



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 04:29 AM UTC

PDB ID : 4V9J / pdb_00004v9j
Title : 70S ribosome translocation intermediate GDPNP-II containing elongation factor EFG/GDPNP, mRNA, and tRNA bound in the pe^{*}/E state.
Authors : Zhou, J.; Lancaster, L.; Donohue, J.P.; Noller, H.F.
Deposited on : 2013-04-23
Resolution : 3.86 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (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

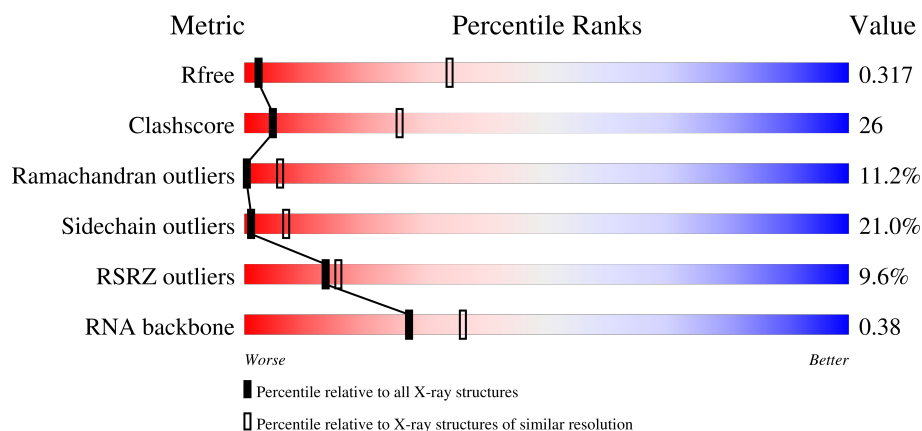
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.86 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	1165 (4.02-3.70)
Clashscore	190562	1207 (4.02-3.70)
Ramachandran outliers	187476	1149 (4.02-3.70)
Sidechain outliers	187428	1142 (4.02-3.70)
RSRZ outliers	180081	1164 (4.02-3.70)
RNA backbone	3983	1012 (4.62-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	AB	235	8% 34% 44% 18% .
1	CB	235	5% 36% 45% 16% .
2	AC	207	3% 38% 46% 15%
2	CC	207	4% 40% 43% 16% .

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Mol	Chain	Length	Quality of chain
3	AD	208	
3	CD	208	
4	AE	151	
4	CE	151	
5	AF	101	
5	CF	101	
6	AG	155	
6	CG	155	
7	AH	138	
7	CH	138	
8	AI	127	
8	CI	127	
9	AJ	99	
9	CJ	99	
10	AK	119	
10	CK	119	
11	AL	125	
11	CL	125	
12	AM	125	
12	CM	125	
13	AN	60	
13	CN	60	
14	AO	88	
14	CO	88	
15	AP	84	

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Mol	Chain	Length	Quality of chain
15	CP	84	
16	AQ	100	
16	CQ	100	
17	AR	70	
17	CR	70	
18	AS	79	
18	CS	79	
19	AT	99	
19	CT	99	
20	AA	1511	
20	CA	1511	
21	AV	18	
21	CV	18	
22	AW	77	
22	CW	77	
23	AY	687	
23	CY	687	
24	AU	6	
24	CU	6	
25	BC	228	
25	DC	228	
26	BD	275	
26	DD	275	
27	BE	205	
27	DE	205	

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Mol	Chain	Length	Quality of chain
28	BF	208	
28	DF	208	
29	BG	181	
29	DG	181	
30	BH	167	
30	DH	167	
31	BJ	170	
31	DJ	170	
32	BK	140	
32	DK	140	
33	BO	122	
33	DO	122	
34	BP	146	
34	DP	146	
35	BQ	141	
35	DQ	141	
36	BR	117	
36	DR	117	
37	BS	99	
37	DS	99	
38	BT	138	
38	DT	138	
39	BU	117	
39	DU	117	
40	BV	101	

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Mol	Chain	Length	Quality of chain
40	DV	101	
41	BW	113	
41	DW	113	
42	BX	93	
42	DX	93	
43	BY	107	
43	DY	107	
44	BZ	185	
44	DZ	185	
45	B0	84	
45	D0	84	
46	B1	93	
46	D1	93	
47	B4	35	
47	D4	35	
48	BN	138	
48	DN	138	
49	B2	71	
49	D2	71	
50	B3	60	
50	D3	60	
51	B5	59	
51	D5	59	
52	B6	50	
52	D6	50	

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Mol	Chain	Length	Quality of chain
53	B7	49	
53	D7	49	
54	B8	64	
54	D8	64	
55	B9	37	
55	D9	37	
56	Be	103	
56	De	103	
57	Bf	31	
57	Bg	31	
57	Df	31	
57	Dg	31	
58	Bh	30	
58	Dh	30	
59	BB	119	
59	DB	119	
60	BA	2879	
60	DA	2879	

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
24	KBE	AU	1	-	-	-	X
24	DPP	AU	2	-	-	X	-
24	5OH	AU	6	-	-	X	-
24	5OH	CU	6	-	-	X	-
61	GNP	CY	702	-	-	X	-

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 308202 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AB	235	Total	C	N	O	S	0	0	0
			1910	1218	342	345	5			
1	CB	235	Total	C	N	O	S	0	0	0
			1910	1218	342	345	5			

- Molecule 2 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AC	207	Total	C	N	O	S	0	0	0
			1621	1022	315	283	1			
2	CC	207	Total	C	N	O	S	0	0	0
			1621	1022	315	283	1			

- Molecule 3 is a protein called 30S ribosomal protein S4.

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

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AE	151	Total	C	N	O	S	0	0	0
			1156	729	218	205	4			
4	CE	151	Total	C	N	O	S	0	0	0
			1156	729	218	205	4			

- Molecule 5 is a protein called 30S ribosomal protein S6.

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

- Molecule 6 is a protein called 30S ribosomal protein S7.

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

- Molecule 7 is a protein called 30S ribosomal protein S8.

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

- Molecule 8 is a protein called 30S ribosomal protein S9.

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

- Molecule 9 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AJ	99	Total	C	N	O	S	0	0	0
			802	504	157	140	1			
9	CJ	99	Total	C	N	O	S	0	0	0
			802	504	157	140	1			

- Molecule 10 is a protein called 30S ribosomal protein S11.

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 11 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AL	125	Total	C	N	O	S	0	0	0
			976	614	196	165	1			
11	CL	125	Total	C	N	O	S	0	0	0
			976	614	196	165	1			

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AM	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			
12	CM	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			

- Molecule 13 is a protein called 30S ribosomal protein S14 type Z.

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

- Molecule 14 is a protein called 30S ribosomal protein S15.

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

- Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AP	84	Total	C	N	O	S	0	0	0
			706	446	140	119	1			
15	CP	84	Total	C	N	O	S	0	0	0
			706	446	140	119	1			

- Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AQ	100	Total	C	N	O	S	0	0	0
			835	534	156	143	2			
16	CQ	100	Total	C	N	O	S	0	0	0
			835	534	156	143	2			

- Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	AR	70	Total	C	N	O	0	0	0
			574	367	112	95			
17	CR	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AS	79	Total	C	N	O	S	0	0	0
			634	405	115	112	2			
18	CS	79	Total	C	N	O	S	0	0	0
			634	405	115	112	2			

- Molecule 19 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AT	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			
19	CT	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

- Molecule 20 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AA	1511	Total	C	N	O	P	0	0	0
			32474	14455	6015	10494	1510			
20	CA	1511	Total	C	N	O	P	0	0	0
			32474	14455	6015	10494	1510			

- Molecule 21 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AV	18	Total	C	N	O	P	0	0	0
			393	177	81	118	17			
21	CV	18	Total	C	N	O	P	0	0	0
			393	177	81	118	17			

- Molecule 22 is a RNA chain called tRNA-Met.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AW	77	Total	C	N	O	P	0	0	0
			1635	732	291	536	76			
22	CW	77	Total	C	N	O	P	0	0	0
			1635	732	291	536	76			

- Molecule 23 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AY	687	Total	C	N	O	S	0	0	0
			5380	3414	922	1024	20			
23	CY	687	Total	C	N	O	S	0	0	0
			5380	3414	922	1024	20			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AY	129	LYS	HIS	conflict	UNP Q72I01
AY	226	ASN	HIS	conflict	UNP Q72I01
CY	129	LYS	HIS	conflict	UNP Q72I01
CY	226	ASN	HIS	conflict	UNP Q72I01

- Molecule 24 is a protein called Viomycin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	AU	6	Total	C	N	O	0	0	0
			48	25	13	10			
24	CU	6	Total	C	N	O	0	0	0
			48	25	13	10			

- Molecule 25 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BC	228	Total	C	N	O	S	0	0	0
			1742	1101	319	319	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	DC	228	Total	C	N	O	S	0	0	0
			1742	1101	319	319	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BC	20	VAL	ILE	conflict	UNP Q72GV9
BC	28	ARG	HIS	conflict	UNP Q72GV9
DC	20	VAL	ILE	conflict	UNP Q72GV9
DC	28	ARG	HIS	conflict	UNP Q72GV9

- Molecule 26 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BD	275	Total	C	N	O	S	0	0	0
			2145	1353	428	361	3			
26	DD	275	Total	C	N	O	S	0	0	0
			2145	1353	428	361	3			

- Molecule 27 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BE	205	Total	C	N	O	S	0	0	0
			1569	991	300	272	6			
27	DE	205	Total	C	N	O	S	0	0	0
			1569	991	300	272	6			

- Molecule 28 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BF	208	Total	C	N	O	S	0	0	0
			1628	1037	304	284	3			
28	DF	208	Total	C	N	O	S	0	0	0
			1628	1037	304	284	3			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BF	2	LYS	-	insertion	UNP Q72I05
BF	3	GLU	-	insertion	UNP Q72I05
BF	4	VAL	-	insertion	UNP Q72I05

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Chain	Residue	Modelled	Actual	Comment	Reference
BF	5	ALA	-	insertion	UNP Q72I05
BF	6	VAL	-	insertion	UNP Q72I05
DF	2	LYS	-	insertion	UNP Q72I05
DF	3	GLU	-	insertion	UNP Q72I05
DF	4	VAL	-	insertion	UNP Q72I05
DF	5	ALA	-	insertion	UNP Q72I05
DF	6	VAL	-	insertion	UNP Q72I05

- Molecule 29 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			
29	DG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BG	5	VAL	LEU	conflict	UNP Q72I16
DG	5	VAL	LEU	conflict	UNP Q72I16

- Molecule 30 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BH	167	Total	C	N	O	S	0	0	0
			1274	806	238	229	1			
30	DH	167	Total	C	N	O	S	0	0	0
			1274	806	238	229	1			

- Molecule 31 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
31	BJ	170	Total	C	N	O	0	0	0
			851	510	170	171			
31	DJ	170	Total	C	N	O	0	0	0
			851	510	170	171			

- Molecule 32 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BK	140	Total	C	N	O	S	0	0	0
			1035	659	183	188	5			
32	DK	140	Total	C	N	O	S	0	0	0
			1035	659	183	188	5			

- Molecule 33 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
33	DO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BO	69	ILE	VAL	conflict	UNP Q72I14
DO	69	ILE	VAL	conflict	UNP Q72I14

- Molecule 34 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			
34	DP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 35 is a protein called 50S ribosomal protein L16.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BQ	32	TYR	PHE	conflict	UNP Q72I11
DQ	32	TYR	PHE	conflict	UNP Q72I11

- Molecule 36 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
36	BR	117	Total	C	N	O	0	0	0
			960	599	202	159			
36	DR	117	Total	C	N	O	0	0	0
			960	599	202	159			

- Molecule 37 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
37	BS	99	Total	C	N	O	0	0	0
			775	488	155	132			
37	DS	99	Total	C	N	O	0	0	0
			775	488	155	132			

- Molecule 38 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BT	138	Total	C	N	O	S	0	0	0
			1147	713	235	198	1			
38	DT	138	Total	C	N	O	S	0	0	0
			1147	713	235	198	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BT	123	GLN	LYS	conflict	UNP Q72JU9
BT	135	ALA	VAL	conflict	UNP Q72JU9
DT	123	GLN	LYS	conflict	UNP Q72JU9
DT	135	ALA	VAL	conflict	UNP Q72JU9

- Molecule 39 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BU	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
39	DU	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 40 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	DV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 41 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BW	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			
41	DW	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			

- Molecule 42 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BX	93	Total	C	N	O	S	0	0	0
			734	477	132	125				
42	DX	93	Total	C	N	O	S	0	0	0
			734	477	132	125				

- Molecule 43 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BY	107	Total	C	N	O	S	0	0	0
			818	524	155	134	5			
43	DY	107	Total	C	N	O	S	0	0	0
			818	524	155	134	5			

- Molecule 44 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BZ	185	Total	C	N	O	S	0	0	0
			1473	939	262	270	2			
44	DZ	185	Total	C	N	O	S	0	0	0
			1473	939	262	270	2			

- Molecule 45 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	B0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			
45	D0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B0	11	ARG	LYS	conflict	UNP Q72HR3
D0	11	ARG	LYS	conflict	UNP Q72HR3

- Molecule 46 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	B1	93	Total	C	N	O	S	0	0	0
			732	460	145	126	1			
46	D1	93	Total	C	N	O	S	0	0	0
			732	460	145	126	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B1	81	LYS	ARG	conflict	UNP Q72G84
D1	81	LYS	ARG	conflict	UNP Q72G84

- Molecule 47 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	B4	35	Total	C	N	O	S	0	0	0
			271	174	44	50	3			
47	D4	35	Total	C	N	O	S	0	0	0
			271	174	44	50	3			

- Molecule 48 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
48	DN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 49 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			
49	D2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B3	60	Total	C	N	O	S	0	0	0
			477	303	91	82	1			
50	D3	60	Total	C	N	O	S	0	0	0
			477	303	91	82	1			

- Molecule 51 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
51	D5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B5	29	THR	ILE	conflict	UNP P62652
D5	29	THR	ILE	conflict	UNP P62652

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B6	50	Total	C	N	O	S	0	0	0
			433	270	88	71	4			
52	D6	50	Total	C	N	O	S	0	0	0
			433	270	88	71	4			

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			
53	D7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	D8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 55 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	B9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
55	D9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 56 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	Be	102	Total	C	N	O		0	0	0
			686	430	119	137				
56	De	102	Total	C	N	O		0	0	0
			686	430	119	137				

- Molecule 57 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	Bf	31	Total	C	N	O		0	0	0
			156	93	31	32				
57	Bg	31	Total	C	N	O		0	0	0
			156	93	31	32				
57	Df	31	Total	C	N	O		0	0	0
			156	93	31	32				
57	Dg	31	Total	C	N	O		0	0	0
			156	93	31	32				

- Molecule 58 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	Bh	30	Total	C	N	O		0	0	0
			151	90	30	31				
58	Dh	30	Total	C	N	O		0	0	0
			151	90	30	31				

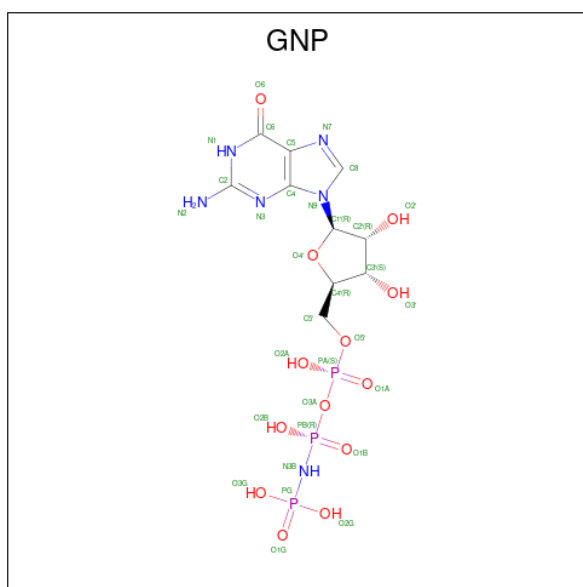
- Molecule 59 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 60 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
60	BA	2879	Total	C	N	O	P	0	0	0
			61997	27594	11582	19943	2878			
60	DA	2879	Total	C	N	O	P	0	0	0
			61997	27594	11582	19943	2878			

- Molecule 61 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
61	AY	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
61	CY	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

- Molecule 62 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	AY	1	Total	Mg	0	0
			1	1		

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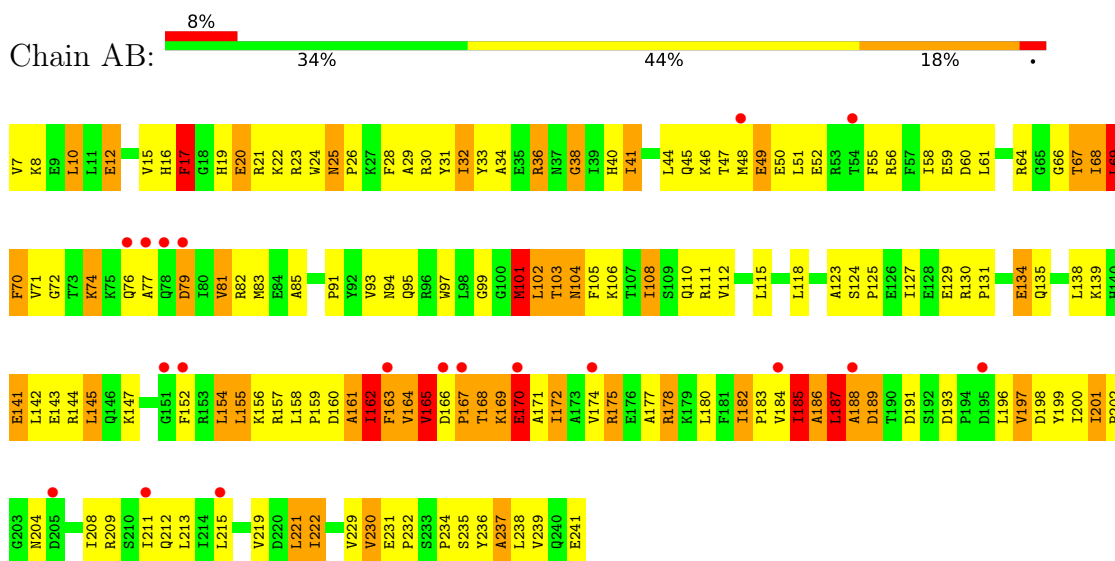
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	CY	1	Total	Mg	0	0
			1	1		

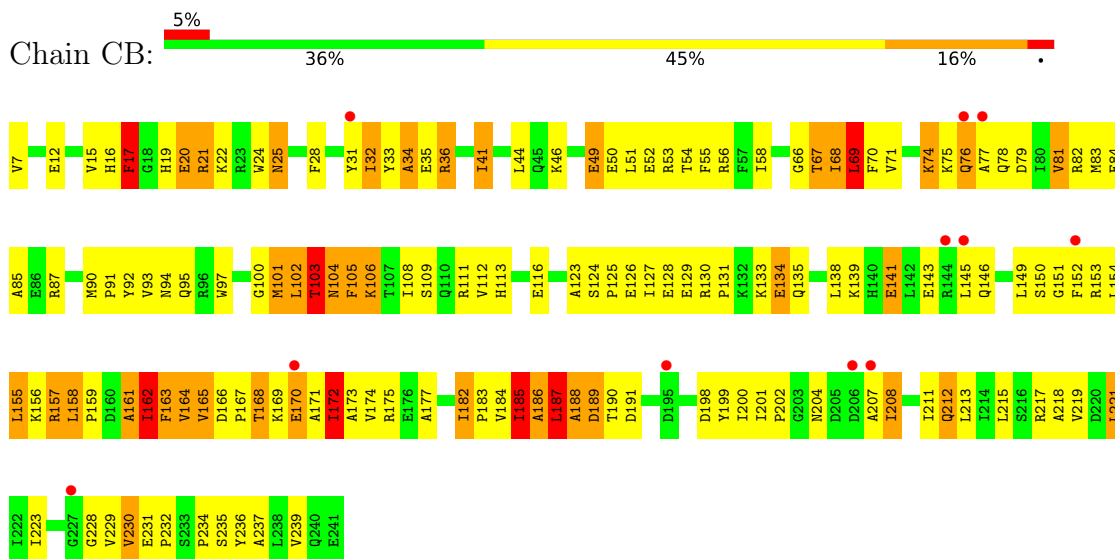
3 Residue-property plots [i](#)

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

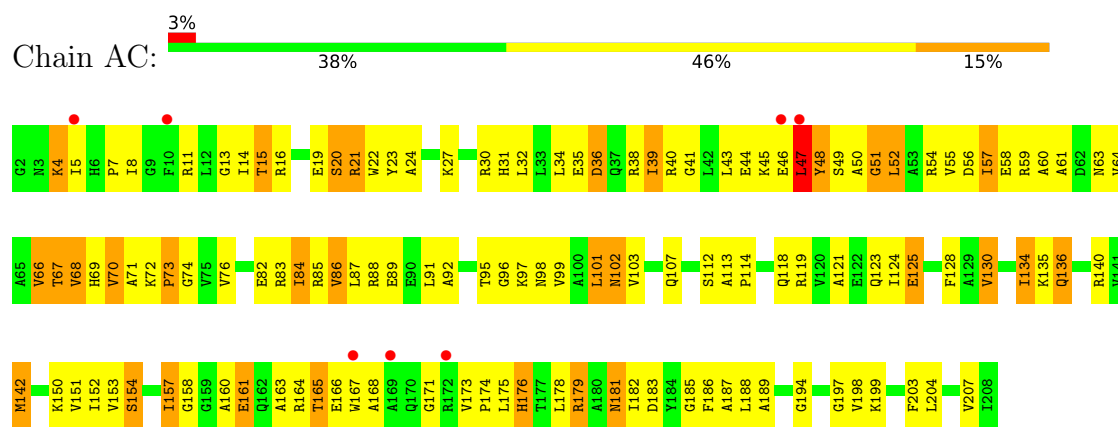
- Molecule 1: 30S ribosomal protein S2



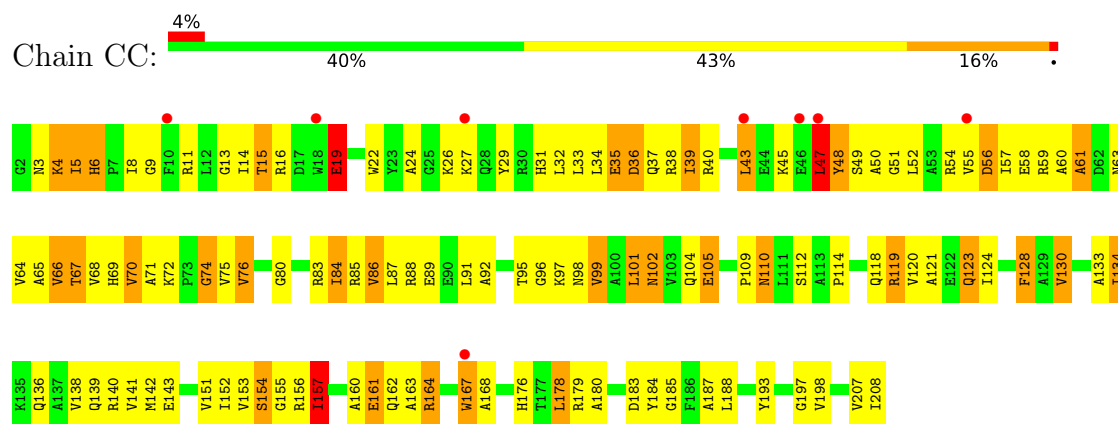
- Molecule 1: 30S ribosomal protein S2



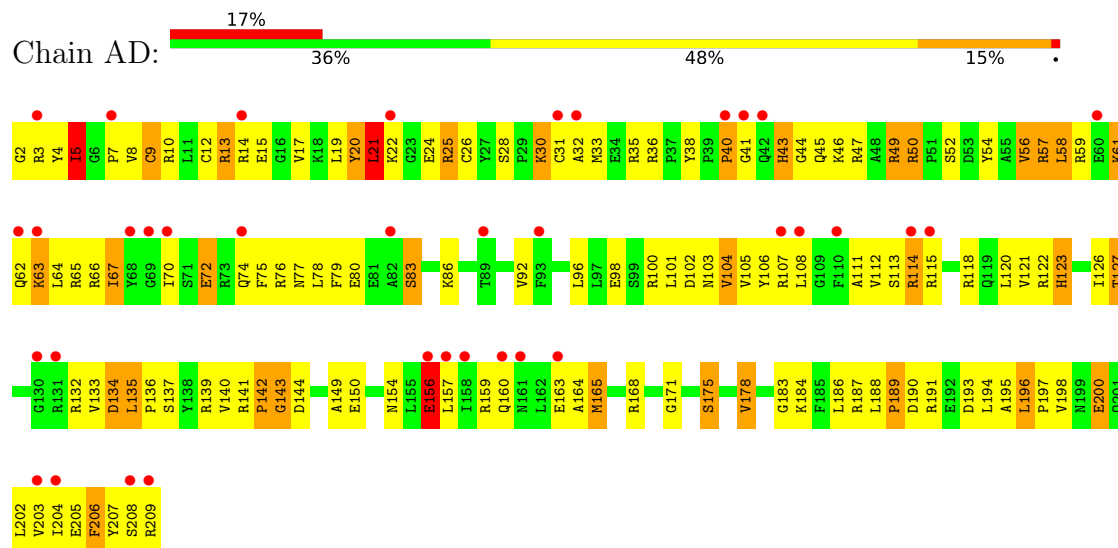
- Molecule 2: 30S ribosomal protein S3



• Molecule 2: 30S ribosomal protein S3

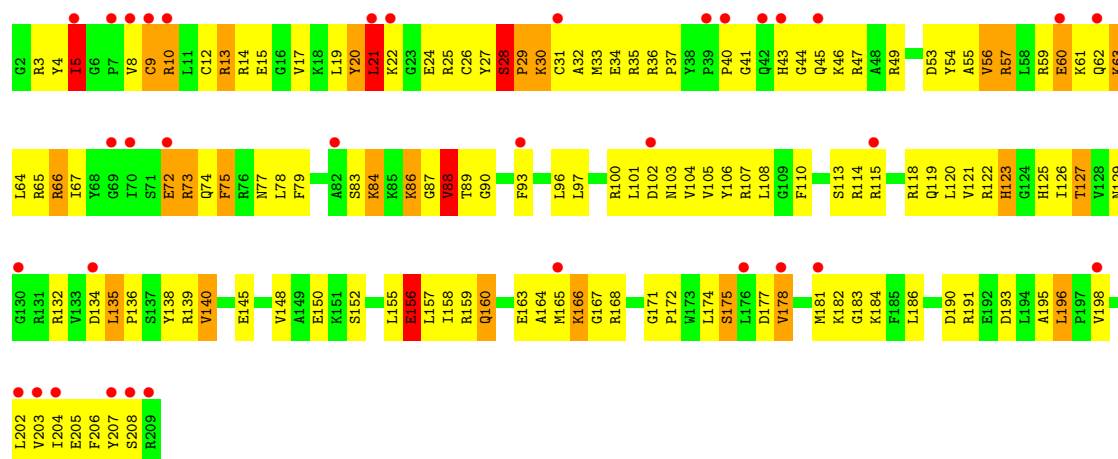


• Molecule 3: 30S ribosomal protein S4

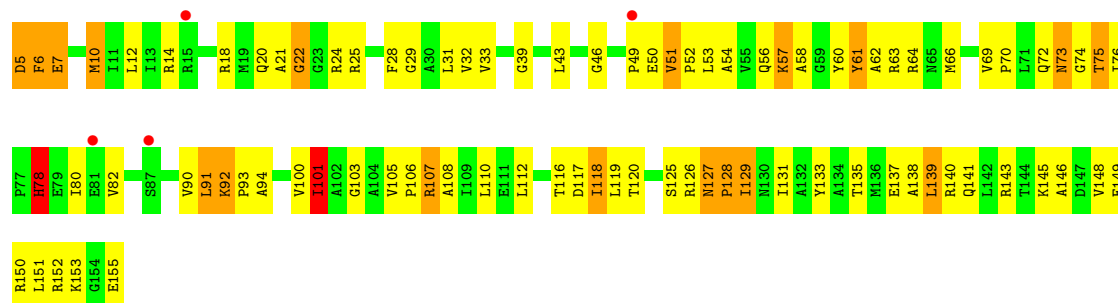
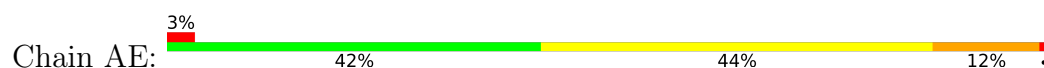


• Molecule 3: 30S ribosomal protein S4

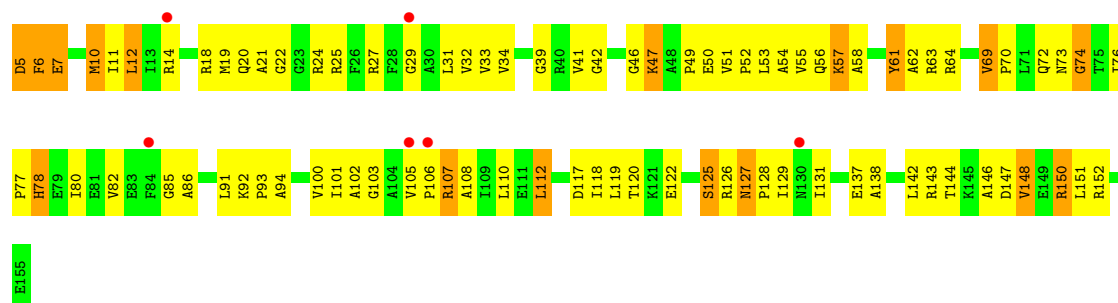




• Molecule 4: 30S ribosomal protein S5



• Molecule 4: 30S ribosomal protein S5

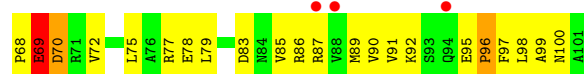


• Molecule 5: 30S ribosomal protein S6

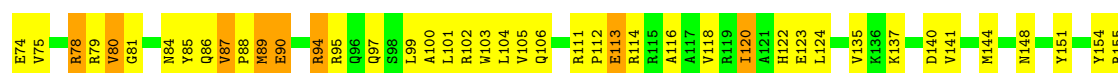
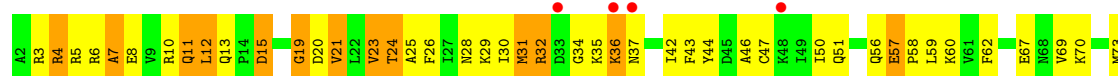
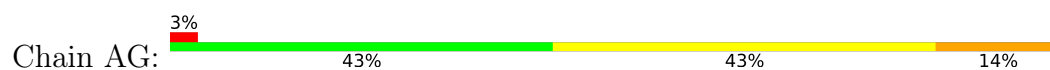




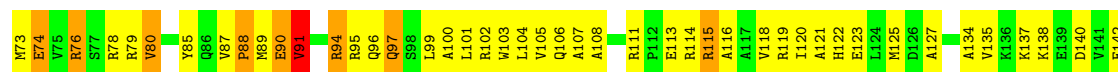
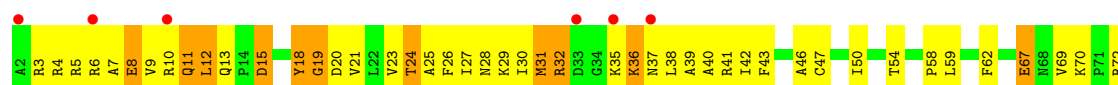
• Molecule 5: 30S ribosomal protein S6



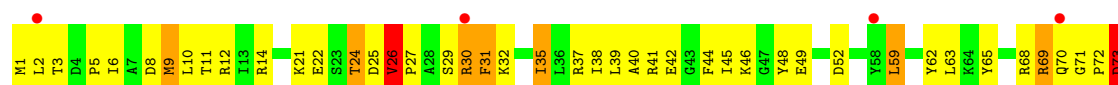
• Molecule 6: 30S ribosomal protein S7



• Molecule 6: 30S ribosomal protein S7

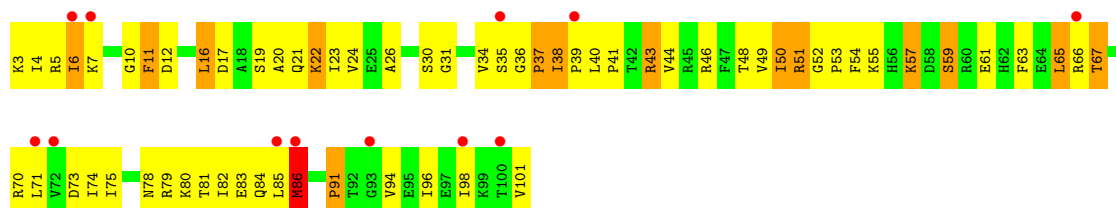


• Molecule 7: 30S ribosomal protein S8



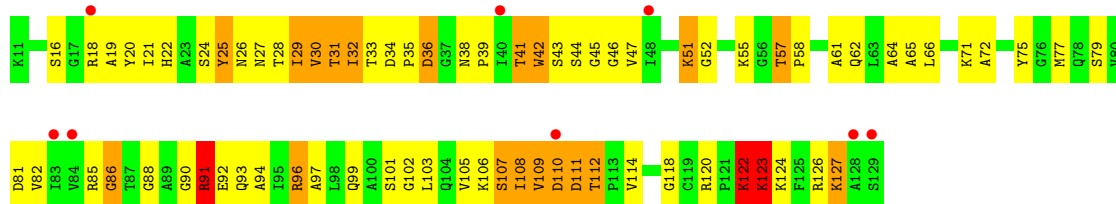
- Molecule 9: 30S ribosomal protein S10

Chain CJ: 



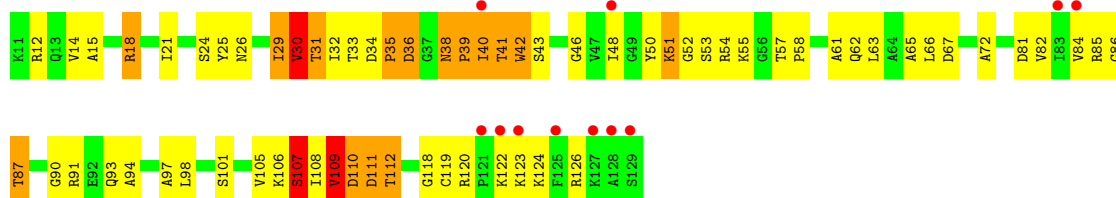
- Molecule 10: 30S ribosomal protein S11

Chain AK: 



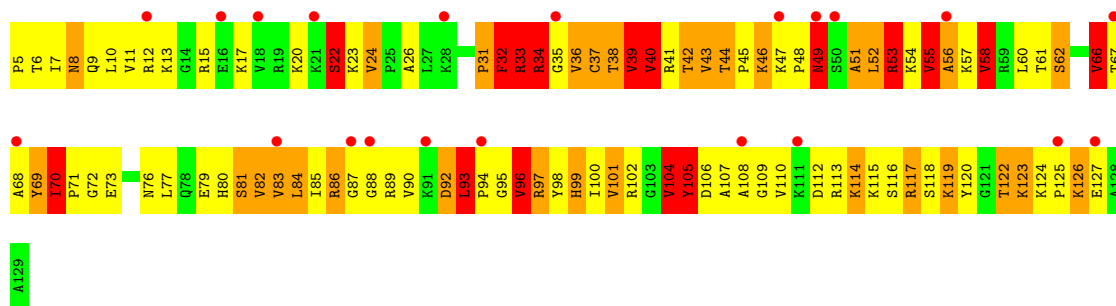
- Molecule 10: 30S ribosomal protein S11

Chain CK: 

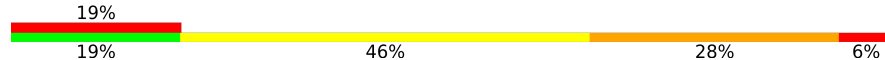


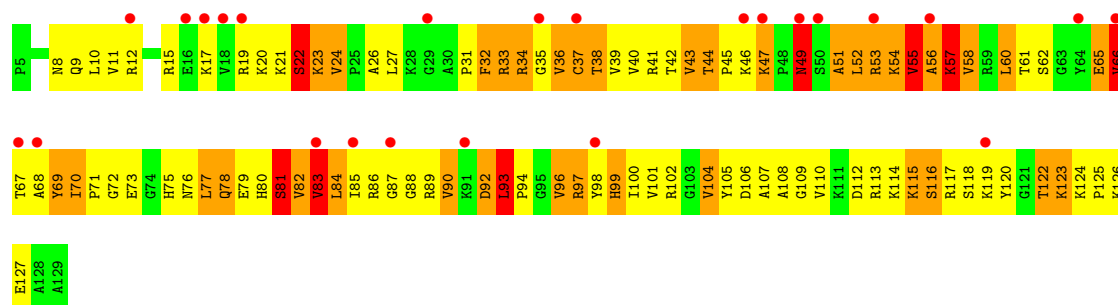
- Molecule 11: 30S ribosomal protein S12

Chain AL: 

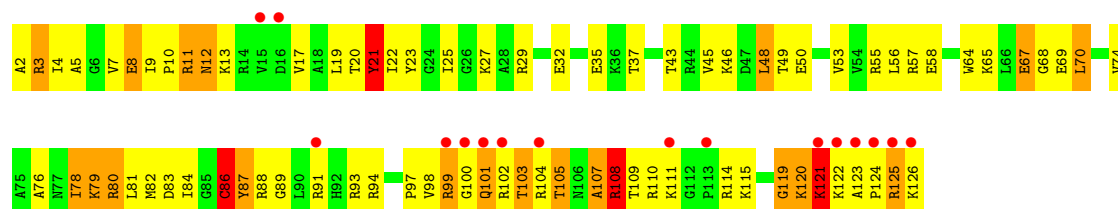


- Molecule 11: 30S ribosomal protein S12

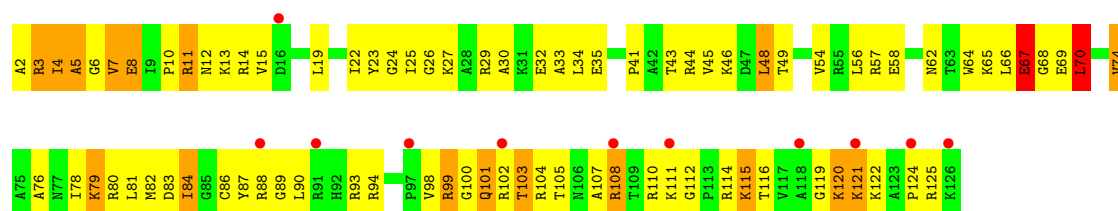
Chain CL: 



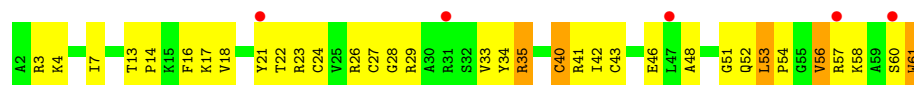
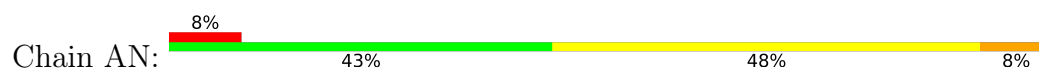
- Molecule 12: 30S ribosomal protein S13



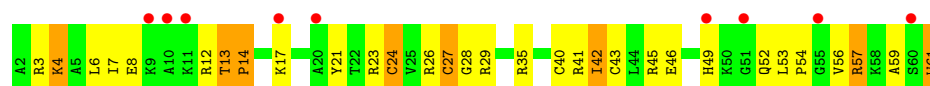
- Molecule 12: 30S ribosomal protein S13



- Molecule 13: 30S ribosomal protein S14 type Z

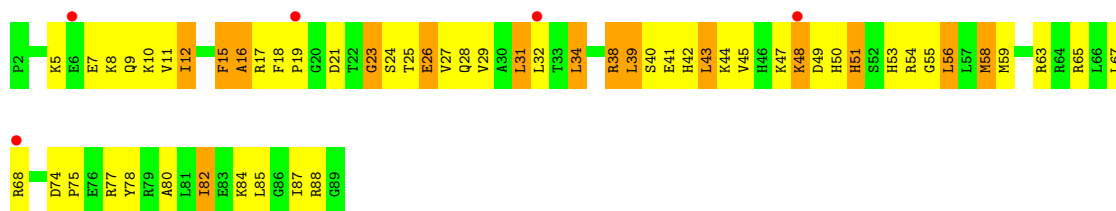


- Molecule 13: 30S ribosomal protein S14 type Z



- Molecule 14: 30S ribosomal protein S15

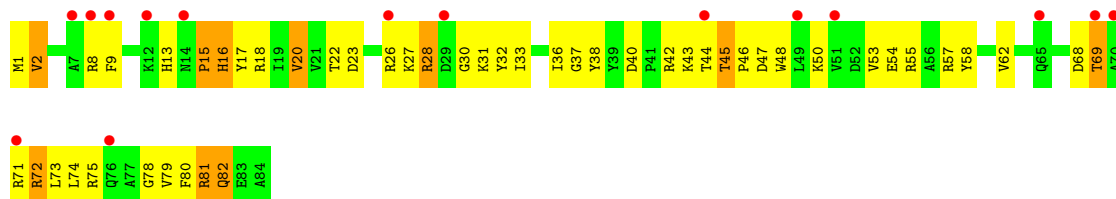
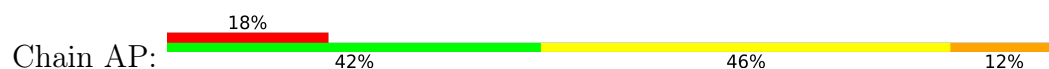




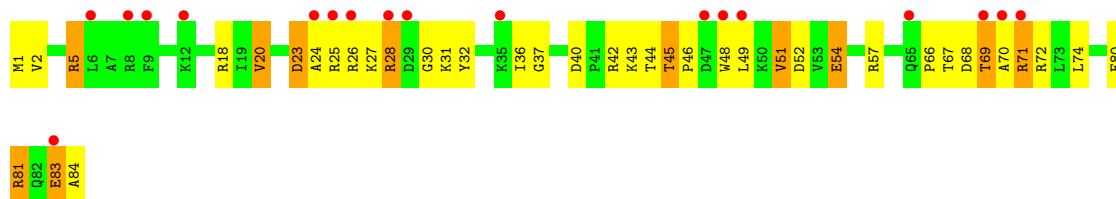
• Molecule 14: 30S ribosomal protein S15



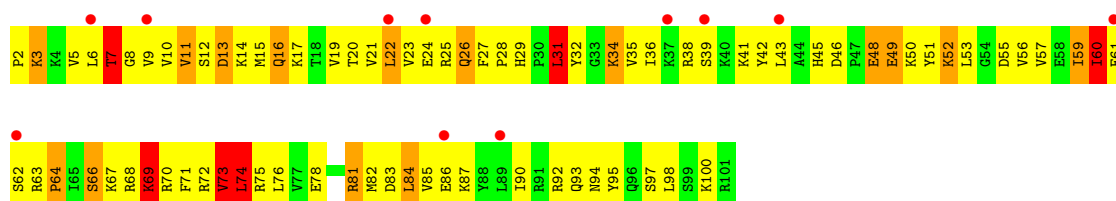
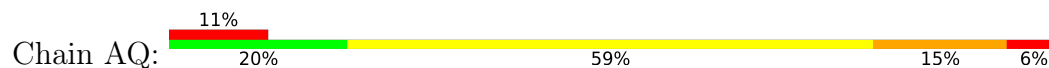
• Molecule 15: 30S ribosomal protein S16



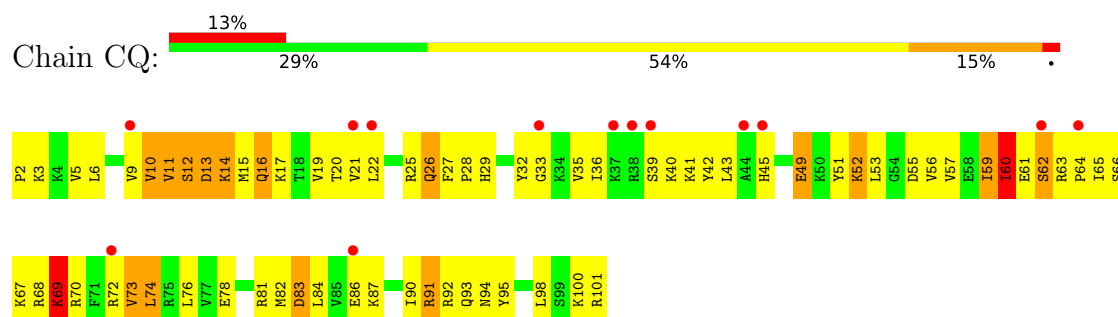
• Molecule 15: 30S ribosomal protein S16



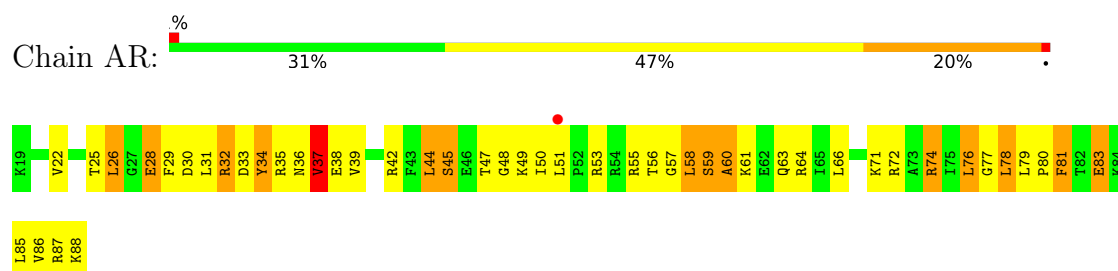
• Molecule 16: 30S ribosomal protein S17



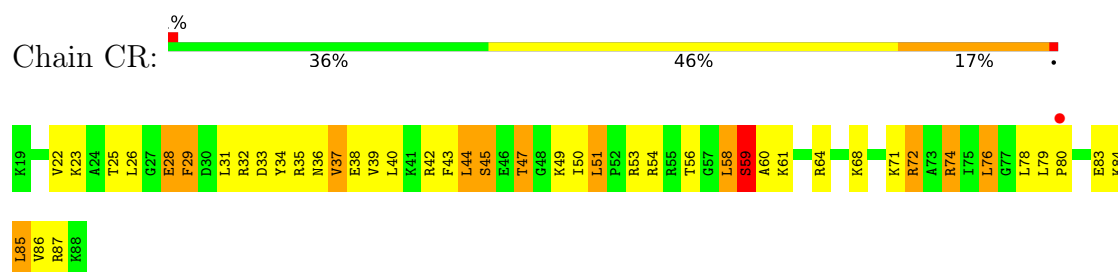
- Molecule 16: 30S ribosomal protein S17



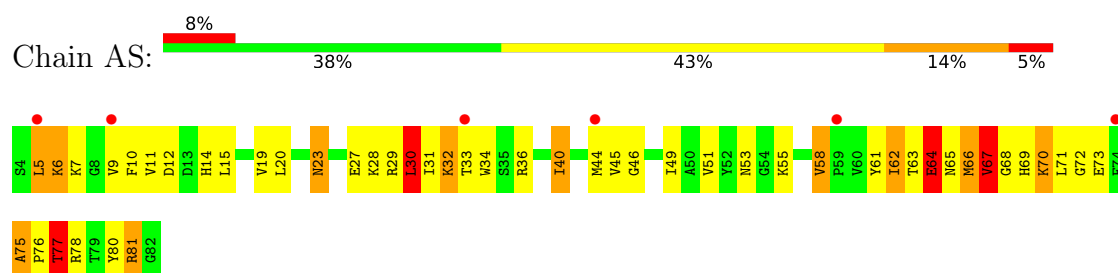
- Molecule 17: 30S ribosomal protein S18



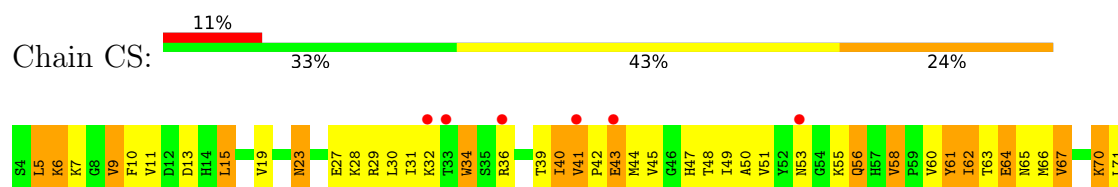
- Molecule 17: 30S ribosomal protein S18



- Molecule 18: 30S ribosomal protein S19



- Molecule 18: 30S ribosomal protein S19

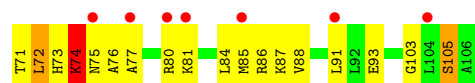
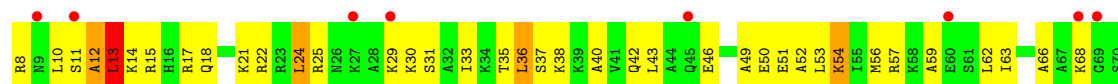
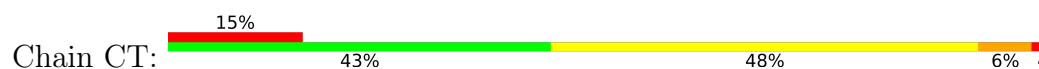




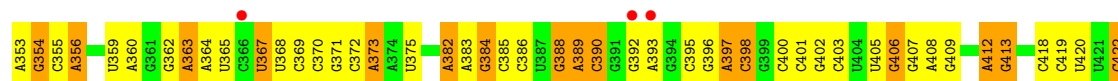
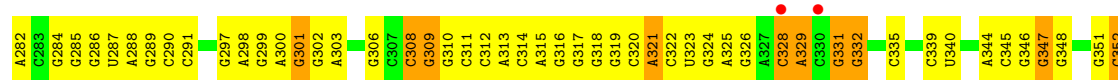
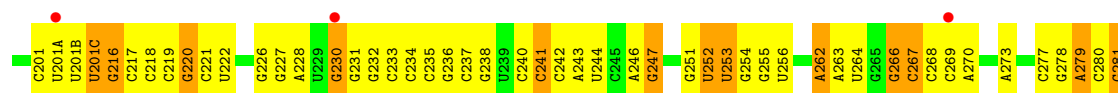
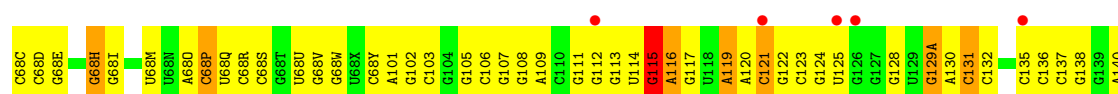
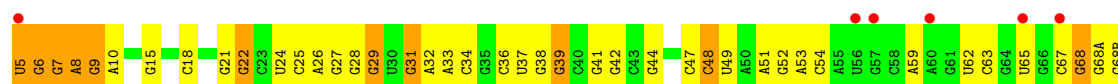
- Molecule 19: 30S ribosomal protein S20

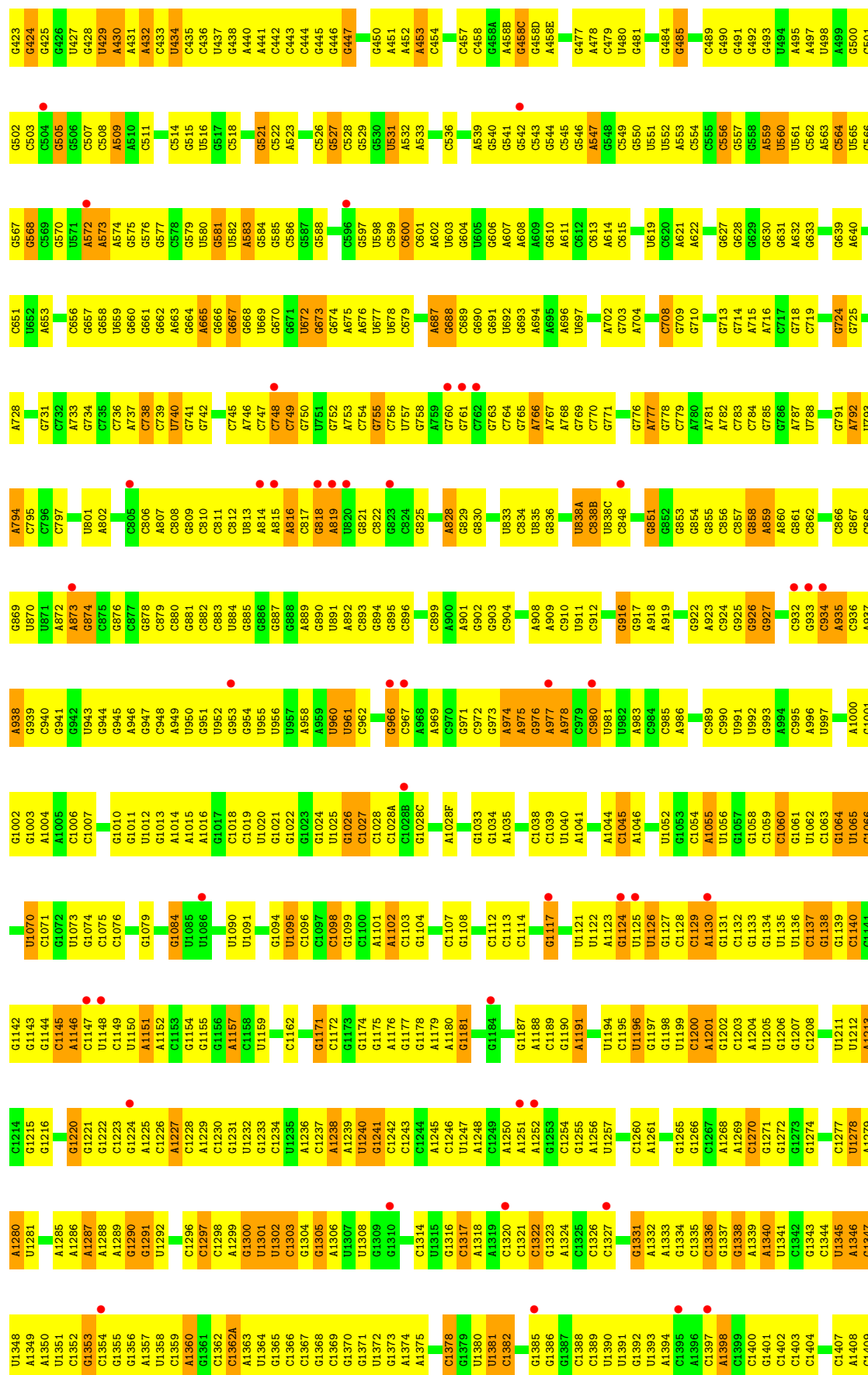


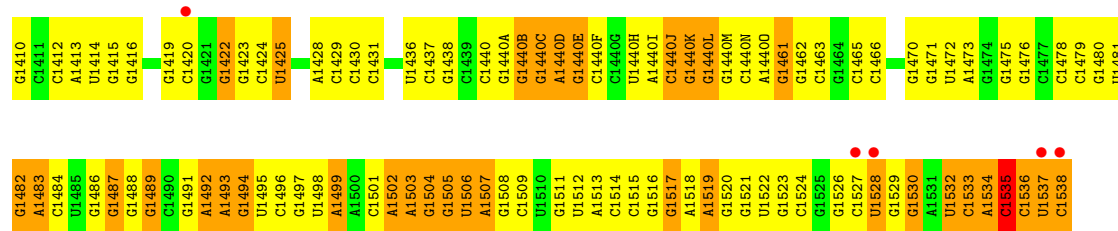
- Molecule 19: 30S ribosomal protein S20



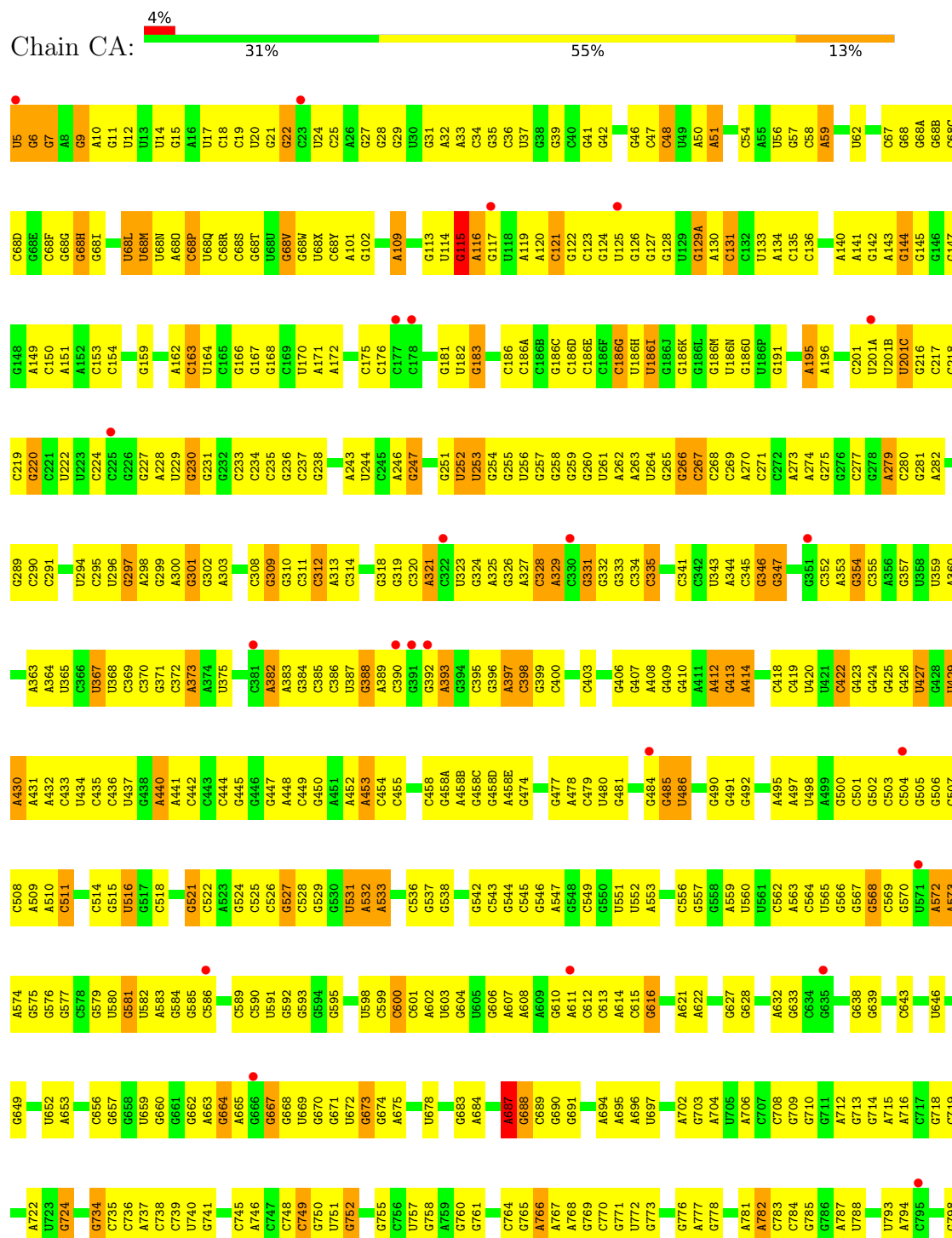
- Molecule 20: 16S ribosomal RNA

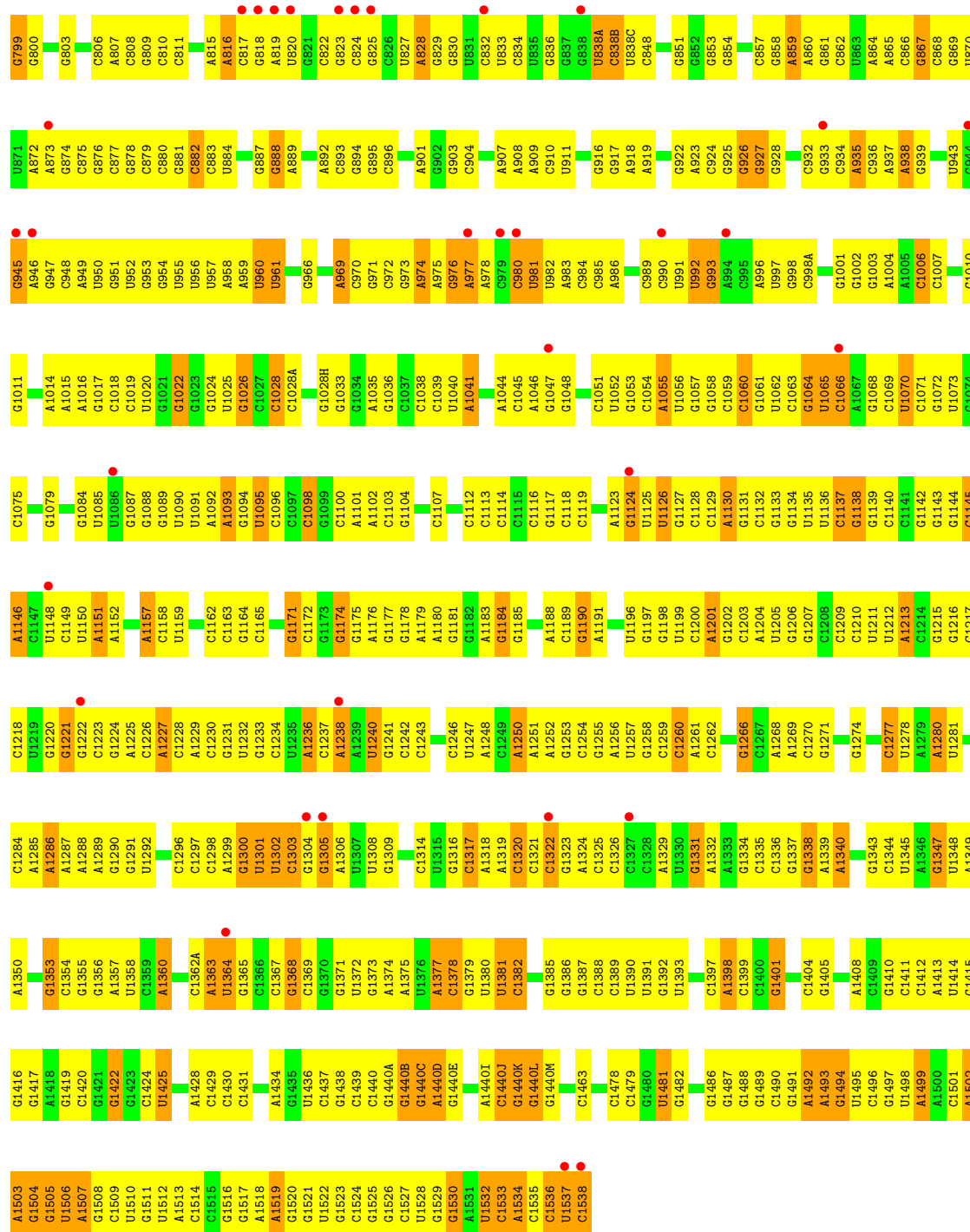




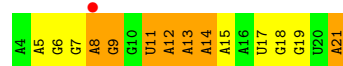


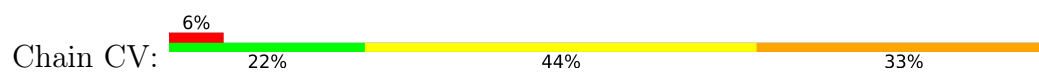
• Molecule 20: 16S ribosomal RNA



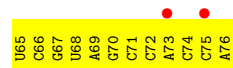
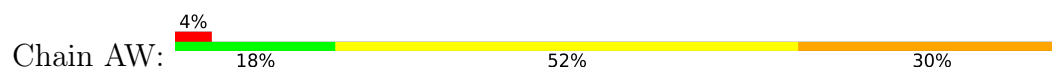


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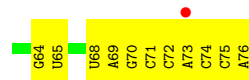
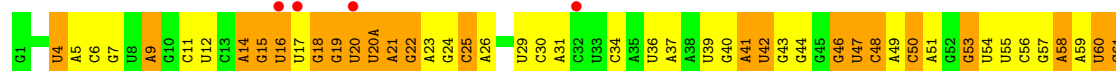




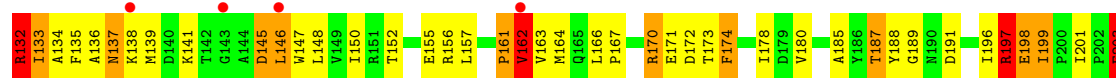
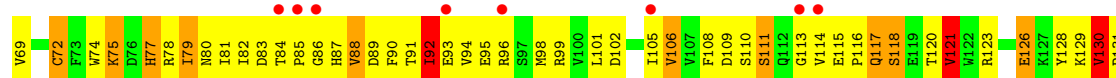
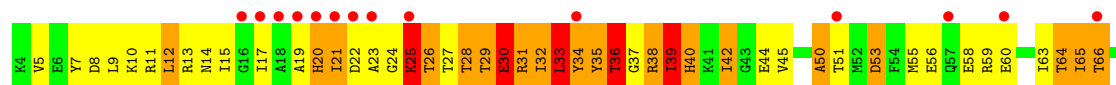
• Molecule 22: tRNA-Met

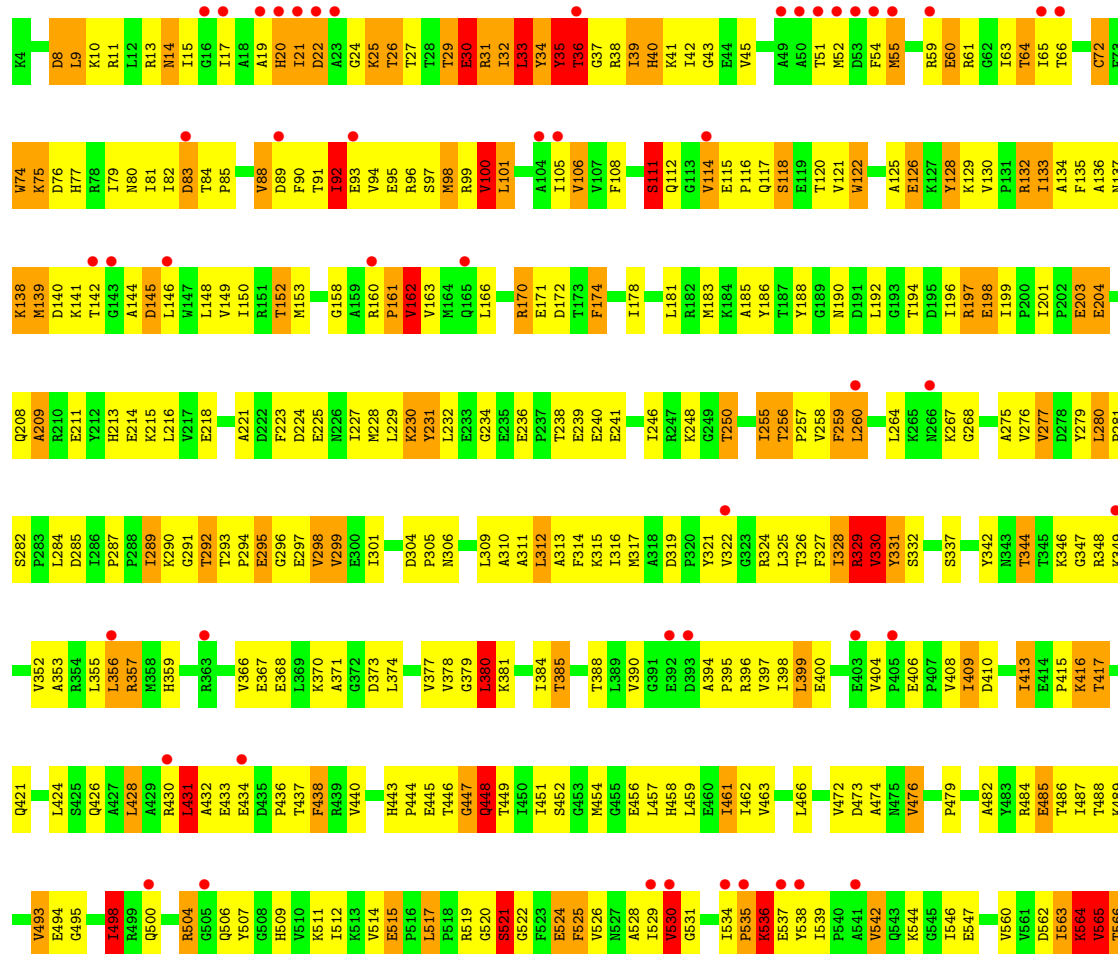


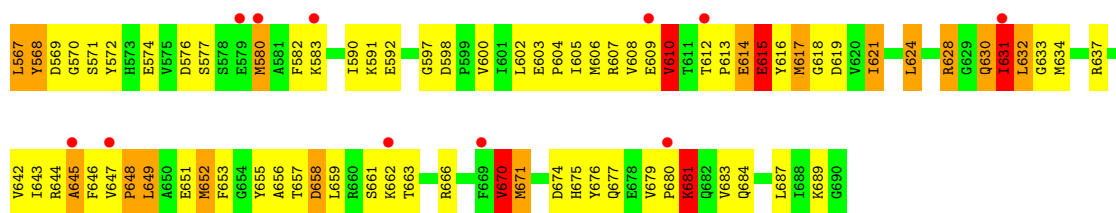
• Molecule 22: tRNA-Met



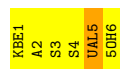
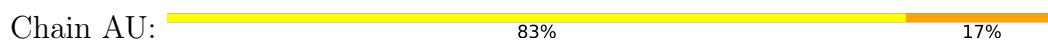
• Molecule 23: Elongation factor G



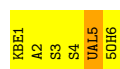
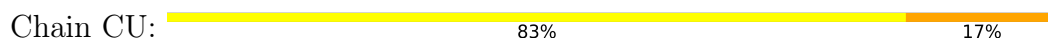




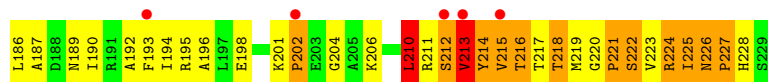
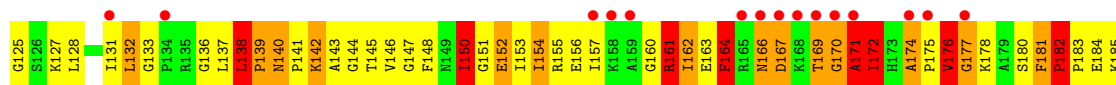
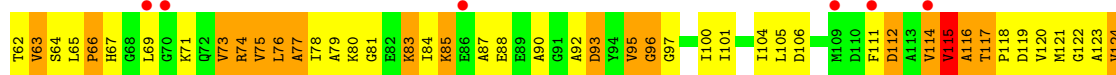
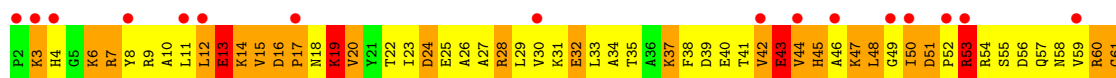
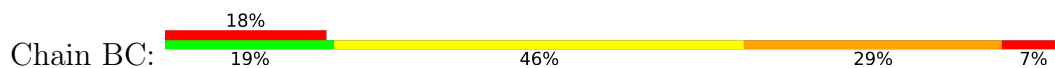
● Molecule 24: Viomycin



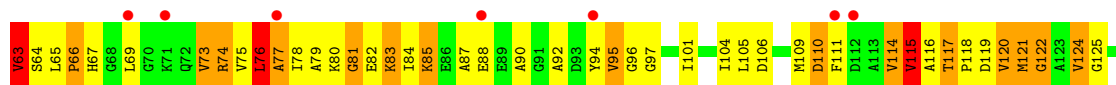
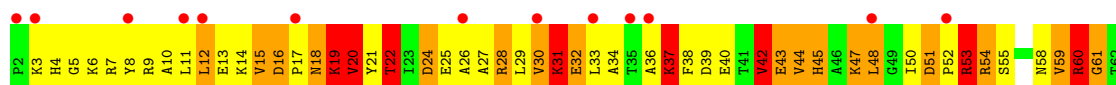
● Molecule 24: Viomycin

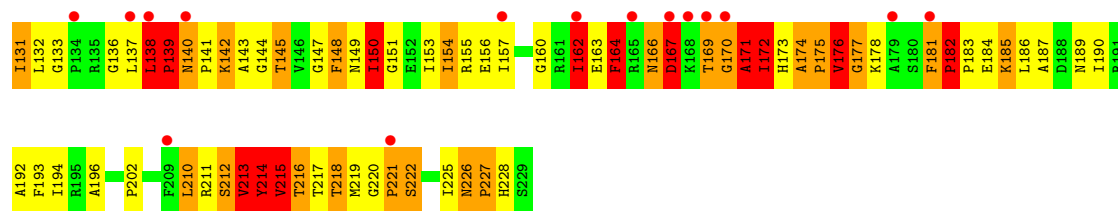


● Molecule 25: 50S ribosomal protein L1

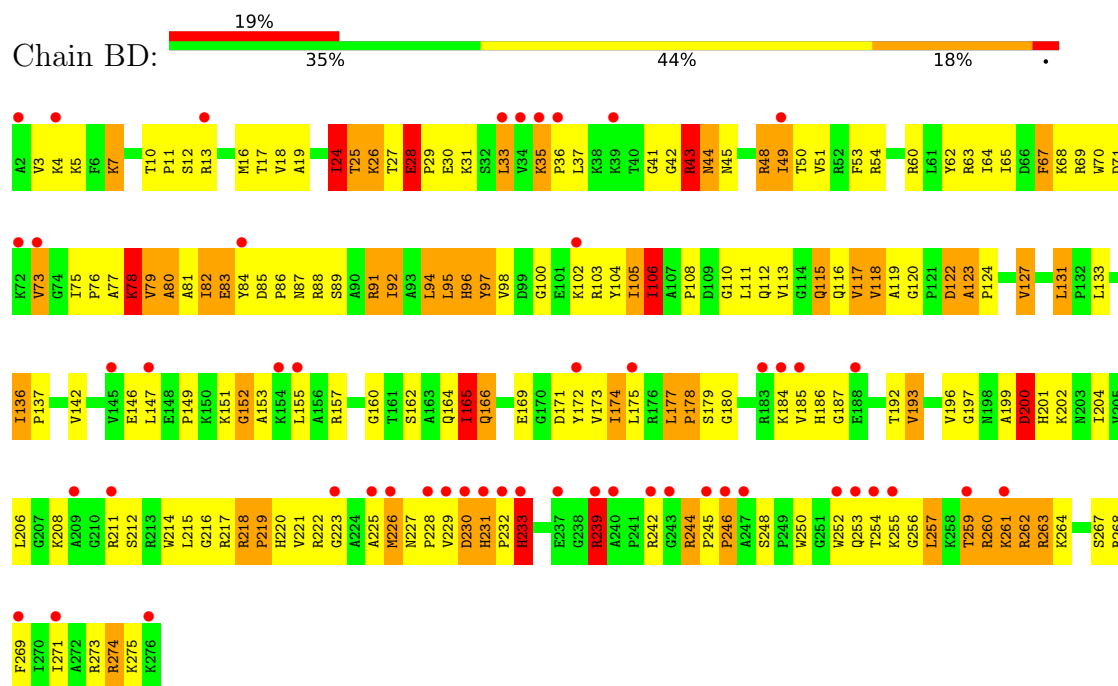


● Molecule 25: 50S ribosomal protein L1

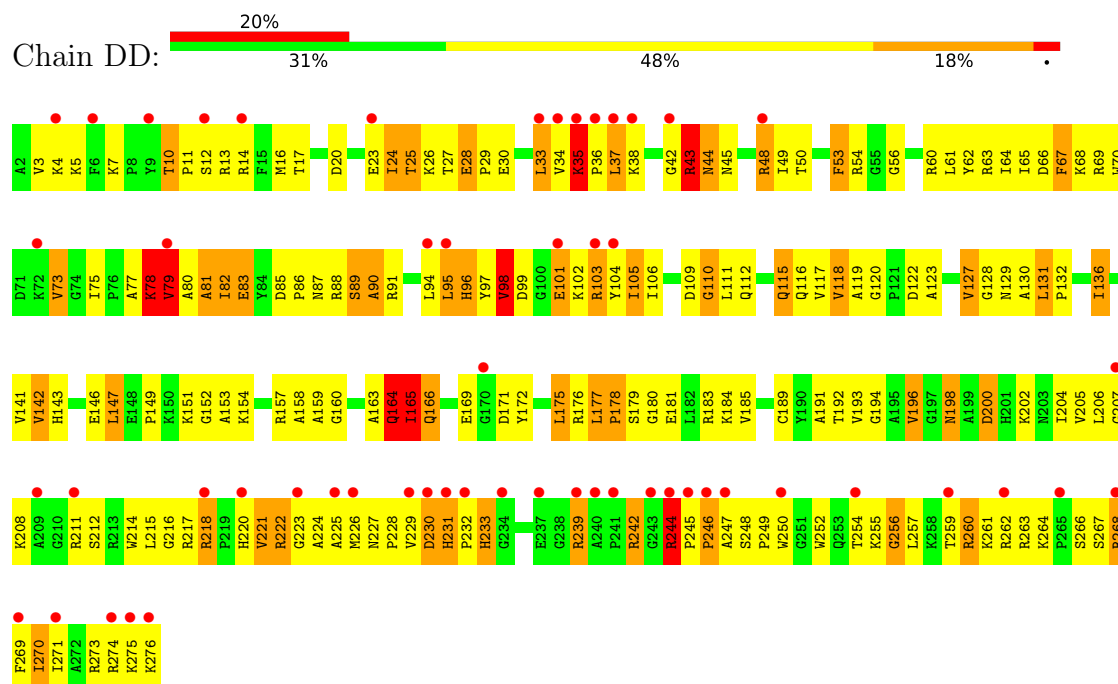




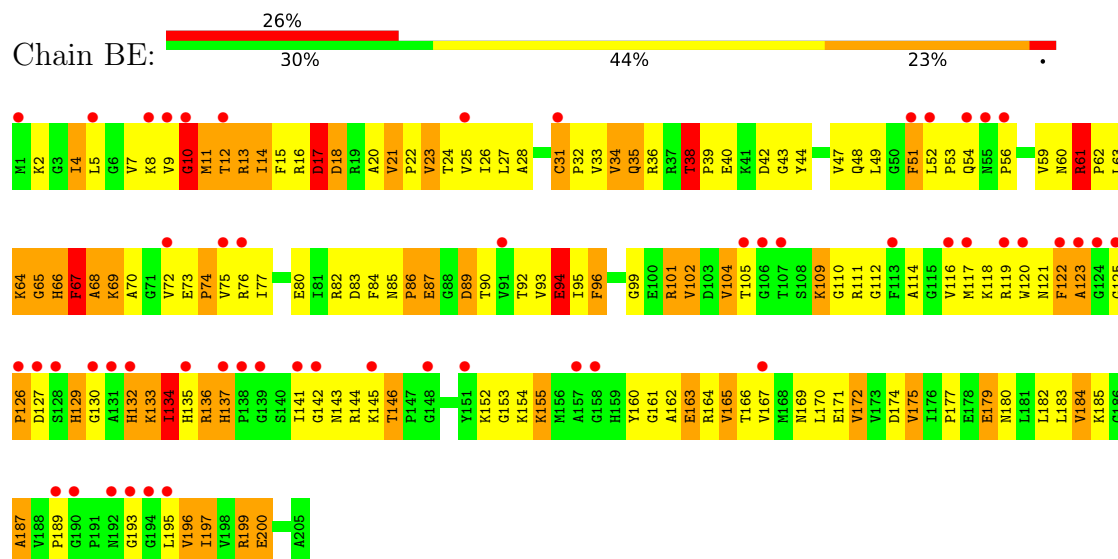
● Molecule 26: 50S ribosomal protein L2



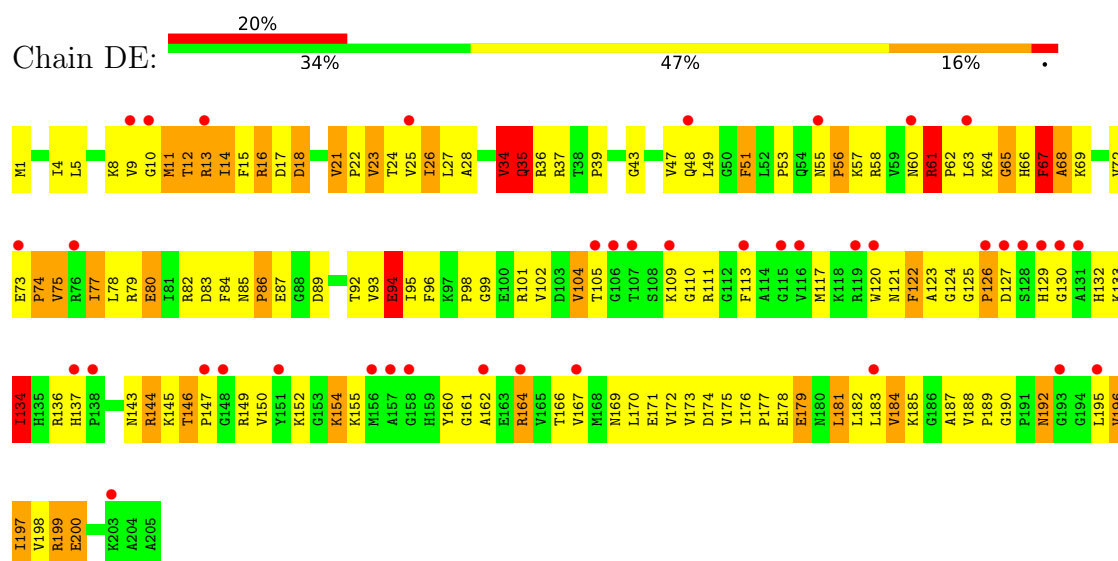
● Molecule 26: 50S ribosomal protein L2



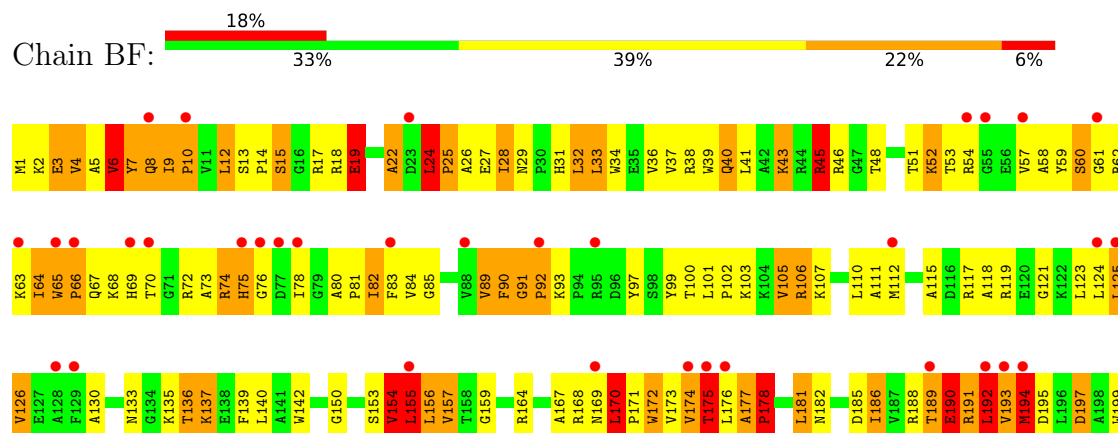
• Molecule 27: 50S ribosomal protein L3

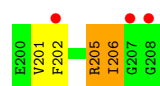


• Molecule 27: 50S ribosomal protein L3

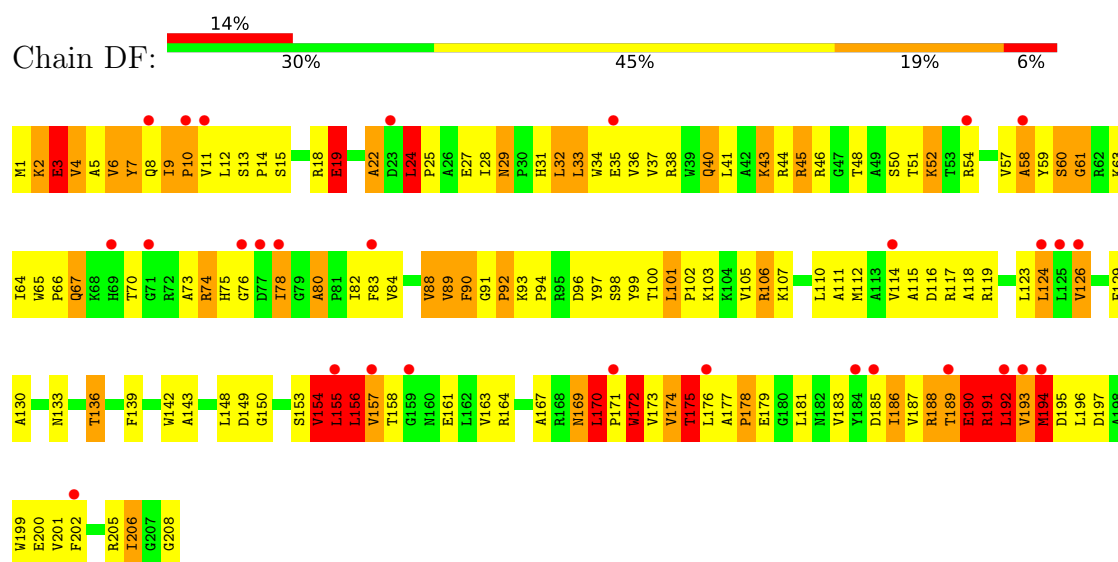


• Molecule 28: 50S ribosomal protein L4

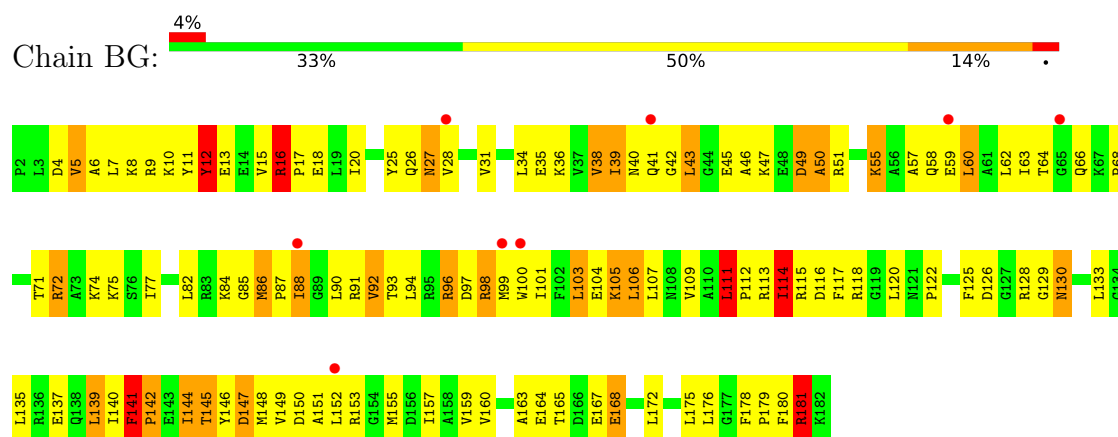




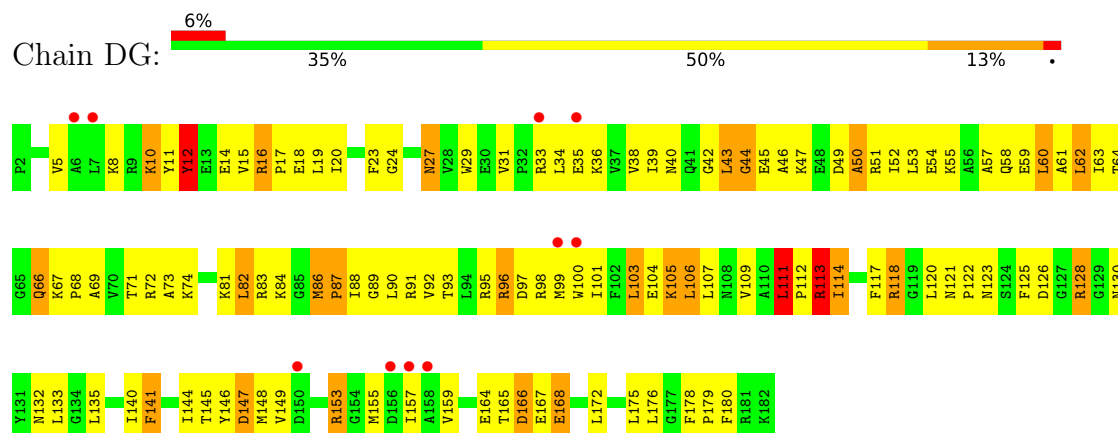
• Molecule 28: 50S ribosomal protein L4



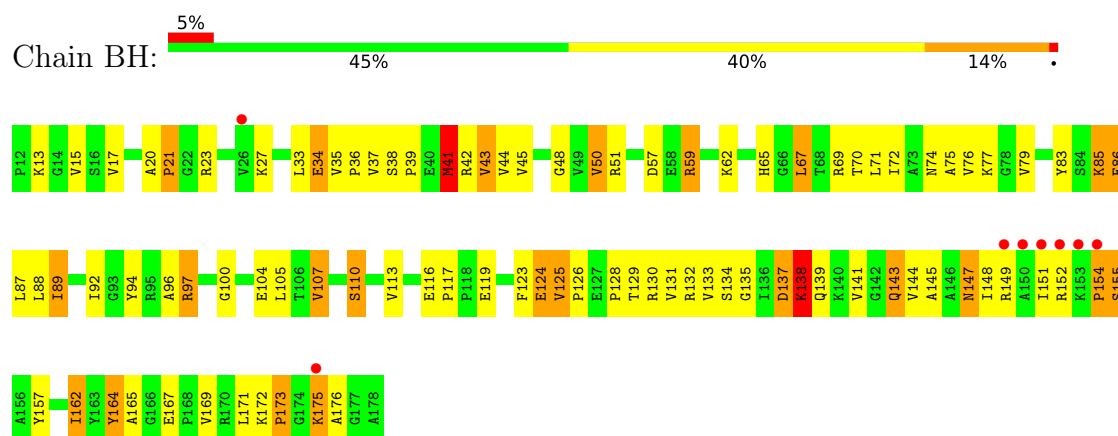
• Molecule 29: 50S ribosomal protein L5



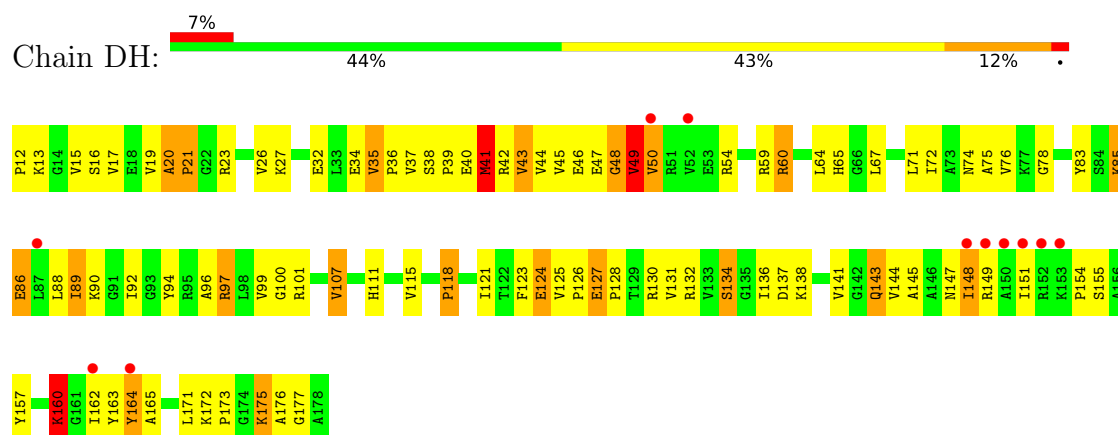
• Molecule 29: 50S ribosomal protein L5



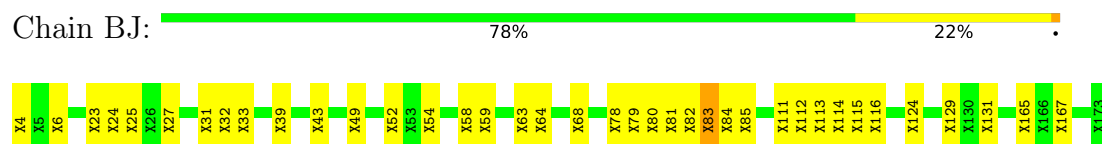
- Molecule 30: 50S ribosomal protein L6



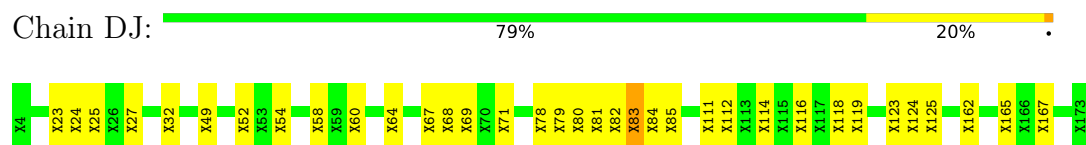
- Molecule 30: 50S ribosomal protein L6



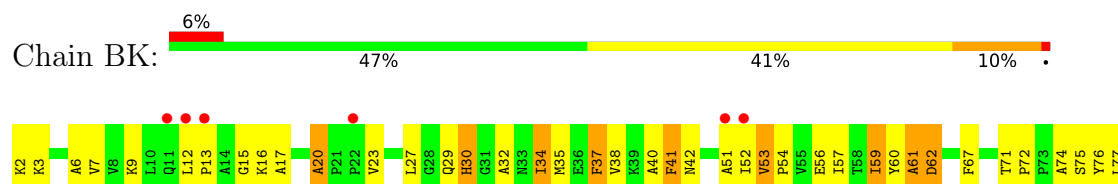
- Molecule 31: 50S ribosomal protein L10



- Molecule 31: 50S ribosomal protein L10



- Molecule 32: 50S ribosomal protein L11

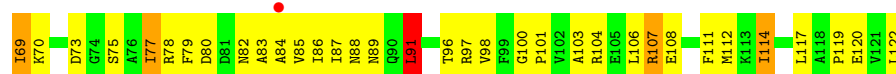
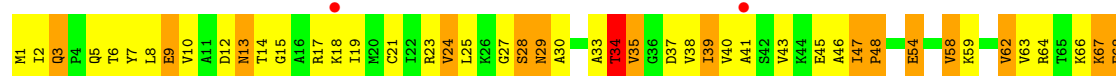




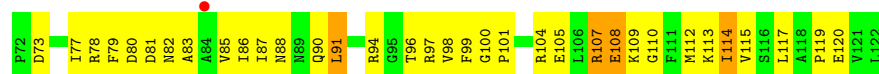
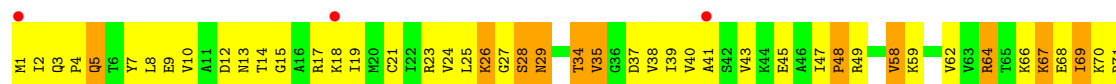
• Molecule 32: 50S ribosomal protein L11



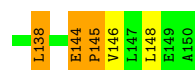
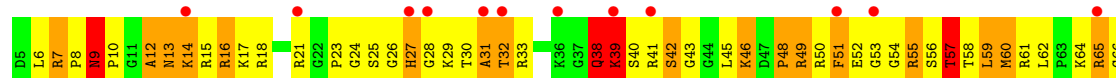
• Molecule 33: 50S ribosomal protein L14



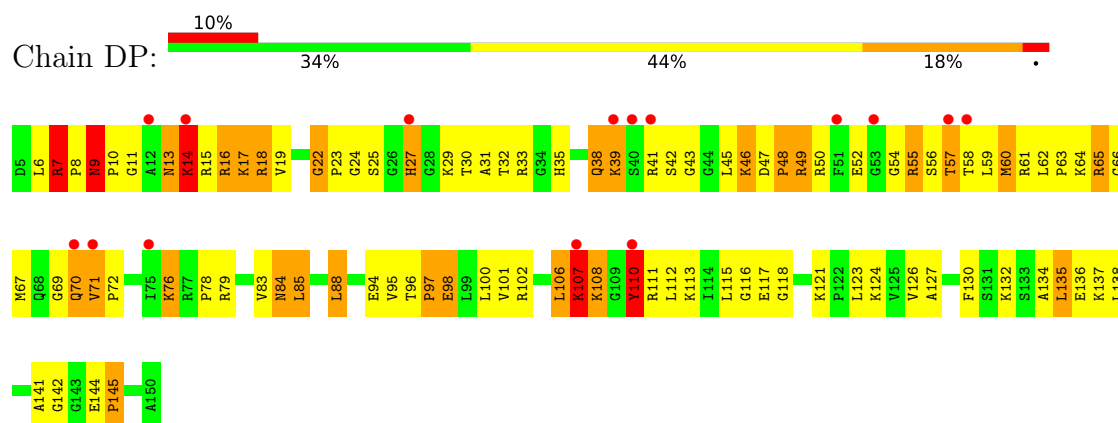
• Molecule 33: 50S ribosomal protein L14



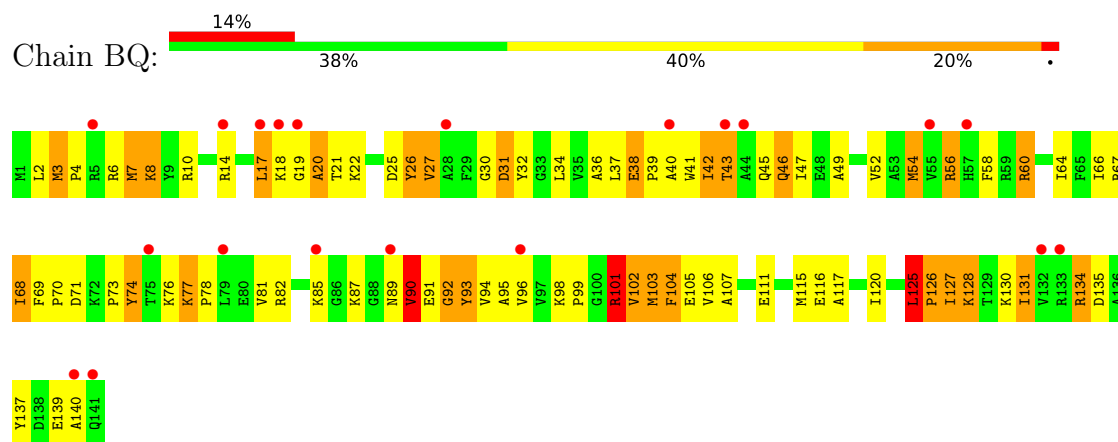
• Molecule 34: 50S ribosomal protein L15



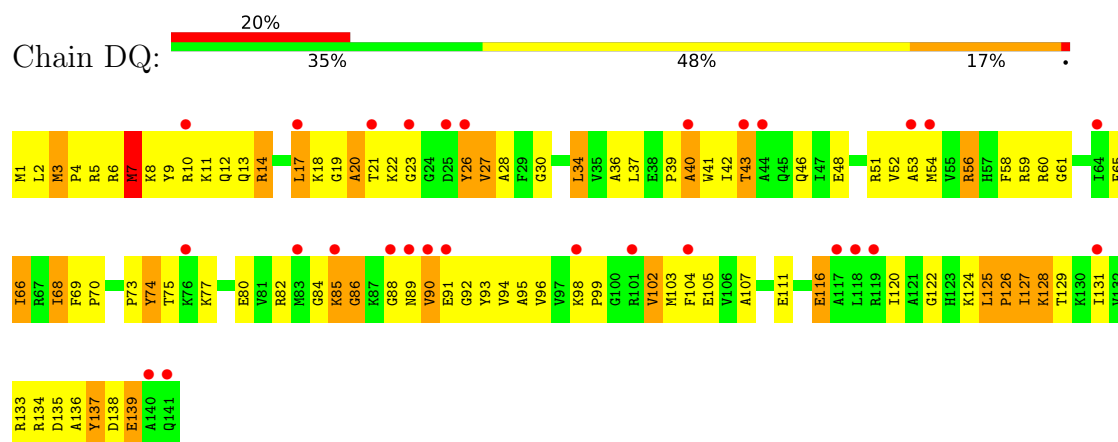
• Molecule 34: 50S ribosomal protein L15



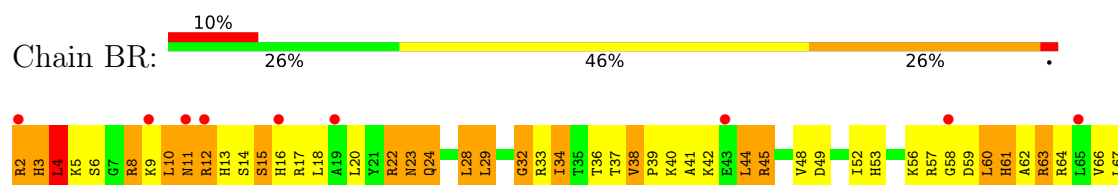
• Molecule 35: 50S ribosomal protein L16

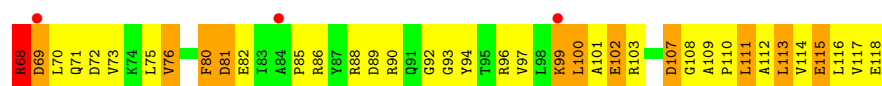


• Molecule 35: 50S ribosomal protein L16

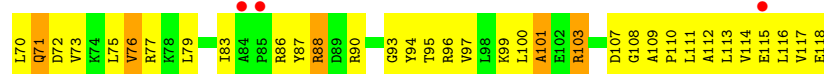


• Molecule 36: 50S ribosomal protein L17

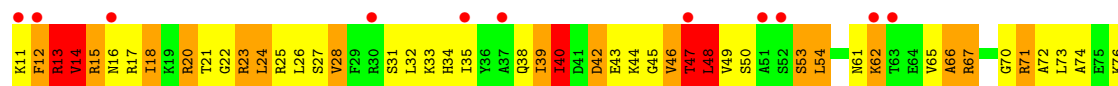




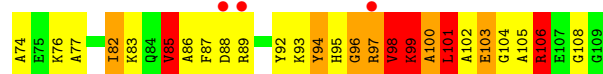
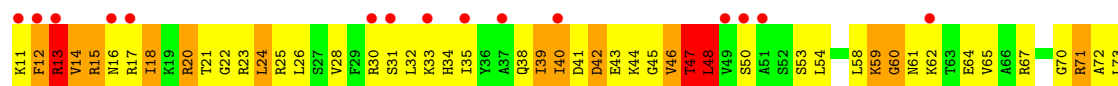
• Molecule 36: 50S ribosomal protein L17



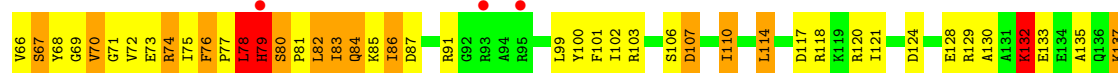
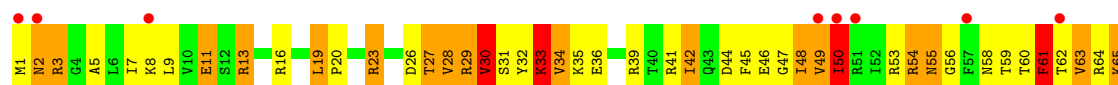
• Molecule 37: 50S ribosomal protein L18



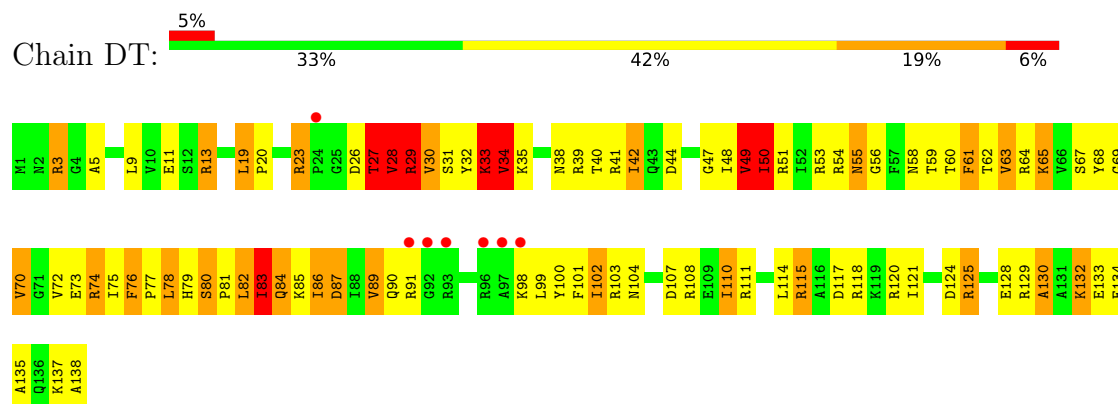
• Molecule 37: 50S ribosomal protein L18



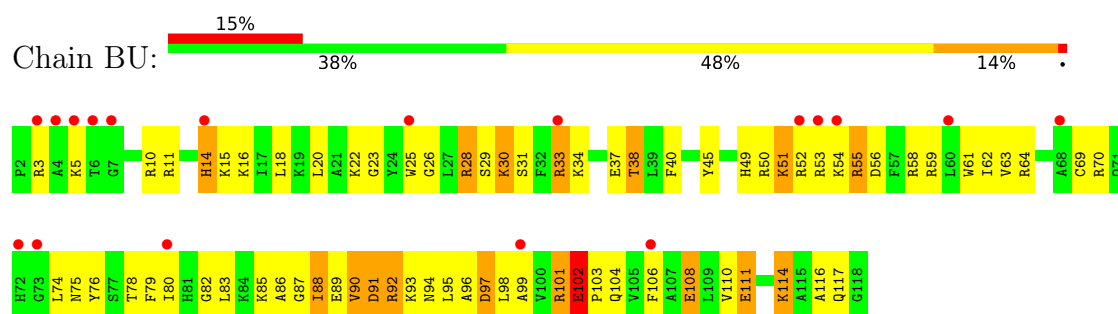
• Molecule 38: 50S ribosomal protein L19



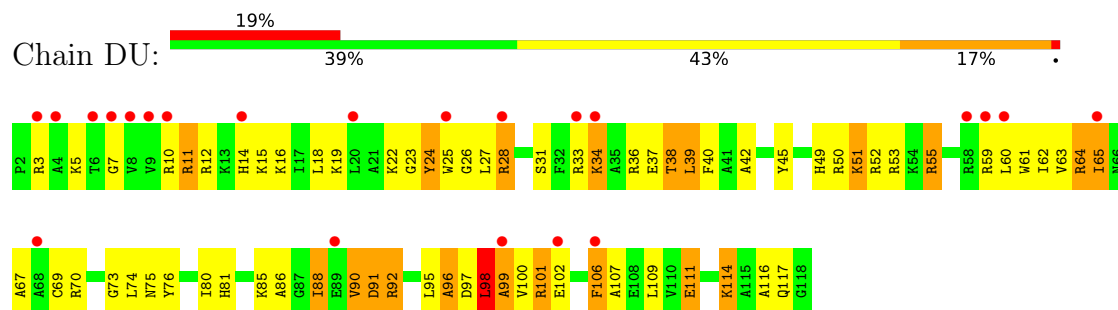
- Molecule 38: 50S ribosomal protein L19



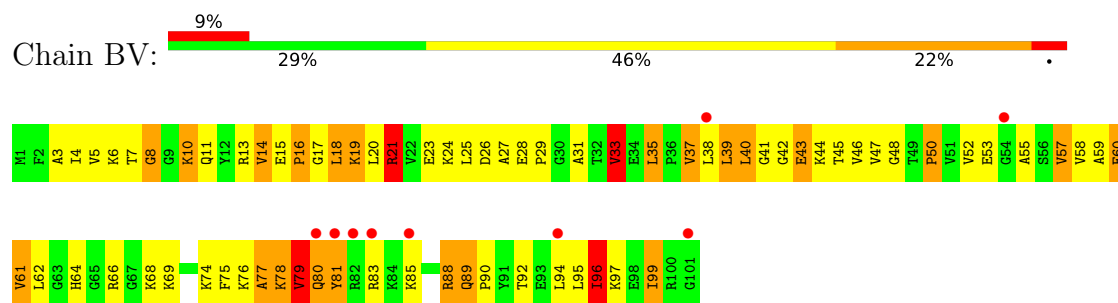
- Molecule 39: 50S ribosomal protein L20



- Molecule 39: 50S ribosomal protein L20

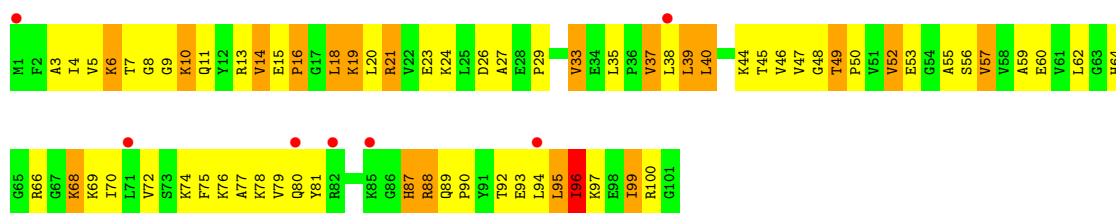


- Molecule 40: 50S ribosomal protein L21

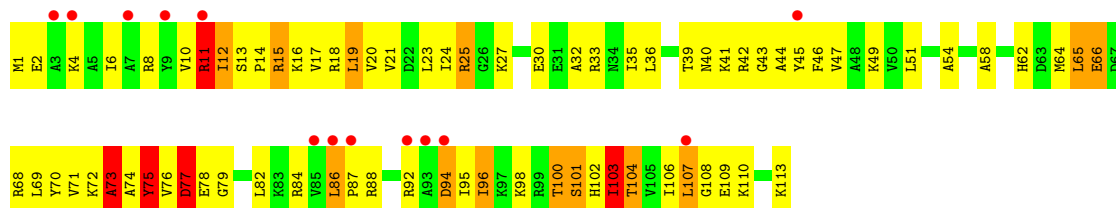


- Molecule 40: 50S ribosomal protein L21

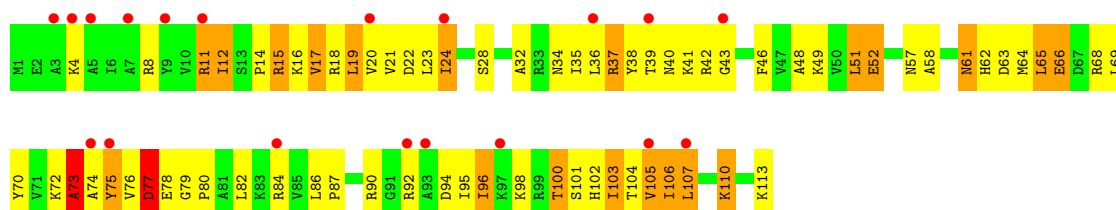




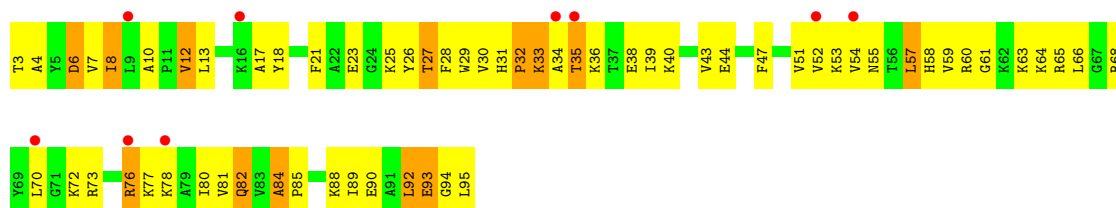
• Molecule 41: 50S ribosomal protein L22



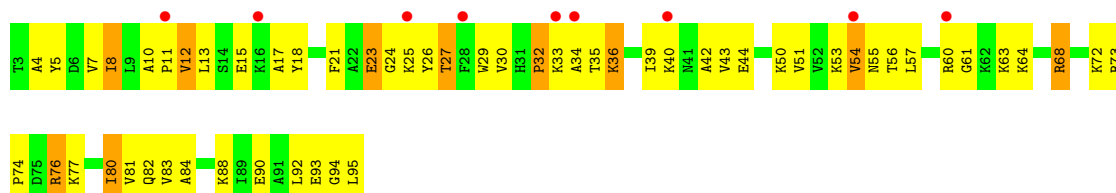
• Molecule 41: 50S ribosomal protein L22



• Molecule 42: 50S ribosomal protein L23

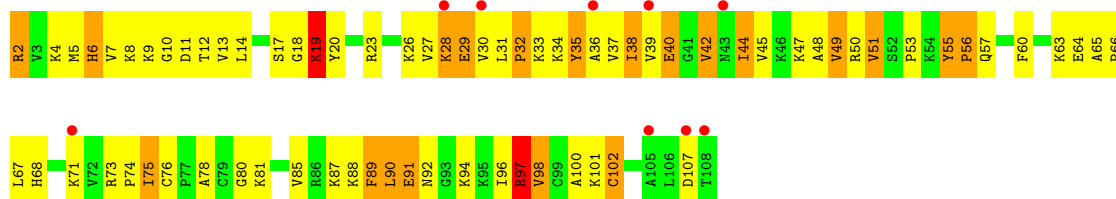


• Molecule 42: 50S ribosomal protein L23



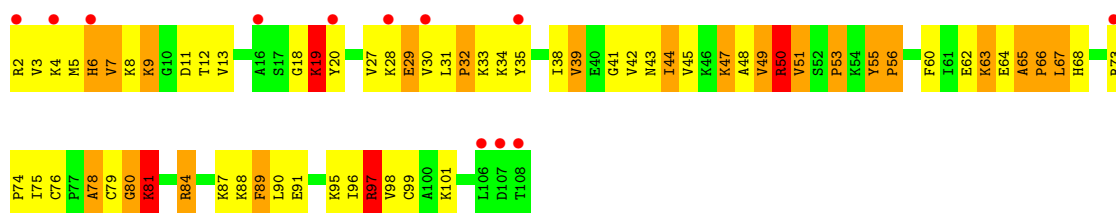
- Molecule 43: 50S ribosomal protein L24

Chain BY: 



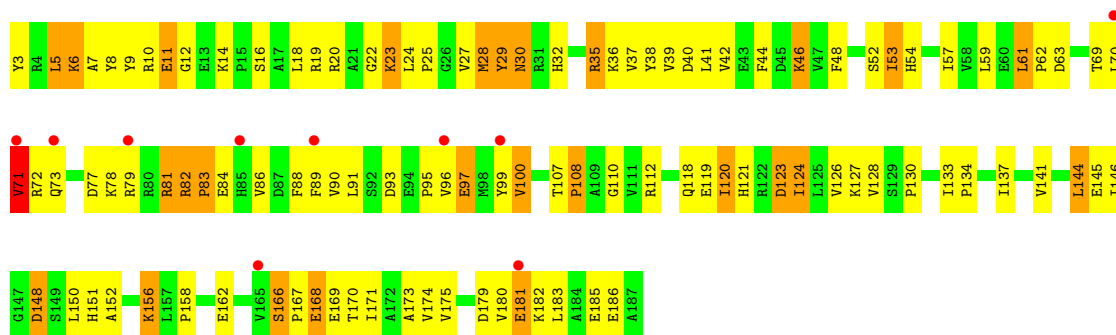
- Molecule 43: 50S ribosomal protein L24

Chain DY: 



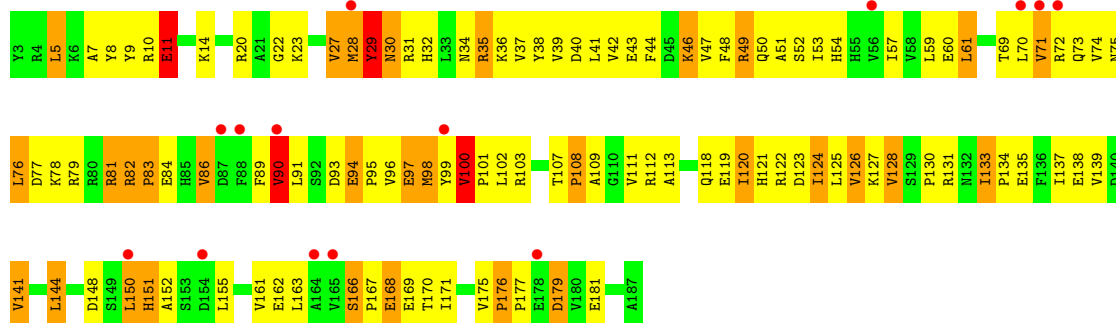
- Molecule 44: 50S ribosomal protein L25

Chain BZ: 

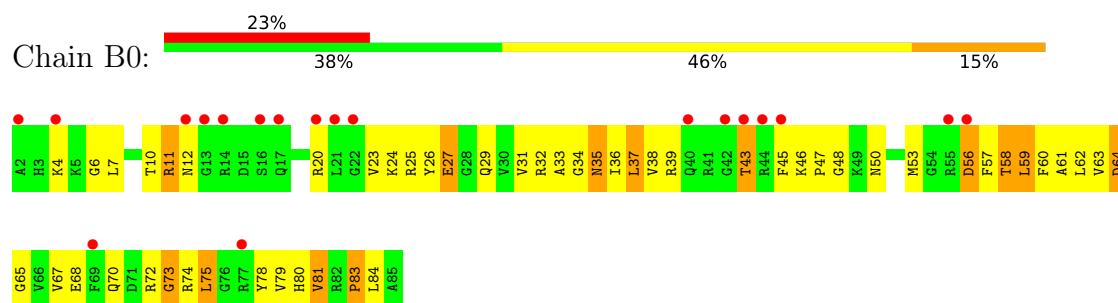


- Molecule 44: 50S ribosomal protein L25

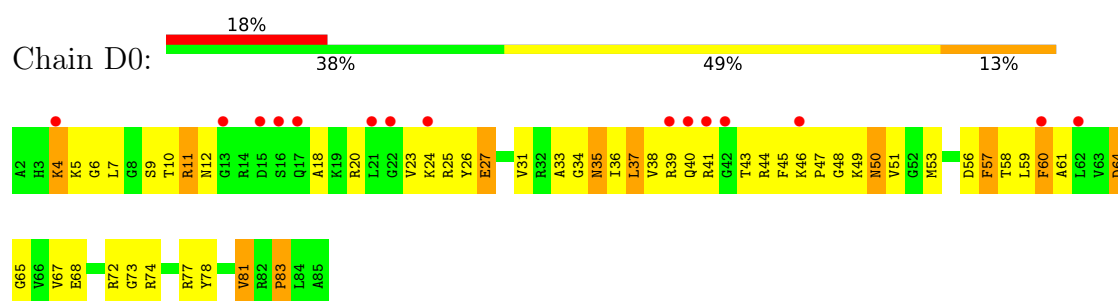
Chain DZ: 



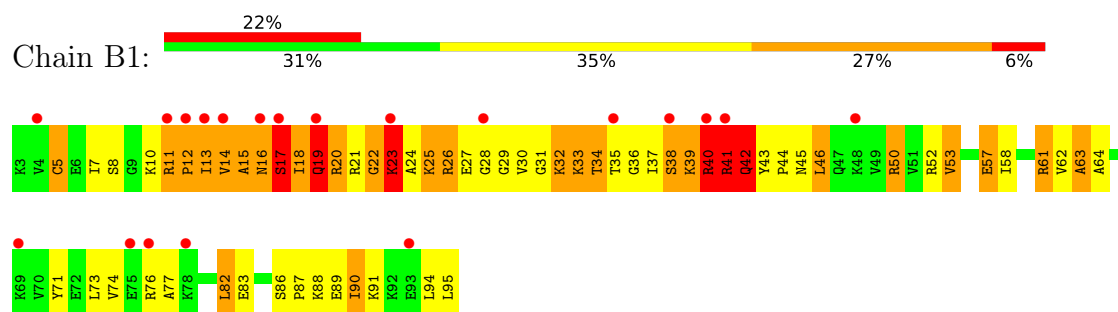
- Molecule 45: 50S ribosomal protein L27



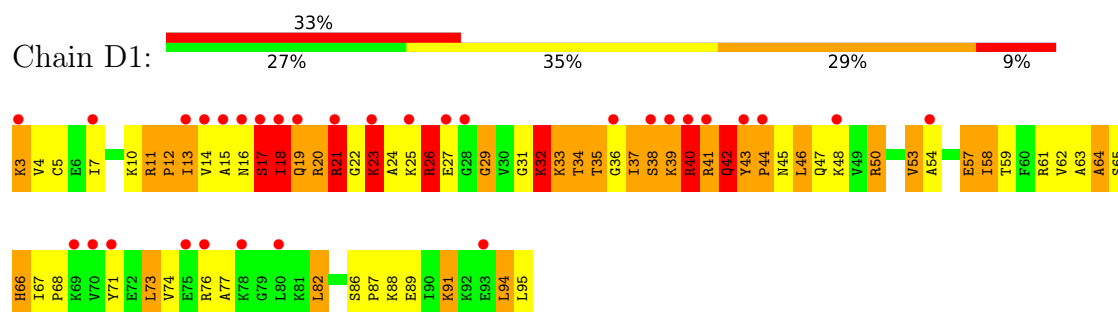
- Molecule 45: 50S ribosomal protein L27



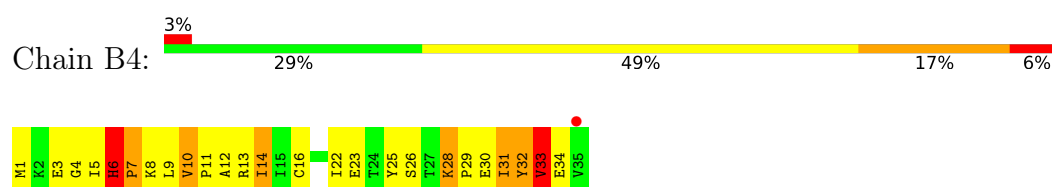
- Molecule 46: 50S ribosomal protein L28



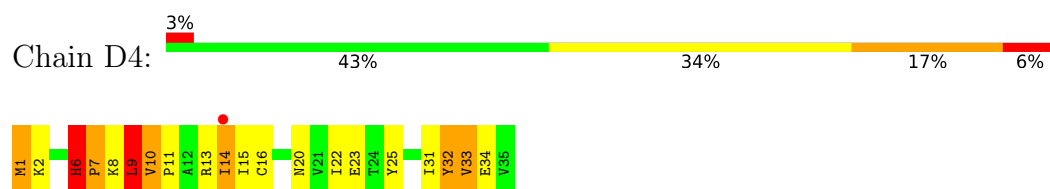
- Molecule 46: 50S ribosomal protein L28



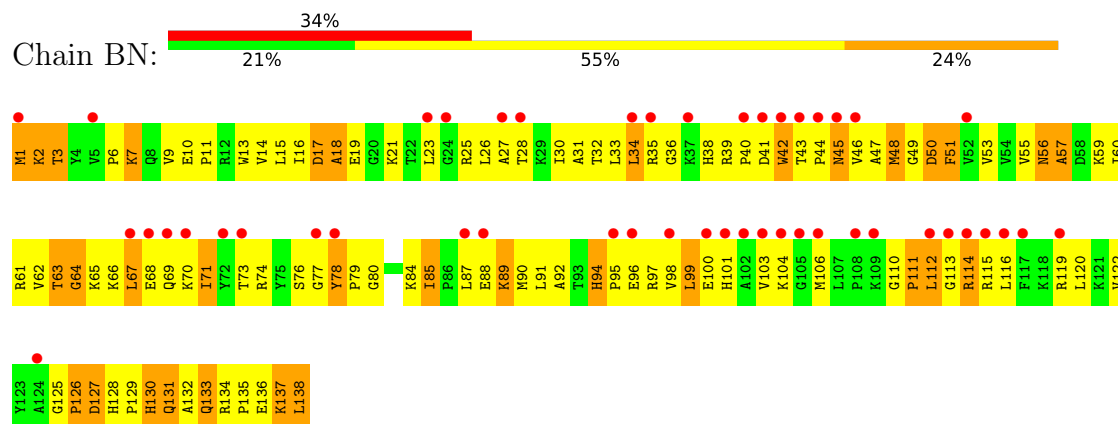
- Molecule 47: 50S ribosomal protein L31



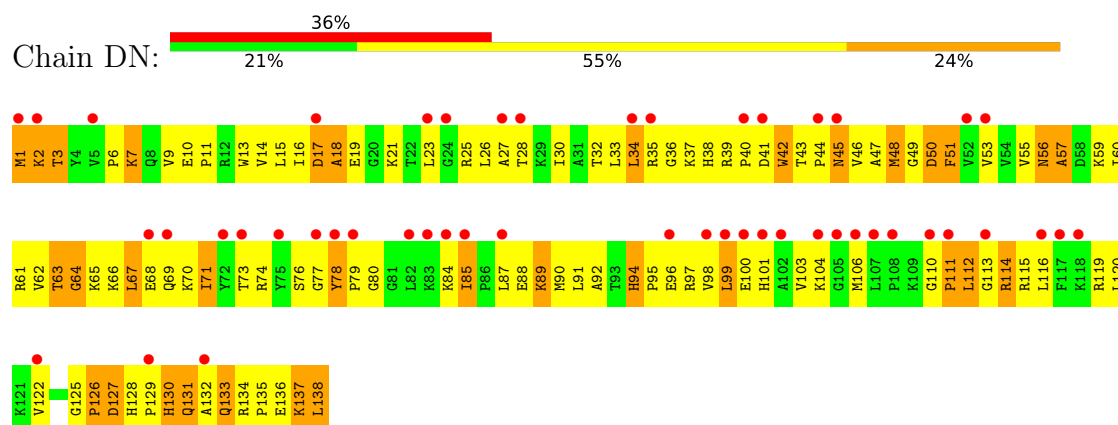
- Molecule 47: 50S ribosomal protein L31



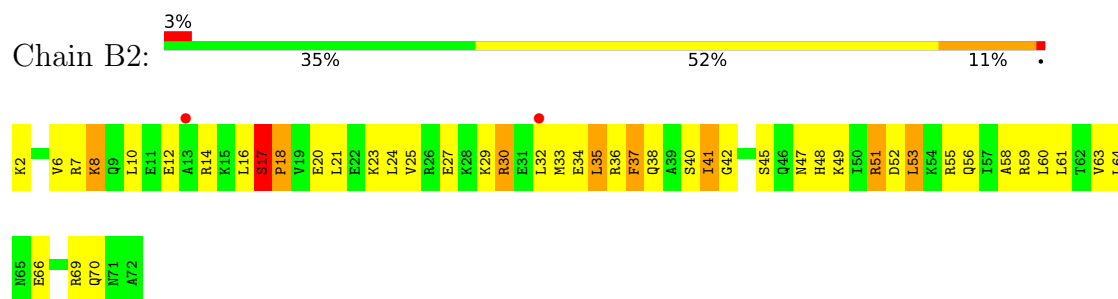
- Molecule 48: 50S ribosomal protein L13



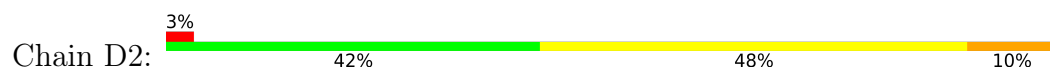
- Molecule 48: 50S ribosomal protein L13



- Molecule 49: 50S ribosomal protein L29



- Molecule 49: 50S ribosomal protein L29

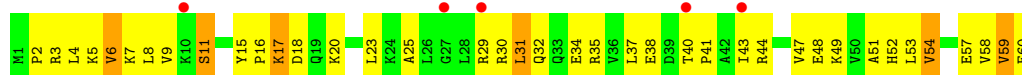




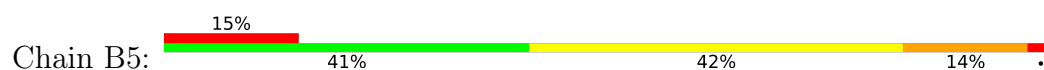
- Molecule 50: 50S ribosomal protein L30



- Molecule 50: 50S ribosomal protein L30



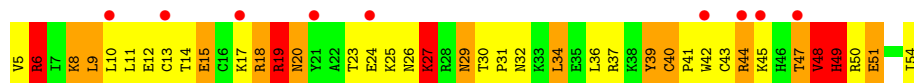
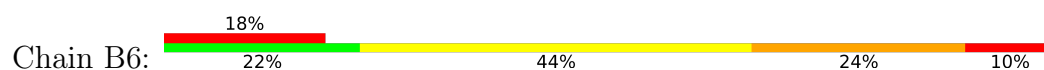
- Molecule 51: 50S ribosomal protein L32



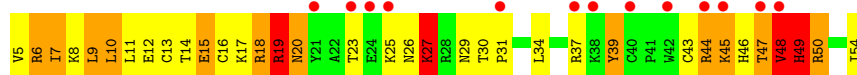
- Molecule 51: 50S ribosomal protein L32



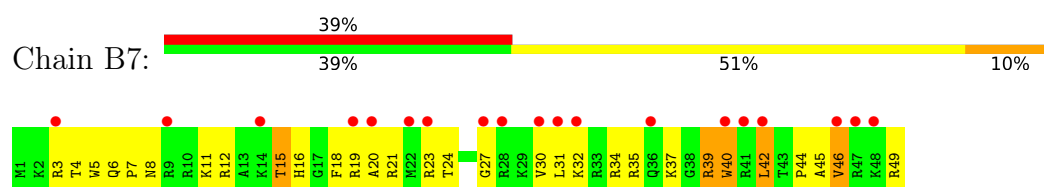
- Molecule 52: 50S ribosomal protein L33



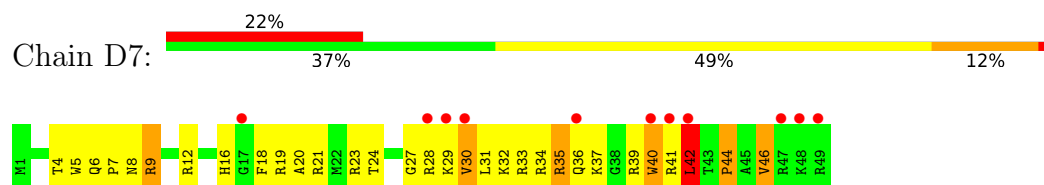
- Molecule 52: 50S ribosomal protein L33



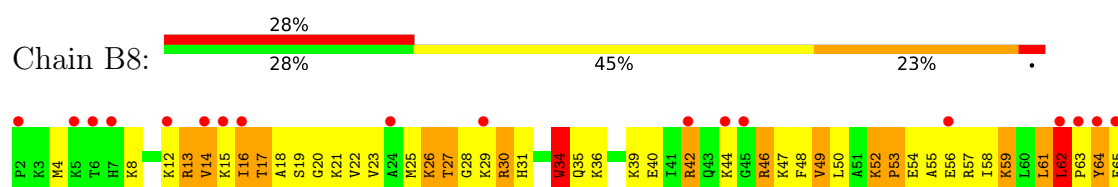
- Molecule 53: 50S ribosomal protein L34



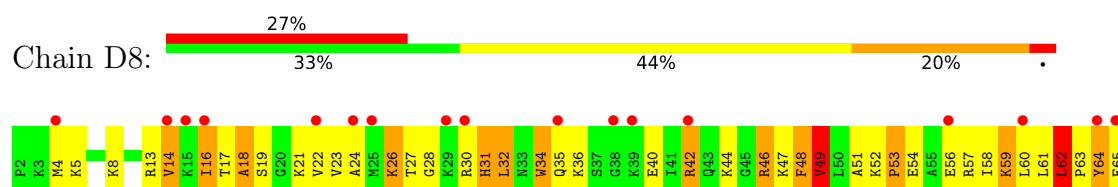
- Molecule 53: 50S ribosomal protein L34



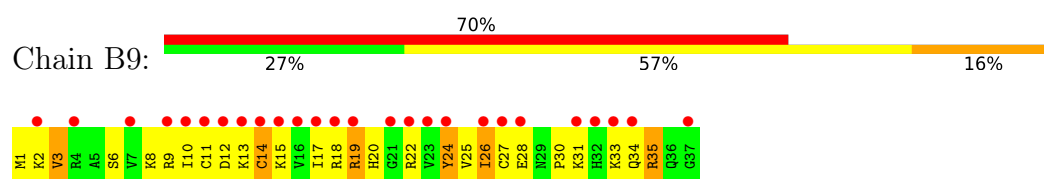
- Molecule 54: 50S ribosomal protein L35



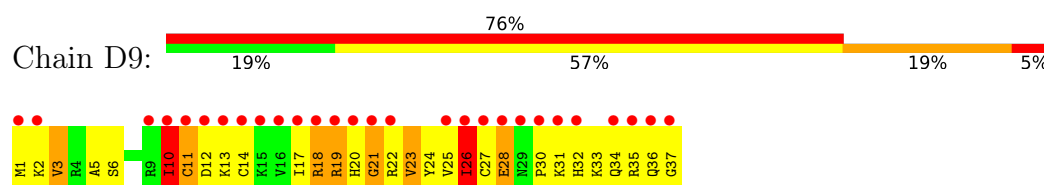
- Molecule 54: 50S ribosomal protein L35



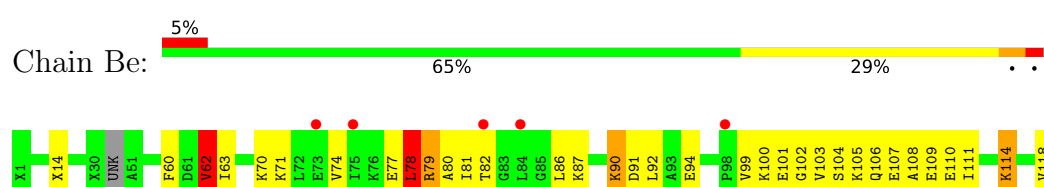
- Molecule 55: 50S ribosomal protein L36



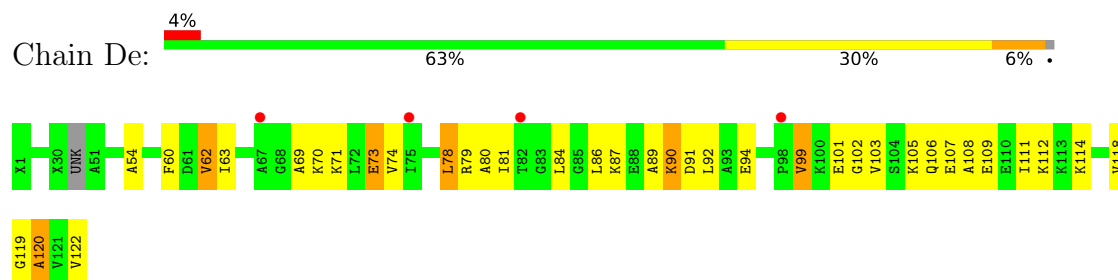
- Molecule 55: 50S ribosomal protein L36



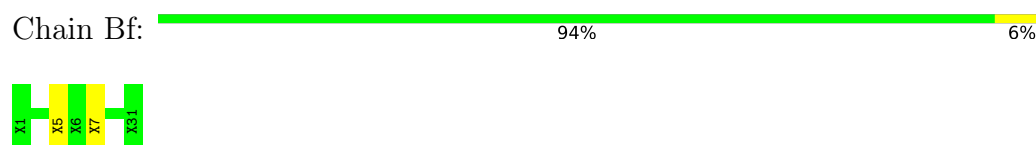
- Molecule 56: 50S ribosomal protein L7/L12



- Molecule 56: 50S ribosomal protein L7/L12



- Molecule 57: 50S ribosomal protein L7/L12



- Molecule 57: 50S ribosomal protein L7/L12



There are no outlier residues recorded for this chain.

- Molecule 57: 50S ribosomal protein L7/L12



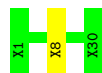
There are no outlier residues recorded for this chain.

- Molecule 57: 50S ribosomal protein L7/L12



There are no outlier residues recorded for this chain.

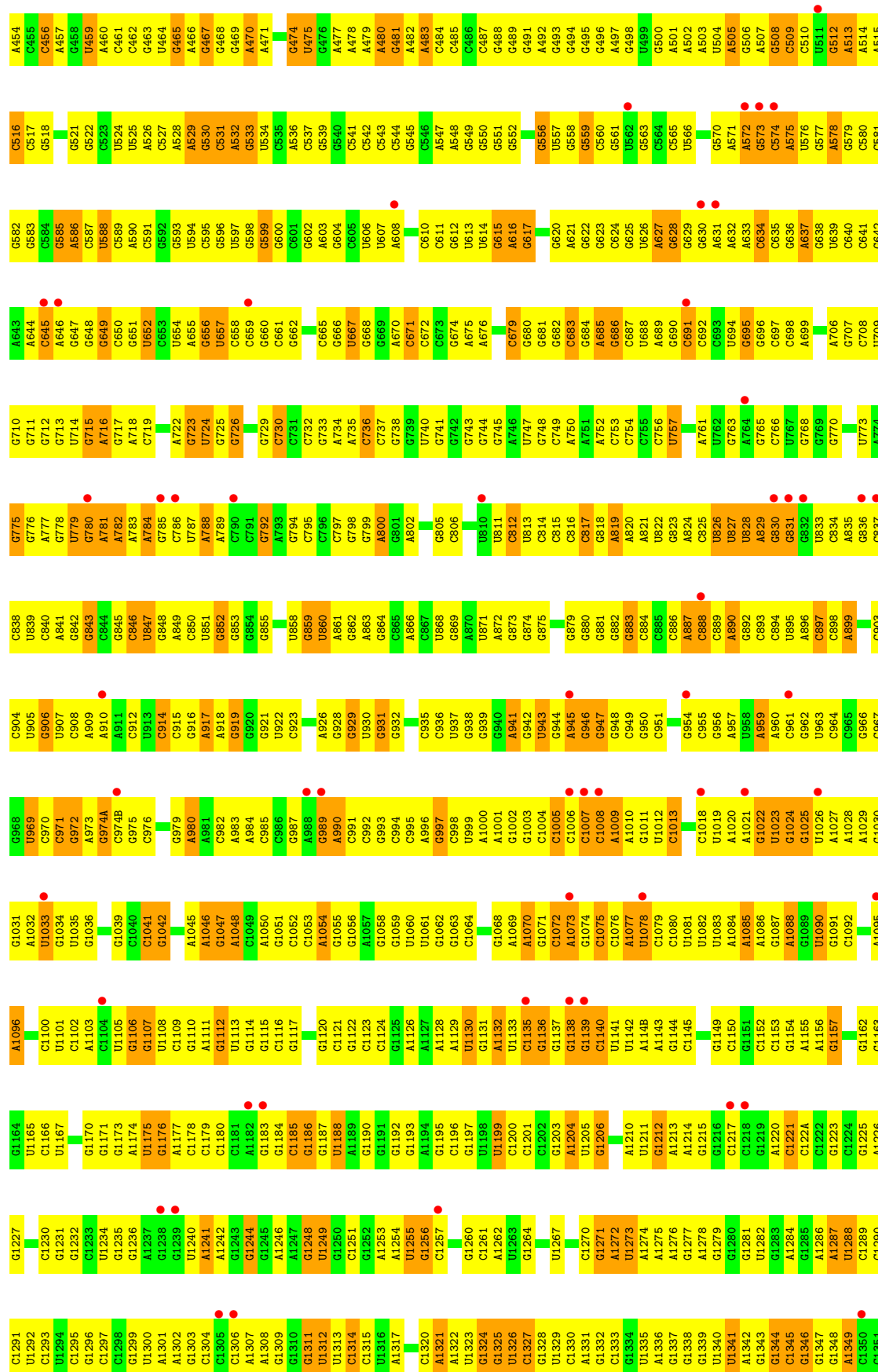
- Molecule 58: 50S ribosomal protein L7/L12



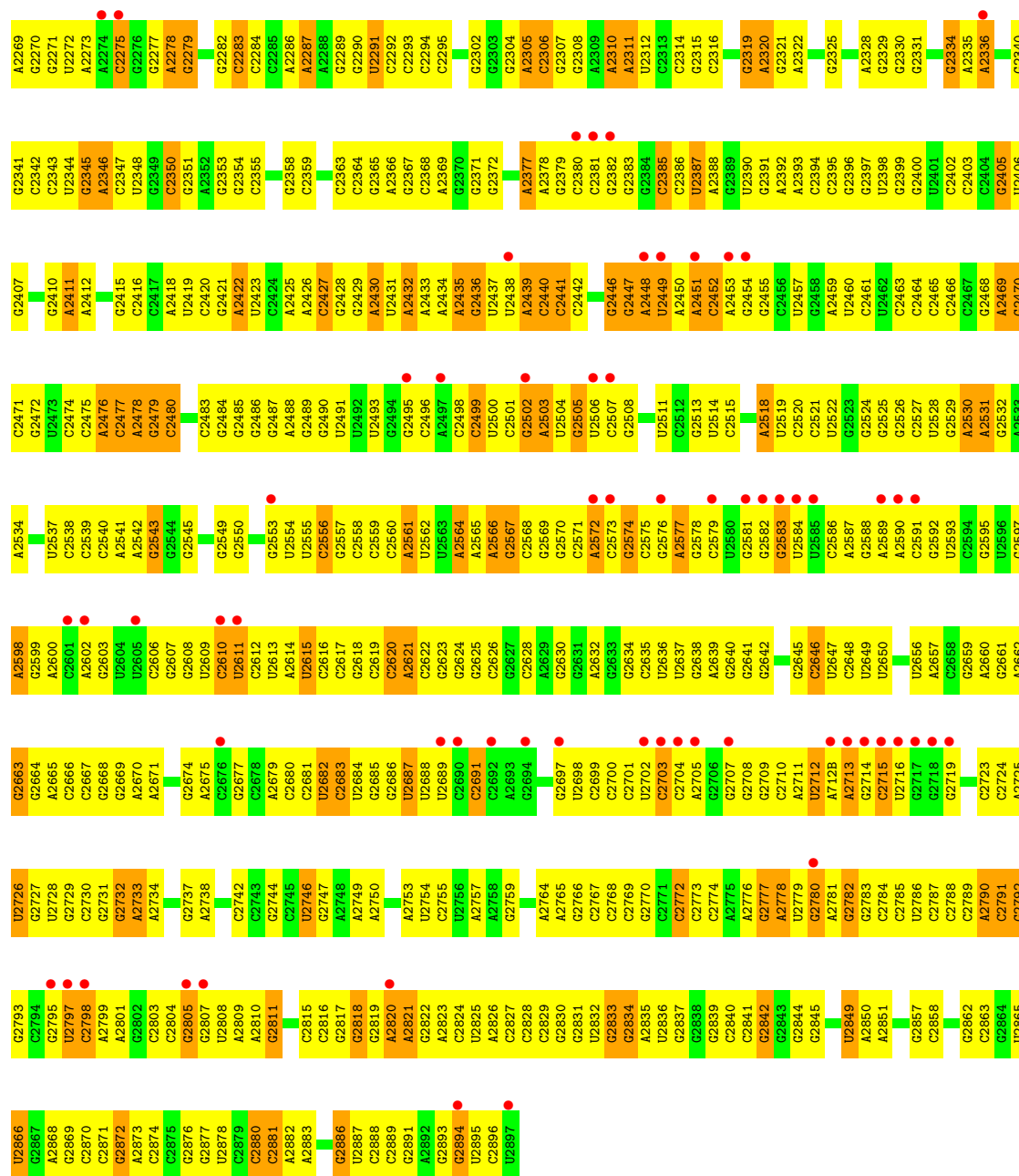
- Molecule 58: 50S ribosomal protein L7/L12



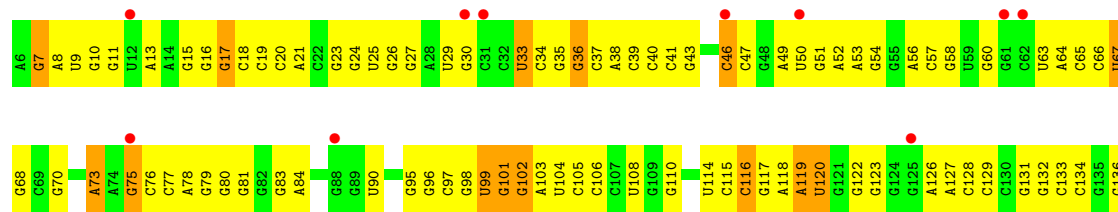
- Molecule 59: 5S ribosomal RNA







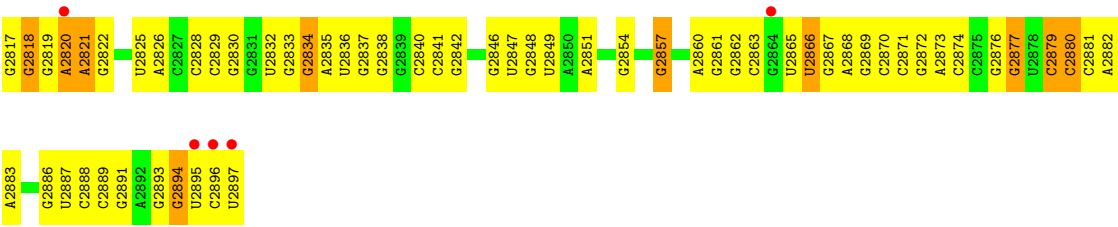
• Molecule 60: 23S ribosomal RNA



C985	C923	U851	C786	C720	C853	C591	G522	C456	C392	C319	U270P	A222	C137A	
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C989	C925	C853	A788	U724	C655	U594	U524	A458	C394	C321	C270R	G224	G138	
A990	A928	C854		C725	C656	C595	U525	U459	U395	A322		G225	G139	
C991	C929	C956	C792	C726	U657	C596	A526	A460	G396	G323	G270T	G226	A140	
C992	U930	C957	A793	A727	C658	U597	C527	C461	C397	A324	G270U	A227	A141A	
C993	C931	C958	C794	C728	C659	C598	A527	C462	G398	G325	C270V	A228	C141B	
C994	C932	C959	C795	C729	C660	C599	A528	C463		G326	G270W	G142	C143	
C995	C933	C960	C796	C730	C661	C600	C530	U464	A401	C327	G270X	U230	C144	
A996	U934	U860	C797		C662	C601	A532	A465	A402	G328	G270Y	C231	C145	
C997	C935	A861	C798	C733		C602	G533	A466	U403	G329	U270Z	G232	G146	
C998		C862	C799	A734	G666	A603	G534	C467	C404	A330	U271A	A233	U147	
C999	C938	A800	A800	A735	U667	C604	U534	C468	U405	A331	C271B		C148	
U1000	C939	C869	C801	C736	G668	C605		C469	G406	A332	G271C	C237	C149	
A1001	A940	A870	A802	C737	G669	U606	C537	A470	G407		U271D	C238	A149	
A941	C941	C871	C805	C738	A670	U607	G539	A471	C408	G271	U239	U239	C150	
A942	U942	A872	C806	C739	C671	A608	G540		C409	G272		G240	C151	
U1002	U943	A873		C740	C672	A609A		C474	C410	C343	G273A	A241	G171	
G1003	U943	C873	U810	C741	C673	G609B	C541	U475	C411	G344	G273B	G242	C172	
C1004	C944	C874	C874	C742	C674		C542		A412	A345	C273C	U243	C173	
C1005	U945	C875	U811	C743	C675	U612	C543		C413	A346	C273D	A244	G174	
C1006	A946	C876	C812	C744	C676	U613	G545		C414	A347	C273E	G245	C175	
C876	C947	C877	U813	C745	G681	U614			A415	G348	U273F	G175	G176	
U1007	C948	U877	C814	A746	G682	C615	A548	A482	C416	G349	U273G	G248	G177	
A1008	C949		C815	C747	C683	A616	G549	A483	C417	U350	G274	C249		
A1009	C950	U880	C816	U747	C684	C617	G550	C484	C418	G351	G275	G250		
U1010	C951	C881	C817	C748	G685	U618A	G551	C485	C419	G352	A276	A251		
C1011	U952	C882	C818	C749	A685		G552	C486	C420	G353	C277	G252		
C883	C952	C883	C819	A750	G686		U553	C487	U421	G354	A278	C253		
A953	A953	C884	A819	C751	C687	C620	U554	C488	A422	G355	C279	G254		
C954	C954	C887	A820	A752	U688	A621	U554	C489	A423	G356	C280	A255		
C955	C955	A887	A821	C753	C689	C622	G556	C490	G424		G281	A256		
C956	C956	C988	U822	C754	G690	U557	C623	A491		G360	A282	A257		
C957	A957	C989	C823	C755	C691	C624	G558	A492	U427	G361	C287	G258	A190	
U958	U958	A890	A824	C756	C692	C625	G559	A493	A429		C288	G260	A191	
A959	C959	G992	C925	U757	C693	U626	C560	C494	G430	A3636	C289	G261	C192	
A960	C960	C993	U826	C758	U694	A627	G561	C495	A429	C364	C289	G262	C193	
C961	C961	C994	U827	C759	G695	C628	U562	C496	G430	A289	G290	G263	G194	
C962	U962	U895	U828	C760	C696	C629	G563	A497	U431	A282		C283	C195	
C963	C963	A896	A829	A761	C697	C630	C564	C498	A432	C366B		G284	A195	
C964	C964	C997	C830	C762	C698	A631	C565	U499	C433	G370	A294	C285		
C965	C965	C998	C831	G763	A699	A632		G500	U434	A371	G295	A265	A196	
C966	C966	A999	G832	A764	C700	C633	A572	A501	C435	G372	C296	G286	C198	
C967	C967	A999	U833	C765	C701	C634	C573	A502	C436	U373	C297	C287	A199	
C968	C968	C903	C834	C766	C702	C635	C574	A503	G438	A374	G298	C288	U200	
U969	C969	C904	A835	C767	C703	C636	U575	U504	C439	U289	A299	C289		
C970	C970	U905	C836	U768	A705	A637	U576	A505	G440	A300	U289	U289		
C971	C971	G906	C837		C705	C638	G577	G506	C441	G301	A300	A270A	G205	
		U907	C838	U773	C707	U639	A578	A507	U442	G302	A270B			
			U839	A774	C708	C640	G579	A508	A443	C303	A270C		C209	
			C840	C775	U709	C641	G580	C509	C444	U302	C270D		C210	
			A841	C776	C710		C581	C510	G382	U305	C270E		A211	
			C842	A777	G711		G582	U511	C445	U306	G270F		G212	
			C843	C778	G712	C645	G583	U384	U447	U307	G270G		A213	
				U779	G713	A646	C584	A513	U448	G308	C270H		G214	
			C844	C780	U714	A646	G585	A513	A449	G309	C270I		G215	
			C845	A781	C715	C647	A586		G386	G270J				
			U846	C782	A716	C648	G587		U387	G270K			A216	
			C847	A783	C717	C649	U588		G388	G270L			G217	
			U848	C784	G717	C650	U588		G389	A311			A218	
			A849	A785	A718	C651	C589						U270M	G219
			C850	C786	C719	U652	A590						U270N	G220

A1872	G1801	U1639	A1572	C1435	G1371	C1305	U1240	A1174	G1110	G1047
G1878	A1802	C1640	G1573	G1436	G1371	C1306	A1241	U1175	A1111	A1048
C1879	A1803	C1574	C1574	C1437	U1372	A1307	A1242	U1176	C1112	C1049
C1880	G1645	G1645	C1575	U1438	A1373	G1308	G1243	A1177	U1113	A1050
C1881	U1805	G1646	U1576	A1511	G1374	G1309	G1244	C1178	G1114	G1051
	G1718	G1647	C1577	G1441	C1375	G1310		C1179	G1115	C1052
A1809	G1725	C1648	G1513	G1442	G1376	G1311	U1248	G1183	C1116	C1053
A1810	G1726	G1649	A1579	G1443	U1312	U1249	G1250	G1184	C1119	A1054
G1888	A1810	G1650	C1515	G1444	C1313	G1251	C1251	G1185	G1120	G1056
A1812	G1581	G1651	G1581	A1448	C1314	C1314	G1251	G1186	G1121	G1057
A1890	G1813	A1652	G1582	C1445	G1381	C1315	G1252	G1187	C1122	G1058
G1891	G1814	G1653	A1583	C1446	U1316	U1253	A1253	G1188	G1123	G1059
C1892	U1730	G1653	A1583	G1447	A1384	U1317	A1254	U1188	C1124	U1060
A1815	G1731	A1654	C1585	G1448	G1385		G1255	A1189	G1125	U1061
C1893	A1732	A1655		A1498	G1389	C1320	G1256	G1190	G1126	G1062
A1817	G1733	C1656	C1588	A1499	U1321	G1320	G1257	G1193	A1126	G1063
G1818	U1818	C1657	G1589	A1453	U1322	A1322	C1258	G1194	A1127	C1064
C1896	U1820	C1658	U1590	U1454	U1391	G1323	G1259	G1195	A1128	U1065
	A1821		G1591	G1455	A1392	G1324	G1260	C1196	A1129	
G1899	G1822	C1662	C1592		A1393	G1325	C1261	G1197	G1131	A1070
A1900	G1750	G1663	G1593	G1459	U1394	C1326	A1262	U1198	G1132	A1069
A1901	C1751	A1664	G1594	G1460	A1395	C1327	U1263	U1199	U1133	A1070
C1902	G1752	A1665	G1595	A1459	A1396	C1328	G1264	U1199	G1135	G1071
G1903	A1825	G1666	A1596	G1461	U1396	G1329	A1265	C1200	G1136	A1072
G1904	G1826	C1667	C1597	C1462	U1397	U1397	A1266	C1201	G1137	C1073
C1905	U1756	A1668	C1598	C1463	C1398	C1330		C1202	G1138	G1074
G1906	U1757	C1669	G1532	C1464	A1399	G1332		G1203	C1139	C1075
A1829	A1758	C1670	G1533	A1465	G1400	A1333	A1269	A1204	U1076	C1076
C1830	A1759	G1671	U1535	G1466	C1401	C1334	C1271	U1205	C1140	A1077
A1913	G1762	G1674	U1602	C1467	C1402	G1334	G1271		U1141	U1078
G1831	G1763	C1675	A1603	C1468	C1403	U1335	A1272		U1142	C1079
	C1763	A1676	C1604	A1469	U1404	A1336	U1273	C1208	U1142	C1079
U1915	G1764	A1677	G1605		U1405	G1337	A1274	G1209	A1148	C1080
U1917	C1765	G1678	C1605		U1406	G1338	A1275	G1215	A1143	U1081
A1918					C1407	G1339	A1276	G1216	G1144	U1082
A1919	C1771		A1608	C1472	U1541	U1340	G1277	G1212	C1145	U1083
C1838	G1772	G1681	A1609	C1474	G1542	U1341	A1278	A1213	C1146	A1084
G1839	A1773	C1682	A1610		A1543	A1342	G1279	A1214	G1147	A1085
G1840	C1774	G1683	C1611	A1477	U1544	U1343	G1280	G1215	C1148	A1086
U1923	U1841	C1684	G1612	G1478	A1545	G1344	G1281	G1216	G1149	G1087
C1924	G1842	C1685	G1613	A1479	A1546	C1344	G1282	C1217	C1150	A1088
C1843	C1778	C1686	A1614	G1480	C154B	C1345	G1283	C1218	G1151	G1089
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G1846	C1781	U1688	A1616		G1416	C1347	A1284	C1220	G1154	C1092
A1847	C1782	A1689	C1617		C1417	G1348	G1285	C1221	C1155	
G1930	A1848	A1690	A1618	A1486	G1418	A1349	G1286	A1152	C1155	
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	U1851	C1693	G1623	A1430	G1421	U1352	C1289	A1095	U1094	
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A1937	U1788	G1695	G1626	G1492	G1423	A1354	C1291	U1097		
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U1939	G1789	G1697	G1628	A1494	G1425	G1356	C1293	C1100	G1162	
U1939	C1790	U1629	U1629	A1495	G1426	U1357	U1294	G1101	G1163	
U1940	A1791	A1698	G1629	A1496	G1427	G1358	G1232	G1164	G1164	
G1941	G1792	G1699	C1631	U1497	A1427	A1359	G1295	G1232	G1165	
C1942	U1700	C1665	A1631	U1497	C1428	A1359	G1296	C1233	U1165	
	A1701	A1566	A1632	C1498	G1429	A1360		U1234	C1104	
G1861	U1702	U1567	A1567	C1499	C1430	G1361	G1299	U1234	U1105	
U1944	G1703	G1568	G1568	G1500	U1431		A1301	G1236	G1166	
	C1636	A1569	G1635	G1501	C1432	G1364	A1301	A1237	U1167	
U1864	G1704	G1636	G1636	C1501	C1432	U1433	A1302	G1238	G1170	
C1947	U1798	A1637	A1637	C1502	U1433	A1365	A1302	G1238	G1171	
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U2746	G2686	A2621	C2560	U2492	G2364	U2291	C2226	U2144	A2082	A2019	U1951
G2747	U2687	G2625	A2561	U2493	G2365	C2292	C2229	C2145	G2083	A2020	A1952
A2748	U2688	C2626	U2562	G2494	A2366	C2293	G2230	C2146	C2084	C2021	A1953
A2749	U2689	G2627	U2563	G2495	G2367	C2294	G2231	C2147	C2085	U2022	G1954
A2750	C2690	G2628	A2564	C2496	C2368	C2295	G2232	G2148	G2086	G2023	U1955
A2753	C2691	A2629	A2565	A2497	A2369	A298	U2232	G2151	G2087	G2024	U1956
U2754	A2692	U2636	A2566	C2498	G2370	G2299	U2233	G2152	G2088	C2025	C1957
U2756	A2693	G2630	C2567	C2499	G2371	G2299	G2234	G2153	U2089	C2026	C1958
U2757	U2694	A2632	U2568	U2500	G2372	G2302	G2235	G2154	G2090	G2027	
	U2695	A2632	C2569	C2501	C2373	G2302	G2236	G2155	U2091	U2028	
	U2696		G2502	G2502	C2374	G2303	G2237	G2156	U2092	G2029	
	G2697	G2635	A2503	A2504	G2375	G2304	G2238	G2157	G2093	A2031	
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A2764	C2700	U2639	C2575	U2506	A2378	G2307	A2241	G2160	U2096	A2033	
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C2767	U2702	U2640	A2577	G2508	G2382	A2310	A2247	G2162	U2098	G2035	
	C2703	G2641	G2578	G2509	G2383	A2311	U2248	G2163	U2099	G2036	
	G2704	G2642	C2579	C2510	G2384	U2312	C2249	C2164	G2100	G2037	
	A2705	G2643	U2580	G2513	U2385	U2313	U2250	G2165	G2101	C2038	
	G2706	G2644	G2581	G2514	G2386	C2314	G2251	U2170	U2102	C2039	
	G2707	G2645	G2582	U2514	A2450	G2315	G2252	G2171	C2103	U2040	
	G2708	C2646	G2583	C2515	U2387		G2253	G2172	G2104	U2041	
	G2709	U2647	U2584	G2516	U2388		G2254	G2173	G2105	A2042	
	G2710	G2648	U2585	G2517	U2389		G2255	G2174	G2106	C2043	
	A2711	U2649	G2586	A2518	G2390		G2256	G2175	C2107	G2044	
G2780	U2712	U2650	A2587	U2519	G2391		G2257	G2176	G2108	C2045	
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G2782	G2714	C2652	A2589	G2521	C2393		U2259	A2178	U2110	U2047	
G2783	G2715	U2653	U2590	U2522	G2394		U2260	G2179	G2111	U2048	
G2784	C2716	A2654	G2591	G2523	C2395		U2261	U2180	C2112	G2049	
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U2786	U2717	G2656	U2593	G2525	G2397		U2263	C2177	G2115	A2051	
G2787	U2718	A2657	G2594	G2526	U2398		U2264	G2178	G2116	G2052	
C2788	A2719	C2658	C2595	G2527	G2399		U2265	U2180	G2117	G2053	
C2789	U2720		U2596	U2528	G2400		U2266	G2186	U2118	A2054	
A2790	G2721	U2662	G2597	G2529	C2401		U2267	G2189	A2119	G2055	
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A2799	C2730	A2670	U2605	C2538	G2410		U2275	C2206	C2063	A2001	
A2801	G2731	A2671	C2606		A2411		G2276	C2207	C2064	G2002	
G2802	G2732	G2672	G2607	A2542	A2412		G2277	C2208	C2065	G2003	
C2803	A2733	G2673	G2608	G2543	G2413		U2278	U2209	G2066	C2006	
C2804	G2734	G2674	U2609	G2544	G2414		G2279	G2210	G2067		
G2805	G2735	A2675	C2610	G2545	G2415		G2280	G2211	U2068	C2009	
G2807	G2736	C2676	U2611	U2546	C2416		G2281	G2212	G2069	G2010	
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A2809	A2738	A2678	U2613	U2552	A2418		C2283	G2214	A2071	U2011	
A2810	U2739	G2679	G2614	G2553	U2419		C2284	G2215	G2072	G2012	
G2811	A2740	C2680	U2615	U2554	G2420		G2285	G2216	G2073	A2013	
G2812	G2741	C2681	G2616	U2555	G2421		U2286	G2217	U2074	A2014	
A2813	G2742	U2682	C2617	C2556	A2422		U2287	G2218	U2075	A2015	
G2814	C2743	U2683	G2618	G2557	A2423		U2288	G2219	G2080	U2016	
G2815	G2744	U2684	C2619	C2558	G2424		G2289	A2225	U2017	U2017	
C2816	C2745	G2685	C2620	C2559	A2425		G2290		C2143	G2018	



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	302.39Å 683.92Å 356.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.86 40.00 – 3.87	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.86) 64.3 (40.00-3.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.34	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 3.89Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.264 , 0.317 0.270 , 0.317	Depositor DCC
R_{free} test set	21652 reflections (3.22%)	wwPDB-VP
Wilson B-factor (Å ²)	76.3	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.15 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.24$, $\langle L^2 \rangle = 0.09$	Xtriage
Estimated twinning fraction	0.320 for h,-k,-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	308202	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: DPP, UAL, MG, KBE, GNP, 5OH

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	AB	0.66	3/1945 (0.2%)	1.26	24/2621 (0.9%)
1	CB	0.61	2/1945 (0.1%)	1.28	26/2621 (1.0%)
2	AC	0.42	0/1645	0.93	1/2216 (0.0%)
2	CC	0.41	0/1645	0.91	2/2216 (0.1%)
3	AD	0.43	0/1733	0.98	6/2318 (0.3%)
3	CD	0.39	0/1733	0.94	6/2318 (0.3%)
4	AE	0.44	0/1172	0.99	5/1576 (0.3%)
4	CE	0.42	0/1172	0.99	4/1576 (0.3%)
5	AF	0.37	0/856	0.90	2/1154 (0.2%)
5	CF	0.38	0/856	0.86	0/1154
6	AG	0.38	0/1276	0.89	1/1709 (0.1%)
6	CG	0.38	0/1276	0.88	1/1709 (0.1%)
7	AH	0.43	0/1136	1.01	5/1527 (0.3%)
7	CH	0.42	0/1136	0.96	2/1527 (0.1%)
8	AI	0.42	0/1029	0.88	1/1378 (0.1%)
8	CI	0.43	0/1029	0.87	0/1378
9	AJ	0.40	0/815	0.94	3/1095 (0.3%)
9	CJ	0.41	0/815	0.93	1/1095 (0.1%)
10	AK	0.52	0/900	1.18	11/1213 (0.9%)
10	CK	0.56	1/900 (0.1%)	1.19	9/1213 (0.7%)
11	AL	0.69	0/992	1.34	19/1327 (1.4%)
11	CL	0.63	0/992	1.29	15/1327 (1.1%)
12	AM	0.42	0/1008	0.98	1/1347 (0.1%)
12	CM	0.39	0/1008	0.98	4/1347 (0.3%)
13	AN	0.37	0/501	0.83	2/664 (0.3%)
13	CN	0.35	0/501	0.75	0/664
14	AO	0.42	0/745	0.85	0/992
14	CO	0.44	0/745	0.95	2/992 (0.2%)
15	AP	0.35	0/722	0.89	1/970 (0.1%)
15	CP	0.36	0/722	0.83	3/970 (0.3%)
16	AQ	0.53	0/848	1.10	7/1131 (0.6%)
16	CQ	0.51	0/848	1.12	5/1131 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AR	0.39	0/579	0.97	3/768 (0.4%)
17	CR	0.37	0/579	1.00	4/768 (0.5%)
18	AS	0.44	0/647	0.93	3/870 (0.3%)
18	CS	0.42	0/647	1.02	2/870 (0.2%)
19	AT	0.44	0/764	0.89	1/1006 (0.1%)
19	CT	0.43	0/764	0.89	2/1006 (0.2%)
20	AA	0.20	0/36351	0.44	3/56736 (0.0%)
20	CA	0.20	0/36351	0.43	4/56736 (0.0%)
21	AV	0.23	0/443	0.45	0/691
21	CV	0.18	0/443	0.39	0/691
22	AW	0.22	0/1827	0.47	0/2845
22	CW	0.20	0/1827	0.46	0/2845
23	AY	0.54	3/5481 (0.1%)	1.05	33/7418 (0.4%)
23	CY	0.59	7/5481 (0.1%)	1.07	34/7418 (0.5%)
24	AU	0.94	0/11	1.89	0/13
24	CU	0.95	0/11	1.89	0/13
25	BC	0.72	1/1774 (0.1%)	1.36	28/2391 (1.2%)
25	DC	0.73	1/1774 (0.1%)	1.40	32/2391 (1.3%)
26	BD	0.50	0/2195	0.97	6/2955 (0.2%)
26	DD	0.47	1/2195 (0.0%)	1.00	10/2955 (0.3%)
27	BE	0.55	2/1602 (0.1%)	1.16	18/2160 (0.8%)
27	DE	0.52	0/1602	1.09	10/2160 (0.5%)
28	BF	0.65	3/1663 (0.2%)	1.30	26/2249 (1.2%)
28	DF	0.61	3/1663 (0.2%)	1.28	26/2249 (1.2%)
29	BG	0.61	1/1499 (0.1%)	1.79	9/2016 (0.4%)
29	DG	0.58	3/1499 (0.2%)	1.09	9/2016 (0.4%)
30	BH	0.40	0/1298	0.98	5/1751 (0.3%)
30	DH	0.41	0/1298	0.98	3/1751 (0.2%)
32	BK	0.43	0/1054	1.01	7/1427 (0.5%)
32	DK	0.40	0/1054	0.97	6/1427 (0.4%)
33	BO	0.40	0/943	1.02	3/1269 (0.2%)
33	DO	0.40	0/943	0.94	3/1269 (0.2%)
34	BP	0.46	0/1131	1.11	7/1504 (0.5%)
34	DP	0.42	0/1131	1.04	11/1504 (0.7%)
35	BQ	0.43	0/1143	0.99	9/1527 (0.6%)
35	DQ	0.44	0/1143	1.03	3/1527 (0.2%)
36	BR	0.43	0/974	0.94	2/1302 (0.2%)
36	DR	0.42	0/974	0.93	1/1302 (0.1%)
37	BS	0.49	0/783	1.10	7/1041 (0.7%)
37	DS	0.50	0/783	1.08	5/1041 (0.5%)
38	BT	0.48	0/1161	1.12	11/1549 (0.7%)
38	DT	0.46	0/1161	1.10	10/1549 (0.6%)
39	BU	0.49	0/982	0.93	3/1306 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	DU	0.50	0/982	0.95	3/1306 (0.2%)
40	BV	0.51	0/790	1.12	7/1057 (0.7%)
40	DV	0.46	0/790	0.98	3/1057 (0.3%)
41	BW	0.52	0/911	1.04	5/1220 (0.4%)
41	DW	0.51	0/911	0.99	3/1220 (0.2%)
42	BX	0.38	0/748	0.96	5/1004 (0.5%)
42	DX	0.37	0/748	0.91	3/1004 (0.3%)
43	BY	0.43	0/831	0.98	4/1108 (0.4%)
43	DY	0.44	0/831	0.97	7/1108 (0.6%)
44	BZ	0.44	0/1505	0.98	4/2042 (0.2%)
44	DZ	0.44	0/1505	1.02	9/2042 (0.4%)
45	B0	0.34	0/671	0.83	1/892 (0.1%)
45	D0	0.35	0/671	0.85	1/892 (0.1%)
46	B1	0.73	1/739 (0.1%)	1.21	10/981 (1.0%)
46	D1	0.80	2/739 (0.3%)	1.33	13/981 (1.3%)
47	B4	0.60	0/276	1.10	2/372 (0.5%)
47	D4	0.60	0/276	1.12	2/372 (0.5%)
48	BN	0.43	0/1131	1.07	9/1525 (0.6%)
48	DN	0.43	0/1131	1.07	9/1525 (0.6%)
49	B2	0.46	0/600	0.97	2/793 (0.3%)
49	D2	0.44	0/600	0.89	0/793
50	B3	0.41	0/482	1.02	4/646 (0.6%)
50	D3	0.41	0/482	0.98	6/646 (0.9%)
51	B5	0.51	0/473	0.99	2/639 (0.3%)
51	D5	0.44	0/473	0.87	0/639
52	B6	0.42	0/440	0.96	2/586 (0.3%)
52	D6	0.46	0/440	0.96	0/586
53	B7	0.38	0/438	0.91	1/575 (0.2%)
53	D7	0.40	0/438	0.87	0/575
54	B8	0.45	0/525	1.07	5/691 (0.7%)
54	D8	0.48	0/525	1.03	3/691 (0.4%)
55	B9	0.47	0/310	1.08	3/407 (0.7%)
55	D9	0.40	0/310	1.07	3/407 (0.7%)
56	Be	0.45	0/538	0.90	1/715 (0.1%)
56	De	0.43	0/538	0.93	2/715 (0.3%)
59	BB	0.20	0/2853	0.43	0/4451
59	DB	0.19	0/2853	0.41	0/4451
60	BA	0.20	0/69437	0.45	1/108401 (0.0%)
60	DA	0.20	0/69437	0.44	3/108401 (0.0%)
All	All	0.33	34/330652 (0.0%)	0.68	666/492274 (0.1%)

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
1	AB	0	3
1	CB	0	3
11	AL	0	1
11	CL	0	2
23	AY	0	4
23	CY	0	4
25	BC	0	5
25	DC	0	3
26	BD	0	2
26	DD	0	2
28	BF	0	1
28	DF	0	1
29	BG	0	2
29	DG	0	2
31	BJ	0	1
31	DJ	0	1
37	BS	0	3
37	DS	0	3
38	DT	0	1
41	BW	0	1
41	DW	0	2
46	B1	0	2
46	D1	0	2
All	All	0	51

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	BG	114	ILE	C-N	17.84	1.58	1.33
29	DG	114	ILE	N-CA	-12.42	1.31	1.46
29	DG	113	ARG	CA-C	-7.21	1.42	1.52
23	CY	140	ASP	C-N	-7.13	1.23	1.33
1	AB	185	ILE	C-O	6.82	1.32	1.24

The worst 5 of 666 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	BG	114	ILE	O-C-N	-66.36	39.62	122.57
29	DG	111	LEU	CA-C-N	-15.70	103.79	119.64
29	DG	111	LEU	C-N-CA	-15.70	103.79	119.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	AA	1535	C	O3'-P-O5'	-14.66	82.00	104.00
1	AB	172	ILE	N-CA-C	-14.51	96.07	110.72

There are no chirality outliers.

5 of 51 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AB	170	GLU	Peptide
1	AB	185	ILE	Peptide
1	AB	68	ILE	Peptide
11	AL	32	PHE	Peptide
23	AY	34	TYR	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	AB	1910	0	1957	123	0
1	CB	1910	0	1957	126	0
2	AC	1621	0	1688	83	0
2	CC	1621	0	1688	88	0
3	AD	1703	0	1763	114	0
3	CD	1703	0	1763	119	0
4	AE	1156	0	1213	58	0
4	CE	1156	0	1213	63	0
5	AF	843	0	857	46	0
5	CF	843	0	857	48	0
6	AG	1257	0	1296	71	0
6	CG	1257	0	1296	83	0
7	AH	1116	0	1177	78	0
7	CH	1116	0	1177	85	0
8	AI	1011	0	1043	61	0
8	CI	1011	0	1043	58	0
9	AJ	802	0	849	55	0
9	CJ	802	0	849	61	0
10	AK	885	0	904	51	0
10	CK	885	0	904	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	AL	976	0	1062	135	0
11	CL	976	0	1062	114	0
12	AM	997	0	1072	71	0
12	CM	997	0	1072	72	0
13	AN	492	0	529	30	0
13	CN	492	0	529	26	0
14	AO	734	0	771	44	0
14	CO	734	0	771	47	0
15	AP	706	0	725	36	0
15	CP	706	0	725	30	0
16	AQ	835	0	906	83	0
16	CQ	835	0	906	72	0
17	AR	574	0	644	44	0
17	CR	574	0	644	44	0
18	AS	634	0	655	39	0
18	CS	634	0	655	42	0
19	AT	762	0	859	47	0
19	CT	762	0	859	46	0
20	AA	32474	0	16393	1072	0
20	CA	32474	0	16393	1056	0
21	AV	393	0	197	18	0
21	CV	393	0	197	14	0
22	AW	1635	0	831	72	0
22	CW	1635	0	831	72	0
23	AY	5380	0	5435	339	0
23	CY	5380	0	5436	330	0
24	AU	48	0	40	42	0
24	CU	48	0	41	16	0
25	BC	1742	0	1798	184	0
25	DC	1742	0	1798	186	0
26	BD	2145	0	2234	177	0
26	DD	2145	0	2234	164	0
27	BE	1569	0	1634	147	0
27	DE	1569	0	1634	133	0
28	BF	1628	0	1680	179	0
28	DF	1628	0	1680	166	0
29	BG	1474	0	1535	92	0
29	DG	1474	0	1535	83	0
30	BH	1274	0	1342	66	0
30	DH	1274	0	1342	55	0
31	BJ	851	0	199	35	0
31	DJ	851	0	203	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	BK	1035	0	1082	51	0
32	DK	1035	0	1082	61	0
33	BO	933	0	996	69	0
33	DO	933	0	996	61	0
34	BP	1114	0	1187	87	0
34	DP	1114	0	1187	80	0
35	BQ	1122	0	1179	69	0
35	DQ	1122	0	1179	79	0
36	BR	960	0	1021	87	0
36	DR	960	0	1021	74	0
37	BS	775	0	835	70	0
37	DS	775	0	835	73	0
38	BT	1147	0	1207	105	0
38	DT	1147	0	1207	84	0
39	BU	964	0	1022	85	0
39	DU	964	0	1022	86	0
40	BV	779	0	852	65	0
40	DV	779	0	852	65	0
41	BW	900	0	964	60	0
41	DW	900	0	964	60	0
42	BX	734	0	789	42	0
42	DX	734	0	789	51	0
43	BY	818	0	908	46	0
43	DY	818	0	908	45	0
44	BZ	1473	0	1497	72	0
44	DZ	1473	0	1497	72	0
45	B0	662	0	688	45	0
45	D0	662	0	688	45	0
46	B1	732	0	808	79	0
46	D1	732	0	808	79	0
47	B4	271	0	284	21	0
47	D4	271	0	284	17	0
48	BN	1104	0	1180	217	0
48	DN	1104	0	1180	230	0
49	B2	598	0	653	34	0
49	D2	598	0	653	30	0
50	B3	477	0	529	20	0
50	D3	477	0	529	24	0
51	B5	459	0	477	31	0
51	D5	459	0	477	40	0
52	B6	433	0	461	37	0
52	D6	433	0	461	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	B7	430	0	480	39	0
53	D7	430	0	480	37	0
54	B8	517	0	582	47	0
54	D8	517	0	582	41	0
55	B9	307	0	336	23	0
55	D9	307	0	338	31	0
56	Be	686	0	620	22	0
56	De	686	0	620	26	0
57	Bf	156	0	37	1	0
57	Bg	156	0	39	0	0
57	Df	156	0	38	0	0
57	Dg	156	0	40	0	0
58	Bh	151	0	39	1	0
58	Dh	151	0	40	1	0
59	BB	2551	0	1295	93	0
59	DB	2551	0	1295	83	0
60	BA	61997	0	31250	2256	0
60	DA	61997	0	31250	2190	0
61	AY	32	0	13	8	0
61	CY	32	0	13	18	0
62	AY	1	0	0	0	0
62	CY	1	0	0	0	0
All	All	308202	0	213207	13289	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 26.

The worst 5 of 13289 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)
48:DN:78:TYR:CD2	60:DA:2642:G:C5'	1.74	1.62
39:DU:64:ARG:CD	48:DN:41:ASP:HA	1.14	1.60
39:BU:64:ARG:CD	48:BN:41:ASP:HA	1.32	1.57
39:DU:64:ARG:HD2	48:DN:41:ASP:CA	1.06	1.52
39:BU:64:ARG:HD2	48:BN:41:ASP:CA	1.37	1.49

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AB	233/235 (99%)	154 (66%)	60 (26%)	19 (8%)	0	11
1	CB	233/235 (99%)	164 (70%)	49 (21%)	20 (9%)	0	10
2	AC	205/207 (99%)	140 (68%)	43 (21%)	22 (11%)	0	6
2	CC	205/207 (99%)	136 (66%)	47 (23%)	22 (11%)	0	6
3	AD	206/208 (99%)	146 (71%)	46 (22%)	14 (7%)	1	14
3	CD	206/208 (99%)	140 (68%)	49 (24%)	17 (8%)	0	11
4	AE	149/151 (99%)	118 (79%)	22 (15%)	9 (6%)	1	16
4	CE	149/151 (99%)	125 (84%)	16 (11%)	8 (5%)	1	17
5	AF	99/101 (98%)	82 (83%)	14 (14%)	3 (3%)	3	26
5	CF	99/101 (98%)	81 (82%)	10 (10%)	8 (8%)	1	11
6	AG	153/155 (99%)	113 (74%)	27 (18%)	13 (8%)	0	10
6	CG	153/155 (99%)	116 (76%)	24 (16%)	13 (8%)	0	10
7	AH	136/138 (99%)	98 (72%)	21 (15%)	17 (12%)	0	4
7	CH	136/138 (99%)	90 (66%)	29 (21%)	17 (12%)	0	4
8	AI	125/127 (98%)	98 (78%)	16 (13%)	11 (9%)	0	10
8	CI	125/127 (98%)	100 (80%)	16 (13%)	9 (7%)	1	13
9	AJ	97/99 (98%)	69 (71%)	22 (23%)	6 (6%)	1	15
9	CJ	97/99 (98%)	71 (73%)	20 (21%)	6 (6%)	1	15
10	AK	117/119 (98%)	81 (69%)	23 (20%)	13 (11%)	0	6
10	CK	117/119 (98%)	82 (70%)	22 (19%)	13 (11%)	0	6
11	AL	123/125 (98%)	55 (45%)	38 (31%)	30 (24%)	0	1
11	CL	123/125 (98%)	54 (44%)	41 (33%)	28 (23%)	0	1
12	AM	123/125 (98%)	85 (69%)	21 (17%)	17 (14%)	0	3
12	CM	123/125 (98%)	85 (69%)	22 (18%)	16 (13%)	0	3
13	AN	58/60 (97%)	46 (79%)	7 (12%)	5 (9%)	0	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	CN	58/60 (97%)	45 (78%)	8 (14%)	5 (9%)	0	10
14	AO	86/88 (98%)	59 (69%)	20 (23%)	7 (8%)	1	11
14	CO	86/88 (98%)	60 (70%)	20 (23%)	6 (7%)	1	14
15	AP	82/84 (98%)	61 (74%)	14 (17%)	7 (8%)	0	10
15	CP	82/84 (98%)	59 (72%)	20 (24%)	3 (4%)	2	22
16	AQ	98/100 (98%)	71 (72%)	14 (14%)	13 (13%)	0	3
16	CQ	98/100 (98%)	72 (74%)	17 (17%)	9 (9%)	0	10
17	AR	68/70 (97%)	43 (63%)	17 (25%)	8 (12%)	0	5
17	CR	68/70 (97%)	49 (72%)	16 (24%)	3 (4%)	2	20
18	AS	77/79 (98%)	45 (58%)	21 (27%)	11 (14%)	0	3
18	CS	77/79 (98%)	38 (49%)	29 (38%)	10 (13%)	0	3
19	AT	97/99 (98%)	77 (79%)	16 (16%)	4 (4%)	2	21
19	CT	97/99 (98%)	79 (81%)	14 (14%)	4 (4%)	2	21
23	AY	685/687 (100%)	474 (69%)	144 (21%)	67 (10%)	0	8
23	CY	685/687 (100%)	476 (70%)	143 (21%)	66 (10%)	0	8
24	AU	2/6 (33%)	2 (100%)	0	0	100	100
24	CU	2/6 (33%)	2 (100%)	0	0	100	100
25	BC	226/228 (99%)	109 (48%)	65 (29%)	52 (23%)	0	1
25	DC	226/228 (99%)	108 (48%)	66 (29%)	52 (23%)	0	1
26	BD	273/275 (99%)	177 (65%)	66 (24%)	30 (11%)	0	6
26	DD	273/275 (99%)	179 (66%)	57 (21%)	37 (14%)	0	3
27	BE	203/205 (99%)	123 (61%)	50 (25%)	30 (15%)	0	3
27	DE	203/205 (99%)	133 (66%)	41 (20%)	29 (14%)	0	3
28	BF	206/208 (99%)	130 (63%)	47 (23%)	29 (14%)	0	3
28	DF	206/208 (99%)	126 (61%)	55 (27%)	25 (12%)	0	4
29	BG	179/181 (99%)	116 (65%)	45 (25%)	18 (10%)	0	8
29	DG	179/181 (99%)	121 (68%)	43 (24%)	15 (8%)	0	10
30	BH	165/167 (99%)	115 (70%)	35 (21%)	15 (9%)	0	10
30	DH	165/167 (99%)	121 (73%)	26 (16%)	18 (11%)	0	6
32	BK	138/140 (99%)	97 (70%)	28 (20%)	13 (9%)	0	9
32	DK	138/140 (99%)	91 (66%)	35 (25%)	12 (9%)	0	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	BO	120/122 (98%)	88 (73%)	25 (21%)	7 (6%)	1	16
33	DO	120/122 (98%)	90 (75%)	22 (18%)	8 (7%)	1	15
34	BP	144/146 (99%)	82 (57%)	41 (28%)	21 (15%)	0	3
34	DP	144/146 (99%)	88 (61%)	35 (24%)	21 (15%)	0	3
35	BQ	139/141 (99%)	93 (67%)	32 (23%)	14 (10%)	0	8
35	DQ	139/141 (99%)	99 (71%)	26 (19%)	14 (10%)	0	8
36	BR	115/117 (98%)	72 (63%)	28 (24%)	15 (13%)	0	3
36	DR	115/117 (98%)	78 (68%)	26 (23%)	11 (10%)	0	8
37	BS	97/99 (98%)	54 (56%)	22 (23%)	21 (22%)	0	1
37	DS	97/99 (98%)	52 (54%)	24 (25%)	21 (22%)	0	1
38	BT	136/138 (99%)	84 (62%)	33 (24%)	19 (14%)	0	3
38	DT	136/138 (99%)	89 (65%)	28 (21%)	19 (14%)	0	3
39	BU	115/117 (98%)	89 (77%)	21 (18%)	5 (4%)	2	20
39	DU	115/117 (98%)	84 (73%)	20 (17%)	11 (10%)	0	8
40	BV	99/101 (98%)	59 (60%)	22 (22%)	18 (18%)	0	2
40	DV	99/101 (98%)	63 (64%)	22 (22%)	14 (14%)	0	3
41	BW	111/113 (98%)	88 (79%)	16 (14%)	7 (6%)	1	15
41	DW	111/113 (98%)	90 (81%)	10 (9%)	11 (10%)	0	8
42	BX	91/93 (98%)	71 (78%)	12 (13%)	8 (9%)	0	10
42	DX	91/93 (98%)	69 (76%)	17 (19%)	5 (6%)	1	17
43	BY	105/107 (98%)	48 (46%)	33 (31%)	24 (23%)	0	1
43	DY	105/107 (98%)	50 (48%)	34 (32%)	21 (20%)	0	1
44	BZ	183/185 (99%)	126 (69%)	42 (23%)	15 (8%)	0	11
44	DZ	183/185 (99%)	120 (66%)	45 (25%)	18 (10%)	0	8
45	B0	82/84 (98%)	59 (72%)	15 (18%)	8 (10%)	0	8
45	D0	82/84 (98%)	55 (67%)	20 (24%)	7 (8%)	0	10
46	B1	91/93 (98%)	55 (60%)	19 (21%)	17 (19%)	0	2
46	D1	91/93 (98%)	55 (60%)	17 (19%)	19 (21%)	0	1
47	B4	33/35 (94%)	17 (52%)	13 (39%)	3 (9%)	0	10
47	D4	33/35 (94%)	17 (52%)	11 (33%)	5 (15%)	0	2
48	BN	136/138 (99%)	95 (70%)	25 (18%)	16 (12%)	0	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	DN	136/138 (99%)	94 (69%)	26 (19%)	16 (12%)	0	5
49	B2	69/71 (97%)	52 (75%)	13 (19%)	4 (6%)	1	16
49	D2	69/71 (97%)	51 (74%)	14 (20%)	4 (6%)	1	16
50	B3	58/60 (97%)	48 (83%)	7 (12%)	3 (5%)	1	18
50	D3	58/60 (97%)	45 (78%)	10 (17%)	3 (5%)	1	18
51	B5	57/59 (97%)	37 (65%)	10 (18%)	10 (18%)	0	2
51	D5	57/59 (97%)	37 (65%)	13 (23%)	7 (12%)	0	4
52	B6	48/50 (96%)	26 (54%)	11 (23%)	11 (23%)	0	1
52	D6	48/50 (96%)	26 (54%)	11 (23%)	11 (23%)	0	1
53	B7	47/49 (96%)	32 (68%)	11 (23%)	4 (8%)	0	10
53	D7	47/49 (96%)	34 (72%)	9 (19%)	4 (8%)	0	10
54	B8	62/64 (97%)	38 (61%)	18 (29%)	6 (10%)	0	8
54	D8	62/64 (97%)	37 (60%)	17 (27%)	8 (13%)	0	4
55	B9	35/37 (95%)	16 (46%)	14 (40%)	5 (14%)	0	3
55	D9	35/37 (95%)	19 (54%)	12 (34%)	4 (11%)	0	5
56	Be	70/103 (68%)	38 (54%)	25 (36%)	7 (10%)	0	8
56	De	70/103 (68%)	40 (57%)	23 (33%)	7 (10%)	0	8
All	All	13304/13578 (98%)	8936 (67%)	2877 (22%)	1491 (11%)	0	6

5 of 1491 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AB	20	GLU
1	AB	67	THR
1	AB	76	GLN
1	AB	103	THR
1	AB	157	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AB	203/203 (100%)	158 (78%)	45 (22%)	1	6
1	CB	203/203 (100%)	168 (83%)	35 (17%)	2	12
2	AC	161/161 (100%)	123 (76%)	38 (24%)	1	5
2	CC	161/161 (100%)	120 (74%)	41 (26%)	0	4
3	AD	180/180 (100%)	141 (78%)	39 (22%)	1	6
3	CD	180/180 (100%)	146 (81%)	34 (19%)	1	10
4	AE	116/116 (100%)	91 (78%)	25 (22%)	1	6
4	CE	116/116 (100%)	93 (80%)	23 (20%)	1	9
5	AF	90/90 (100%)	72 (80%)	18 (20%)	1	9
5	CF	90/90 (100%)	73 (81%)	17 (19%)	1	10
6	AG	126/126 (100%)	110 (87%)	16 (13%)	4	20
6	CG	126/126 (100%)	106 (84%)	20 (16%)	2	14
7	AH	119/119 (100%)	93 (78%)	26 (22%)	1	6
7	CH	119/119 (100%)	99 (83%)	20 (17%)	2	13
8	AI	98/98 (100%)	76 (78%)	22 (22%)	1	6
8	CI	98/98 (100%)	82 (84%)	16 (16%)	2	14
9	AJ	89/89 (100%)	68 (76%)	21 (24%)	1	5
9	CJ	89/89 (100%)	71 (80%)	18 (20%)	1	8
10	AK	90/90 (100%)	72 (80%)	18 (20%)	1	9
10	CK	90/90 (100%)	79 (88%)	11 (12%)	5	21
11	AL	104/104 (100%)	73 (70%)	31 (30%)	0	2
11	CL	104/104 (100%)	77 (74%)	27 (26%)	0	3
12	AM	100/100 (100%)	81 (81%)	19 (19%)	1	10
12	CM	100/100 (100%)	84 (84%)	16 (16%)	2	14
13	AN	49/49 (100%)	39 (80%)	10 (20%)	1	8
13	CN	49/49 (100%)	40 (82%)	9 (18%)	1	11
14	AO	79/79 (100%)	60 (76%)	19 (24%)	1	4
14	CO	79/79 (100%)	62 (78%)	17 (22%)	1	6
15	AP	72/72 (100%)	58 (81%)	14 (19%)	1	9
15	CP	72/72 (100%)	58 (81%)	14 (19%)	1	9
16	AQ	95/95 (100%)	74 (78%)	21 (22%)	1	6
16	CQ	95/95 (100%)	79 (83%)	16 (17%)	2	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	AR	61/61 (100%)	49 (80%)	12 (20%)	1	9
17	CR	61/61 (100%)	49 (80%)	12 (20%)	1	9
18	AS	69/69 (100%)	49 (71%)	20 (29%)	0	2
18	CS	69/69 (100%)	52 (75%)	17 (25%)	1	4
19	AT	76/76 (100%)	66 (87%)	10 (13%)	4	19
19	CT	76/76 (100%)	67 (88%)	9 (12%)	5	21
23	AY	579/579 (100%)	460 (79%)	119 (21%)	1	8
23	CY	579/579 (100%)	453 (78%)	126 (22%)	1	6
24	AU	2/2 (100%)	2 (100%)	0	100	100
24	CU	2/2 (100%)	2 (100%)	0	100	100
25	BC	180/180 (100%)	132 (73%)	48 (27%)	0	3
25	DC	180/180 (100%)	132 (73%)	48 (27%)	0	3
26	BD	217/217 (100%)	161 (74%)	56 (26%)	0	3
26	DD	217/217 (100%)	165 (76%)	52 (24%)	1	4
27	BE	165/165 (100%)	126 (76%)	39 (24%)	1	5
27	DE	165/165 (100%)	130 (79%)	35 (21%)	1	7
28	BF	165/165 (100%)	126 (76%)	39 (24%)	1	5
28	DF	165/165 (100%)	123 (74%)	42 (26%)	0	4
29	BG	155/155 (100%)	117 (76%)	38 (24%)	1	4
29	DG	155/155 (100%)	122 (79%)	33 (21%)	1	6
30	BH	136/136 (100%)	109 (80%)	27 (20%)	1	9
30	DH	136/136 (100%)	112 (82%)	24 (18%)	2	12
32	BK	105/105 (100%)	91 (87%)	14 (13%)	4	19
32	DK	105/105 (100%)	90 (86%)	15 (14%)	3	17
33	BO	100/100 (100%)	78 (78%)	22 (22%)	1	6
33	DO	100/100 (100%)	85 (85%)	15 (15%)	3	16
34	BP	112/112 (100%)	84 (75%)	28 (25%)	0	4
34	DP	112/112 (100%)	92 (82%)	20 (18%)	2	12
35	BQ	111/111 (100%)	83 (75%)	28 (25%)	0	4
35	DQ	111/111 (100%)	87 (78%)	24 (22%)	1	6
36	BR	100/100 (100%)	74 (74%)	26 (26%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	DR	100/100 (100%)	81 (81%)	19 (19%)	1	10
37	BS	77/77 (100%)	52 (68%)	25 (32%)	0	2
37	DS	77/77 (100%)	56 (73%)	21 (27%)	0	3
38	BT	120/120 (100%)	97 (81%)	23 (19%)	1	9
38	DT	120/120 (100%)	95 (79%)	25 (21%)	1	7
39	BU	93/93 (100%)	77 (83%)	16 (17%)	2	12
39	DU	93/93 (100%)	74 (80%)	19 (20%)	1	8
40	BV	82/82 (100%)	62 (76%)	20 (24%)	1	4
40	DV	82/82 (100%)	61 (74%)	21 (26%)	0	4
41	BW	92/92 (100%)	72 (78%)	20 (22%)	1	6
41	DW	92/92 (100%)	72 (78%)	20 (22%)	1	6
42	BX	75/75 (100%)	59 (79%)	16 (21%)	1	6
42	DX	75/75 (100%)	62 (83%)	13 (17%)	2	12
43	BY	88/88 (100%)	67 (76%)	21 (24%)	1	5
43	DY	88/88 (100%)	69 (78%)	19 (22%)	1	6
44	BZ	162/162 (100%)	132 (82%)	30 (18%)	1	11
44	DZ	162/162 (100%)	123 (76%)	39 (24%)	1	4
45	B0	66/66 (100%)	56 (85%)	10 (15%)	3	15
45	D0	66/66 (100%)	55 (83%)	11 (17%)	2	13
46	B1	78/78 (100%)	62 (80%)	16 (20%)	1	8
46	D1	78/78 (100%)	54 (69%)	24 (31%)	0	2
47	B4	31/31 (100%)	20 (64%)	11 (36%)	0	1
47	D4	31/31 (100%)	24 (77%)	7 (23%)	1	5
48	BN	117/117 (100%)	101 (86%)	16 (14%)	3	18
48	DN	117/117 (100%)	101 (86%)	16 (14%)	3	18
49	B2	66/66 (100%)	55 (83%)	11 (17%)	2	13
49	D2	66/66 (100%)	57 (86%)	9 (14%)	3	18
50	B3	52/52 (100%)	44 (85%)	8 (15%)	2	15
50	D3	52/52 (100%)	42 (81%)	10 (19%)	1	9
51	B5	51/51 (100%)	43 (84%)	8 (16%)	2	15
51	D5	51/51 (100%)	40 (78%)	11 (22%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	B6	49/49 (100%)	35 (71%)	14 (29%)	0	2
52	D6	49/49 (100%)	35 (71%)	14 (29%)	0	2
53	B7	42/42 (100%)	39 (93%)	3 (7%)	13	40
53	D7	42/42 (100%)	36 (86%)	6 (14%)	3	17
54	B8	54/54 (100%)	39 (72%)	15 (28%)	0	3
54	D8	54/54 (100%)	43 (80%)	11 (20%)	1	8
55	B9	34/34 (100%)	27 (79%)	7 (21%)	1	8
55	D9	34/34 (100%)	25 (74%)	9 (26%)	0	3
56	Be	54/54 (100%)	45 (83%)	9 (17%)	2	13
56	De	54/54 (100%)	46 (85%)	8 (15%)	3	16
All	All	11174/11174 (100%)	8829 (79%)	2345 (21%)	1	7

5 of 2345 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
28	DF	35	GLU
51	D5	23	HIS
29	DG	147	ASP
28	DF	32	LEU
39	DU	28	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 164 such sidechains are listed below:

Mol	Chain	Res	Type
23	CY	137	ASN
37	DS	34	HIS
23	CY	448	GLN
27	DE	169	ASN
39	DU	81	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
20	AA	1511/1511 (100%)	330 (21%)	21 (1%)
20	CA	1511/1511 (100%)	304 (20%)	18 (1%)
21	AV	17/18 (94%)	8 (47%)	1 (5%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	CV	17/18 (94%)	8 (47%)	1 (5%)
22	AW	76/77 (98%)	27 (35%)	2 (2%)
22	CW	76/77 (98%)	22 (28%)	2 (2%)
59	BB	118/119 (99%)	26 (22%)	2 (1%)
59	DB	118/119 (99%)	19 (16%)	1 (0%)
60	BA	2878/2879 (99%)	730 (25%)	26 (0%)
60	DA	2878/2879 (99%)	693 (24%)	22 (0%)
All	All	9200/9208 (99%)	2167 (23%)	96 (1%)

5 of 2167 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
20	AA	6	G
20	AA	7	G
20	AA	8	A
20	AA	9	G
20	AA	22	G

5 of 96 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
20	CA	429	U
22	CW	20(A)	U
20	CA	531	U
20	CA	1145	C
60	DA	271(C)	G

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
24	KBE	AU	1	24	8,8,9	1.04	0	6,8,10	2.15	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	DPP	CU	2	24	4,5,6	0.65	0	1,5,7	0.27	0
24	UAL	AU	5	24	6,8,9	2.79	3 (50%)	4,9,11	2.19	1 (25%)
24	5OH	AU	6	24	7,12,13	0.75	0	4,16,18	0.94	0
24	KBE	CU	1	24	8,8,9	1.05	0	6,8,10	2.16	1 (16%)
24	5OH	CU	6	24	7,12,13	0.75	0	4,16,18	0.94	0
24	DPP	AU	2	24	4,5,6	0.65	0	1,5,7	0.28	0
24	UAL	CU	5	24	6,8,9	2.78	3 (50%)	4,9,11	2.20	1 (25%)

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
24	KBE	AU	1	24	-	3/7/7/8	-
24	DPP	CU	2	24	-	2/2/4/6	-
24	UAL	AU	5	24	-	0/3/7/9	-
24	5OH	AU	6	24	-	0/2/18/20	0/1/1/1
24	KBE	CU	1	24	-	3/7/7/8	-
24	5OH	CU	6	24	-	0/2/18/20	0/1/1/1
24	DPP	AU	2	24	-	2/2/4/6	-
24	UAL	CU	5	24	-	0/3/7/9	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AU	5	UAL	C-CA	5.31	1.54	1.45
24	CU	5	UAL	C-CA	5.28	1.54	1.45
24	AU	5	UAL	C1-N1	-3.51	1.34	1.40
24	CU	5	UAL	C1-N1	-3.48	1.35	1.40
24	AU	5	UAL	CB-N1	-2.29	1.30	1.35

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	CU	1	KBE	CB-CA-C	4.95	120.16	112.17
24	AU	1	KBE	CB-CA-C	4.94	120.14	112.17
24	CU	5	UAL	O-C-CA	-4.27	120.03	125.39
24	AU	5	UAL	O-C-CA	-4.25	120.06	125.39

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	AU	1	KBE	C-CA-CB-N
24	AU	1	KBE	C-CA-CB-CG
24	CU	1	KBE	C-CA-CB-N
24	CU	1	KBE	C-CA-CB-CG
24	AU	2	DPP	N-CA-CB-NG

There are no ring outliers.

6 monomers are involved in 53 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	CU	2	DPP	2	0
24	AU	5	UAL	1	0
24	AU	6	5OH	27	0
24	CU	6	5OH	12	0
24	AU	2	DPP	12	0
24	CU	5	UAL	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
61	GNP	AY	701	62	34,34,34	1.47	4 (11%)	47,54,54	1.36	8 (17%)
61	GNP	CY	702	62	34,34,34	1.47	4 (11%)	47,54,54	1.36	8 (17%)

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
61	GNP	AY	701	62	-	7/18/38/38	0/3/3/3
61	GNP	CY	702	62	-	7/18/38/38	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	CY	702	GNP	PG-O1G	5.00	1.53	1.46
61	AY	701	GNP	PG-O1G	4.98	1.53	1.46
61	AY	701	GNP	PA-O3A	-4.14	1.55	1.59
61	CY	702	GNP	PA-O3A	-4.13	1.55	1.59
61	AY	701	GNP	PB-O3A	-2.57	1.55	1.59

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	CY	702	GNP	O2B-PB-O1B	3.42	117.21	109.87
61	AY	701	GNP	O2B-PB-O1B	3.41	117.18	109.87
61	AY	701	GNP	O2G-PG-O3G	3.30	116.47	107.59
61	CY	702	GNP	O2G-PG-O3G	3.30	116.45	107.59
61	CY	702	GNP	O3G-PG-O1G	-2.99	105.95	113.45

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

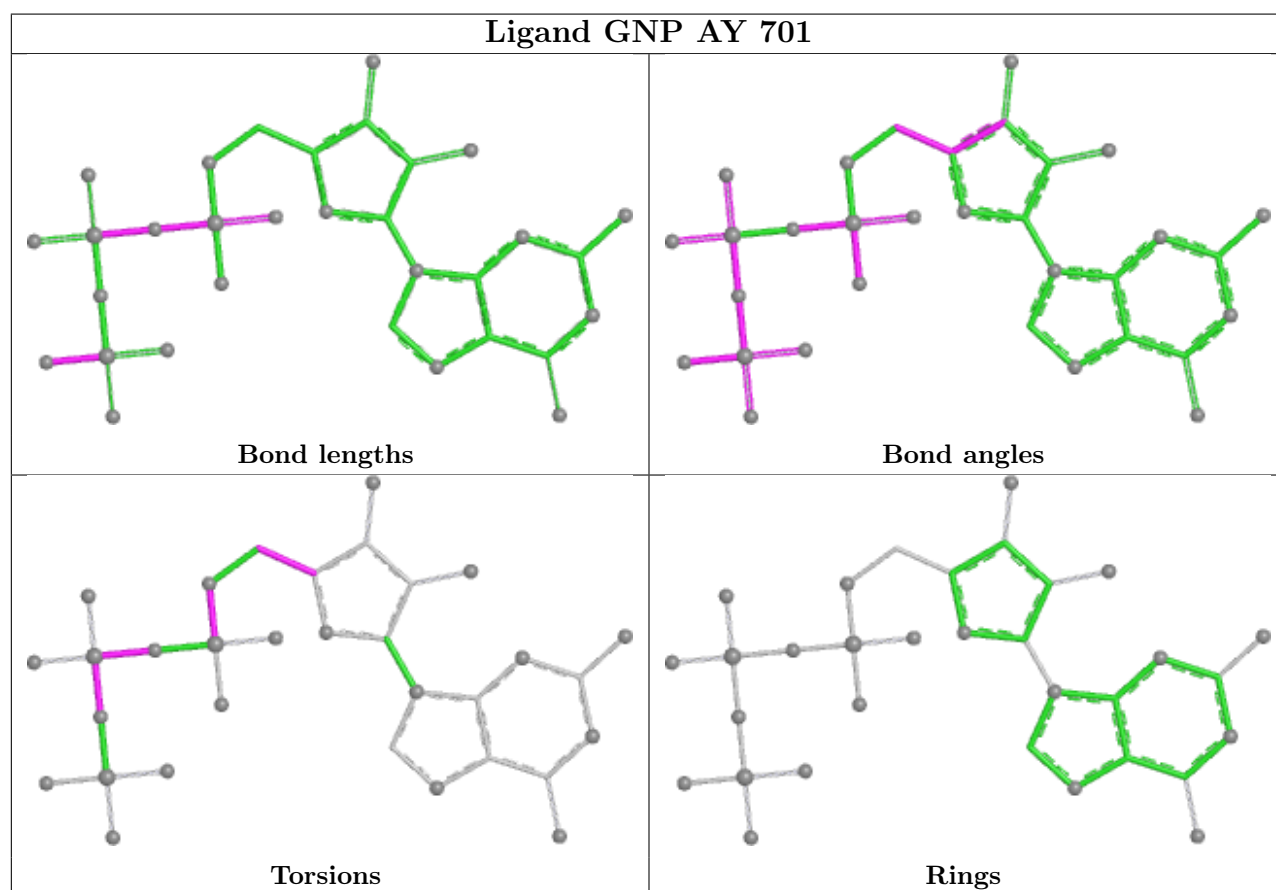
Mol	Chain	Res	Type	Atoms
61	AY	701	GNP	PG-N3B-PB-O1B
61	AY	701	GNP	PG-N3B-PB-O3A
61	AY	701	GNP	PA-O3A-PB-O2B
61	AY	701	GNP	C5'-O5'-PA-O3A
61	AY	701	GNP	C5'-O5'-PA-O1A

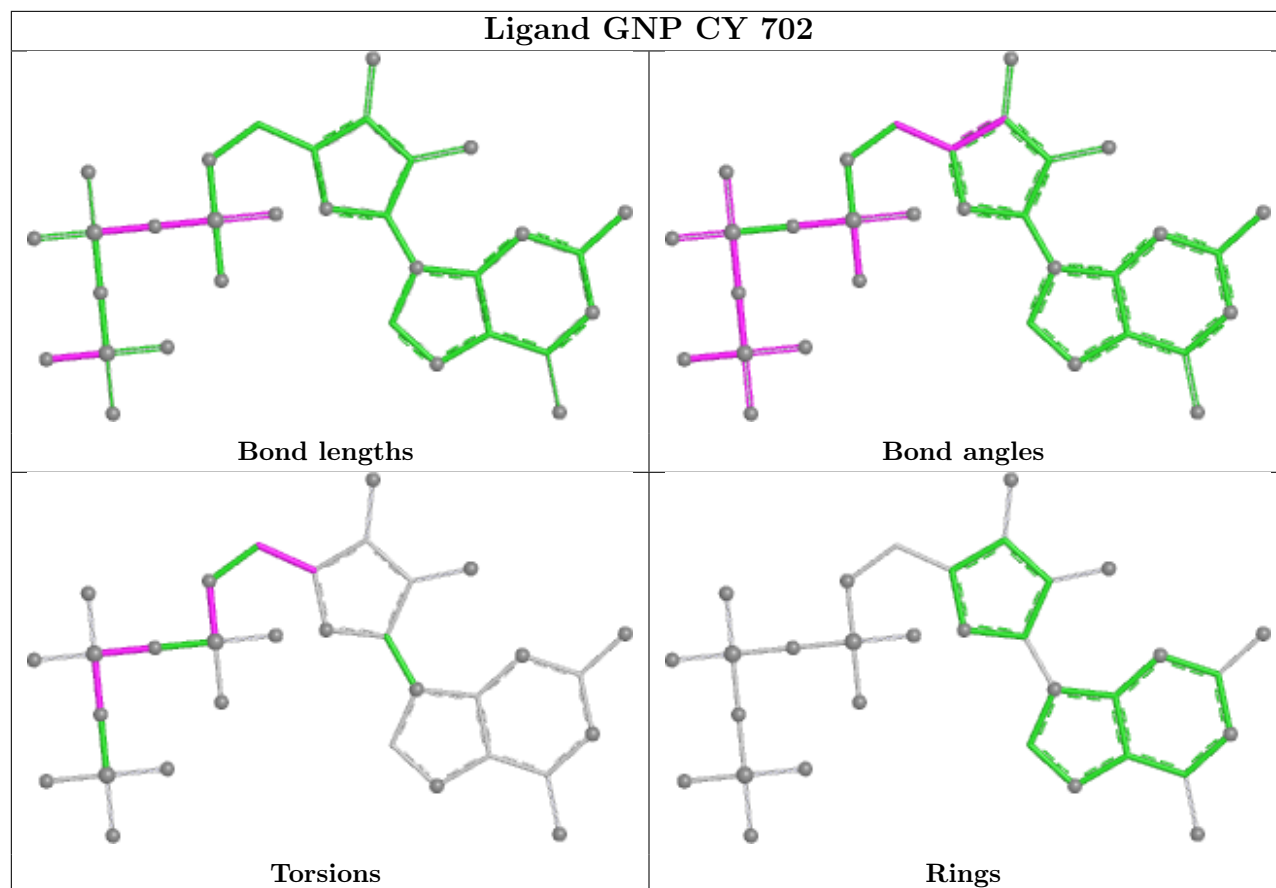
There are no ring outliers.

2 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	AY	701	GNP	8	0
61	CY	702	GNP	18	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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AB	235/235 (100%)	0.27	19 (8%) 18 18	13, 75, 147, 218	0
1	CB	235/235 (100%)	0.13	11 (4%) 36 27	26, 78, 150, 182	0
2	AC	207/207 (100%)	-0.05	7 (3%) 48 34	21, 64, 129, 194	0
2	CC	207/207 (100%)	-0.07	8 (3%) 43 31	33, 66, 122, 164	0
3	AD	208/208 (100%)	0.68	36 (17%) 4 6	24, 71, 131, 187	0
3	CD	208/208 (100%)	0.68	35 (16%) 4 7	16, 79, 141, 186	0
4	AE	151/151 (100%)	-0.04	4 (2%) 57 39	10, 57, 124, 176	0
4	CE	151/151 (100%)	0.09	6 (3%) 42 31	23, 71, 126, 185	0
5	AF	101/101 (100%)	0.08	4 (3%) 42 31	36, 69, 131, 173	0
5	CF	101/101 (100%)	0.22	7 (6%) 23 20	29, 64, 127, 176	0
6	AG	155/155 (100%)	-0.21	4 (2%) 57 39	20, 84, 135, 192	0
6	CG	155/155 (100%)	-0.16	6 (3%) 43 31	39, 86, 144, 209	0
7	AH	138/138 (100%)	-0.06	6 (4%) 40 29	21, 64, 118, 145	0
7	CH	138/138 (100%)	-0.04	3 (2%) 62 44	33, 67, 126, 179	0
8	AI	127/127 (100%)	0.43	13 (10%) 12 15	13, 74, 122, 146	0
8	CI	127/127 (100%)	0.31	14 (11%) 10 13	16, 69, 128, 177	0
9	AJ	99/99 (100%)	0.38	11 (11%) 10 13	34, 74, 129, 147	0
9	CJ	99/99 (100%)	0.67	12 (12%) 8 12	24, 81, 132, 167	0
10	AK	119/119 (100%)	0.25	8 (6%) 24 21	17, 68, 129, 145	0
10	CK	119/119 (100%)	0.39	11 (9%) 14 16	37, 83, 128, 165	0
11	AL	125/125 (100%)	0.77	21 (16%) 4 7	22, 64, 128, 177	0
11	CL	125/125 (100%)	1.19	24 (19%) 3 5	21, 72, 139, 179	0
12	AM	125/125 (100%)	0.41	16 (12%) 7 11	54, 96, 167, 207	0
12	CM	125/125 (100%)	0.22	11 (8%) 15 16	58, 97, 159, 195	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AN	60/60 (100%)	0.56	5 (8%) 17 17	3, 48, 113, 131	0
13	CN	60/60 (100%)	0.82	9 (15%) 5 9	30, 54, 113, 147	0
14	AO	88/88 (100%)	0.36	5 (5%) 29 23	24, 64, 113, 158	0
14	CO	88/88 (100%)	0.25	7 (7%) 18 18	32, 73, 127, 165	0
15	AP	84/84 (100%)	1.00	15 (17%) 3 6	35, 82, 143, 179	0
15	CP	84/84 (100%)	0.69	18 (21%) 2 5	29, 73, 132, 175	0
16	AQ	100/100 (100%)	0.48	11 (11%) 10 13	24, 66, 120, 137	0
16	CQ	100/100 (100%)	0.51	13 (13%) 7 10	42, 74, 130, 159	0
17	AR	70/70 (100%)	-0.16	1 (1%) 73 52	28, 54, 107, 143	0
17	CR	70/70 (100%)	0.02	1 (1%) 73 52	26, 69, 132, 198	0
18	AS	79/79 (100%)	0.38	6 (7%) 20 18	25, 95, 172, 193	0
18	CS	79/79 (100%)	0.42	9 (11%) 10 13	26, 89, 165, 199	0
19	AT	99/99 (100%)	0.42	5 (5%) 33 26	16, 66, 130, 188	0
19	CT	99/99 (100%)	0.52	15 (15%) 5 8	27, 80, 144, 169	0
20	AA	1511/1511 (100%)	-0.03	70 (4%) 37 28	11, 79, 165, 273	0
20	CA	1511/1511 (100%)	0.01	56 (3%) 45 32	6, 84, 166, 265	0
21	AV	18/18 (100%)	0.36	1 (5%) 30 24	41, 113, 170, 197	0
21	CV	18/18 (100%)	0.52	1 (5%) 30 24	33, 135, 179, 181	0
22	AW	77/77 (100%)	-0.08	3 (3%) 43 31	24, 109, 168, 243	0
22	CW	77/77 (100%)	-0.09	5 (6%) 25 21	43, 116, 183, 208	0
23	AY	687/687 (100%)	0.16	43 (6%) 26 22	26, 80, 149, 224	0
23	CY	687/687 (100%)	0.22	61 (8%) 15 16	25, 86, 158, 217	0
24	AU	2/6 (33%)	0.28	0 100 100	66, 66, 66, 66	0
24	CU	2/6 (33%)	-0.53	0 100 100	66, 66, 66, 66	0
25	BC	228/228 (100%)	0.81	42 (18%) 3 6	77, 137, 202, 235	0
25	DC	228/228 (100%)	0.93	35 (15%) 5 8	73, 140, 196, 228	0
26	BD	275/275 (100%)	0.84	51 (18%) 3 6	12, 58, 126, 156	0
26	DD	275/275 (100%)	0.92	55 (20%) 3 5	18, 59, 122, 191	0
27	BE	205/205 (100%)	0.83	53 (25%) 1 4	16, 58, 123, 159	0
27	DE	205/205 (100%)	0.97	40 (19%) 3 5	20, 74, 138, 209	0
28	BF	208/208 (100%)	0.82	37 (17%) 4 6	41, 78, 145, 195	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DF	208/208 (100%)	0.81	29 (13%) 6 10	26, 76, 155, 199	0
29	BG	181/181 (100%)	0.18	8 (4%) 39 29	24, 87, 153, 191	0
29	DG	181/181 (100%)	0.15	10 (5%) 30 24	40, 94, 165, 199	0
30	BH	167/167 (100%)	0.11	8 (4%) 35 27	7, 68, 133, 171	0
30	DH	167/167 (100%)	0.20	11 (6%) 24 21	11, 67, 139, 168	0
31	BJ	0/170	-	-	-	-
31	DJ	0/170	-	-	-	-
32	BK	140/140 (100%)	0.03	8 (5%) 29 23	24, 91, 182, 225	0
32	DK	140/140 (100%)	0.19	13 (9%) 14 16	30, 110, 178, 234	0
33	BO	122/122 (100%)	-0.07	3 (2%) 58 41	24, 45, 123, 162	0
33	DO	122/122 (100%)	-0.00	4 (3%) 49 34	20, 58, 106, 159	0
34	BP	146/146 (100%)	0.58	16 (10%) 10 13	22, 76, 132, 175	0
34	DP	146/146 (100%)	0.46	15 (10%) 12 14	28, 78, 141, 189	0
35	BQ	141/141 (100%)	0.68	20 (14%) 6 9	17, 63, 130, 200	0
35	DQ	141/141 (100%)	0.84	28 (19%) 3 5	22, 68, 140, 174	0
36	BR	117/117 (100%)	0.47	12 (10%) 12 14	15, 57, 119, 178	0
36	DR	117/117 (100%)	0.53	12 (10%) 12 14	18, 69, 143, 195	0
37	BS	99/99 (100%)	0.82	15 (15%) 5 8	22, 104, 172, 208	0
37	DS	99/99 (100%)	0.79	18 (18%) 3 6	18, 106, 167, 216	0
38	BT	138/138 (100%)	0.06	11 (7%) 18 18	22, 71, 133, 179	0
38	DT	138/138 (100%)	0.18	7 (5%) 33 26	19, 75, 153, 238	0
39	BU	117/117 (100%)	0.96	18 (15%) 5 8	40, 57, 131, 184	0
39	DU	117/117 (100%)	0.89	22 (18%) 3 6	24, 61, 118, 158	0
40	BV	101/101 (100%)	0.47	9 (8%) 15 16	13, 54, 114, 146	0
40	DV	101/101 (100%)	0.39	7 (6%) 23 20	20, 72, 127, 200	0
41	BW	113/113 (100%)	0.46	13 (11%) 9 13	16, 55, 121, 147	0
41	DW	113/113 (100%)	0.86	19 (16%) 4 7	5, 65, 136, 178	0
42	BX	93/93 (100%)	0.37	9 (9%) 13 15	18, 60, 114, 149	0
42	DX	93/93 (100%)	0.41	9 (9%) 13 15	34, 63, 128, 170	0
43	BY	107/107 (100%)	0.36	9 (8%) 17 17	8, 86, 151, 180	0
43	DY	107/107 (100%)	0.47	12 (11%) 10 13	35, 76, 151, 176	0
44	BZ	185/185 (100%)	-0.01	10 (5%) 31 25	30, 76, 142, 176	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
44	DZ	185/185 (100%)	0.18	14 (7%)	20	18	36, 82, 147, 226	0
45	B0	84/84 (100%)	0.80	19 (22%)	2	4	18, 92, 159, 181	0
45	D0	84/84 (100%)	0.77	15 (17%)	3	6	19, 85, 145, 160	0
46	B1	93/93 (100%)	1.03	20 (21%)	2	4	26, 91, 161, 204	0
46	D1	93/93 (100%)	1.55	31 (33%)	1	2	38, 92, 166, 194	0
47	B4	35/35 (100%)	0.01	1 (2%)	53	37	49, 106, 171, 203	0
47	D4	35/35 (100%)	-0.06	1 (2%)	53	37	82, 115, 164, 187	0
48	BN	138/138 (100%)	1.56	47 (34%)	1	2	59, 83, 108, 111	0
48	DN	138/138 (100%)	1.48	49 (35%)	1	2	58, 84, 107, 116	0
49	B2	71/71 (100%)	0.15	2 (2%)	55	38	38, 79, 143, 185	0
49	D2	71/71 (100%)	0.05	2 (2%)	55	38	42, 70, 130, 187	0
50	B3	60/60 (100%)	0.44	6 (10%)	12	15	34, 62, 117, 150	0
50	D3	60/60 (100%)	0.64	5 (8%)	17	17	53, 68, 130, 150	0
51	B5	59/59 (100%)	1.04	9 (15%)	5	8	26, 56, 131, 149	0
51	D5	59/59 (100%)	0.91	9 (15%)	5	8	16, 83, 166, 185	0
52	B6	50/50 (100%)	0.76	9 (18%)	3	6	63, 99, 159, 175	0
52	D6	50/50 (100%)	1.25	13 (26%)	1	4	61, 118, 161, 188	0
53	B7	49/49 (100%)	1.79	19 (38%)	1	2	18, 47, 122, 156	0
53	D7	49/49 (100%)	1.27	11 (22%)	2	4	33, 61, 140, 186	0
54	B8	64/64 (100%)	1.15	18 (28%)	1	3	29, 63, 152, 160	0
54	D8	64/64 (100%)	1.44	17 (26%)	1	4	28, 75, 142, 191	0
55	B9	37/37 (100%)	3.67	26 (70%)	0	0	71, 109, 177, 183	0
55	D9	37/37 (100%)	4.11	28 (75%)	0	0	102, 132, 185, 210	0
56	Be	72/103 (69%)	0.19	5 (6%)	23	20	40, 109, 188, 239	0
56	De	72/103 (69%)	0.16	4 (5%)	30	24	46, 118, 183, 199	0
57	Bf	0/31	-	-			-	-
57	Bg	0/31	-	-			-	-
57	Df	0/31	-	-			-	-
57	Dg	0/31	-	-			-	-
58	Bh	0/30	-	-			-	-
58	Dh	0/30	-	-			-	-
59	BB	119/119 (100%)	-0.04	6 (5%)	34	26	27, 111, 173, 186	0
59	DB	119/119 (100%)	-0.07	6 (5%)	34	26	35, 118, 182, 220	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
60	BA	2879/2879 (100%)	0.18	227 (7%) 18 18	7, 78, 171, 308	0
60	DA	2879/2879 (100%)	0.15	201 (6%) 22 20	5, 79, 177, 310	0
All	All	22716/23310 (97%)	0.32	2175 (9%) 13 15	3, 79, 161, 310	0

The worst 5 of 2175 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
60	BA	2250	G	20.1
60	DA	2250	G	16.2
55	D9	15	LYS	15.3
60	DA	2573	C	12.9
60	DA	2581	G	12.8

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
24	KBE	AU	1	9/10	0.44	0.42	65,65,65,65	0
24	UAL	AU	5	9/10	0.61	0.13	65,65,65,65	0
24	5OH	AU	6	12/13	0.71	0.13	99,101,102,102	0
24	KBE	CU	1	9/10	0.80	0.22	65,65,65,65	0
24	DPP	CU	2	6/7	0.82	0.10	65,65,65,65	0
24	DPP	AU	2	6/7	0.84	0.08	65,65,65,65	0
24	UAL	CU	5	9/10	0.85	0.09	65,65,65,65	0
24	5OH	CU	6	12/13	0.92	0.11	99,101,102,102	0

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, 95th percentile and maximum values of B factors of atoms in the group. The column

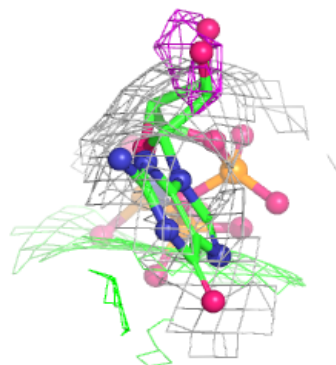
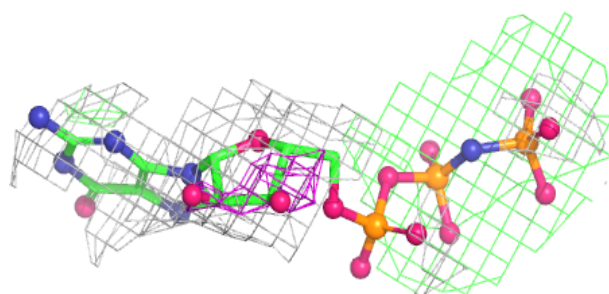
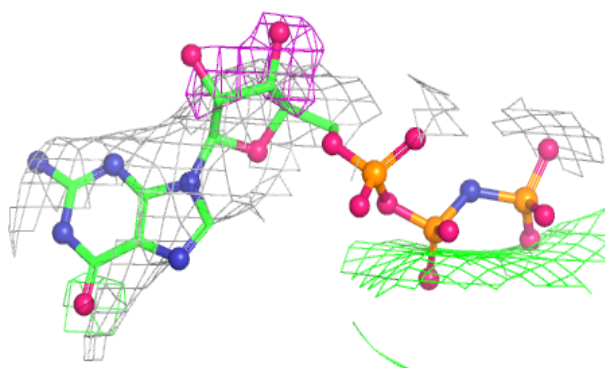
labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
61	GNP	AY	701	32/32	0.78	0.13	58,71,81,83	0
62	MG	AY	702	1/1	0.81	0.10	124,124,124,124	0
61	GNP	CY	702	32/32	0.91	0.10	58,71,81,83	0
62	MG	CY	701	1/1	0.95	0.07	104,104,104,104	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.

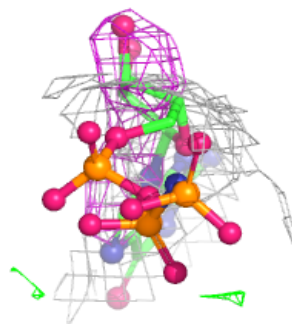
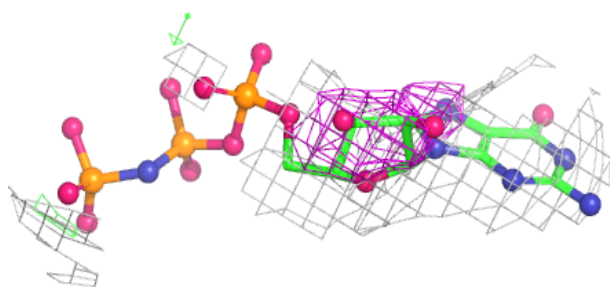
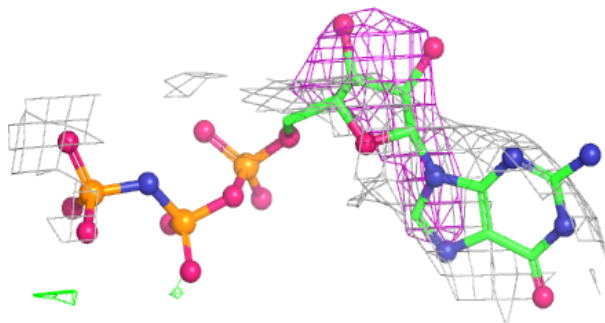
Electron density around GNP AY 701:

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 GNP CY 702:

$2mF_o - DF_c$ (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.