0 100 100	39, 65, 89, 109	0
45	DX	92/92 (100%)	0.02	1 (1%) 78 65	33, 55, 88, 115	0
46	CY	100/100 (100%)	1.57	24 (24%) 2 3	58, 94, 168, 214	0
46	DY	100/100 (100%)	1.13	22 (22%) 2 4	48, 81, 193, 251	0
47	CZ	176/176 (100%)	0.74	10 (5%) 29 22	76, 118, 157, 233	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
47	DZ	176/176 (100%)	0.90	18 (10%) 12 12	69, 119, 173, 203	0
48	Ca	84/84 (100%)	0.68	10 (11%) 9 10	44, 67, 127, 170	0
48	Da	84/84 (100%)	1.11	16 (19%) 3 4	49, 82, 137, 167	0
49	CH	93/93 (100%)	-0.00	2 (2%) 62 47	30, 54, 102, 140	0
49	DH	93/93 (100%)	0.28	1 (1%) 78 65	29, 66, 121, 179	0
50	CK	71/71 (100%)	0.46	6 (8%) 16 15	42, 85, 125, 180	0
50	DK	71/71 (100%)	0.31	5 (7%) 22 18	37, 68, 124, 179	0
51	CL	59/59 (100%)	0.30	1 (1%) 69 54	45, 72, 111, 223	0
51	DL	59/59 (100%)	0.53	1 (1%) 69 54	48, 79, 120, 213	0
52	C5	30/30 (100%)	0.22	0 100 100	76, 99, 130, 155	0
52	D5	30/30 (100%)	0.97	2 (6%) 24 19	99, 128, 155, 167	0
53	C6	59/59 (100%)	0.50	5 (8%) 16 15	34, 63, 160, 206	0
53	D6	59/59 (100%)	0.37	5 (8%) 16 15	28, 65, 172, 205	0
54	C7	44/44 (100%)	1.22	9 (20%) 2 4	54, 101, 146, 183	0
54	D7	44/44 (100%)	1.62	14 (31%) 1 1	84, 125, 165, 181	0
55	C8	48/48 (100%)	0.04	3 (6%) 26 20	26, 40, 79, 139	0
55	D8	48/48 (100%)	-0.14	2 (4%) 40 29	21, 34, 77, 135	0
56	C9	63/63 (100%)	0.68	8 (12%) 8 9	34, 54, 90, 123	0
56	D9	63/63 (100%)	0.83	8 (12%) 8 9	39, 66, 102, 136	0
57	C0	36/36 (100%)	1.60	12 (33%) 1 1	93, 125, 175, 177	0
57	D0	36/36 (100%)	1.66	10 (27%) 1 2	73, 106, 141, 145	0
58	C1	2807/2899 (96%)	-0.56	21 (0%) 84 73	21, 54, 148, 279	0
58	D1	2807/2899 (96%)	-0.49	33 (1%) 76 63	16, 52, 155, 267	0
59	Cs	119/119 (100%)	-0.13	3 (2%) 58 43	58, 83, 138, 197	0
59	Ds	119/119 (100%)	0.48	4 (3%) 48 35	62, 104, 147, 172	0
60	D2	20/20 (100%)	0.90	1 (5%) 34 25	133, 235, 281, 283	0
61	D4	76/76 (100%)	-0.16	1 (1%) 75 61	37, 79, 120, 201	0
62	DA	87/206 (42%)	1.41	17 (19%) 3 4	118, 190, 257, 309	0
63	DW	113/113 (100%)	-0.02	1 (0%) 81 68	33, 51, 100, 159	0
64	DV	55/55 (100%)	1.22	9 (16%) 4 6	110, 248, 297, 345	0
All	All	20982/21697 (96%)	0.13	1017 (4%) 35 26	16, 77, 159, 377	0

The worst 5 of 1017 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
31	CE	2	PRO	10.5
40	CR	54	LEU	8.2
13	AM	124	PRO	7.8
22	Bb	85	C	7.8
4	AD	49	ARG	7.6

## 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 oligosaccharides in this entry.

## 6.4 Ligands [i](#)

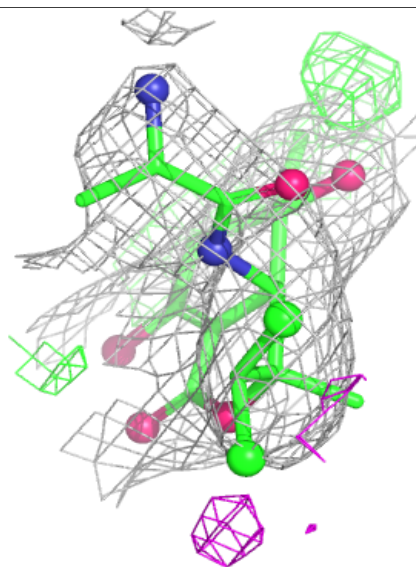
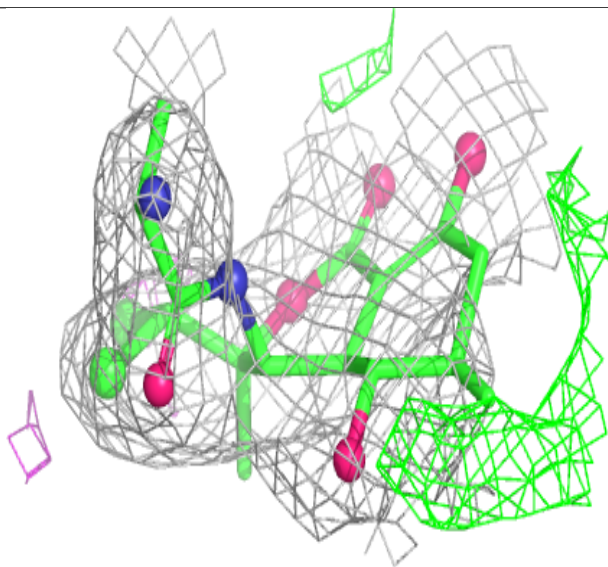
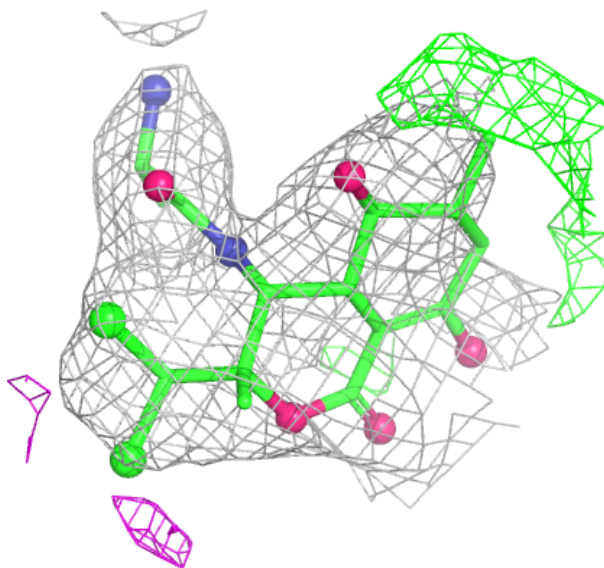
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
66	3V6	C1	3001	24/24	0.87	0.17	46,63,76,91	0
67	MG	D1	3002	1/1	0.89	0.13	40,40,40,40	0
65	PAR	Ab	1601	42/42	0.91	0.14	51,65,75,91	0
66	3V6	D1	3001	24/24	0.92	0.13	32,55,75,86	0
67	MG	C1	3002	1/1	0.93	0.13	41,41,41,41	0
65	PAR	Bb	1601	42/42	0.95	0.10	42,50,56,67	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

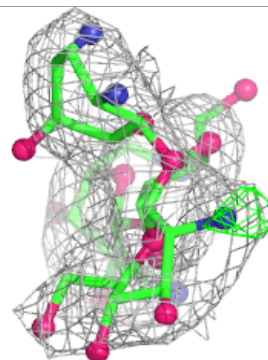
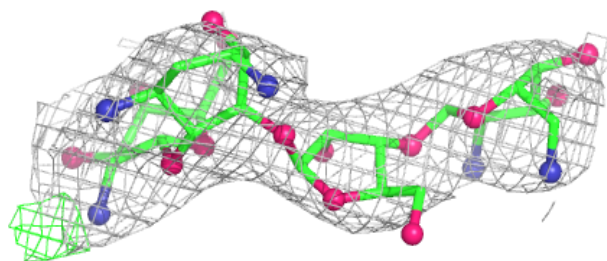
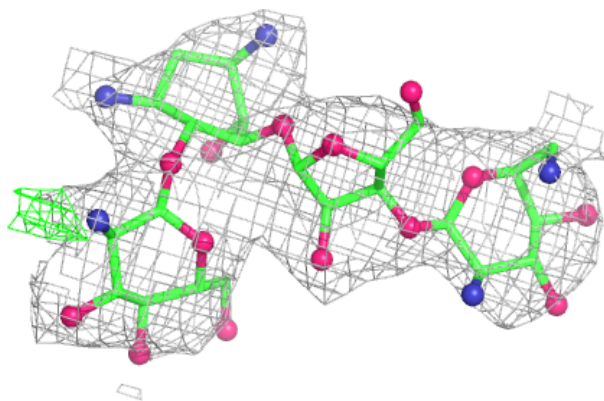
**Electron density around 3V6 C1 3001:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



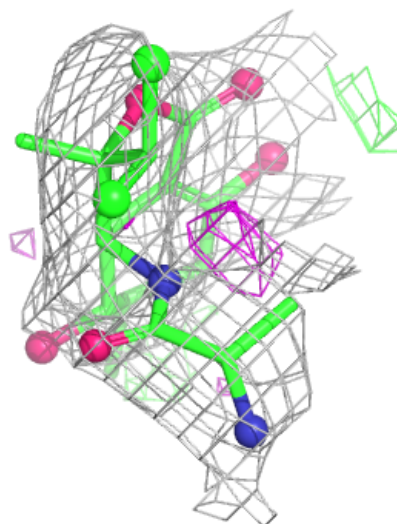
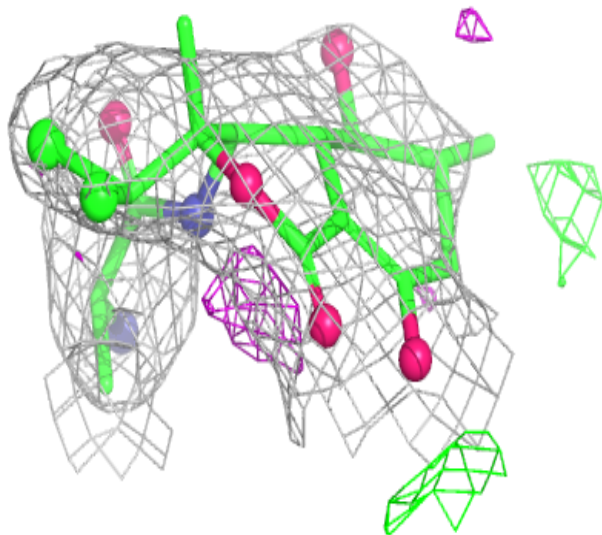
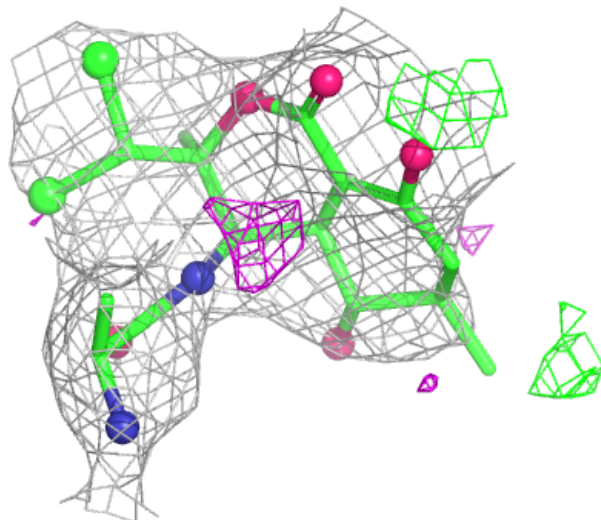
**Electron density around PAR Ab 1601:**

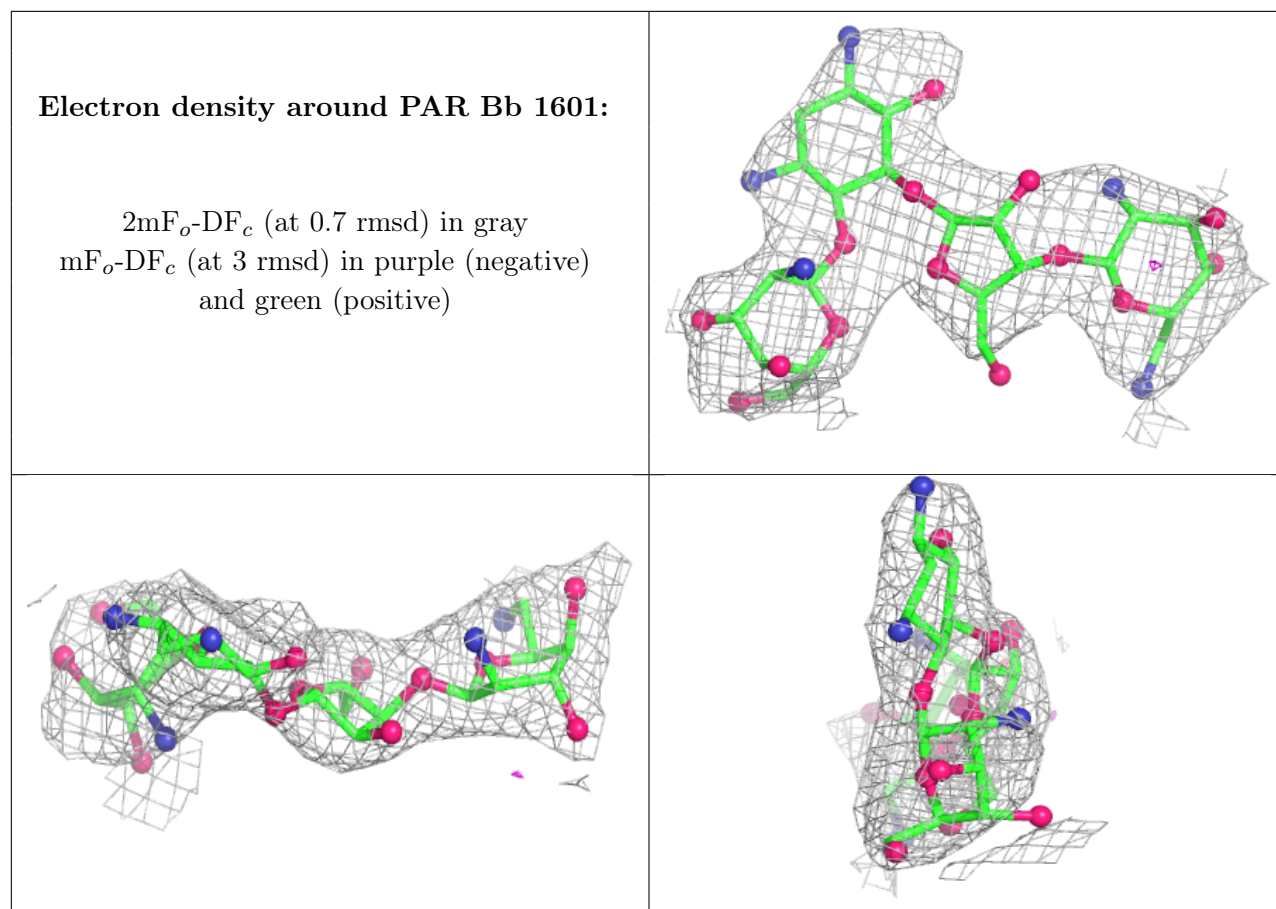
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 3V6 D1 3001:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.