



wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 03:47 am BST

PDB ID : 4V9M
Title : 70S Ribosome translocation intermediate FA-4.2A containing elongation factor EFG/FUSIDIC ACID/GDP, mRNA, and tRNA bound in the pe^{*}/E state.
Authors : Zhou, J.; Lancaster, L.; Donohue, J.P.; Noller, H.F.
Deposited on : 2013-04-25
Resolution : 4.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

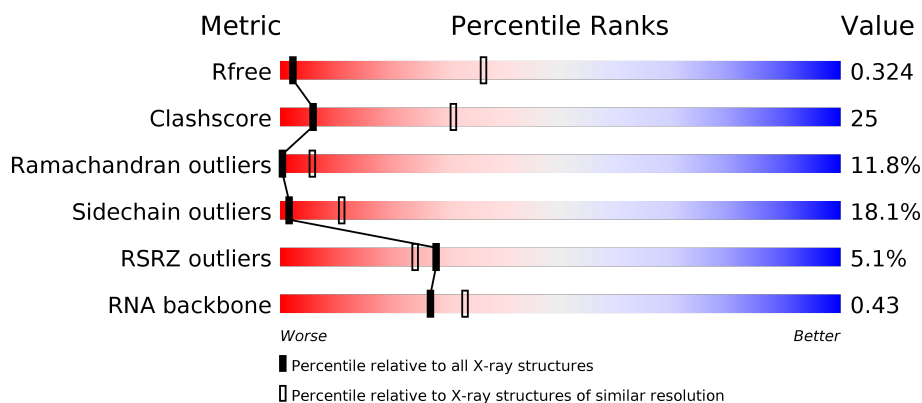
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)
RNA backbone	3102	1048 (5.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	<div> <div>35%</div> <div>45%</div> <div>18%</div> <div>•</div> </div>
1	CB	235	<div> <div>33%</div> <div>48%</div> <div>17%</div> <div>•</div> </div>
2	AC	207	<div> <div>12%</div> <div>42%</div> <div>47%</div> <div>10%</div> </div>
2	CC	207	<div> <div>13%</div> <div>50%</div> <div>39%</div> <div>11%</div> </div>

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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	



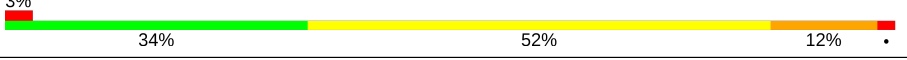
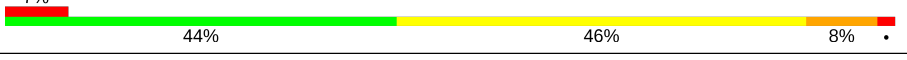

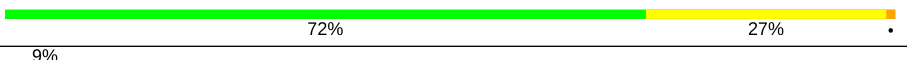
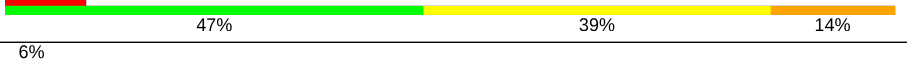
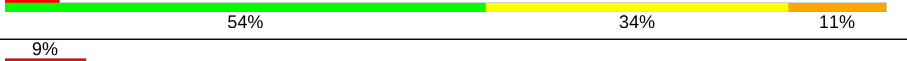
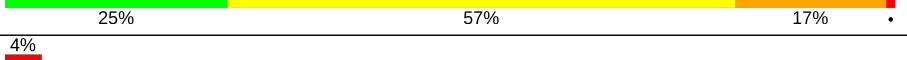
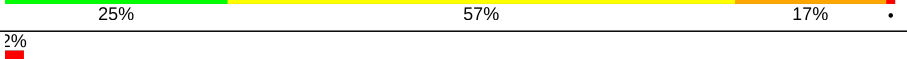
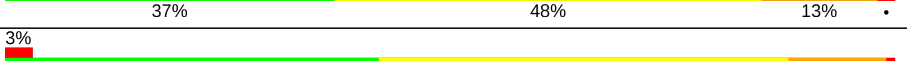
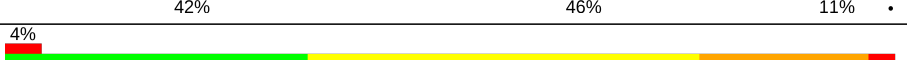
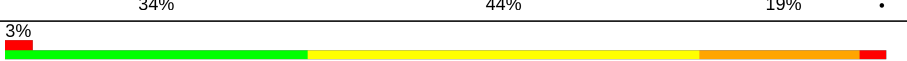
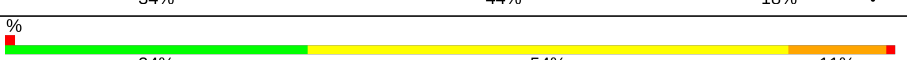
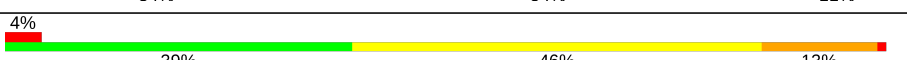
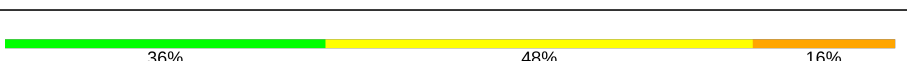
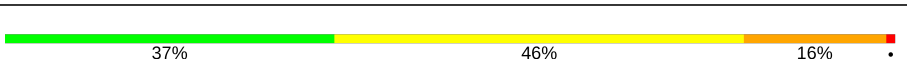
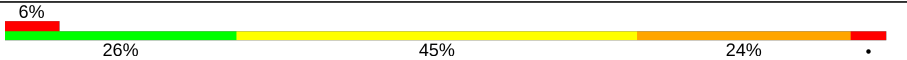
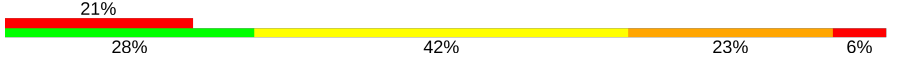
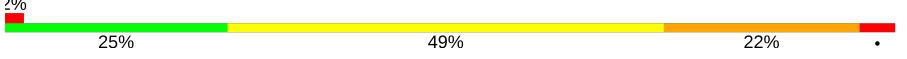
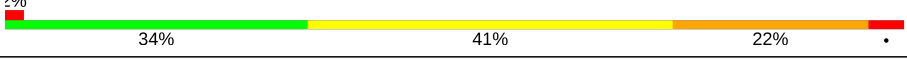
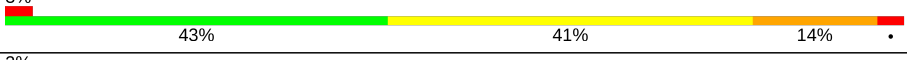

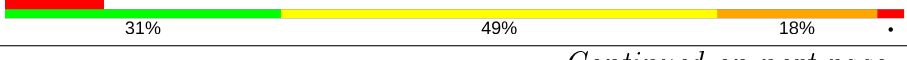

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Mol	Chain	Length	Quality of chain
15	CP	84	
16	AQ	100	
16	CQ	100	
17	AR	70	
17	CR	70	
18	AS	79	
18	CS	79	
19	AT	99	
19	CT	99	
20	AA	1511	
20	CA	1511	
21	AW	77	
21	CW	77	
22	AV	23	
22	CV	23	
23	AY	687	
23	CY	687	
24	BC	228	
24	DC	228	
25	BD	275	
25	DD	275	
26	BE	205	
26	DE	205	
27	BF	208	
27	DF	208	

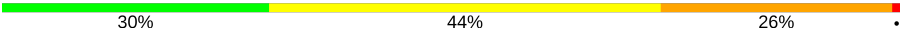

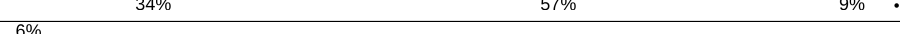
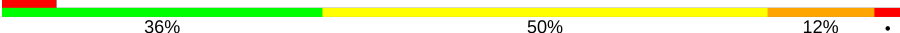
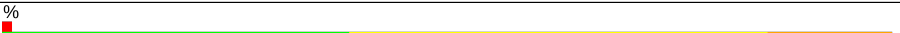
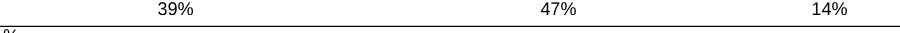

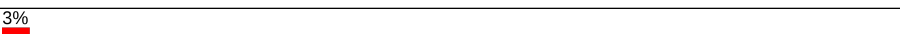
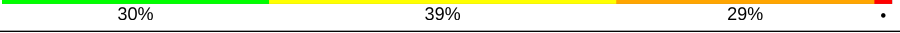
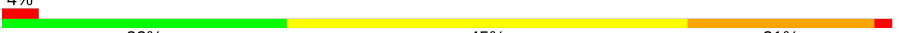



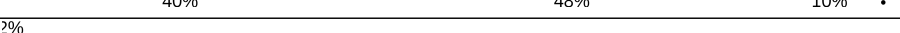
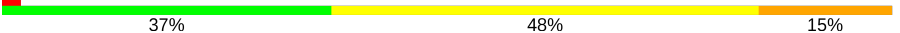

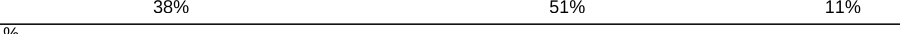




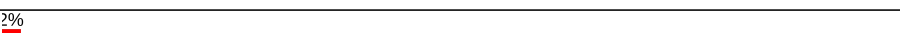



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Mol	Chain	Length	Quality of chain
28	BG	181	
28	DG	181	
29	BH	167	
29	DH	167	
30	BJ	170	
30	DJ	170	
31	BK	140	
31	DK	140	
32	BN	138	
32	DN	138	
33	BO	122	
33	DO	122	
34	BP	146	
34	DP	146	
35	BQ	141	
35	DQ	141	
36	BR	117	
36	DR	117	
37	BS	99	
37	DS	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	B2	71	
46	D2	71	
47	B3	60	
47	D3	60	
48	B5	59	
48	D5	59	
49	B6	50	
49	D6	50	
50	B7	49	
50	D7	49	
51	B8	64	
51	D8	64	
52	B9	37	
52	D9	37	

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Mol	Chain	Length	Quality of chain
53	Be	102	
53	De	102	
54	Bf	31	
54	Bg	31	
54	Df	31	
54	Dg	31	
55	Bh	30	
55	Dh	30	
56	B1	93	
56	D1	93	
57	B4	35	
57	D4	35	
58	BA	2879	
58	DA	2879	
59	BB	119	
59	DB	119	

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 308068 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
			1010	639	197	174			
8	CI	127	Total	C	N	O	0	0	0
			1010	639	197	174			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	58	HIS	ARG	CONFLICT	UNP P62669
CI	58	HIS	ARG	CONFLICT	UNP P62669

- 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			
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	155	144	2			
16	CQ	100	Total	C	N	O	S	0	0	0
			835	534	155	144	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AQ	96	GLU	GLN	CONFLICT	UNP P62658
CQ	96	GLU	GLN	CONFLICT	UNP P62658

- 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
			763	470	162	129	2			
19	CT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AT	41	ILE	VAL	CONFLICT	UNP P62661
CT	41	ILE	VAL	CONFLICT	UNP P62661

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

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 transfer RNA.

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

- Molecule 22 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	23	Total	C	N	O	P	0	0	0
			503	227	106	148	22			
22	CV	23	Total	C	N	O	P	0	0	0
			503	227	106	148	22			

- Molecule 23 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AY	667	Total	C	N	O	S	0	0	0
			5219	3318	893	990	18			
23	CY	667	Total	C	N	O	S	0	0	0
			5219	3318	893	990	18			

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

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Chain	Residue	Modelled	Actual	Comment	Reference
CY	226	ASN	HIS	CONFLICT	UNP Q72I01

- Molecule 24 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	BC	228	Total	C	N	O	S	0	0	0
			1742	1101	319	319	3			
24	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 25 is a protein called 50S ribosomal protein L2.

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

- Molecule 26 is a protein called 50S ribosomal protein L3.

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

- Molecule 27 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BF	208	Total	C	N	O	S	0	0	0
			1628	1037	304	284	3			
27	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
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 28 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			
28	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 29 is a protein called 50S ribosomal protein L6.

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

- Molecule 30 is a protein called 50S ribosomal protein L10.

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

- Molecule 31 is a protein called 50S ribosomal protein L11.

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

- Molecule 32 is a protein called 50S ribosomal protein L13.

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

- 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			

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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 L29.

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

- Molecule 47 is a protein called 50S ribosomal protein L30.

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

- Molecule 48 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	B5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
48	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 49 is a protein called 50S ribosomal protein L33.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			
51	D8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 52 is a protein called 50S ribosomal protein L36.

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

- Molecule 53 is a protein called 50S ribosomal protein L7/L12.

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

- Molecule 54 is a protein called 50S ribosomal protein L7/L12.

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

- Molecule 55 is a protein called 50S ribosomal protein L7/L12.

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

- Molecule 56 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	B1	93	Total	C	N	O	S	0	0	0
			732	460	145	126	1			
56	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 57 is a protein called 50S ribosomal protein L31.

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

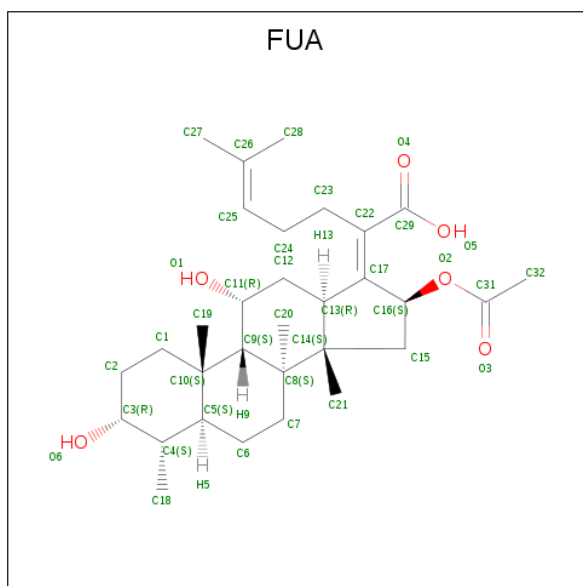
- Molecule 58 is a RNA chain called 23S ribosomal RNA.

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

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

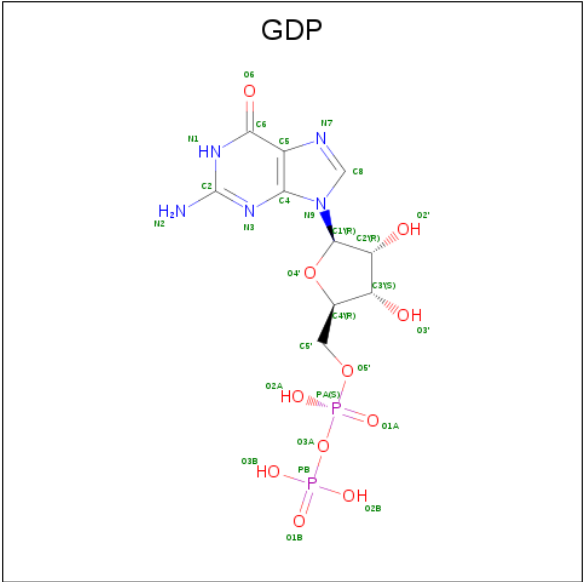
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	BB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			
59	DB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

- Molecule 60 is FUSIDIC ACID (three-letter code: FUA) (formula: $C_{31}H_{48}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
60	AY	1	Total	C	O	0	0
			37	31	6		
60	CY	1	Total	C	O	0	0
			37	31	6		

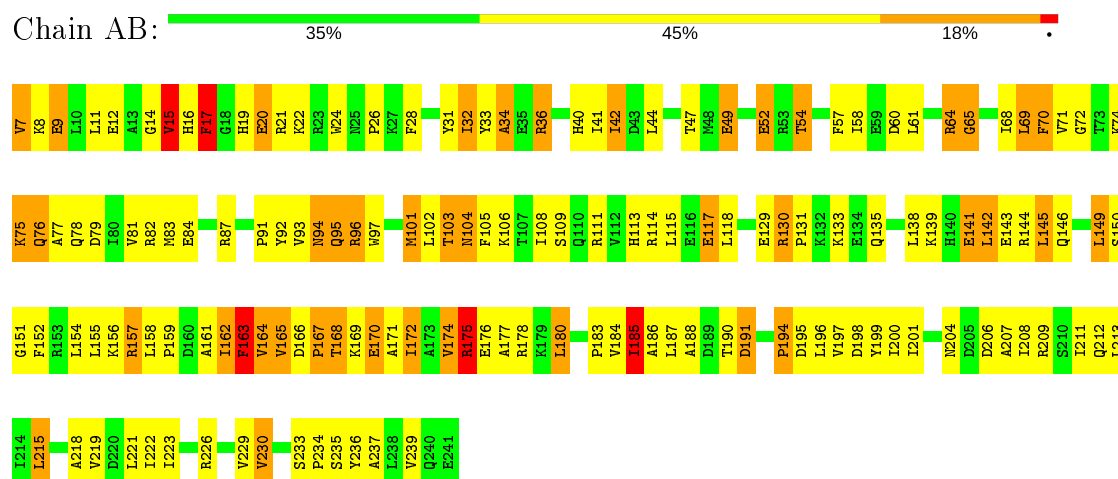
- Molecule 61 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



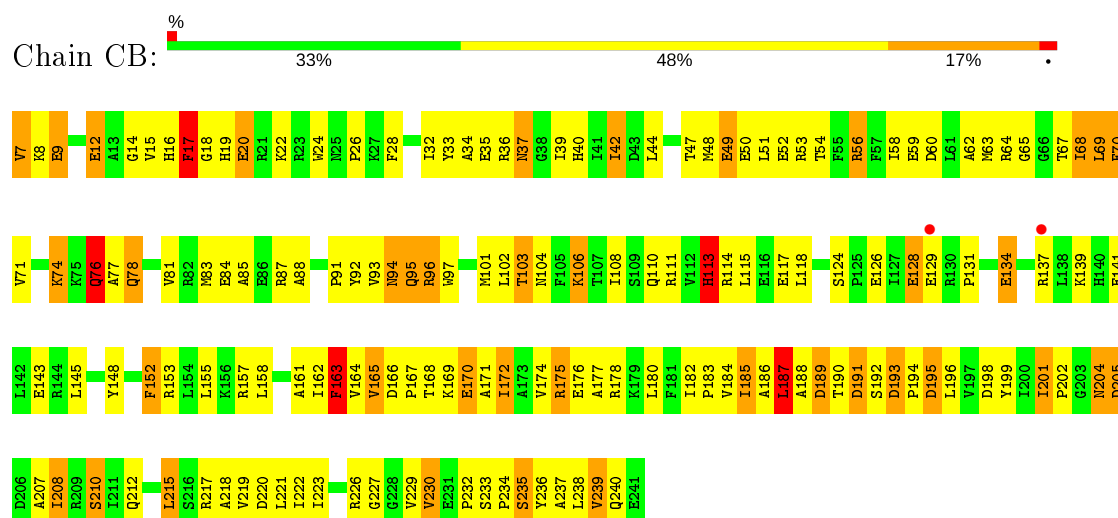
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

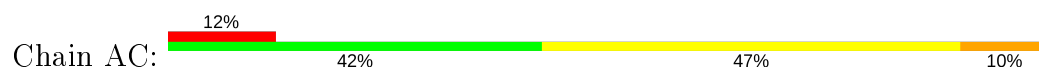
• Molecule 1: 30S ribosomal protein S2

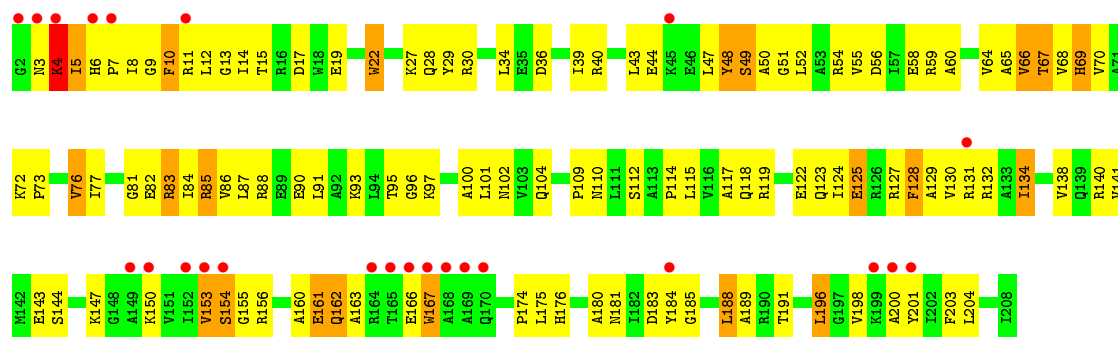


• Molecule 1: 30S ribosomal protein S2

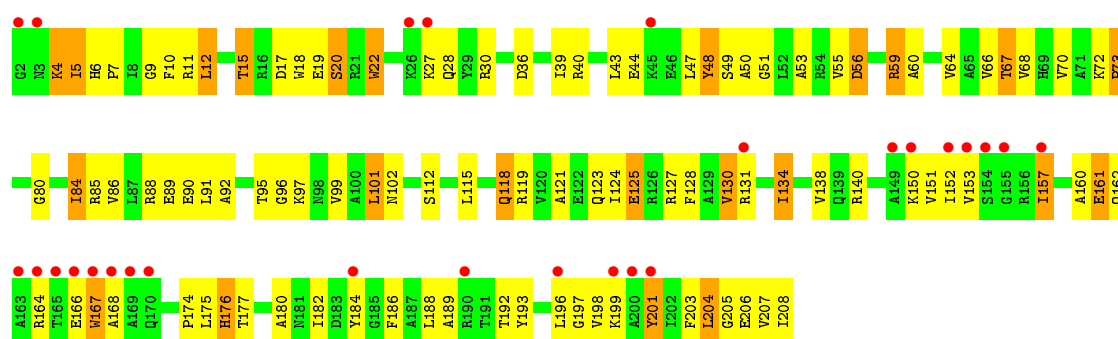


• Molecule 2: 30S ribosomal protein S3

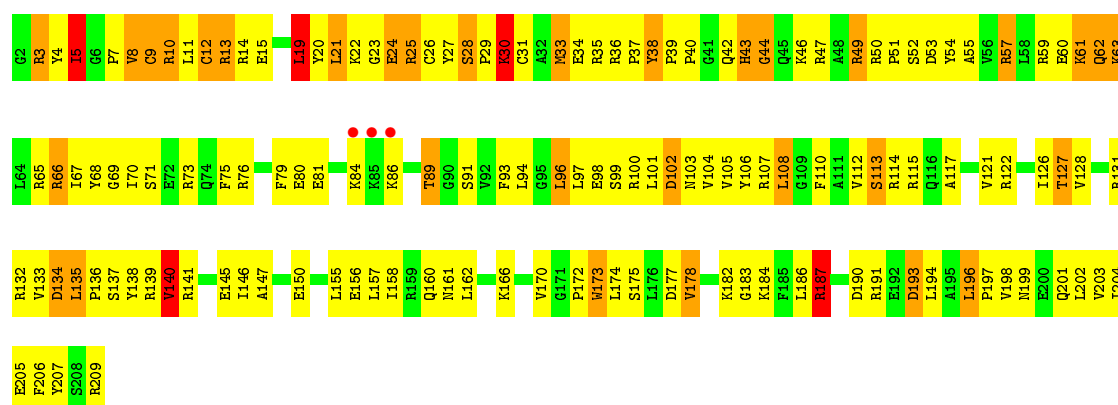




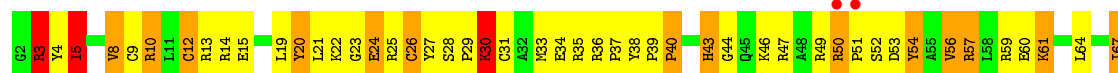
• Molecule 2: 30S ribosomal protein S3

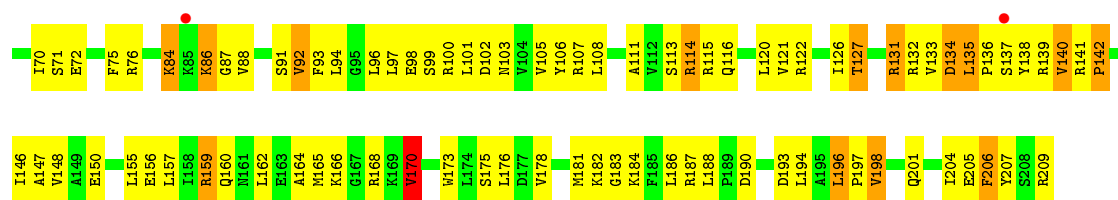


• Molecule 3: 30S ribosomal protein S4

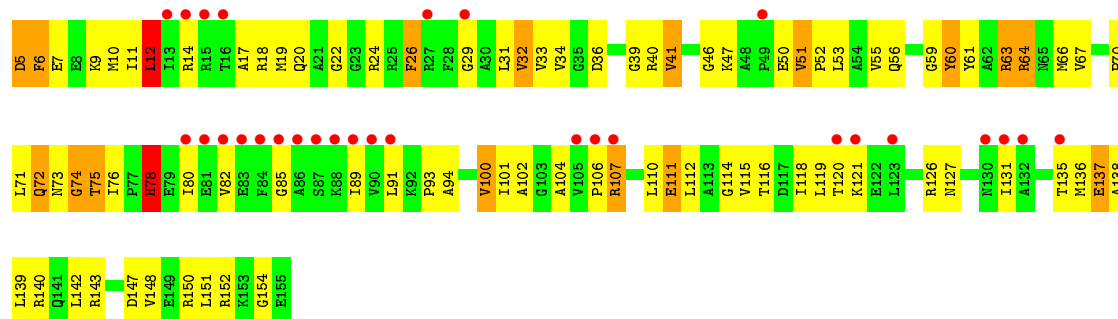
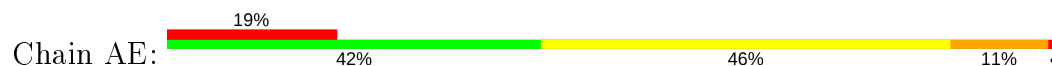


• Molecule 3: 30S ribosomal protein S4

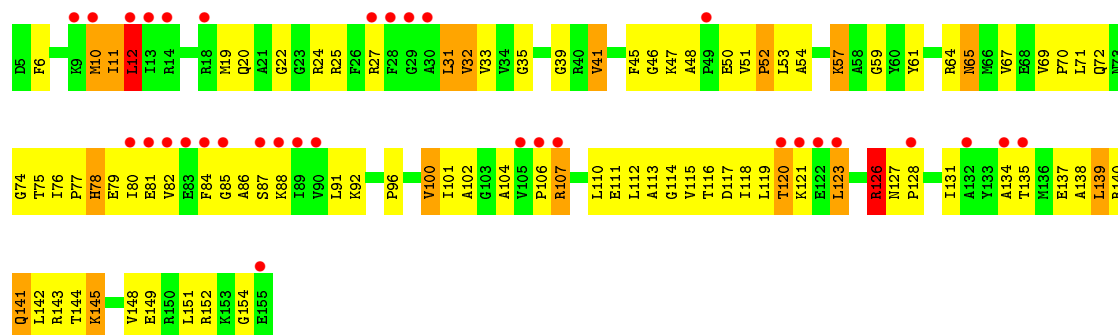




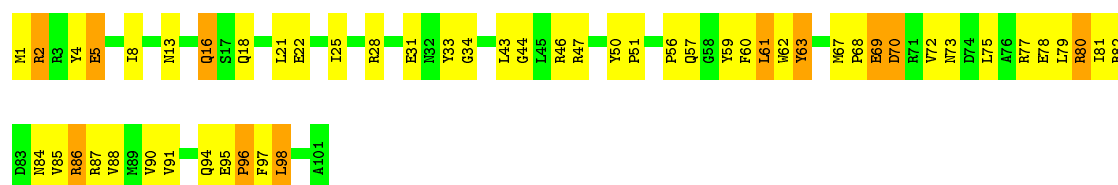
• Molecule 4: 30S ribosomal protein S5



• Molecule 4: 30S ribosomal protein S5

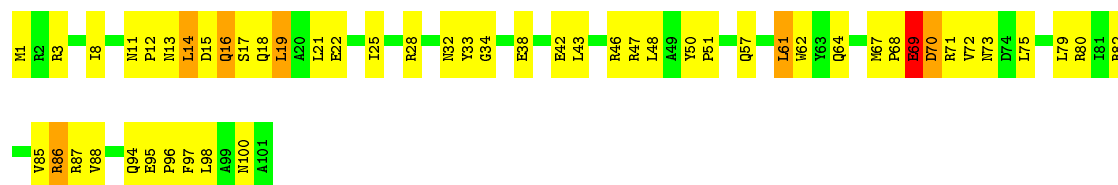


• Molecule 5: 30S ribosomal protein S6

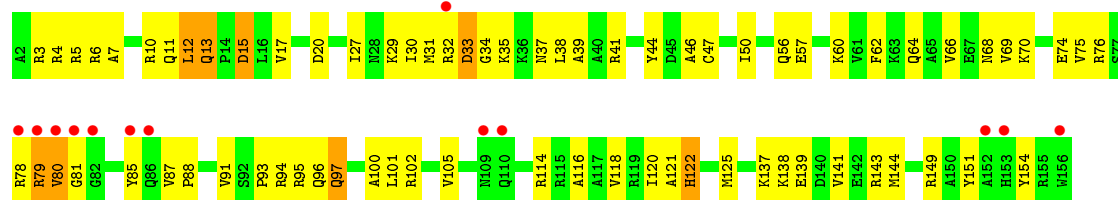


• Molecule 5: 30S ribosomal protein S6

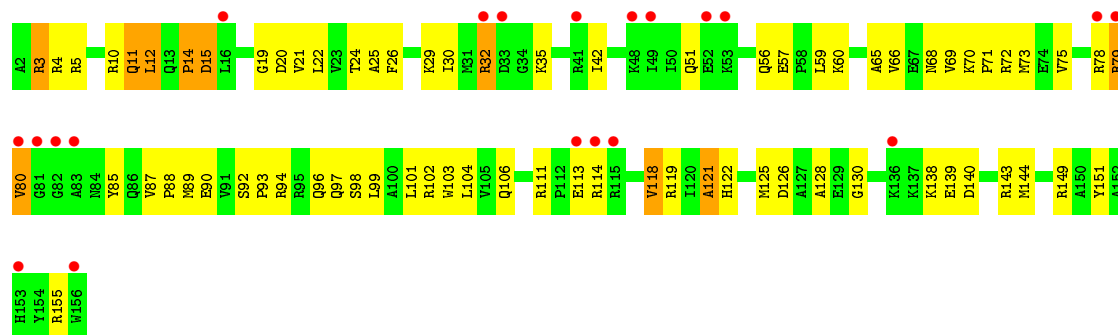




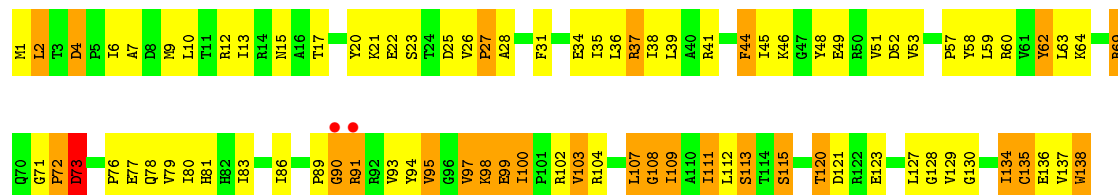
• Molecule 6: 30S ribosomal protein S7



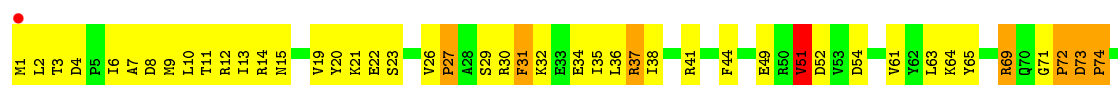
• Molecule 6: 30S ribosomal protein S7



• Molecule 7: 30S ribosomal protein S8

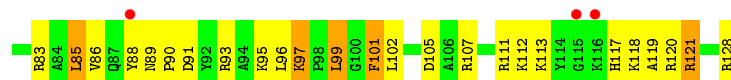
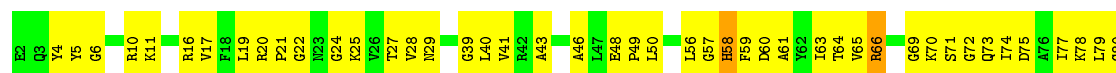


• Molecule 7: 30S ribosomal protein S8





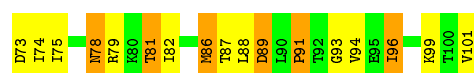
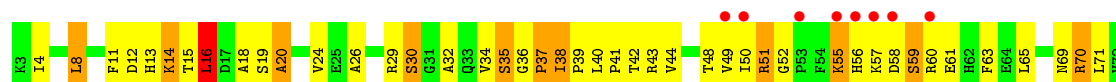
• Molecule 8: 30S ribosomal protein S9



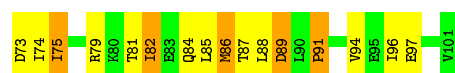
• Molecule 8: 30S ribosomal protein S9



• Molecule 9: 30S ribosomal protein S10

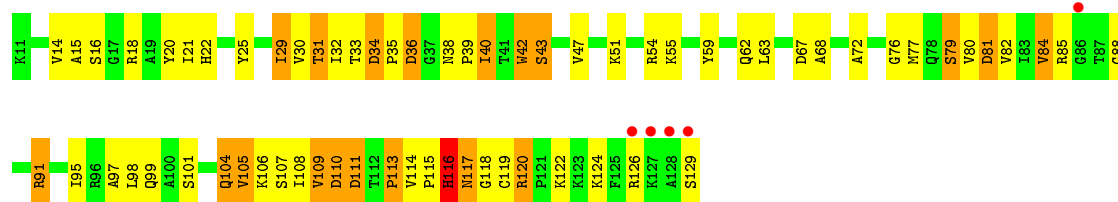


• Molecule 9: 30S ribosomal protein S10

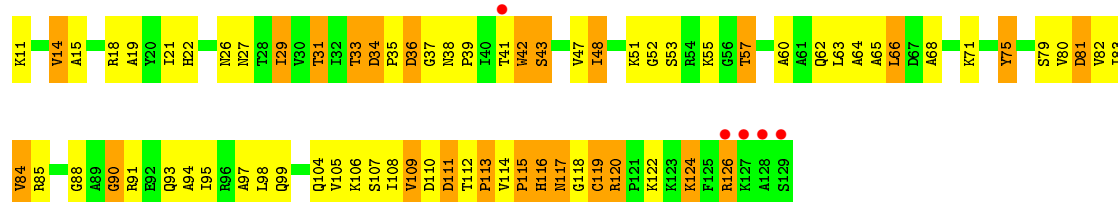


• Molecule 10: 30S ribosomal protein S11

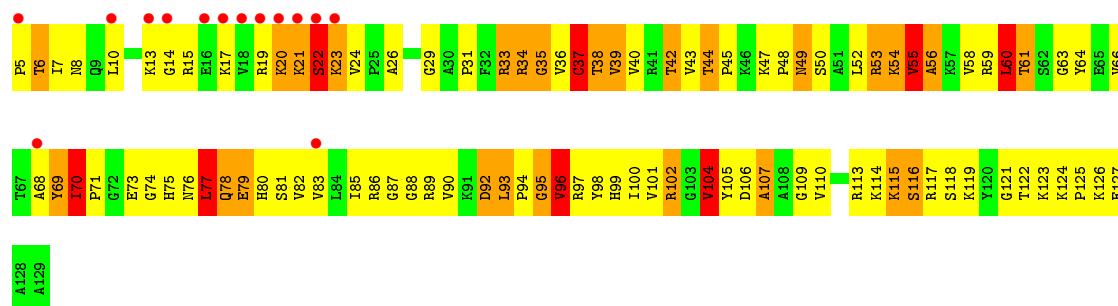




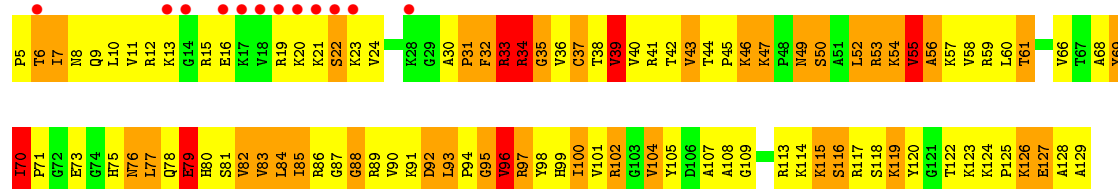
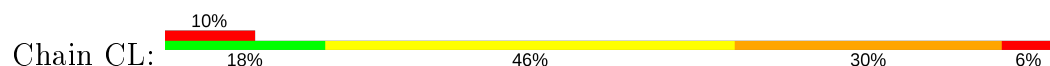
• Molecule 10: 30S ribosomal protein S11



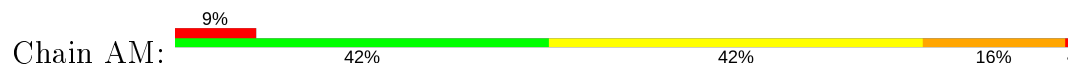
• Molecule 11: 30S ribosomal protein S12

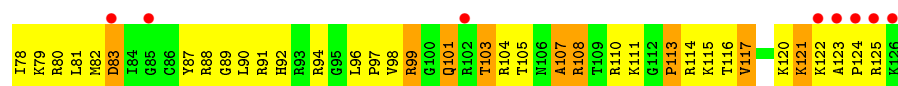


• Molecule 11: 30S ribosomal protein S12

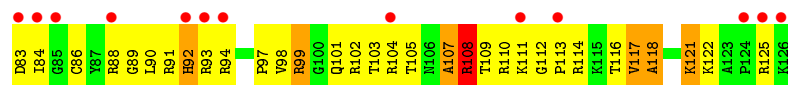
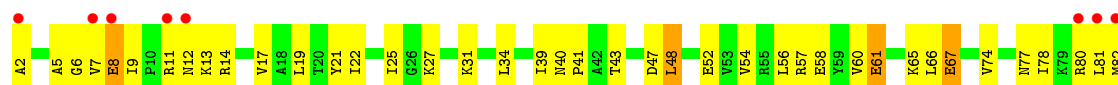
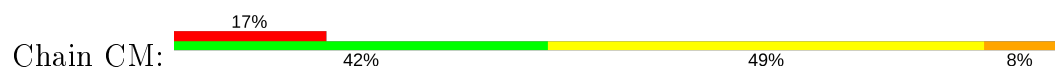


• Molecule 12: 30S ribosomal protein S13





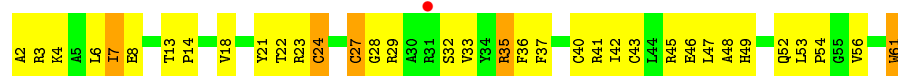
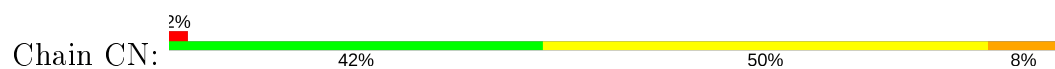
- Molecule 12: 30S ribosomal protein S13



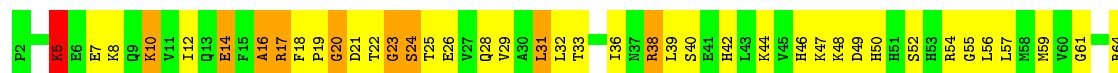
- Molecule 13: 30S ribosomal protein S14 type Z



- Molecule 13: 30S ribosomal protein S14 type Z



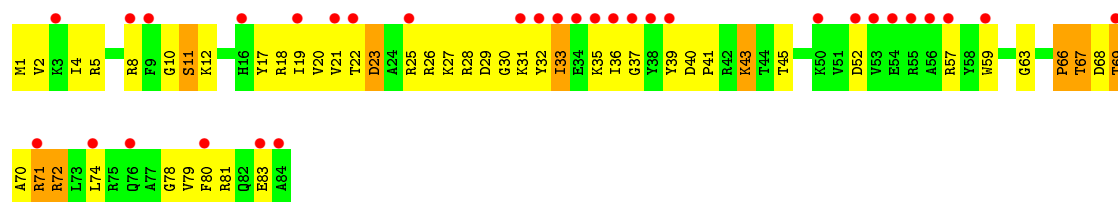

- Molecule 14: 30S ribosomal protein S15



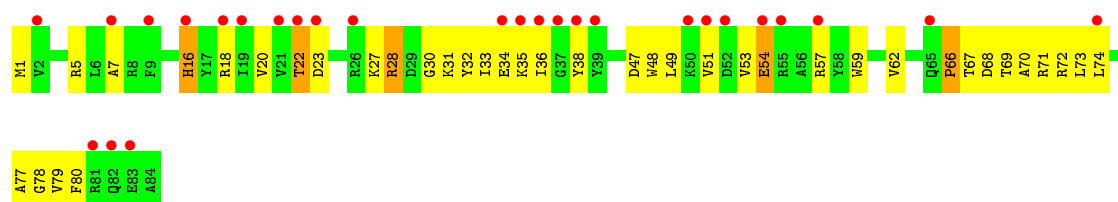
- Molecule 14: 30S ribosomal protein S15



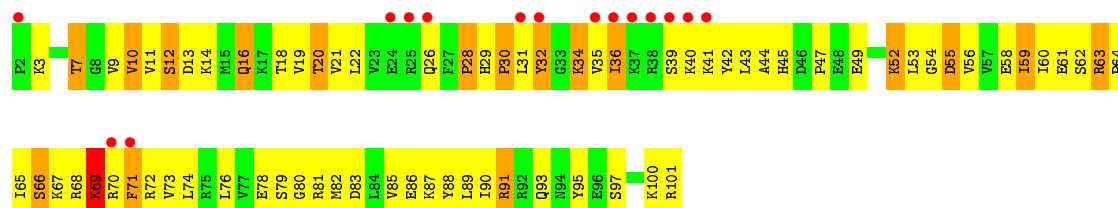

● Molecule 15: 30S ribosomal protein S16

Chain AP: 

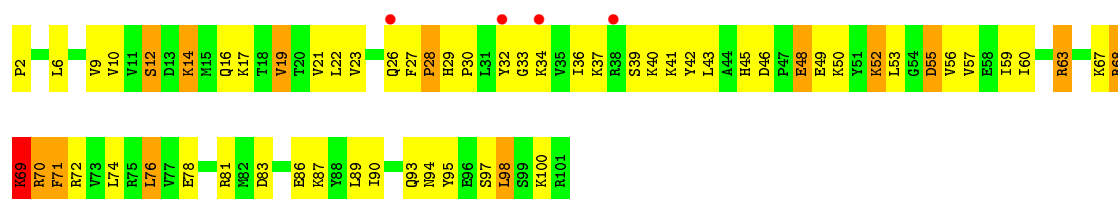
● Molecule 15: 30S ribosomal protein S16

Chain CP: 

● Molecule 16: 30S ribosomal protein S17

Chain AQ: 

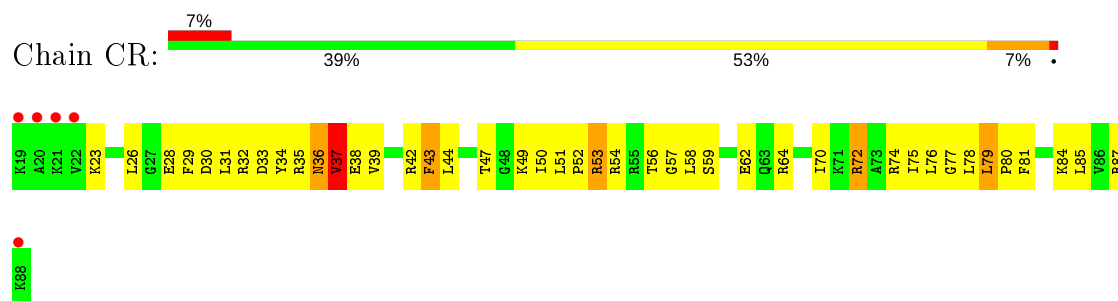
● Molecule 16: 30S ribosomal protein S17

Chain CQ: 

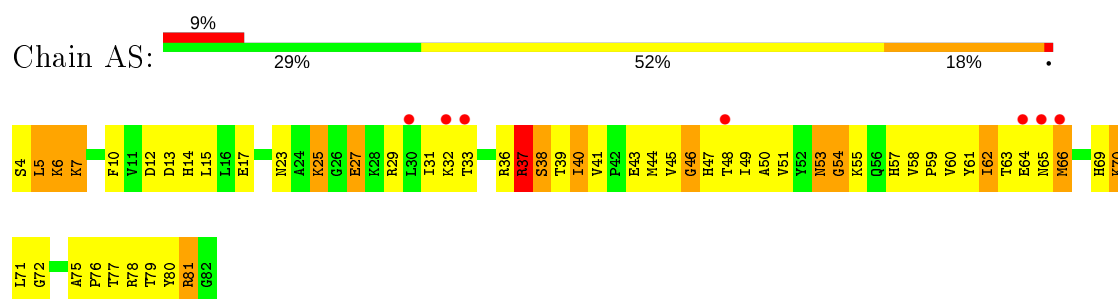
● Molecule 17: 30S ribosomal protein S18

Chain AR: 

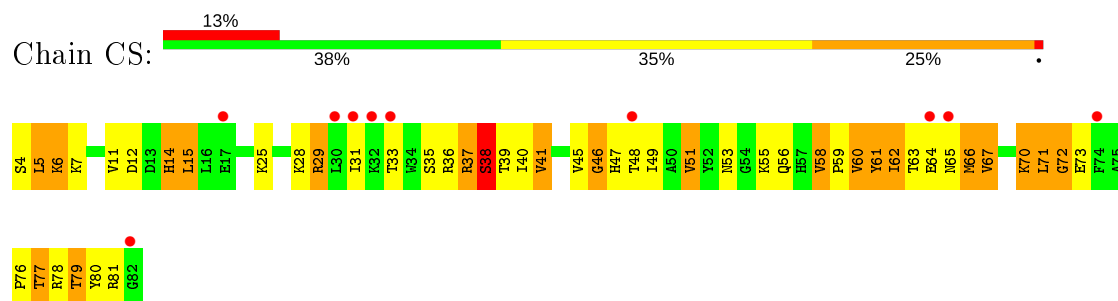
- Molecule 17: 30S ribosomal protein S18



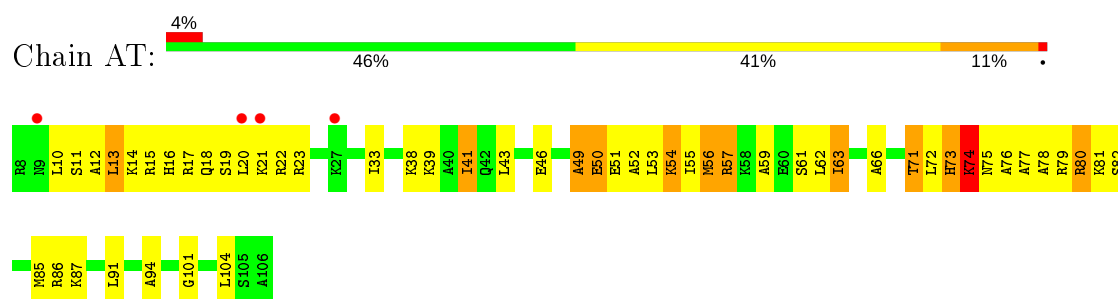
- Molecule 18: 30S ribosomal protein S19



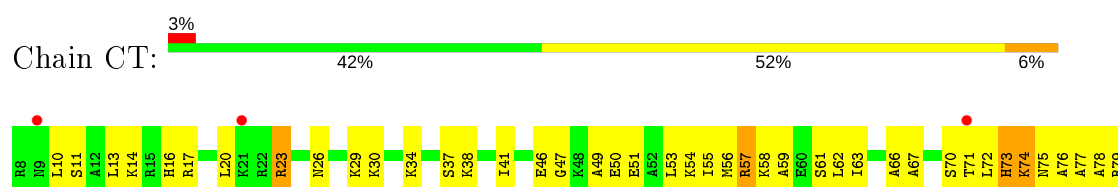
- Molecule 18: 30S ribosomal protein S19

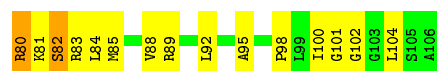


- Molecule 19: 30S ribosomal protein S20

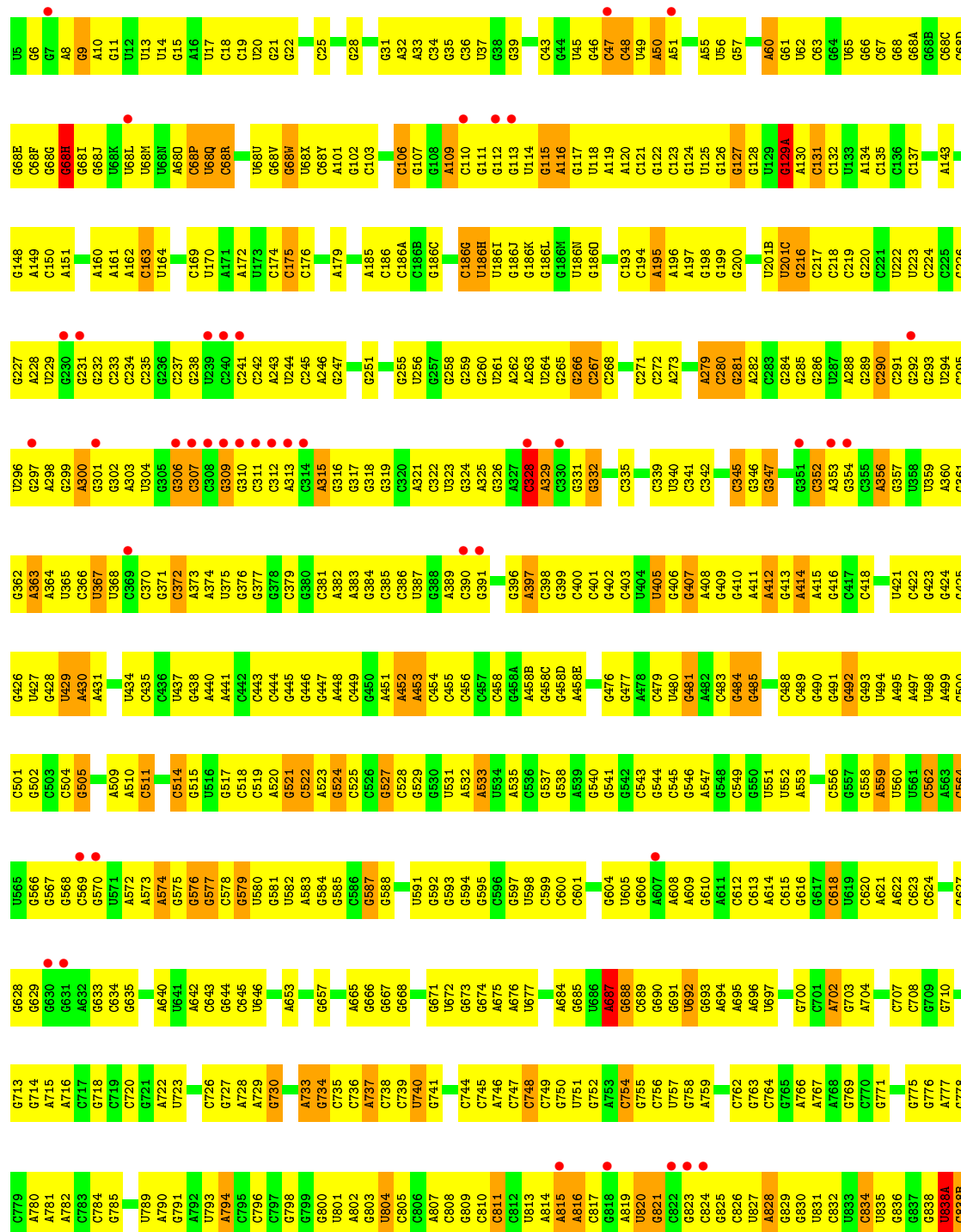


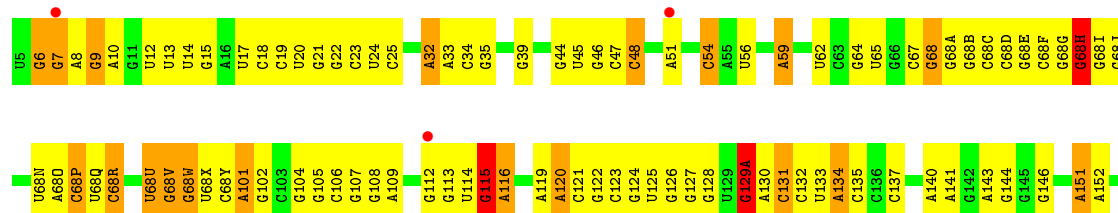
- Molecule 19: 30S ribosomal protein S20



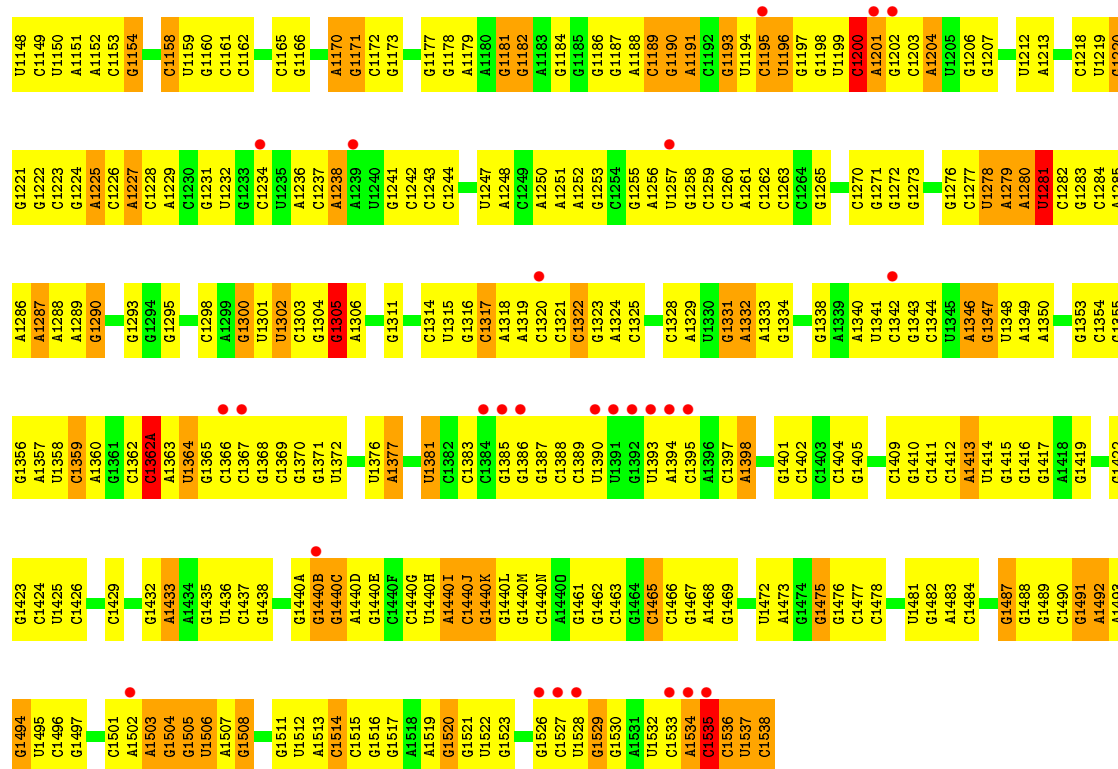


• Molecule 20: ribosomal RNA 16S

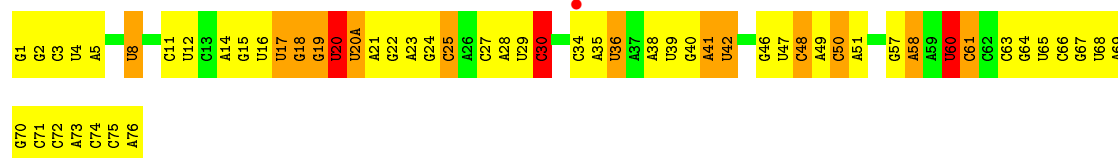




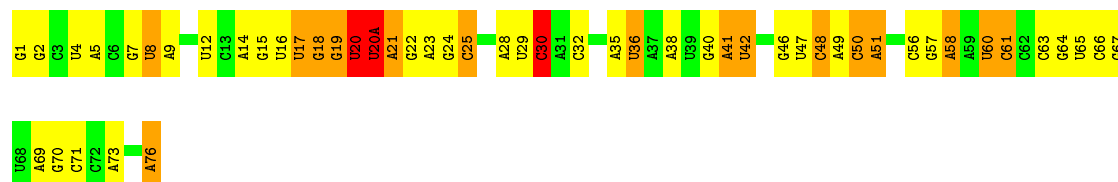
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A1081	C940	G876	G803	G726	G581	A520	C442		U304	C235	
A1005	G941	C877	G804	G727	G582	C521	C443	C372	G305	G236	
G1082	G942	C878	C805	A728	G583	A522	C444	A373	G309	C237	
G1084	U943	C879	C806	A729	G584	A523	C445	A374	G310	G238	
U1085	G944	C880	C807	G730	G585	G524	G446	G375	G311		
	G945	C881	G808	G731	C586	C525	G447	G376	G312		
U1012	C882	G732	C809	G733	G587	C526	A448		C313		
G1013	A946	A733	G809	A734	G588	G527	A449	A383	C314	A243	C174
U1090	A1014		C810	C736	A663	C528	G450	A384	C315	U244	C175
U1091	C948			A737	G664	G529	A451	C385	C316	C245	C176
A1015	A949	G885	G886	A738	G665	G530	A452	C386	G317	A246	C177
G1016	A949	G887	G887	A739	G666	G531	A453	U387	A318	G251	C178
U1094	G950	C888	A814	C738	G667	U531	C454	U388	G319	U252	
U1095	G951	C889	A815	C739	G667	G532		G388	G320	G253	
C1019	U952	A889	C816	G740	G668	A533		U389	C321	G254	
C1097	G953	G890	A817	U741	G669	G534		C390	A322	G255	
C1098	G954	U891	C817	G742	G670	C541		A397	G323	G256	
	U955	A892	C818	G743	G671	G542		C398	C324	G257	
C1028B	U956	C893	A819	U744	G672	C543		G399	G325	G258	
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A1101	A1028D	G894	C821	G745	G674	C545		G402	G327		
A1102	G1028E	G895	C822	A746	G675	G546		C403	G328		
A1028F	A959	C896	G823	G747	A676	A547		G406	G329		
U960	U960		C824	C748	U678	G548		G407	G330		
U961	U961		G825	C749	G679	C549		G408	G331		
	G966	G902	C826	G750	G680	G550		G409	G332		
C1038	C967	G903	U827		G681	G551		U480	G333		
U1040	A968	C904	A828		A684	G552		G401	G334		
A1041	A969	U905	C754	A753	G754	A547		G402	G335		
G1036	C970	G906	U831	G755	A687	G548		C403	G336		
C1037	G971	A907	C832	G756	G688	C549		G406	G337		
C1045	C972	A908	U833	U757	C612	G550		G407	G338		
A1046	G973	A909	C834	G758	C613	G551		G408	G339		
	A974	C910	U835		A614	U552		A409	G340		
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C1054	G976	G912			G615	G553		A411	C341		
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C1062	C984	U920	G852		G703	U561		A499	U421		
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G1064	A986	G922	G854	G778	U705	A563		G423	C343		
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U1067	G990	G926			G633	G567		U427	G354		
G1068	C990	G927	C862	U788	G713	G568		G428	C355		
G1069	U991	G927	U789	A787	G714	C569		U429	G356		
U1070	G992		A864	U790	G635	U571		A510	C357		
C1071	G993	C930	C863	A790	U715	G570		A431	U358		
G1072	A994	G931	A865	G791	A716	U572		A432	U359		
U1073	C995	C932	C866	A792	U719	A573		G433	A360		
G1074	A996	G933	G867	U793	C719	U574		U434	G361		
C1075	U997	C934	U794	A794	U641	G575		C435	A363		
G1076		U871	C795	G721	A642	G576		C436	A364		
U1077	A1000	A872	C796	A722	C643	G577		U437	U365		
A1078	C936	A873	U797	C797	C644	C578		A438	A366		
	U932		A874		U723						



• Molecule 21: transfer RNA



• Molecule 21: transfer RNA



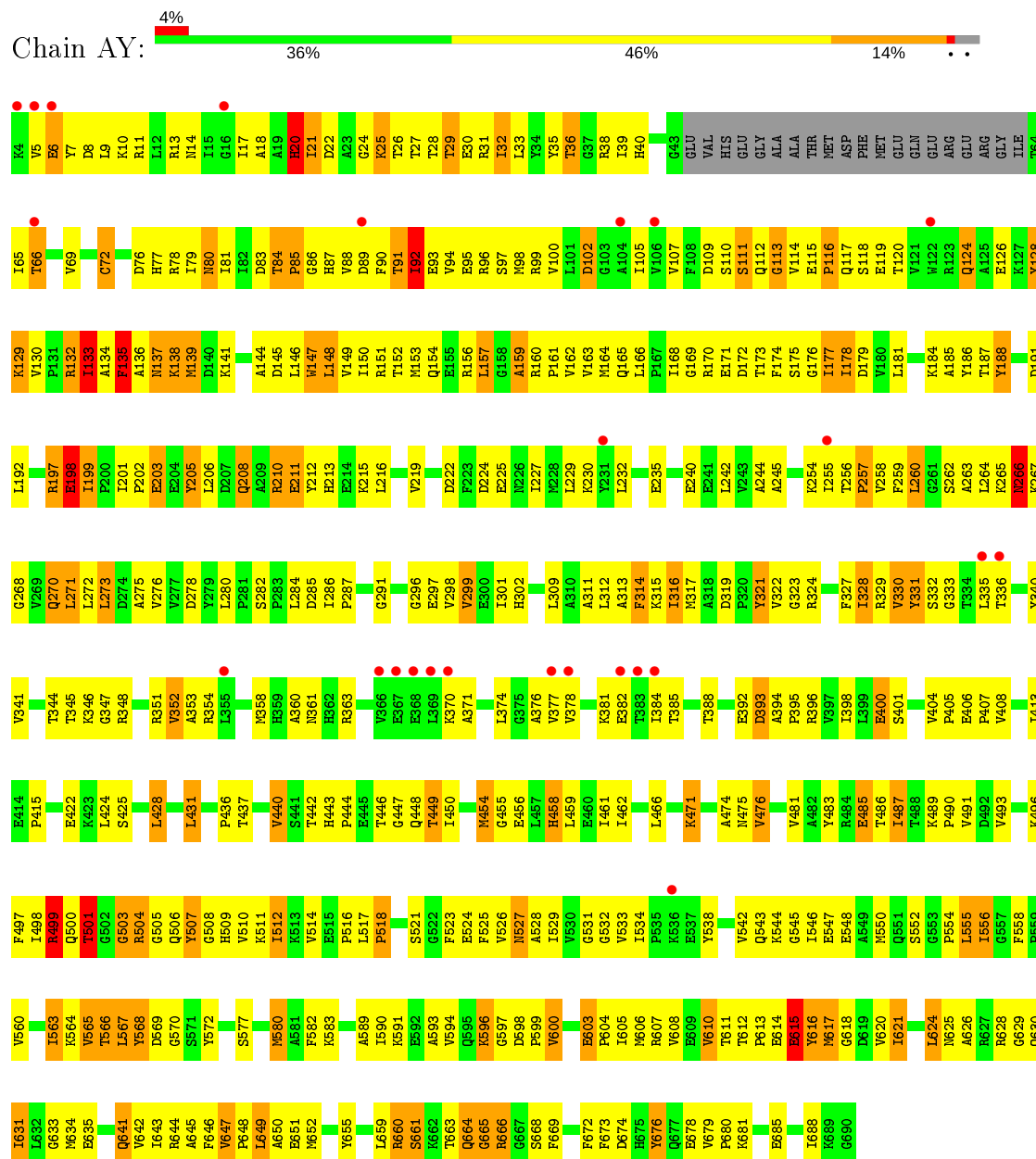
• Molecule 22: messenger RNA



- Molecule 22: messenger RNA

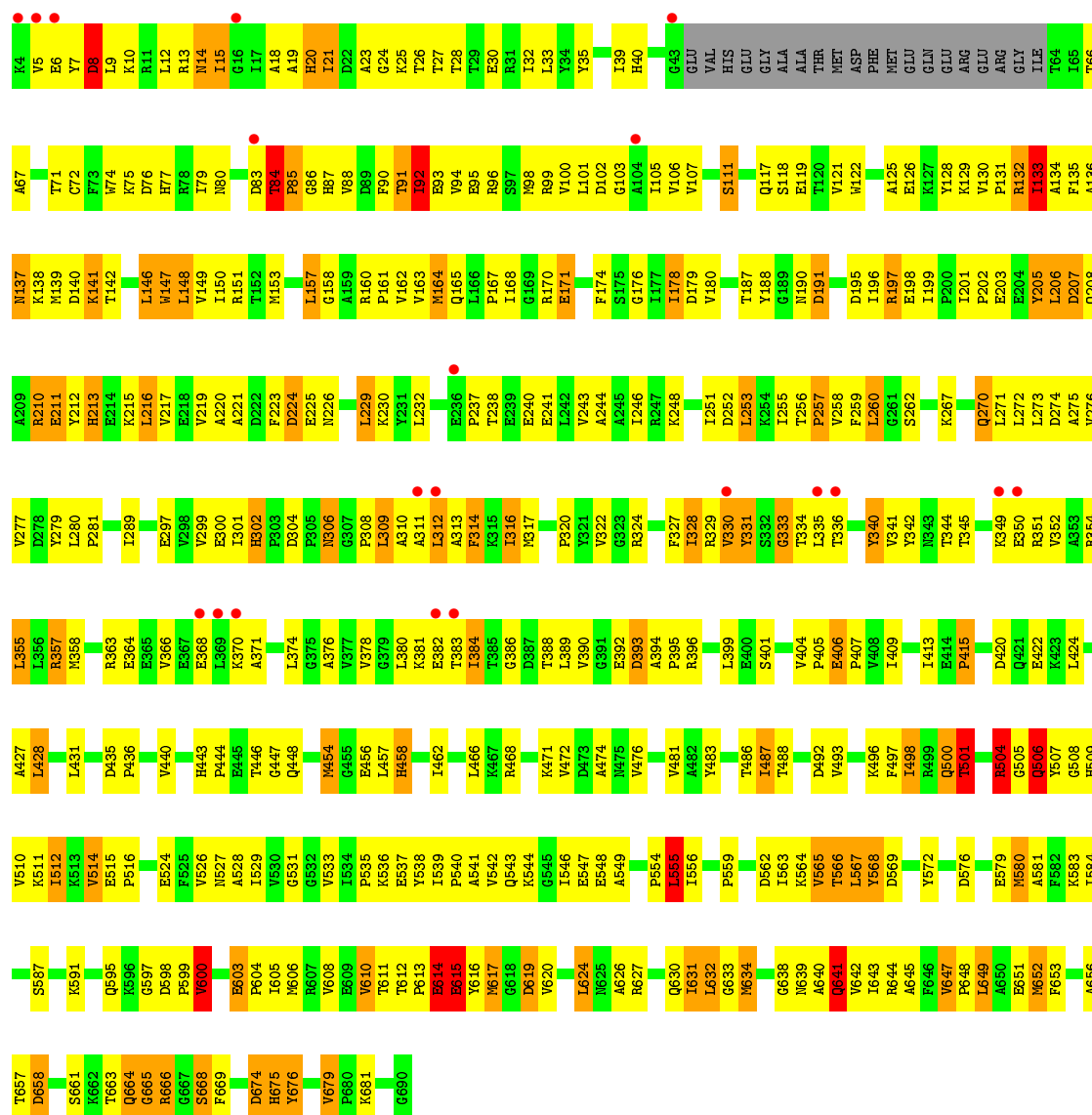


- Molecule 23: Elongation factor G

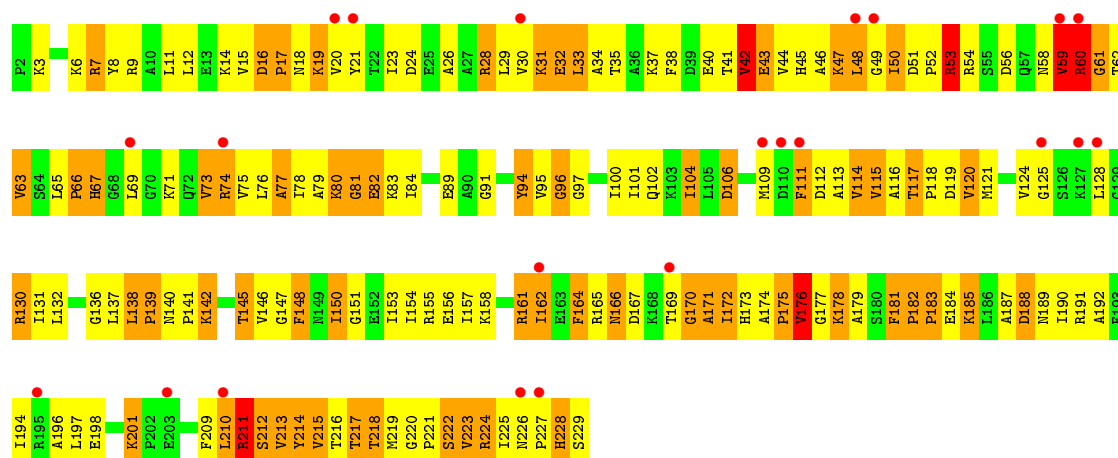


- Molecule 23: Elongation factor G

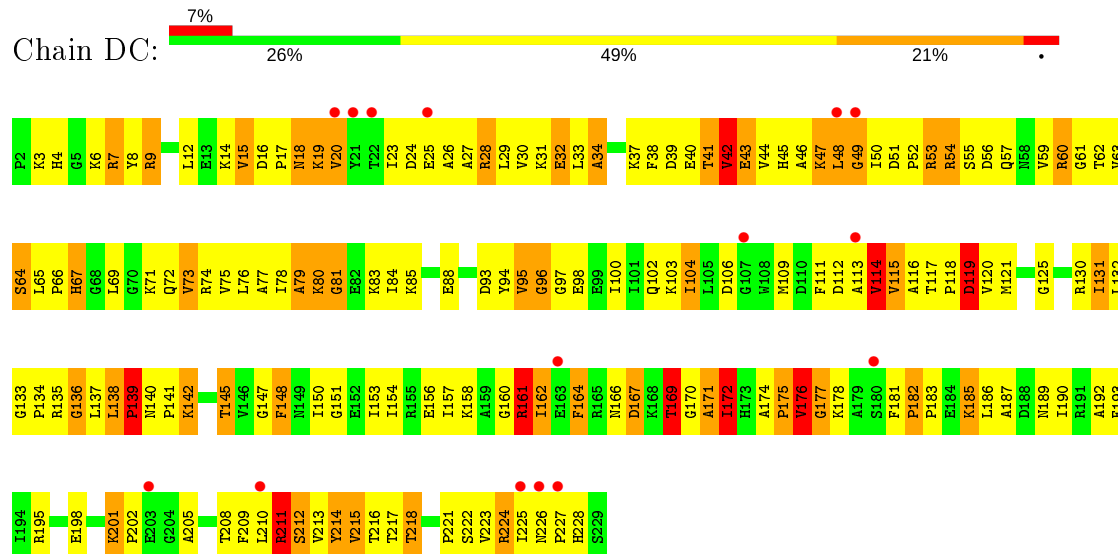




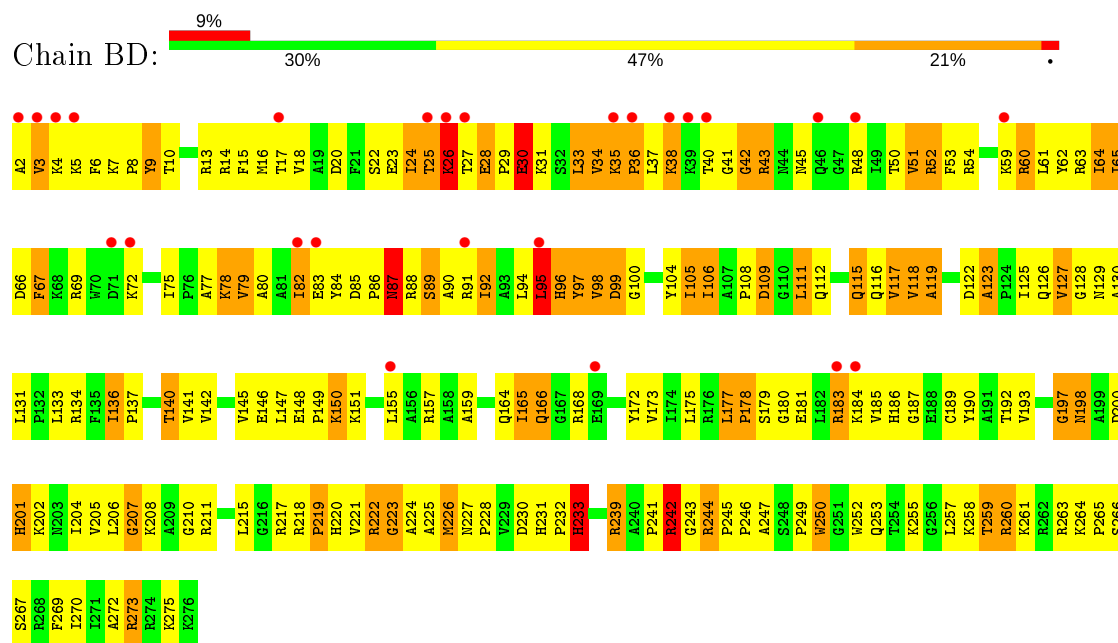
• Molecule 24: 50S ribosomal protein L1



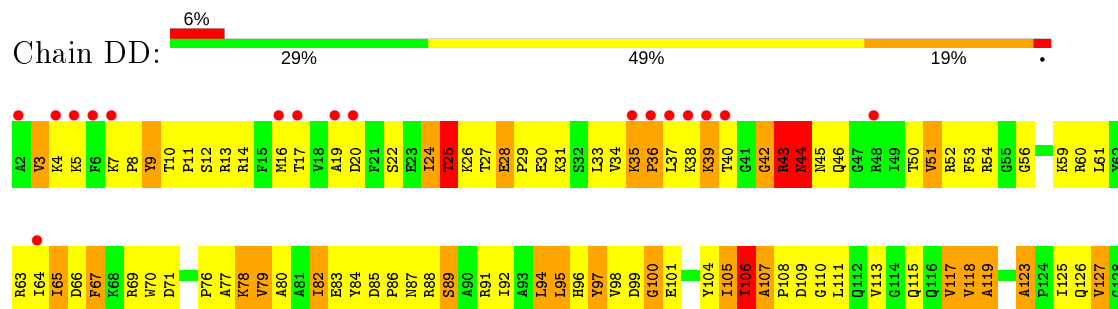
- Molecule 24: 50S ribosomal protein L1

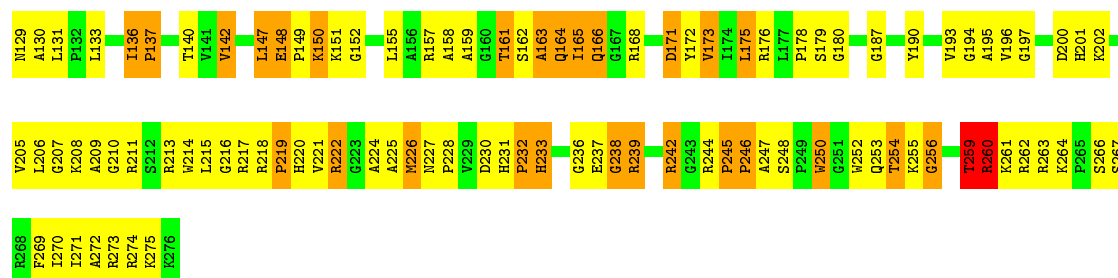


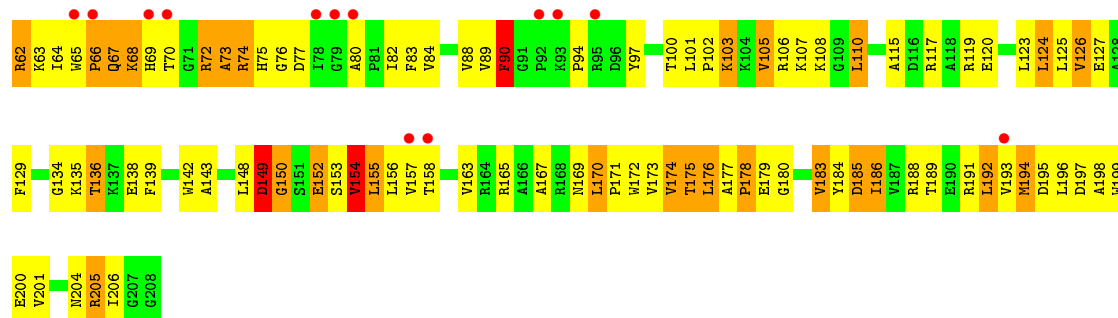
- Molecule 25: 50S ribosomal protein L2



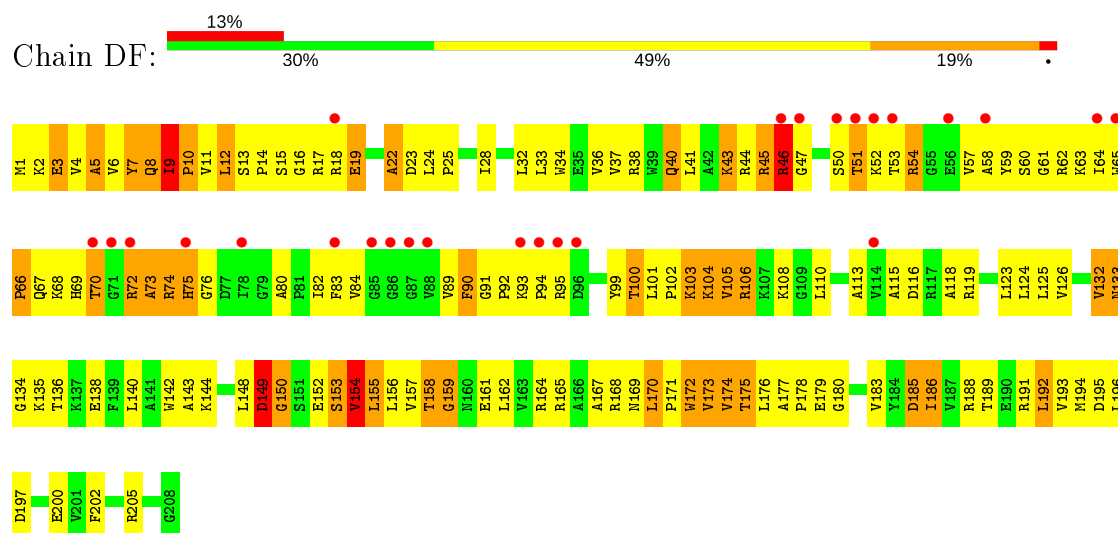
- Molecule 25: 50S ribosomal protein L2



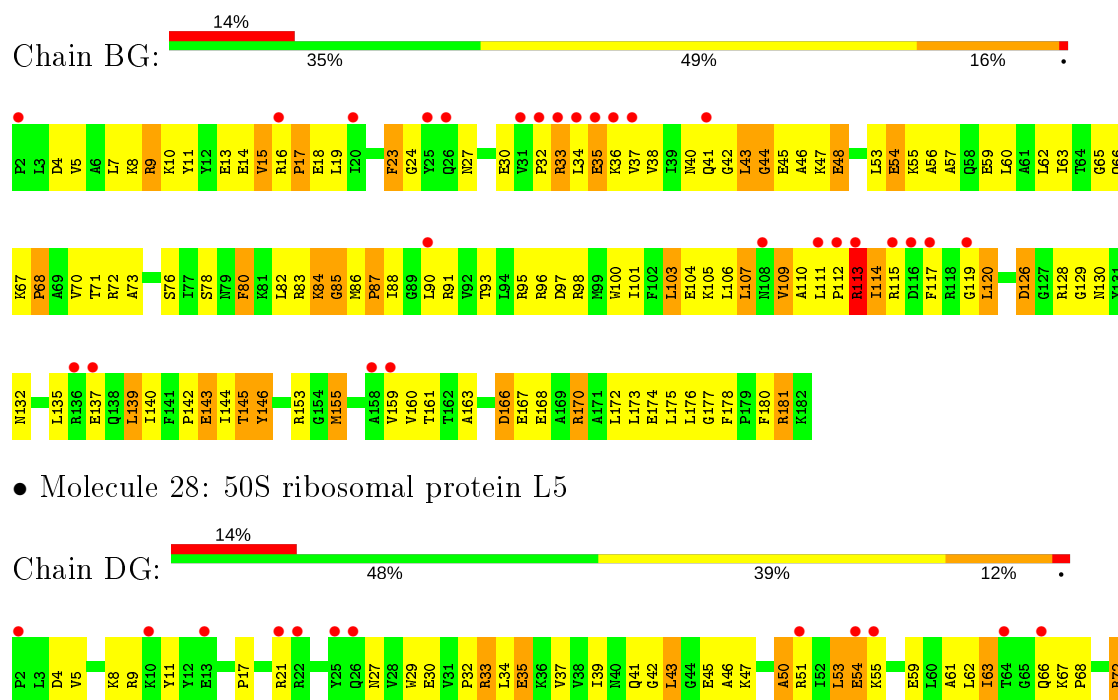




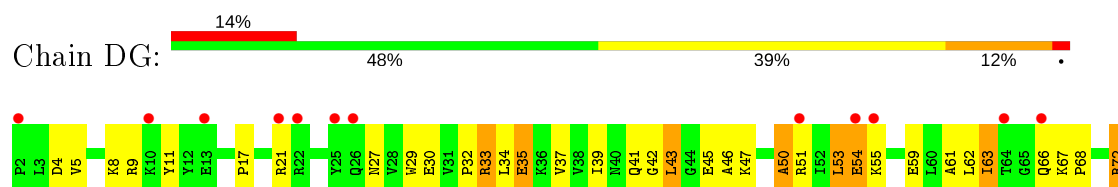
• Molecule 27: 50S ribosomal protein L4

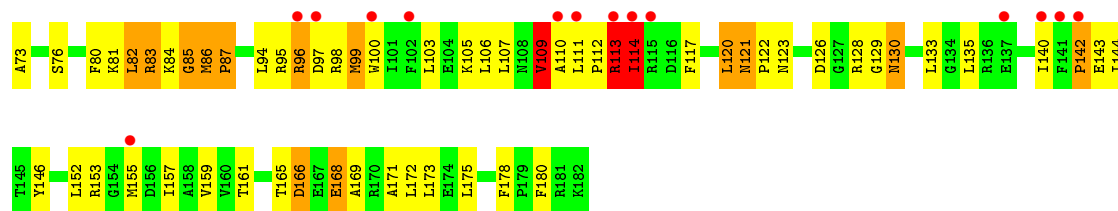


• Molecule 28: 50S ribosomal protein L5

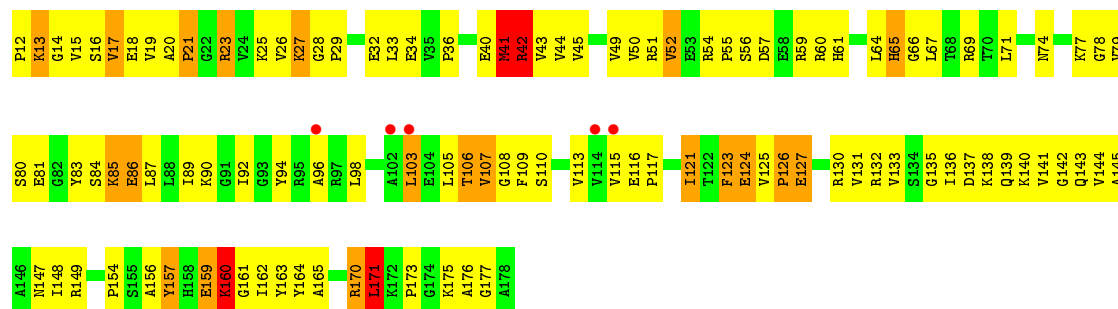


• Molecule 28: 50S ribosomal protein L5

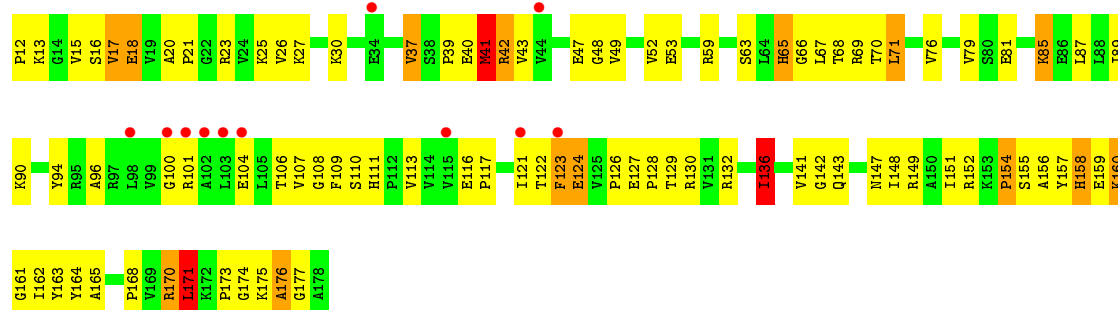




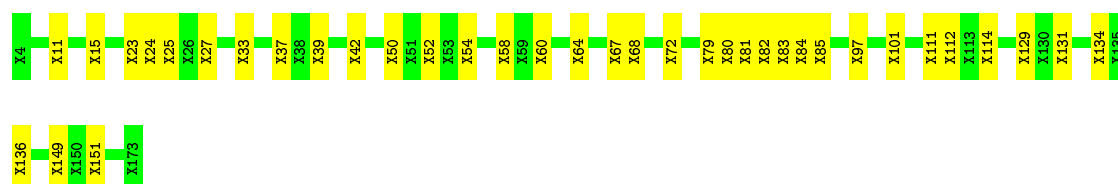
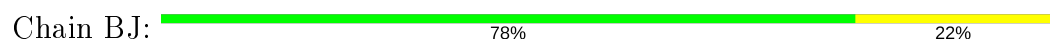
• Molecule 29: 50S ribosomal protein L6



• Molecule 29: 50S ribosomal protein L6

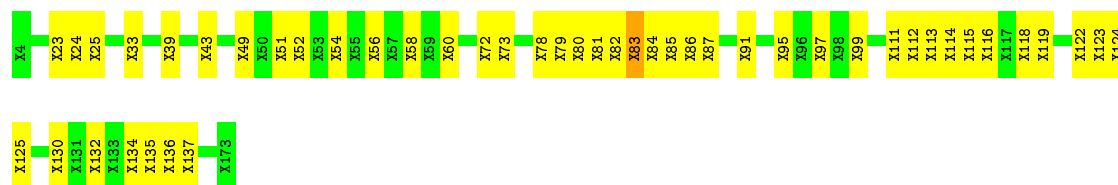


• Molecule 30: 50S ribosomal protein L10

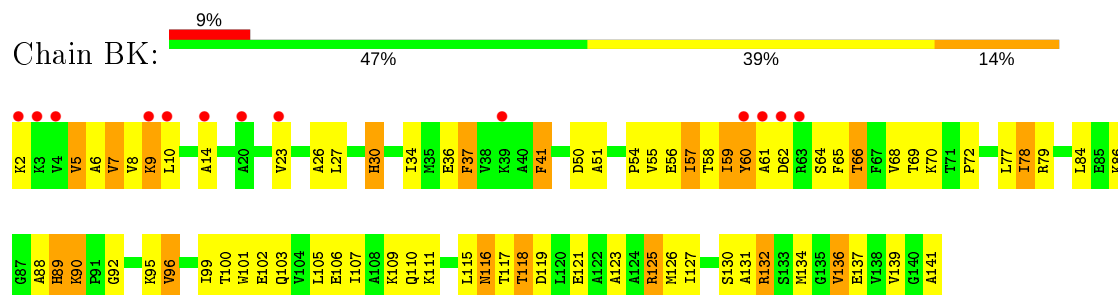


• Molecule 30: 50S ribosomal protein L10

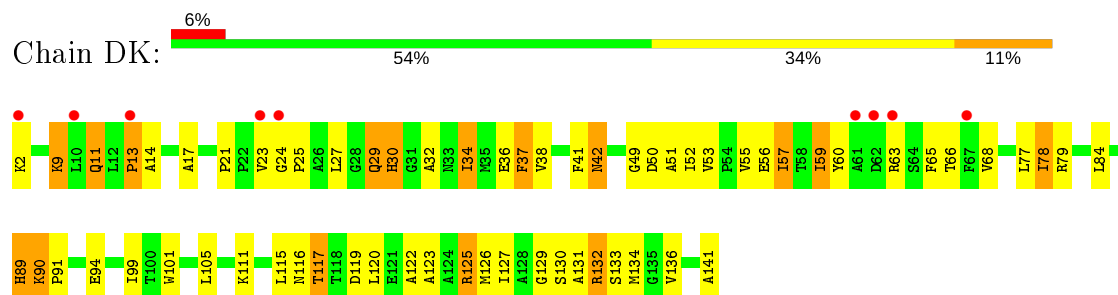




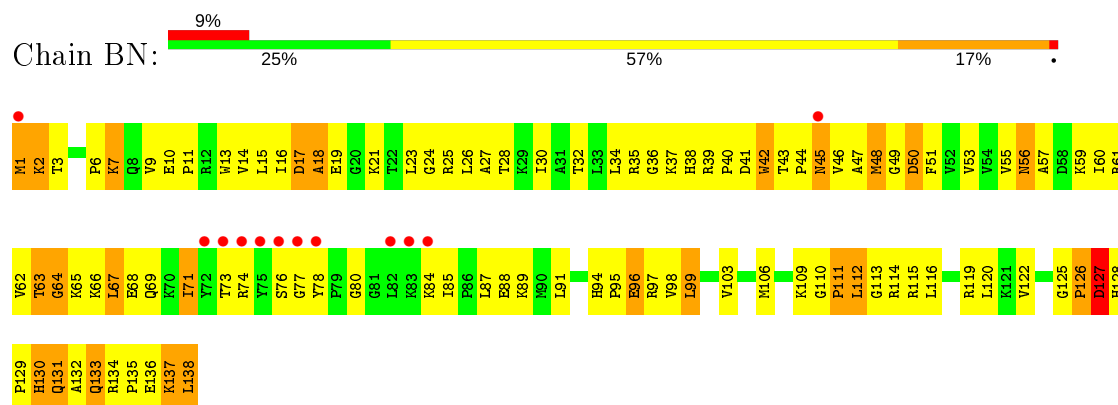
• Molecule 31: 50S ribosomal protein L11



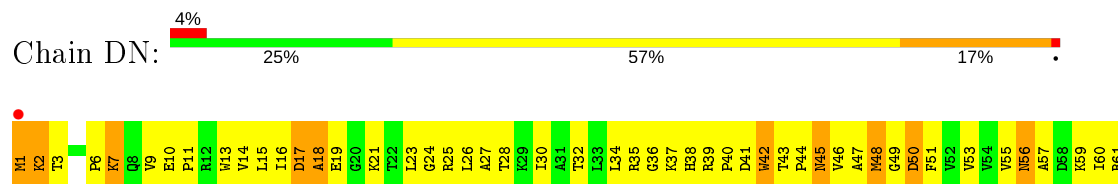
• Molecule 31: 50S ribosomal protein L11

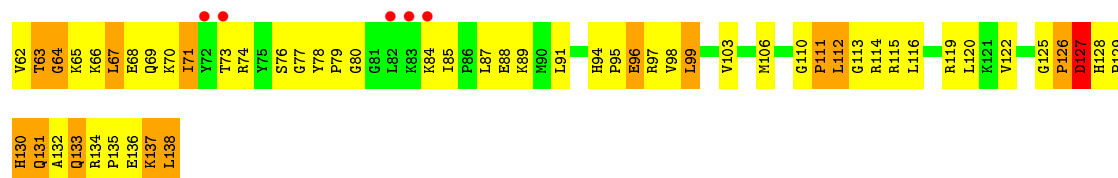


• Molecule 32: 50S ribosomal protein L13

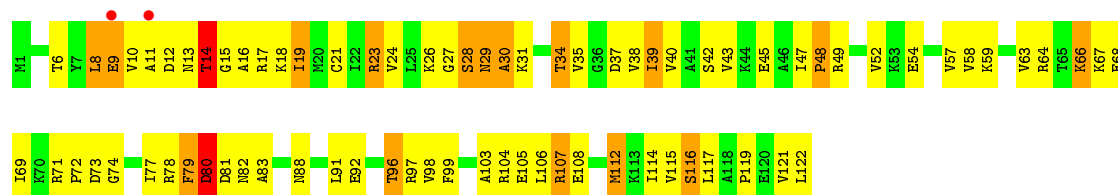


• Molecule 32: 50S ribosomal protein L13

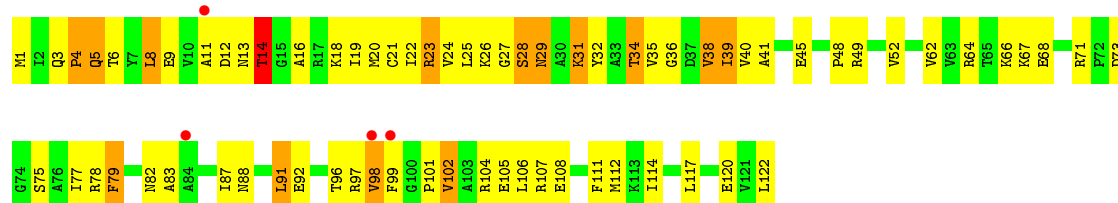
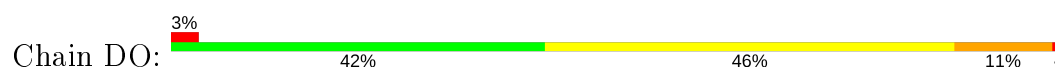




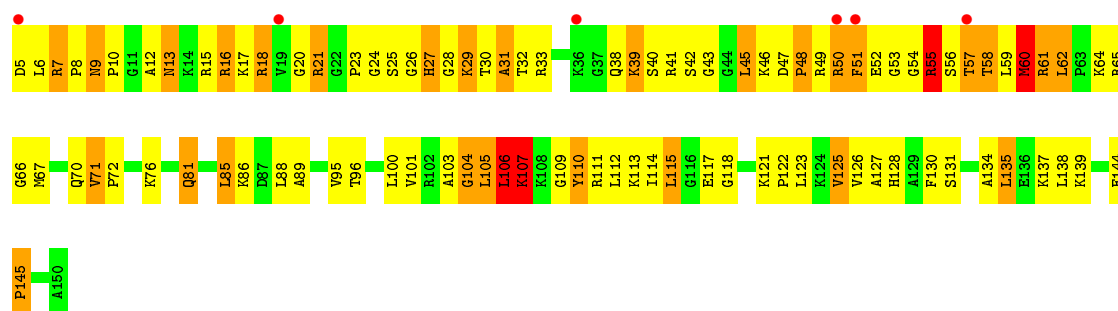
- Molecule 33: 50S ribosomal protein L14



- Molecule 33: 50S ribosomal protein L14

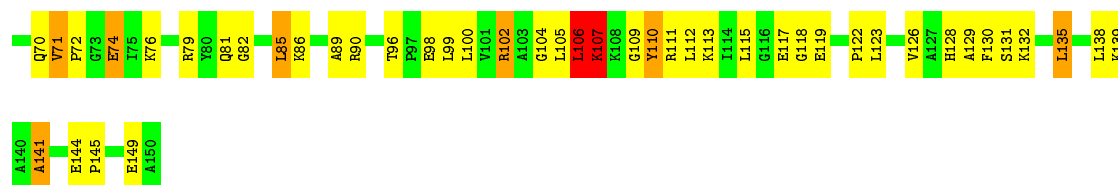


- Molecule 34: 50S ribosomal protein L15

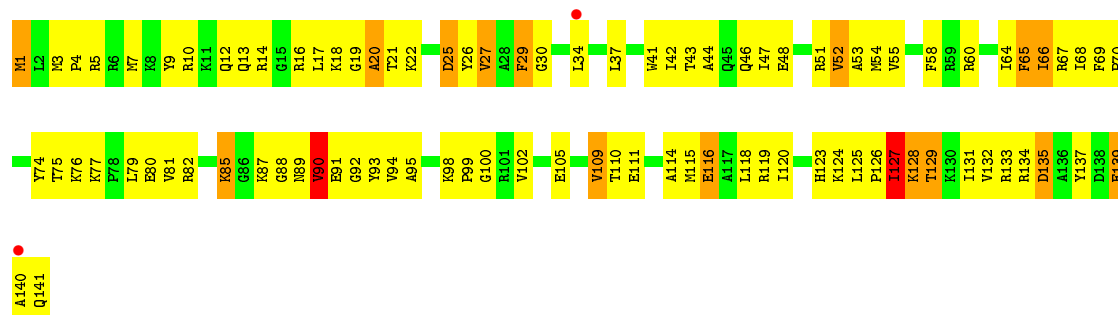


- Molecule 34: 50S ribosomal protein L15

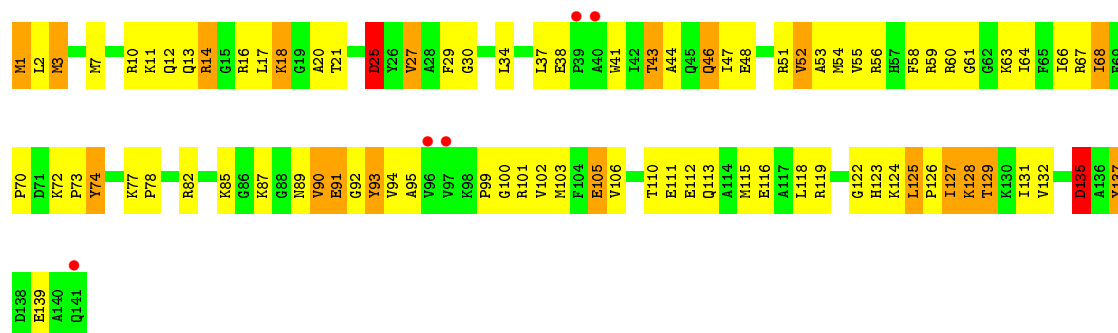
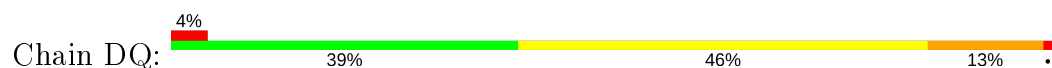




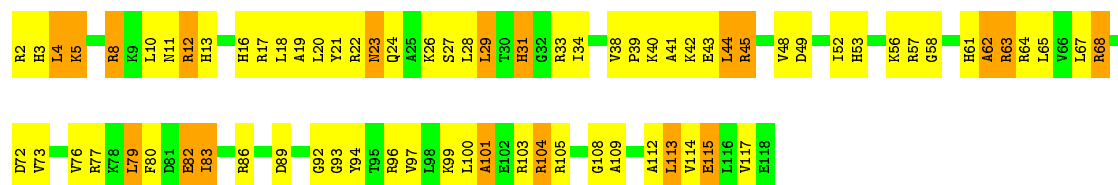
- Molecule 35: 50S ribosomal protein L16



- Molecule 35: 50S ribosomal protein L16

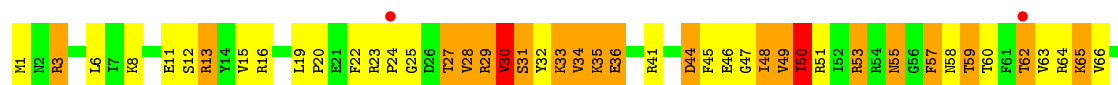


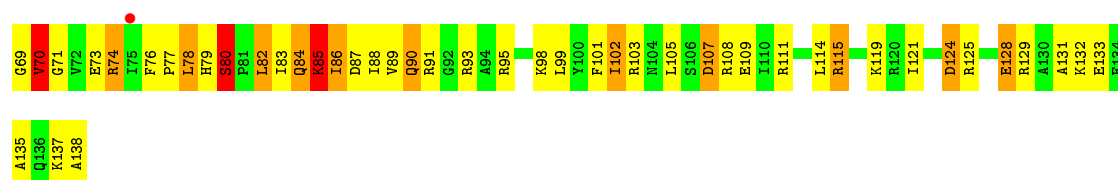
- Molecule 36: 50S ribosomal protein L17



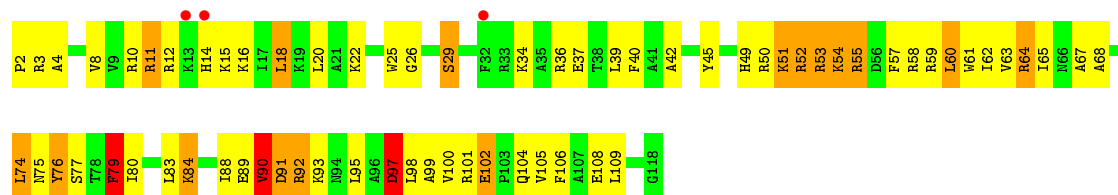
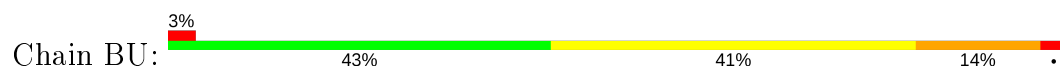
- Molecule 36: 50S ribosomal protein L17



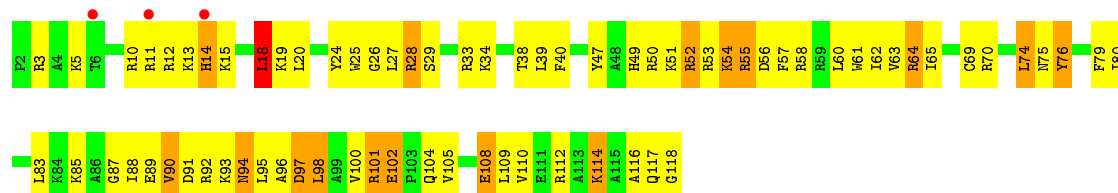




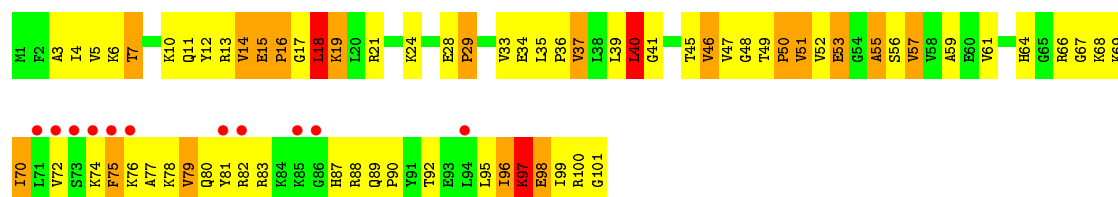
• Molecule 39: 50S ribosomal protein L20



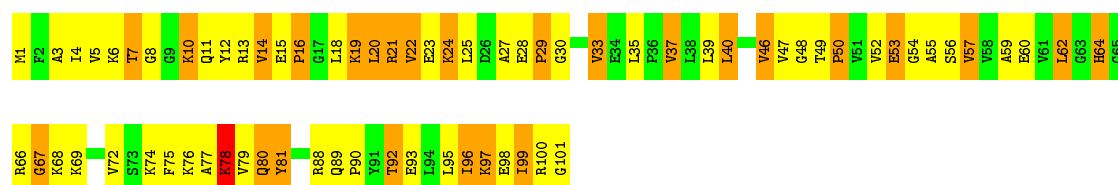
• Molecule 39: 50S ribosomal protein L20



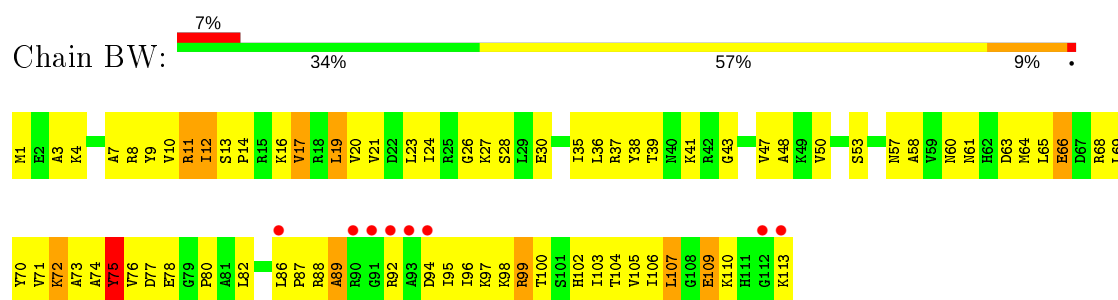
• Molecule 40: 50S ribosomal protein L21



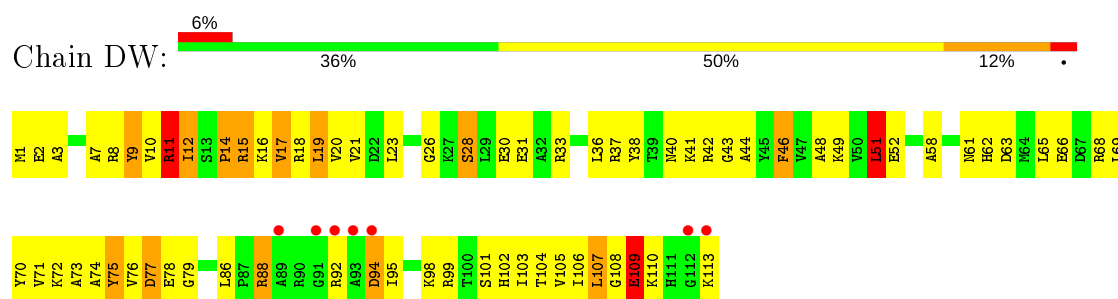
• Molecule 40: 50S ribosomal protein L21



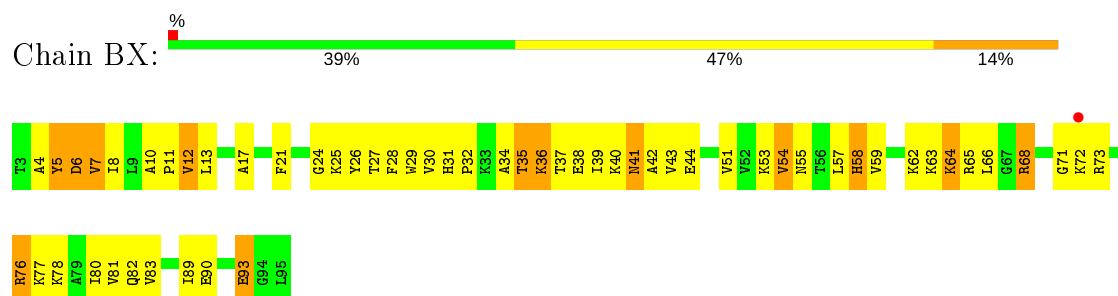
• Molecule 41: 50S ribosomal protein L22



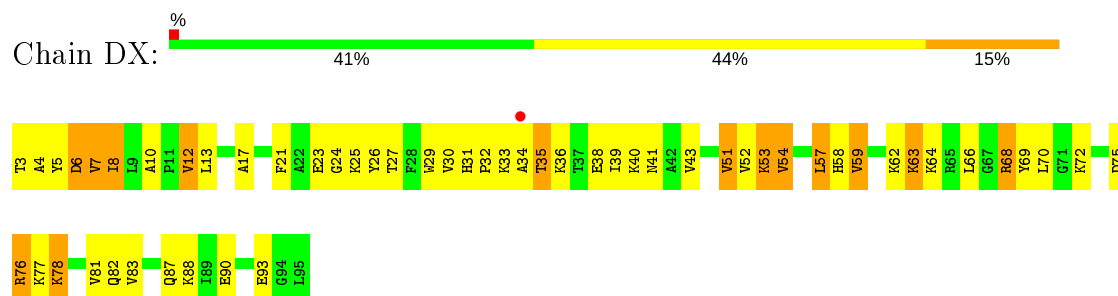
- Molecule 41: 50S ribosomal protein L22



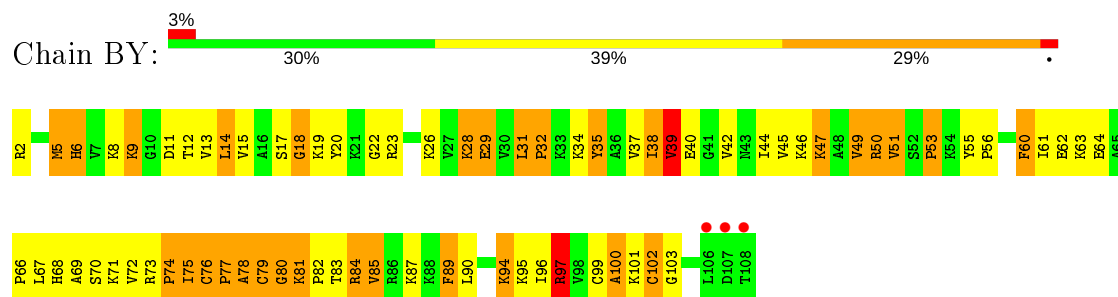
- Molecule 42: 50S ribosomal protein L23



- Molecule 42: 50S ribosomal protein L23

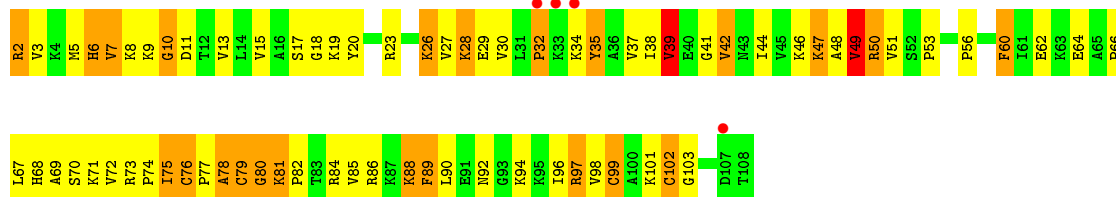


- Molecule 43: 50S ribosomal protein L24



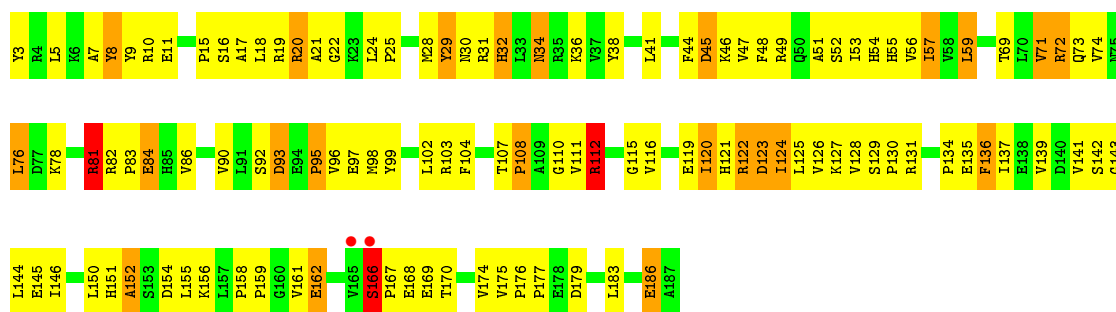
- Molecule 43: 50S ribosomal protein L24

Chain DY: 



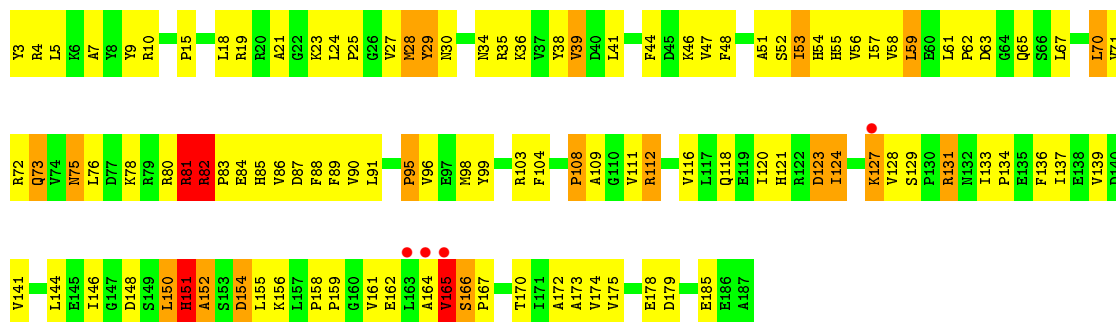
- Molecule 44: 50S ribosomal protein L25

Chain BZ: 



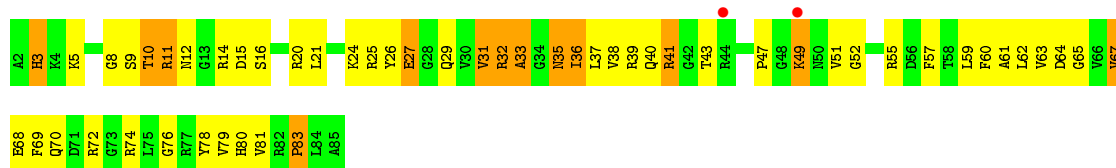
- Molecule 44: 50S ribosomal protein L25

Chain DZ: 

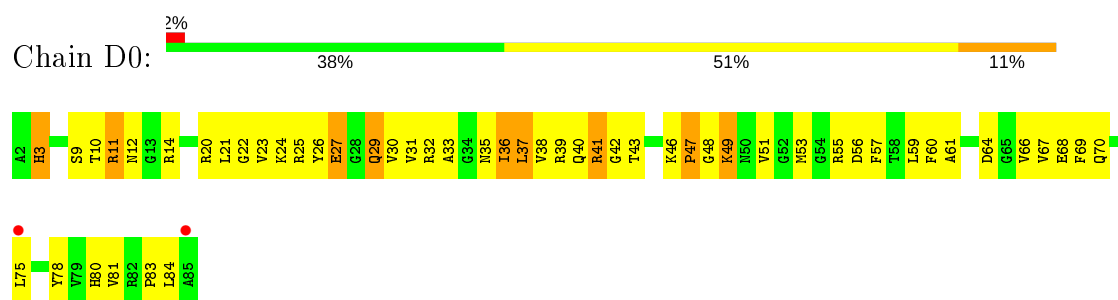


- Molecule 45: 50S ribosomal protein L27

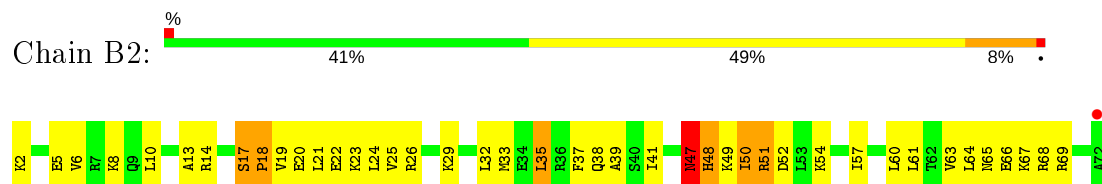
Chain B0: 



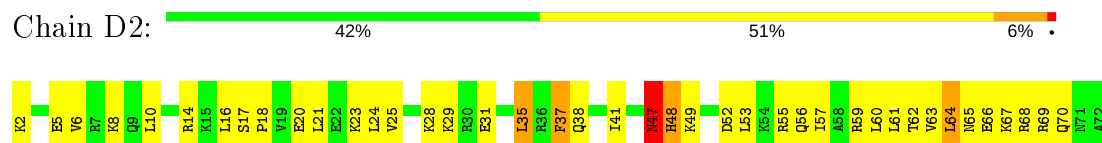
- Molecule 45: 50S ribosomal protein L27



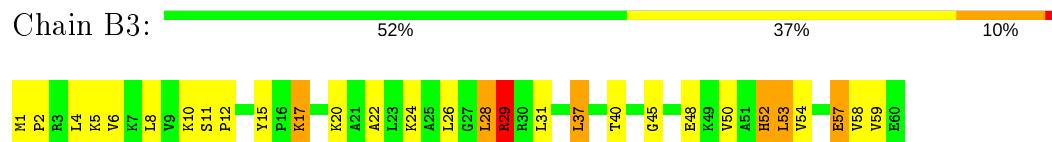
- Molecule 46: 50S ribosomal protein L29



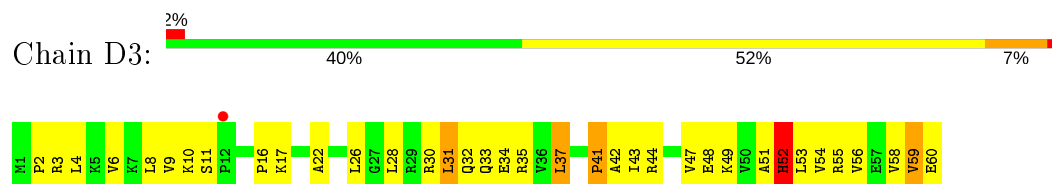
- Molecule 46: 50S ribosomal protein L29



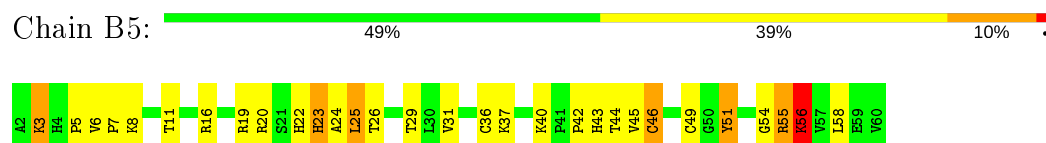
- Molecule 47: 50S ribosomal protein L30



- Molecule 47: 50S ribosomal protein L30

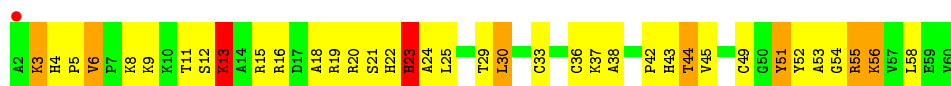


- Molecule 48: 50S ribosomal protein L32



- Molecule 48: 50S ribosomal protein L32





- Molecule 49: 50S ribosomal protein L33



- Molecule 49: 50S ribosomal protein L33



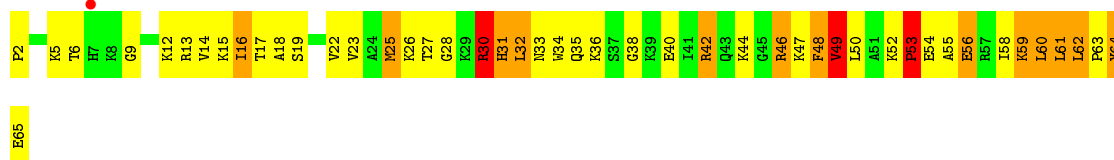
- Molecule 50: 50S ribosomal protein L34



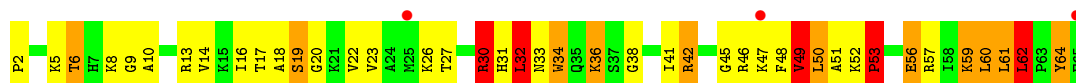
- Molecule 50: 50S ribosomal protein L34



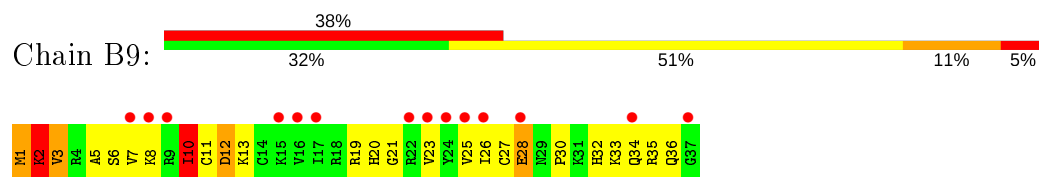
- Molecule 51: 50S ribosomal protein L35



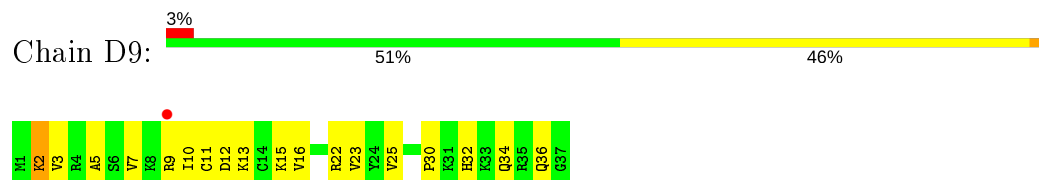
- Molecule 51: 50S ribosomal protein L35



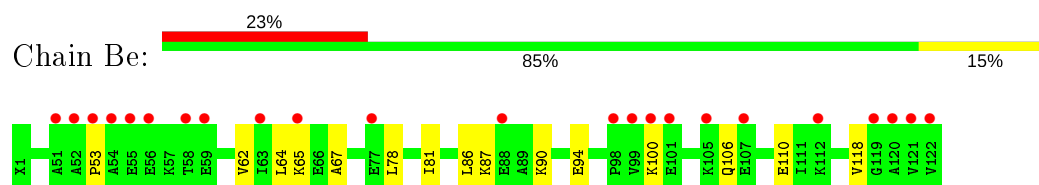
- Molecule 52: 50S ribosomal protein L36



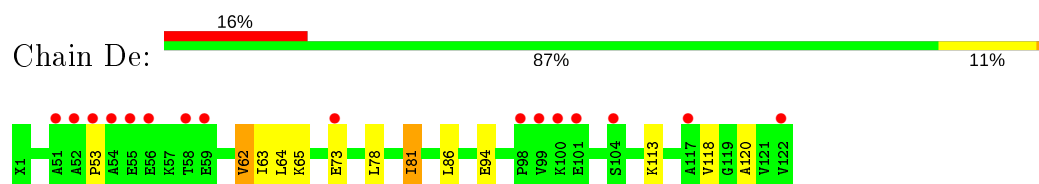
- Molecule 52: 50S ribosomal protein L36



- Molecule 53: 50S ribosomal protein L7/L12



- Molecule 53: 50S ribosomal protein L7/L12



- Molecule 54: 50S ribosomal protein L7/L12



There are no outlier residues recorded for this chain.

- Molecule 54: 50S ribosomal protein L7/L12



There are no outlier residues recorded for this chain.

- Molecule 54: 50S ribosomal protein L7/L12



There are no outlier residues recorded for this chain.

- Molecule 54: 50S ribosomal protein L7/L12



There are no outlier residues recorded for this chain.

- Molecule 55: 50S ribosomal protein L7/L12

Chain Bh:  100%

There are no outlier residues recorded for this chain.

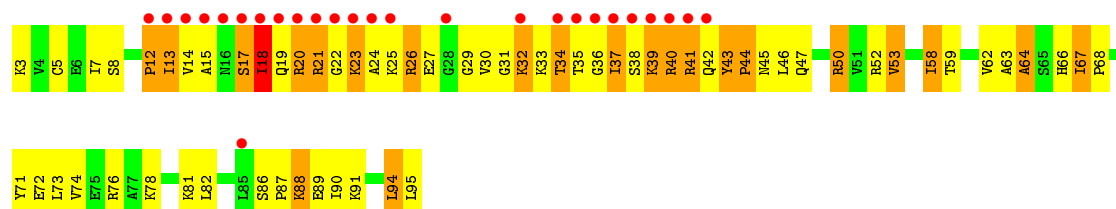
- Molecule 55: 50S ribosomal protein L7/L12

Chain Dh:  100%

There are no outlier residues recorded for this chain.

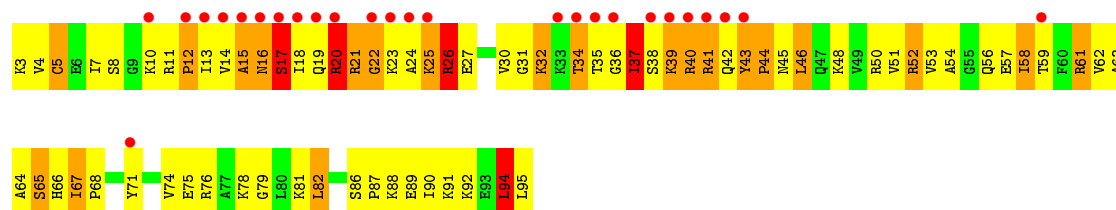
- Molecule 56: 50S ribosomal protein L28

Chain B1:  28%
30% 45% 24%



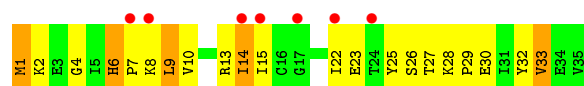
- Molecule 56: 50S ribosomal protein L28

Chain D1:  28%
20% 52% 23% 5%



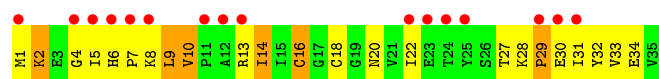
- Molecule 57: 50S ribosomal protein L31

Chain B4:  20%
40% 46% 14%



- Molecule 57: 50S ribosomal protein L31

Chain D4:  46%
34% 49% 17%

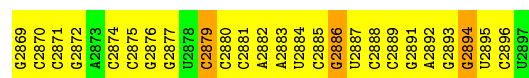


- Molecule 58: 23S ribosomal RNA



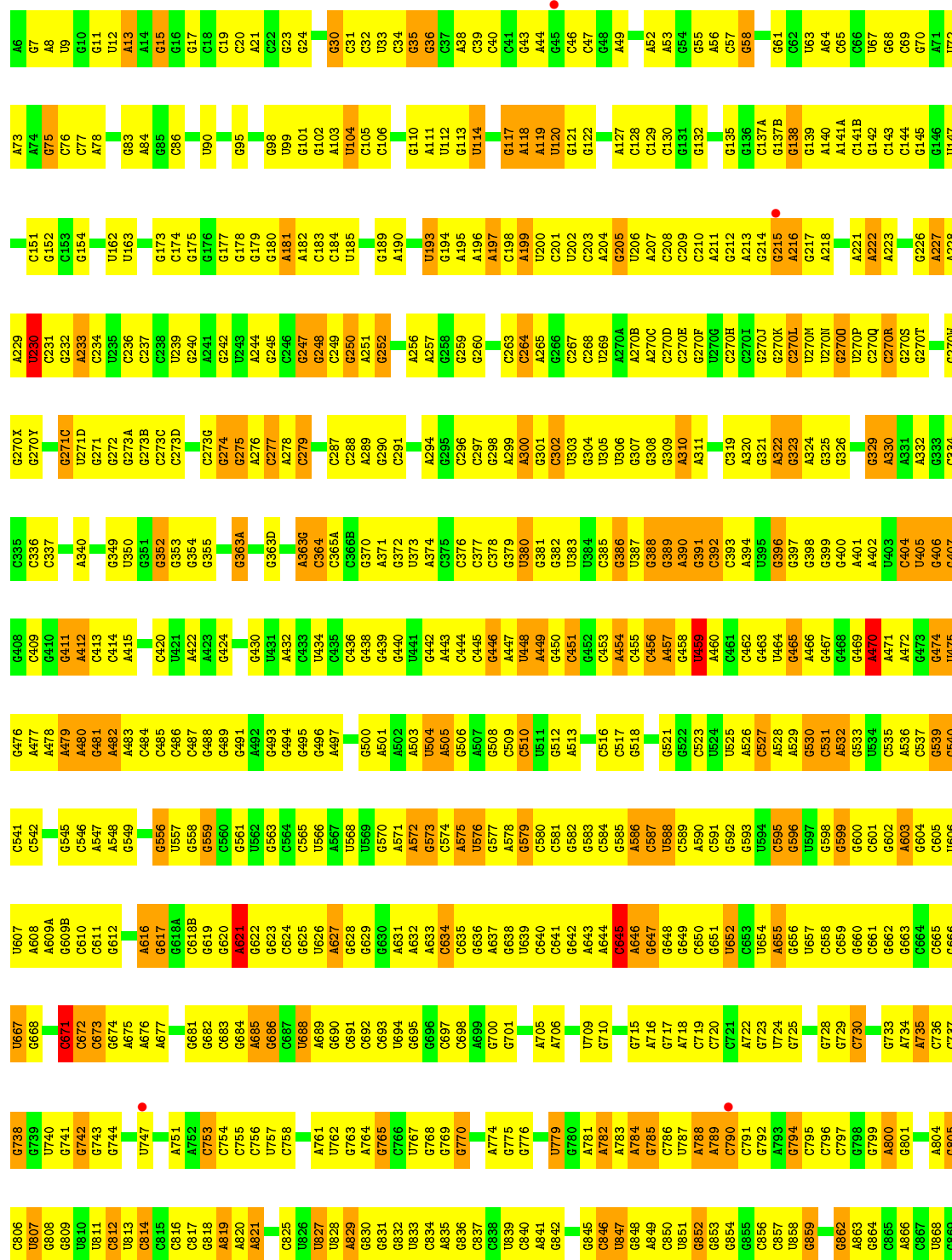
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G1339	A1677	G1613	G1545	G1483	C1411	C1333	U1267	G1206	G1139	C1072	G1002	A941
G1340	G1678	A1614	C1547			G1334	A1268	C1207	G1140	A1073	G1003	G942
U1841	U1679	C1615		A1486	G1416	U1335	A1269	G1208	U1141	G1074	G1004	U943
G1942	U1680	G1616	G1551	G1487	C1417	G1336	A1270	A1306	U1142	C1075	G1005	G944
	G1681	C1617	G1552	G1488	G1418	G1337	G1271	A1210	U1143	C1076	G1006	A945
	G1682	A1618	A1553	U1489	U1419		A1272	U1211	A1143	A1077	G1007	G946
	C1683	G1619	A1554	A1490	U1420		U1273	G1212	U1144	U1078	C1008	G947
	C1684			G1491	U1421	U1341	U1273	G1213	C1145	C1079	A1009	G948
		G1622	C1557	G1492	G1422	U1342	A1275	A1214	C1146	C1080	A1010	G949
		G1623	A1558	C1493	G1423	G1343	A1276	G1215	C1147	U1081	G1011	G950
		G1624	G1559	A1494	G1424	G1344	G1277	G1216	A1148	U1082	U1012	G951
		G1625	G1560	A1495	G1425	C1345	A1278	C1217	G1149	U1083	G1013	G952
		G1626		A1496	G1426	A1349	G1279		C1150	A1084	U1014	A953
		G1627	G1563	U1497	A1427		G1280	A1220	G1151	A1085	G1015	G954
		G1628	C1564	C1498	C1428	U1352	G1281	C1221	C1152	A1086	G1016	C955
			C1565	C1499	G1429	A1353			G1153	G1087	G1017	G956
			A1566	G1500	C1430	A1354	G1285	G1223	G1154	A1088	G1018	A957
			A1567	C1501	C1431	G1355	A1286	C1224	G1155	G1089	U1019	U958
			G1568	C1502	A1434	G1356	A1287	G1225	A1156	U1090	A1020	A959
					G1435	U1357	U1288	A1226	G1157	G1091	A1021	A960
			A1569	C1505	G1436	G1358	C1289	G1227		C1092	G1022	C961
			A1570	C1506	C1437	A1359	G1290	G1228	C1161	G1093	U1023	G962
			A1571	A1508	C1438	A1360	G1229	G1229	G1162		G1024	U963
			A1572	A1509	U1439	G1361	C1230	C1230	G1163		G1025	C964
				A1510	A1439	C1362	U1294	G1231	G1164	A1096	U1026	G965
			C1575	A1511	G1442		C1295	G1232	U1165	U1101	A1027	G966
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			C1577	C1513	G1444	A1366	C1297	U1234	U1167	A1103	A1029	G968
			A1578	U1514	A1448	A1367	C1298	G1235		C1104		U969
			A1580	C1515	A1445	G1368	G1299	G1236	G1171	U1105	A1032	C970
			G1581	U1516	C1446	G1369	U1300	A1237	C1173	G1106	U1033	C971
			C1582	G1517	G1447	G1370	A1301	G1238	A1174	U1107	G1034	G972
			A1583	C1518		G1371	U1240	U1239	U1175	C1108	G1035	A973
			C1585	G1519	C1451	U1372	A1302	U1241	G1176	C1109	G1036	C974A
			A1586	U1520	A1453		C1305	A1242	A1177	G1110	G1037	C974B
			A1587	G1521	U1454	C1375	C1306	A1243	G1178	A1111		G975
			C1588	G1522	G1455	C1376	A1307	G1243	C1179	G1112	G1041	C976
			C1589	U1523		G1377	A1308	G1244	C1180	U1113	G1042	G977
			U1590	G1524	C1458	A1378	G1309	G1245		G1114	C1043	G978
			G1591	G1525	A1459	A1379	G1310	G1246	G1183		G1044	G979
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			G1593	G1527	G1461		U1312	U1248	G1185	C1119	A1046	A981
			G1594	A1528	C1462	A1384	U1313	U1249	G1186	G1120	G1047	C982
			G1595	A1529	C1463	G1385	C1314	G1250	G1187	C1121	A1048	A984
			A1596	G1530	G1464	C1386	C1315	C1251		G1122		
			A1597	C1531	G1465	C1387	U1316	A1252	G1190	C1123	G1053	G987
			G1598	C1532	G1466	G1388	A1317	A1253	G1191	C1124	A1054	A988
			C1599		C1467		A1321	U1254	G1192	G1125	G1057	G989
			G1600	U1533	C1468	U1394	A1322	U1255		A1126	A1057	A990
			G1601	A1536	C1469	A1395	U1323	G1256	C1196	A1127	G1058	
			U1602	C1537	G1470	U1396	A1324	C1257	G1197	A1128	G1059	G993
			A1603	G1538	A1471		G1325	G1258	U1198	A1129	U1060	C994
			C1604	G1539	A1472	C1399	G1326	G1259	U1199	U1130	U1061	C995
			G1605	G1540	G1473	G1400	U1326	C1261	G1200	G1131	G1062	A996
			U1606	U1541			C1327	A1262	G1201	A1132	G1063	G997
			G1607	G1542	A1477	U1406	G1328	U1263	C1202	U1133	G1069	C998
			A1608	C1543	G1478	C1407	U1329	G1264	G1203	G1135	A1069	U999
			A1609	C1544	G1479	C1408	U1330	U1265	G1137	A1136		
				A1545	G1480	C1409	A1331	A1265			A1070	A1000

A2801	G2802	C2803	G2804	G2805	G2807	U2808	A2809	A2810	G2811	C2815	C2816	G2817	C2818	A2819	A2820	A2821	G2822	A2823	A2824	U2825	A2826	C2827	C2828	C2829	G2830	A2834	A2835	U2836	G2837	C2838	G2839	C2840	C2841	G2845	G2846	U2847	G2848	U2849	A2850	A2851	G2852	C2853	G2854	C2855	G2856	G2857	C2858	A2859	A2860	C2863	G2864	U2865	U2866	C2867	C2868	A2869																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
G2731	G2732	A2733	A2734	G2737	A2738	A2741	C2742	C2743	G2744	C2745	U2746	G2747	A2748	A2749	A2750	G2751	C2752	A2753	U2754	C2755	U2756	A2757	A2758	G2759	C2760	A2764	A2765	G2768	C2769	G2770	C2771	C2772	G2777	U2778	U2779	G2780	A2781	G2782	G2783	C2784	G2785	U2786	C2787	C2788	C2789	A2790	C2791	G2792	G2793	C2794	G2795	U2796	C2797	U2798	U2799																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
G2535	G2536	U2537	C2538	C2539	C2540	A2541	A2542	G2545	G2548	G2549	U2552	G2553	U2554	U2555	C2556	G2557	C2558	C2559	C2560	A2561	U2562	A2565	A2566	G2567	C2568	G2569	C2570	A2571	C2572	A2573	G2574	C2575	G2576	A2577	G2578	C2579	U2580	G2581	C2582	G2583	U2584	U2585	C2586	A2587	G2588	U2589	C2590	G2591	C2592	U2593	U2594	G2595	C2596	G2597	U2598	A2598																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
A2469	G2470	C2471	U2472	U2473	C2474	G2475	A2476	C2477	G2478	A2479	C2480	G2481	C2482	G2483	U2484	G2485	G2486	G2487	A2488	U2493	G2494	C2495	G2496	A2497	C2498	G2499	U2500	C2501	G2502	A2503	U2504	G2505	U2506	C2507	C2508	G2509	C2512	G2513	U2514	C2515	C2516	G2517	U2518	U2519	C2520	G2523	G2524	G2525	G2526	C2527	U2528	G2529	A2530	A2531	G2532																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
C2402	C2403	U2406	A2407	U2408	C2409	G2410	A2411	G2414	G2415	C2416	C2417	A2418	U2419	C2420	G2421	A2422	U2423	C2424	A2425	A2426	C2427	G2428	G2429	A2430	U2431	A2432	A2433	A2434	A2435	G2436	A2439	C2440	C2441	G2442	C2443	G2446	A2447	U2448	U2449	A2450	A2451	C2452	A2453	G2454	U2457	G2458	A2459	C2460	U2461	C2465	C2466	C2467	G2468																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
G2341	C2342	C2343	U2344	G2345	A2346	C2347	C2349	C2350	C2351	G2352	G2353	C2354	C2355	C2356	U2357	G2358	C2359	C2360	A2361	C2362	C2363	C2364	G2365	A2366	G2367	C2368	A2369	G2370	G2371	C2372	G2373	C2374	G2375	A2376	A2377	U2378	G2379	C2380	C2381	G2382	C2383	G2384	C2385	U2387	A2388	G2389	U2390	C2391	A2392	G2393	C2394	C2395	G2396	G2397	U2398	G2399																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
G2270	G2273	A2274	C2275	C2278	G2282	C2283	C2284	C2285	A2286	A2287	A2288	C2289	G2290	U2291	C2292	C2293	C2294	C2295	A2298	G2299	G2300	C2301	G2302	G2303	G2304	A2305	C2306	G2307	C2308	G2309	A2310	A2311	U2312	C2313	C2314	G2315	C2316	C2317	G2318	G2319	A2320	G2325	C2326	A2327	A2328	G2329	G2330	G2331	U2332	A2333	G2334	A2335	A2336																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
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A2119	G2120	U2121	U2122	G2125	A2126	G2127	G2128	G2129	U2130	U2131	U2132	G2133	A2134	A2135	C2136	G2137	C2138	C2139	C2140	U2144	C2145	C2146	G2147	G2148	G2152	G2153	G2154	G2155	G2156	G2157	A2158	A2159	G2160	C2163	G2166	A2170	A2171	U2172	A2173	C2174	C2175	A2176	C2177	C2178	C2179	U2180	G2181	G2182	C2183	G2184	A2185	G2186	U2187	U2188																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
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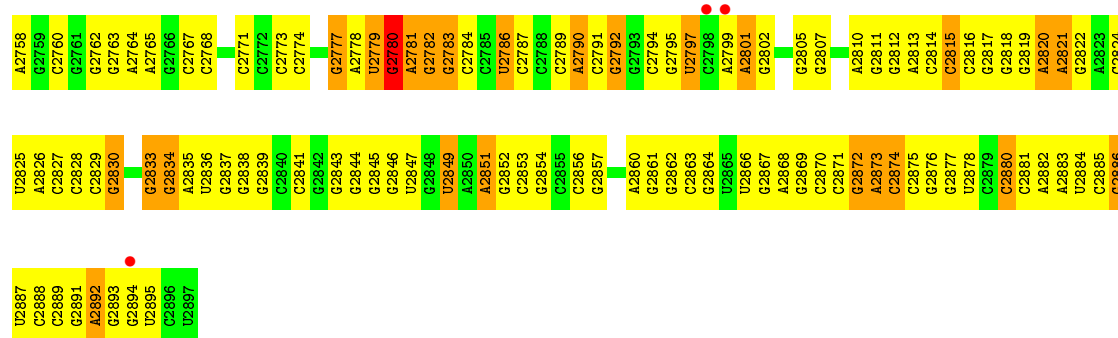
• Molecule 58: 23S ribosomal RNA

Chain DA: 27% 56% 16%



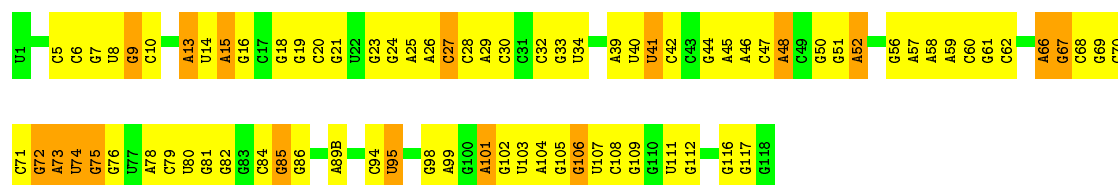
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C2760	U2693	G2629	U2560	C2497	G2434	A2371	U2237	G2237	U2160	U2094	U2029	C1801	G1801
G2761	G2694	G2630	G2561	A2498	G2435	U2372	G2238	G2238	U2161	U2095	U2030	G1802	A1802
U2762	U2695	U2631	U2562	A2499	G2436	U2373	G2239	G2239	U2162	U2096	U2031	G1803	A1803
C2763	C2696	U2632	U2563	C2499	G2437	U2374	G2240	G2240	U2163	U2097	U2032	A1804	A1804
U2764	U2697	G2633	G2564	U2500	G2438	U2375	G2241	G2241	U2164	U2098	U2033	A1805	A1805
G2765	G2698	G2634	U2565	U2501	G2439	U2376	G2242	G2242	U2165	U2099	U2034	A1806	A1806
C2766	C2699	U2634	U2566	A2499	G2440	U2377	G2243	G2243	U2166	U2100	U2035	A1807	A1807
U2767	U2699	U2635	U2567	C2499	A2441	U2378	U2244	G2244	U2167	U2101	U2036	A1808	A1808
C2768	G2700	G2635	U2568	U2500	G2442	U2379	U2245	U2245	U2168	U2102	U2037	A1809	A1809
U2769	U2701	U2636	G2569	G2501	G2443	U2380	G2246	U2246	U2169	U2103	U2038	A1810	A1810
G2770	C2702	U2637	U2570	A2502	G2444	U2381	G2247	G2247	U2170	U2104	U2039	A1811	A1811
A2771	U2703	U2638	G2571	G2503	A2503	U2382	A2248	G2248	U2171	U2105	U2040	A1812	A1812
C2772	G2704	G2639	A2572	U2504	A2504	U2383	U2249	G2249	U2172	U2106	U2041	A1813	A1813
U2773	U2705	U2640	G2573	U2505	A2505	U2384	U2250	G2250	U2173	U2107	U2042	A1814	A1814
G2774	C2706	G2641	U2574	G2506	G2445	U2385	U2251	G2251	U2174	U2108	U2043	A1815	A1815
U2775	U2707	U2642	G2575	U2507	G2446	U2386	U2252	G2252	U2175	U2109	U2044	A1816	A1816
A2776	G2708	G2643	U2576	G2508	G2447	U2387	U2253	G2253	U2176	U2110	U2045	A1817	A1817
C2777	U2709	G2644	A2577	G2509	G2448	U2388	U2254	G2254	U2177	U2111	U2046	A1818	A1818
U2778	U2710	G2645	C2578	C2510	G2449	U2389	U2255	G2255	U2178	U2112	U2047	A1819	A1819
G2779	G2711	U2646	U2579	U2511	A2448	U2390	U2256	G2256	U2179	U2113	U2048	A1820	A1820
C2780	U2712	U2647	U2580	C2512	G2449	U2391	U2257	G2257	U2180	U2114	U2049	A1821	A1821
U2781	C2713	G2648	G2581	G2513	U2449	U2392	U2258	G2258	U2181	U2115	U2050	A1822	A1822
G2782	U2714	U2649	U2582	U2514	U2450	U2393	U2259	G2259	U2182	U2116	U2051	A1823	A1823
U2783	U2715	U2650	G2583	U2515	C2451	U2394	U2260	G2260	U2183	U2117	U2052	A1824	A1824
C2													



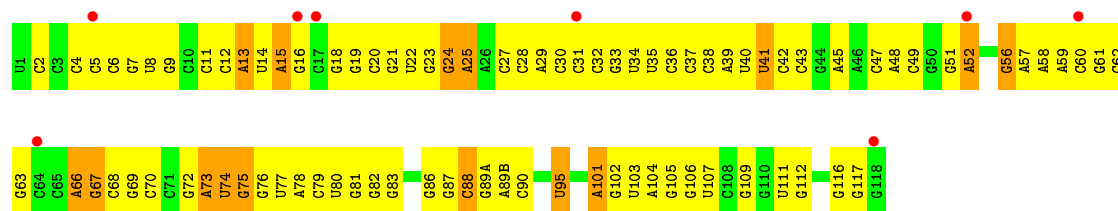
- Molecule 59: 5S ribosomal RNA

Chain BB: 32% 54% 14%



- Molecule 59: 5S ribosomal RNA

Chain DB: 7% 26% 61% 13%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	307.21Å 670.44Å 350.40Å 90.00° 92.37° 90.00°	Depositor
Resolution (Å)	40.00 – 4.00 145.84 – 3.98	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-4.00) 77.8 (145.84-3.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 4.01Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.281 , 0.329 0.285 , 0.324	Depositor DCC
R_{free} test set	25982 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	74.5	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 14.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.24$, $\langle L^2 \rangle = 0.09$	Xtriage
Estimated twinning fraction	0.249 for h,-k,-l	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	308068	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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: GDP, FUA

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	0.37	0/1945	0.70	1/2621 (0.0%)
1	CB	0.37	0/1945	0.70	1/2621 (0.0%)
2	AC	0.27	0/1645	0.53	0/2216
2	CC	0.27	0/1645	0.55	0/2216
3	AD	0.29	0/1733	0.61	1/2318 (0.0%)
3	CD	0.29	0/1733	0.57	0/2318
4	AE	0.28	0/1172	0.58	1/1576 (0.1%)
4	CE	0.30	0/1172	0.57	1/1576 (0.1%)
5	AF	0.28	0/856	0.59	1/1154 (0.1%)
5	CF	0.29	0/856	0.57	1/1154 (0.1%)
6	AG	0.27	0/1276	0.52	0/1709
6	CG	0.28	0/1276	0.53	0/1709
7	AH	0.29	0/1136	0.61	0/1527
7	CH	0.28	0/1136	0.58	0/1527
8	AI	0.28	0/1029	0.51	0/1379
8	CI	0.26	0/1029	0.52	0/1379
9	AJ	0.25	0/815	0.56	1/1095 (0.1%)
9	CJ	0.27	0/815	0.58	1/1095 (0.1%)
10	AK	0.33	0/900	0.66	1/1213 (0.1%)
10	CK	0.35	0/900	0.63	0/1213
11	AL	0.39	0/992	0.86	1/1327 (0.1%)
11	CL	0.38	0/992	0.83	1/1327 (0.1%)
12	AM	0.28	0/1008	0.62	1/1347 (0.1%)
12	CM	0.25	0/1008	0.55	0/1347
13	AN	0.28	0/501	0.49	0/664
13	CN	0.28	0/501	0.47	0/664
14	AO	0.31	0/745	0.56	0/992
14	CO	0.28	0/745	0.56	0/992
15	AP	0.28	0/722	0.51	0/970
15	CP	0.26	0/722	0.50	0/970
16	AQ	0.37	0/848	0.71	0/1131
16	CQ	0.36	0/848	0.72	0/1131

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AR	0.29	0/579	0.60	0/768
17	CR	0.27	0/579	0.62	0/768
18	AS	0.28	0/647	0.60	1/870 (0.1%)
18	CS	0.28	0/647	0.64	0/870
19	AT	0.32	0/765	0.57	0/1007
19	CT	0.31	0/765	0.57	0/1007
20	AA	0.35	0/36351	1.03	78/56736 (0.1%)
20	CA	0.34	0/36351	1.01	66/56736 (0.1%)
21	AW	0.35	0/1827	1.09	6/2845 (0.2%)
21	CW	0.36	0/1827	1.10	8/2845 (0.3%)
22	AV	0.26	0/568	0.83	0/886
22	CV	0.28	0/568	0.90	0/886
23	AY	0.33	1/5317 (0.0%)	0.70	10/7198 (0.1%)
23	CY	0.34	1/5317 (0.0%)	0.71	6/7198 (0.1%)
24	BC	0.39	0/1774	0.75	0/2391
24	DC	0.41	0/1774	0.75	1/2391 (0.0%)
25	BD	0.33	0/2195	0.68	2/2955 (0.1%)
25	DD	0.34	0/2195	0.67	1/2955 (0.0%)
26	BE	0.31	0/1602	0.66	0/2160
26	DE	0.31	0/1602	0.67	0/2160
27	BF	0.34	0/1663	0.74	2/2249 (0.1%)
27	DF	0.35	0/1663	0.76	2/2249 (0.1%)
28	BG	0.27	0/1499	0.56	0/2016
28	DG	0.33	1/1499 (0.1%)	0.63	3/2016 (0.1%)
29	BH	0.29	0/1298	0.61	0/1751
29	DH	0.31	0/1298	0.59	0/1751
31	BK	0.26	0/1054	0.50	0/1427
31	DK	0.26	0/1054	0.49	0/1427
32	BN	0.34	0/1131	0.66	0/1525
32	DN	0.34	0/1131	0.66	0/1525
33	BO	0.29	0/943	0.57	0/1269
33	DO	0.27	0/943	0.55	0/1269
34	BP	0.29	0/1131	0.61	0/1504
34	DP	0.29	0/1131	0.66	0/1504
35	BQ	0.32	0/1143	0.64	0/1527
35	DQ	0.32	0/1143	0.61	0/1527
36	BR	0.30	0/974	0.63	0/1302
36	DR	0.31	0/974	0.65	0/1302
37	BS	0.33	0/783	0.69	0/1041
37	DS	0.34	0/783	0.73	0/1041
38	BT	0.34	0/1161	0.70	1/1549 (0.1%)
38	DT	0.33	0/1161	0.66	0/1549
39	BU	0.37	0/982	0.62	0/1306

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	DU	0.37	0/982	0.62	1/1306 (0.1%)
40	BV	0.34	0/790	0.71	0/1057
40	DV	0.36	0/790	0.70	0/1057
41	BW	0.30	0/911	0.60	0/1220
41	DW	0.31	0/911	0.65	2/1220 (0.2%)
42	BX	0.27	0/748	0.55	0/1004
42	DX	0.29	0/748	0.58	0/1004
43	BY	0.31	0/831	0.60	0/1108
43	DY	0.30	0/831	0.65	0/1108
44	BZ	0.27	0/1505	0.60	0/2042
44	DZ	0.28	0/1505	0.60	0/2042
45	B0	0.25	0/671	0.51	0/892
45	D0	0.26	0/671	0.56	0/892
46	B2	0.32	0/600	0.59	0/793
46	D2	0.31	0/600	0.61	0/793
47	B3	0.26	0/482	0.54	0/646
47	D3	0.24	0/482	0.54	0/646
48	B5	0.27	0/473	0.55	0/639
48	D5	0.26	0/473	0.58	0/639
49	B6	0.31	0/440	0.72	1/586 (0.2%)
49	D6	0.31	0/440	0.68	1/586 (0.2%)
50	B7	0.32	0/438	0.64	0/575
50	D7	0.30	0/438	0.59	0/575
51	B8	0.31	0/525	0.67	0/691
51	D8	0.29	0/525	0.63	2/691 (0.3%)
52	B9	0.27	0/310	0.55	0/407
52	D9	0.27	0/310	0.50	0/407
53	Be	0.45	1/538 (0.2%)	0.55	0/715
53	De	0.26	0/538	0.51	0/715
56	B1	0.46	0/739	0.84	0/981
56	D1	0.46	0/739	0.86	0/981
57	B4	0.33	0/276	0.62	0/372
57	D4	0.34	0/276	0.58	0/372
58	BA	0.37	3/69437 (0.0%)	1.06	184/108401 (0.2%)
58	DA	0.37	1/69437 (0.0%)	1.05	153/108401 (0.1%)
59	BB	0.35	0/2853	1.07	9/4451 (0.2%)
59	DB	0.34	0/2853	1.03	11/4451 (0.2%)
All	All	0.35	8/330554 (0.0%)	0.94	564/492202 (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	2
1	CB	0	3
11	CL	0	1
23	AY	0	5
23	CY	0	1
24	BC	0	2
24	DC	0	3
25	BD	0	2
27	BF	0	2
27	DF	0	2
30	BJ	0	1
30	DJ	0	1
37	BS	0	2
37	DS	0	4
41	BW	0	1
41	DW	0	1
56	B1	0	1
56	D1	0	2
All	All	0	36

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	BA	1914	C	O3'-P	-10.49	1.48	1.61
53	Be	87	LYS	C-N	8.65	1.53	1.34
58	BA	1911	U	O3'-P	-6.43	1.53	1.61
58	BA	1006	C	N1-C2	5.82	1.46	1.40
58	DA	1911	U	O3'-P	-5.77	1.54	1.61

The worst 5 of 564 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	CY	500	GLN	CA-C-N	17.19	155.01	117.20
58	BA	1006	C	C6-N1-C2	-16.88	113.55	120.30
58	BA	1006	C	N3-C2-O2	-14.80	111.54	121.90
23	CY	500	GLN	C-N-CA	14.70	158.44	121.70
58	BA	1006	C	N1-C2-O2	13.47	126.98	118.90

There are no chirality outliers.

5 of 36 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AB	163	PHE	Peptide
1	AB	170	GLU	Peptide
23	AY	133	ILE	Peptide
23	AY	135	PHE	Mainchain
23	AY	499	ARG	Mainchain

5.2 Too-close contacts

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	137	0
1	CB	1910	0	1957	134	0
2	AC	1621	0	1688	88	0
2	CC	1621	0	1688	70	0
3	AD	1703	0	1763	134	0
3	CD	1703	0	1763	105	0
4	AE	1156	0	1213	66	0
4	CE	1156	0	1213	71	0
5	AF	843	0	857	45	0
5	CF	843	0	857	43	0
6	AG	1257	0	1296	49	0
6	CG	1257	0	1296	49	0
7	AH	1116	0	1177	71	0
7	CH	1116	0	1177	73	0
8	AI	1010	0	1037	56	0
8	CI	1010	0	1037	60	0
9	AJ	802	0	849	52	0
9	CJ	802	0	849	48	0
10	AK	885	0	904	56	0
10	CK	885	0	904	55	0
11	AL	976	0	1062	97	0
11	CL	976	0	1062	110	0
12	AM	997	0	1072	55	0
12	CM	997	0	1072	56	0
13	AN	492	0	529	37	0
13	CN	492	0	529	29	0
14	AO	734	0	771	51	0
14	CO	734	0	771	41	0
15	AP	706	0	725	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	CP	706	0	725	37	0
16	AQ	835	0	904	60	0
16	CQ	835	0	904	65	0
17	AR	574	0	644	35	0
17	CR	574	0	644	43	0
18	AS	634	0	655	38	0
18	CS	634	0	655	43	0
19	AT	763	0	861	43	0
19	CT	763	0	861	45	0
20	AA	32474	0	16393	1058	0
20	CA	32474	0	16393	1056	0
21	AW	1635	0	831	68	0
21	CW	1635	0	831	51	0
22	AV	503	0	252	13	0
22	CV	503	0	252	16	0
23	AY	5219	0	5290	335	0
23	CY	5219	0	5290	319	0
24	BC	1742	0	1798	162	0
24	DC	1742	0	1798	172	0
25	BD	2145	0	2234	214	0
25	DD	2145	0	2234	202	0
26	BE	1569	0	1634	132	0
26	DE	1569	0	1634	142	0
27	BF	1628	0	1680	141	0
27	DF	1628	0	1680	141	0
28	BG	1474	0	1535	96	0
28	DG	1474	0	1535	80	0
29	BH	1274	0	1342	79	0
29	DH	1274	0	1342	66	0
30	BJ	851	0	196	31	0
30	DJ	851	0	196	41	0
31	BK	1035	0	1082	53	0
31	DK	1035	0	1082	51	0
32	BN	1104	0	1179	205	0
32	DN	1104	0	1180	217	0
33	BO	933	0	996	62	0
33	DO	933	0	996	69	0
34	BP	1114	0	1187	96	0
34	DP	1114	0	1187	97	0
35	BQ	1122	0	1179	68	0
35	DQ	1122	0	1179	69	0
36	BR	960	0	1021	72	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	DR	960	0	1021	79	0
37	BS	775	0	835	77	0
37	DS	775	0	835	68	0
38	BT	1147	0	1207	107	0
38	DT	1147	0	1207	90	0
39	BU	964	0	1020	95	0
39	DU	964	0	1022	103	1
40	BV	779	0	852	70	0
40	DV	779	0	852	72	0
41	BW	900	0	964	53	0
41	DW	900	0	964	56	0
42	BX	734	0	789	42	0
42	DX	734	0	789	50	0
43	BY	818	0	908	59	0
43	DY	818	0	908	53	0
44	BZ	1473	0	1497	83	0
44	DZ	1473	0	1497	76	0
45	B0	662	0	688	41	0
45	D0	662	0	688	42	0
46	B2	598	0	653	30	0
46	D2	598	0	653	38	0
47	B3	477	0	529	19	0
47	D3	477	0	529	30	0
48	B5	459	0	477	27	0
48	D5	459	0	477	45	0
49	B6	433	0	461	27	0
49	D6	433	0	461	29	0
50	B7	430	0	480	37	0
50	D7	430	0	480	30	0
51	B8	517	0	582	49	0
51	D8	517	0	582	43	0
52	B9	307	0	338	22	0
52	D9	307	0	335	14	0
53	Be	686	0	617	0	0
53	De	686	0	615	0	0
54	Bf	156	0	41	0	0
54	Bg	156	0	38	0	0
54	Df	156	0	42	0	0
54	Dg	156	0	40	0	0
55	Bh	151	0	41	0	0
55	Dh	151	0	40	0	0
56	B1	732	0	808	72	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	D1	732	0	808	78	0
57	B4	271	0	284	17	0
57	D4	271	0	284	15	0
58	BA	61997	0	31250	2049	1
58	DA	61997	0	31250	2317	0
59	BB	2551	0	1295	93	0
59	DB	2551	0	1295	94	0
60	AY	37	0	47	13	0
60	CY	37	0	47	10	0
61	AY	28	0	12	6	0
61	CY	28	0	12	6	0
All	All	308068	0	213012	12886	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

The worst 5 of 12886 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)
20:CA:1494:G:C5'	58:DA:1913:A:N6	1.79	1.45
32:BN:1:MET:HG2	40:BV:13:ARG:NH1	1.30	1.39
23:AY:580:MET:HE2	58:BA:1913:A:N1	1.37	1.35
58:BA:2681:C:N4	58:BA:2725:A:H62	1.22	1.35
23:AY:580:MET:CE	58:BA:1913:A:N1	1.91	1.34

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:BA:1015:G:O2'	39:DU:118:GLY:O[3_545]	2.10	0.10

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

The Analysed column shows the number of residues for which the backbone conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AB	233/235 (99%)	155 (66%)	52 (22%)	26 (11%)	0	7
1	CB	233/235 (99%)	152 (65%)	55 (24%)	26 (11%)	0	7
2	AC	205/207 (99%)	156 (76%)	33 (16%)	16 (8%)	1	14
2	CC	205/207 (99%)	148 (72%)	41 (20%)	16 (8%)	1	14
3	AD	206/208 (99%)	145 (70%)	37 (18%)	24 (12%)	0	6
3	CD	206/208 (99%)	150 (73%)	32 (16%)	24 (12%)	0	6
4	AE	149/151 (99%)	124 (83%)	17 (11%)	8 (5%)	2	21
4	CE	149/151 (99%)	116 (78%)	25 (17%)	8 (5%)	2	21
5	AF	99/101 (98%)	73 (74%)	20 (20%)	6 (6%)	1	19
5	CF	99/101 (98%)	75 (76%)	18 (18%)	6 (6%)	1	19
6	AG	153/155 (99%)	122 (80%)	23 (15%)	8 (5%)	2	21
6	CG	153/155 (99%)	116 (76%)	28 (18%)	9 (6%)	1	19
7	AH	136/138 (99%)	93 (68%)	29 (21%)	14 (10%)	0	8
7	CH	136/138 (99%)	101 (74%)	22 (16%)	13 (10%)	0	10
8	AI	125/127 (98%)	93 (74%)	28 (22%)	4 (3%)	4	31
8	CI	125/127 (98%)	97 (78%)	22 (18%)	6 (5%)	2	23
9	AJ	97/99 (98%)	73 (75%)	14 (14%)	10 (10%)	0	8
9	CJ	97/99 (98%)	78 (80%)	13 (13%)	6 (6%)	1	18
10	AK	117/119 (98%)	85 (73%)	16 (14%)	16 (14%)	0	4
10	CK	117/119 (98%)	79 (68%)	21 (18%)	17 (14%)	0	3
11	AL	123/125 (98%)	42 (34%)	45 (37%)	36 (29%)	0	0
11	CL	123/125 (98%)	43 (35%)	41 (33%)	39 (32%)	0	0
12	AM	123/125 (98%)	88 (72%)	24 (20%)	11 (9%)	1	12
12	CM	123/125 (98%)	90 (73%)	24 (20%)	9 (7%)	1	15
13	AN	58/60 (97%)	43 (74%)	8 (14%)	7 (12%)	0	5
13	CN	58/60 (97%)	44 (76%)	8 (14%)	6 (10%)	0	8
14	AO	86/88 (98%)	62 (72%)	15 (17%)	9 (10%)	0	8
14	CO	86/88 (98%)	62 (72%)	20 (23%)	4 (5%)	2	23
15	AP	82/84 (98%)	64 (78%)	14 (17%)	4 (5%)	2	22
15	CP	82/84 (98%)	62 (76%)	16 (20%)	4 (5%)	2	22
16	AQ	98/100 (98%)	70 (71%)	18 (18%)	10 (10%)	0	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	CQ	98/100 (98%)	68 (69%)	21 (21%)	9 (9%)	1	11
17	AR	68/70 (97%)	52 (76%)	11 (16%)	5 (7%)	1	15
17	CR	68/70 (97%)	47 (69%)	19 (28%)	2 (3%)	4	32
18	AS	77/79 (98%)	41 (53%)	24 (31%)	12 (16%)	0	3
18	CS	77/79 (98%)	50 (65%)	11 (14%)	16 (21%)	0	1
19	AT	97/99 (98%)	81 (84%)	10 (10%)	6 (6%)	1	18
19	CT	97/99 (98%)	76 (78%)	17 (18%)	4 (4%)	3	25
23	AY	663/687 (96%)	436 (66%)	147 (22%)	80 (12%)	0	5
23	CY	663/687 (96%)	454 (68%)	139 (21%)	70 (11%)	0	7
24	BC	226/228 (99%)	106 (47%)	70 (31%)	50 (22%)	0	1
24	DC	226/228 (99%)	114 (50%)	68 (30%)	44 (20%)	0	2
25	BD	273/275 (99%)	177 (65%)	52 (19%)	44 (16%)	0	3
25	DD	273/275 (99%)	171 (63%)	56 (20%)	46 (17%)	0	3
26	BE	203/205 (99%)	127 (63%)	45 (22%)	31 (15%)	0	3
26	DE	203/205 (99%)	128 (63%)	40 (20%)	35 (17%)	0	3
27	BF	206/208 (99%)	132 (64%)	53 (26%)	21 (10%)	0	9
27	DF	206/208 (99%)	131 (64%)	42 (20%)	33 (16%)	0	3
28	BG	179/181 (99%)	126 (70%)	40 (22%)	13 (7%)	1	15
28	DG	179/181 (99%)	131 (73%)	35 (20%)	13 (7%)	1	15
29	BH	165/167 (99%)	113 (68%)	32 (19%)	20 (12%)	0	5
29	DH	165/167 (99%)	102 (62%)	42 (26%)	21 (13%)	0	5
31	BK	138/140 (99%)	98 (71%)	30 (22%)	10 (7%)	1	16
31	DK	138/140 (99%)	100 (72%)	31 (22%)	7 (5%)	2	22
32	BN	136/138 (99%)	95 (70%)	25 (18%)	16 (12%)	0	6
32	DN	136/138 (99%)	95 (70%)	25 (18%)	16 (12%)	0	6
33	BO	120/122 (98%)	84 (70%)	20 (17%)	16 (13%)	0	4
33	DO	120/122 (98%)	86 (72%)	24 (20%)	10 (8%)	1	13
34	BP	144/146 (99%)	82 (57%)	36 (25%)	26 (18%)	0	2
34	DP	144/146 (99%)	81 (56%)	35 (24%)	28 (19%)	0	2
35	BQ	139/141 (99%)	94 (68%)	33 (24%)	12 (9%)	1	12
35	DQ	139/141 (99%)	99 (71%)	30 (22%)	10 (7%)	1	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	BR	115/117 (98%)	80 (70%)	21 (18%)	14 (12%)	0	5
36	DR	115/117 (98%)	81 (70%)	22 (19%)	12 (10%)	0	8
37	BS	97/99 (98%)	57 (59%)	18 (19%)	22 (23%)	0	1
37	DS	97/99 (98%)	48 (50%)	26 (27%)	23 (24%)	0	1
38	BT	136/138 (99%)	85 (62%)	22 (16%)	29 (21%)	0	1
38	DT	136/138 (99%)	90 (66%)	22 (16%)	24 (18%)	0	2
39	BU	115/117 (98%)	91 (79%)	18 (16%)	6 (5%)	2	21
39	DU	115/117 (98%)	90 (78%)	21 (18%)	4 (4%)	3	29
40	BV	99/101 (98%)	65 (66%)	16 (16%)	18 (18%)	0	2
40	DV	99/101 (98%)	63 (64%)	22 (22%)	14 (14%)	0	3
41	BW	111/113 (98%)	84 (76%)	17 (15%)	10 (9%)	1	12
41	DW	111/113 (98%)	85 (77%)	14 (13%)	12 (11%)	0	7
42	BX	91/93 (98%)	66 (72%)	19 (21%)	6 (7%)	1	17
42	DX	91/93 (98%)	70 (77%)	15 (16%)	6 (7%)	1	17
43	BY	105/107 (98%)	44 (42%)	38 (36%)	23 (22%)	0	1
43	DY	105/107 (98%)	47 (45%)	28 (27%)	30 (29%)	0	0
44	BZ	183/185 (99%)	129 (70%)	34 (19%)	20 (11%)	0	7
44	DZ	183/185 (99%)	121 (66%)	44 (24%)	18 (10%)	0	10
45	B0	82/84 (98%)	58 (71%)	17 (21%)	7 (8%)	1	12
45	D0	82/84 (98%)	51 (62%)	24 (29%)	7 (8%)	1	12
46	B2	69/71 (97%)	50 (72%)	13 (19%)	6 (9%)	1	12
46	D2	69/71 (97%)	50 (72%)	16 (23%)	3 (4%)	2	25
47	B3	58/60 (97%)	45 (78%)	10 (17%)	3 (5%)	2	21
47	D3	58/60 (97%)	46 (79%)	9 (16%)	3 (5%)	2	21
48	B5	57/59 (97%)	41 (72%)	12 (21%)	4 (7%)	1	16
48	D5	57/59 (97%)	36 (63%)	18 (32%)	3 (5%)	2	21
49	B6	48/50 (96%)	27 (56%)	13 (27%)	8 (17%)	0	3
49	D6	48/50 (96%)	28 (58%)	11 (23%)	9 (19%)	0	2
50	B7	47/49 (96%)	31 (66%)	14 (30%)	2 (4%)	2	25
50	D7	47/49 (96%)	36 (77%)	6 (13%)	5 (11%)	0	7
51	B8	62/64 (97%)	32 (52%)	22 (36%)	8 (13%)	0	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	D8	62/64 (97%)	38 (61%)	14 (23%)	10 (16%)	0	3
52	B9	35/37 (95%)	23 (66%)	7 (20%)	5 (14%)	0	3
52	D9	35/37 (95%)	26 (74%)	8 (23%)	1 (3%)	4	32
53	Be	70/102 (69%)	35 (50%)	28 (40%)	7 (10%)	0	9
53	De	70/102 (69%)	39 (56%)	24 (34%)	7 (10%)	0	9
56	B1	91/93 (98%)	53 (58%)	19 (21%)	19 (21%)	0	1
56	D1	91/93 (98%)	57 (63%)	15 (16%)	19 (21%)	0	1
57	B4	33/35 (94%)	17 (52%)	11 (33%)	5 (15%)	0	3
57	D4	33/35 (94%)	15 (46%)	9 (27%)	9 (27%)	0	0
All	All	13256/13564 (98%)	8908 (67%)	2779 (21%)	1569 (12%)	0	6

5 of 1569 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AB	76	GLN
1	AB	94	ASN
1	AB	95	GLN
1	AB	165	VAL
1	AB	194	PRO

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%)	161 (79%)	42 (21%)	1	6
1	CB	203/203 (100%)	158 (78%)	45 (22%)	1	6
2	AC	161/161 (100%)	136 (84%)	25 (16%)	2	16
2	CC	161/161 (100%)	136 (84%)	25 (16%)	2	16
3	AD	180/180 (100%)	142 (79%)	38 (21%)	1	6
3	CD	180/180 (100%)	150 (83%)	30 (17%)	2	14
4	AE	116/116 (100%)	95 (82%)	21 (18%)	1	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	CE	116/116 (100%)	92 (79%)	24 (21%)	1	6
5	AF	90/90 (100%)	80 (89%)	10 (11%)	6	26
5	CF	90/90 (100%)	85 (94%)	5 (6%)	21	49
6	AG	126/126 (100%)	112 (89%)	14 (11%)	6	26
6	CG	126/126 (100%)	114 (90%)	12 (10%)	8	31
7	AH	119/119 (100%)	97 (82%)	22 (18%)	1	10
7	CH	119/119 (100%)	104 (87%)	15 (13%)	4	22
8	AI	98/98 (100%)	83 (85%)	15 (15%)	2	16
8	CI	98/98 (100%)	82 (84%)	16 (16%)	2	15
9	AJ	89/89 (100%)	73 (82%)	16 (18%)	1	11
9	CJ	89/89 (100%)	70 (79%)	19 (21%)	1	6
10	AK	90/90 (100%)	76 (84%)	14 (16%)	2	16
10	CK	90/90 (100%)	71 (79%)	19 (21%)	1	6
11	AL	104/104 (100%)	82 (79%)	22 (21%)	1	6
11	CL	104/104 (100%)	74 (71%)	30 (29%)	0	2
12	AM	100/100 (100%)	81 (81%)	19 (19%)	1	9
12	CM	100/100 (100%)	88 (88%)	12 (12%)	5	23
13	AN	49/49 (100%)	40 (82%)	9 (18%)	1	10
13	CN	49/49 (100%)	42 (86%)	7 (14%)	3	19
14	AO	79/79 (100%)	70 (89%)	9 (11%)	5	25
14	CO	79/79 (100%)	68 (86%)	11 (14%)	3	20
15	AP	72/72 (100%)	65 (90%)	7 (10%)	8	30
15	CP	72/72 (100%)	69 (96%)	3 (4%)	30	56
16	AQ	95/95 (100%)	78 (82%)	17 (18%)	2	11
16	CQ	95/95 (100%)	82 (86%)	13 (14%)	3	20
17	AR	61/61 (100%)	53 (87%)	8 (13%)	4	21
17	CR	61/61 (100%)	51 (84%)	10 (16%)	2	14
18	AS	69/69 (100%)	53 (77%)	16 (23%)	1	5
18	CS	69/69 (100%)	53 (77%)	16 (23%)	1	5
19	AT	76/76 (100%)	64 (84%)	12 (16%)	2	16
19	CT	76/76 (100%)	69 (91%)	7 (9%)	9	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	AY	563/579 (97%)	466 (83%)	97 (17%)	2	13
23	CY	563/579 (97%)	460 (82%)	103 (18%)	1	11
24	BC	180/180 (100%)	135 (75%)	45 (25%)	0	4
24	DC	180/180 (100%)	139 (77%)	41 (23%)	1	5
25	BD	217/217 (100%)	173 (80%)	44 (20%)	1	7
25	DD	217/217 (100%)	171 (79%)	46 (21%)	1	6
26	BE	165/165 (100%)	134 (81%)	31 (19%)	1	10
26	DE	165/165 (100%)	133 (81%)	32 (19%)	1	9
27	BF	165/165 (100%)	127 (77%)	38 (23%)	1	5
27	DF	165/165 (100%)	133 (81%)	32 (19%)	1	9
28	BG	155/155 (100%)	126 (81%)	29 (19%)	1	10
28	DG	155/155 (100%)	127 (82%)	28 (18%)	1	11
29	BH	136/136 (100%)	111 (82%)	25 (18%)	1	10
29	DH	136/136 (100%)	120 (88%)	16 (12%)	5	24
31	BK	105/105 (100%)	85 (81%)	20 (19%)	1	9
31	DK	105/105 (100%)	88 (84%)	17 (16%)	2	15
32	BN	117/117 (100%)	100 (86%)	17 (14%)	3	18
32	DN	117/117 (100%)	100 (86%)	17 (14%)	3	18
33	BO	100/100 (100%)	84 (84%)	16 (16%)	2	15
33	DO	100/100 (100%)	87 (87%)	13 (13%)	4	22
34	BP	112/112 (100%)	92 (82%)	20 (18%)	2	11
34	DP	112/112 (100%)	88 (79%)	24 (21%)	1	6
35	BQ	111/111 (100%)	88 (79%)	23 (21%)	1	6
35	DQ	111/111 (100%)	87 (78%)	24 (22%)	1	6
36	BR	100/100 (100%)	83 (83%)	17 (17%)	2	13
36	DR	100/100 (100%)	83 (83%)	17 (17%)	2	13
37	BS	77/77 (100%)	63 (82%)	14 (18%)	1	11
37	DS	77/77 (100%)	59 (77%)	18 (23%)	1	4
38	BT	120/120 (100%)	95 (79%)	25 (21%)	1	6
38	DT	120/120 (100%)	91 (76%)	29 (24%)	0	4
39	BU	93/93 (100%)	71 (76%)	22 (24%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	DU	93/93 (100%)	75 (81%)	18 (19%)	1	9
40	BV	82/82 (100%)	65 (79%)	17 (21%)	1	6
40	DV	82/82 (100%)	62 (76%)	20 (24%)	0	4
41	BW	92/92 (100%)	71 (77%)	21 (23%)	1	5
41	DW	92/92 (100%)	76 (83%)	16 (17%)	2	12
42	BX	75/75 (100%)	61 (81%)	14 (19%)	1	10
42	DX	75/75 (100%)	60 (80%)	15 (20%)	1	8
43	BY	88/88 (100%)	65 (74%)	23 (26%)	0	3
43	DY	88/88 (100%)	71 (81%)	17 (19%)	1	9
44	BZ	162/162 (100%)	132 (82%)	30 (18%)	1	10
44	DZ	162/162 (100%)	134 (83%)	28 (17%)	2	13
45	B0	66/66 (100%)	52 (79%)	14 (21%)	1	6
45	D0	66/66 (100%)	53 (80%)	13 (20%)	1	8
46	B2	66/66 (100%)	59 (89%)	7 (11%)	6	27
46	D2	66/66 (100%)	60 (91%)	6 (9%)	9	33
47	B3	52/52 (100%)	42 (81%)	10 (19%)	1	9
47	D3	52/52 (100%)	48 (92%)	4 (8%)	13	40
48	B5	51/51 (100%)	41 (80%)	10 (20%)	1	8
48	D5	51/51 (100%)	40 (78%)	11 (22%)	1	6
49	B6	49/49 (100%)	43 (88%)	6 (12%)	5	23
49	D6	49/49 (100%)	38 (78%)	11 (22%)	1	6
50	B7	42/42 (100%)	36 (86%)	6 (14%)	3	19
50	D7	42/42 (100%)	36 (86%)	6 (14%)	3	19
51	B8	54/54 (100%)	37 (68%)	17 (32%)	0	2
51	D8	54/54 (100%)	40 (74%)	14 (26%)	0	4
52	B9	34/34 (100%)	30 (88%)	4 (12%)	5	24
52	D9	34/34 (100%)	32 (94%)	2 (6%)	19	48
53	Be	54/54 (100%)	47 (87%)	7 (13%)	4	22
53	De	54/54 (100%)	46 (85%)	8 (15%)	3	17
56	B1	78/78 (100%)	64 (82%)	14 (18%)	2	11
56	D1	78/78 (100%)	59 (76%)	19 (24%)	0	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
57	B4	31/31 (100%)	26 (84%)	5 (16%)	2	15
57	D4	31/31 (100%)	25 (81%)	6 (19%)	1	9
All	All	11138/11170 (100%)	9124 (82%)	2014 (18%)	1	11

5 of 2014 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
44	BZ	112	ARG
4	CE	31	LEU
42	DX	57	LEU
45	B0	67	VAL
57	B4	23	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 87 such sidechains are listed below:

Mol	Chain	Res	Type
42	BX	58	HIS
11	CL	8	ASN
40	DV	64	HIS
44	BZ	30	ASN
3	CD	116	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
20	AA	1510/1511 (99%)	291 (19%)	17 (1%)
20	CA	1510/1511 (99%)	294 (19%)	16 (1%)
21	AW	76/77 (98%)	21 (27%)	2 (2%)
21	CW	76/77 (98%)	24 (31%)	2 (2%)
22	AV	22/23 (95%)	11 (50%)	1 (4%)
22	CV	22/23 (95%)	8 (36%)	2 (9%)
58	BA	2878/2879 (99%)	665 (23%)	22 (0%)
58	DA	2878/2879 (99%)	658 (22%)	23 (0%)
59	BB	118/119 (99%)	17 (14%)	2 (1%)
59	DB	118/119 (99%)	14 (11%)	1 (0%)
All	All	9208/9218 (99%)	2003 (21%)	88 (0%)

5 of 2003 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
20	AA	9	G
20	AA	13	U
20	AA	32	A
20	AA	39	G
20	AA	47	C

5 of 88 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
58	BA	2750	A
20	CA	484	G
58	DA	2212	A
58	BA	2780	G
20	CA	115	G

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 ligands 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
61	GDP	CY	702	-	24,30,30	1.35	3 (12%)	31,47,47	1.99	9 (29%)
60	FUA	CY	701	-	36,40,40	1.76	4 (11%)	46,64,64	2.41	12 (26%)
60	FUA	AY	701	-	36,40,40	1.73	6 (16%)	46,64,64	2.10	11 (23%)
61	GDP	AY	702	-	24,30,30	1.34	3 (12%)	31,47,47	1.99	8 (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
61	GDP	CY	702	-	-	3/12/32/32	0/3/3/3
60	FUA	CY	701	-	-	7/11/92/92	0/4/4/4
60	FUA	AY	701	-	-	8/11/92/92	0/4/4/4
61	GDP	AY	702	-	-	3/12/32/32	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	CY	701	FUA	C23-C22	-6.59	1.39	1.51
60	AY	701	FUA	C23-C22	-6.44	1.40	1.51
60	CY	701	FUA	C23-C24	-4.36	1.39	1.53
60	AY	701	FUA	C23-C24	-4.30	1.39	1.53
61	CY	702	GDP	C6-N1	4.12	1.40	1.33

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	CY	701	FUA	C13-C12-C11	-7.76	101.03	111.90
60	AY	701	FUA	C13-C12-C11	-7.72	101.09	111.90
60	CY	701	FUA	C5-C4-C3	-6.75	98.38	110.60
61	AY	702	GDP	C2-N3-C4	5.35	121.47	115.36
61	CY	702	GDP	C2-N3-C4	5.34	121.45	115.36

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

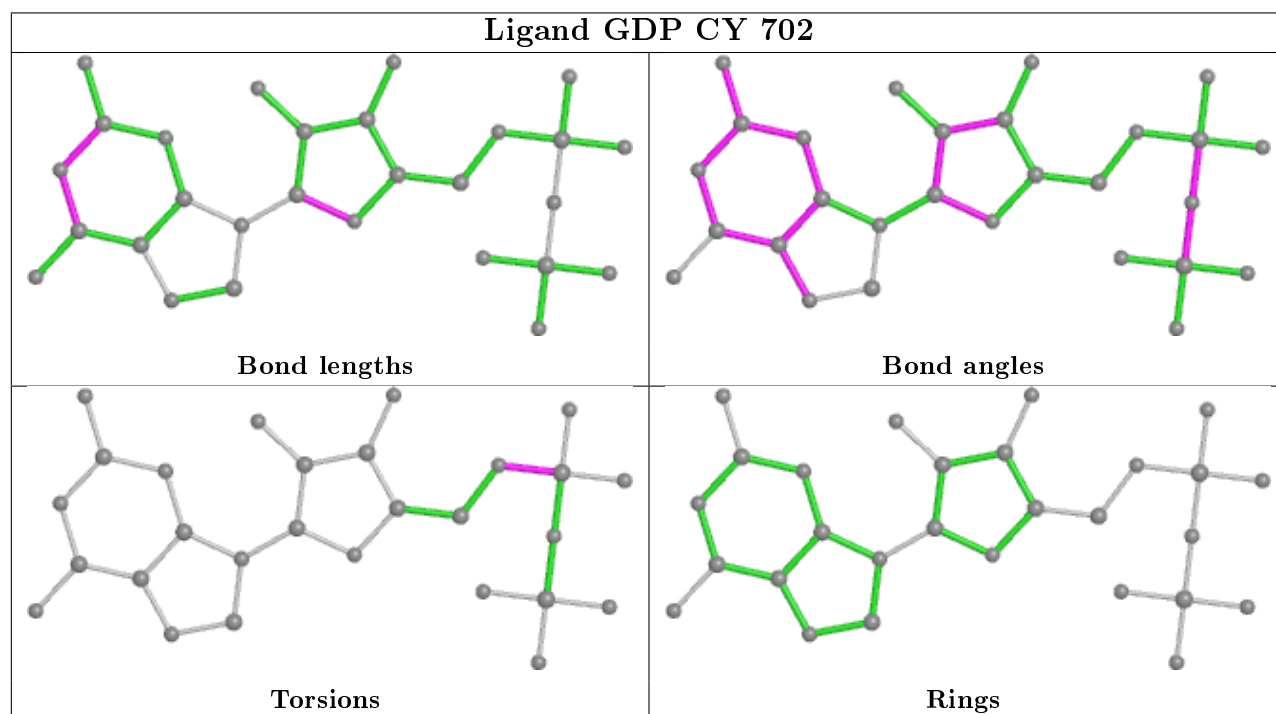
Mol	Chain	Res	Type	Atoms
61	CY	702	GDP	C5'-O5'-PA-O3A
61	CY	702	GDP	C5'-O5'-PA-O1A
60	CY	701	FUA	C13-C17-C22-C29
60	CY	701	FUA	C17-C22-C23-C24
60	CY	701	FUA	C29-C22-C23-C24

There are no ring outliers.

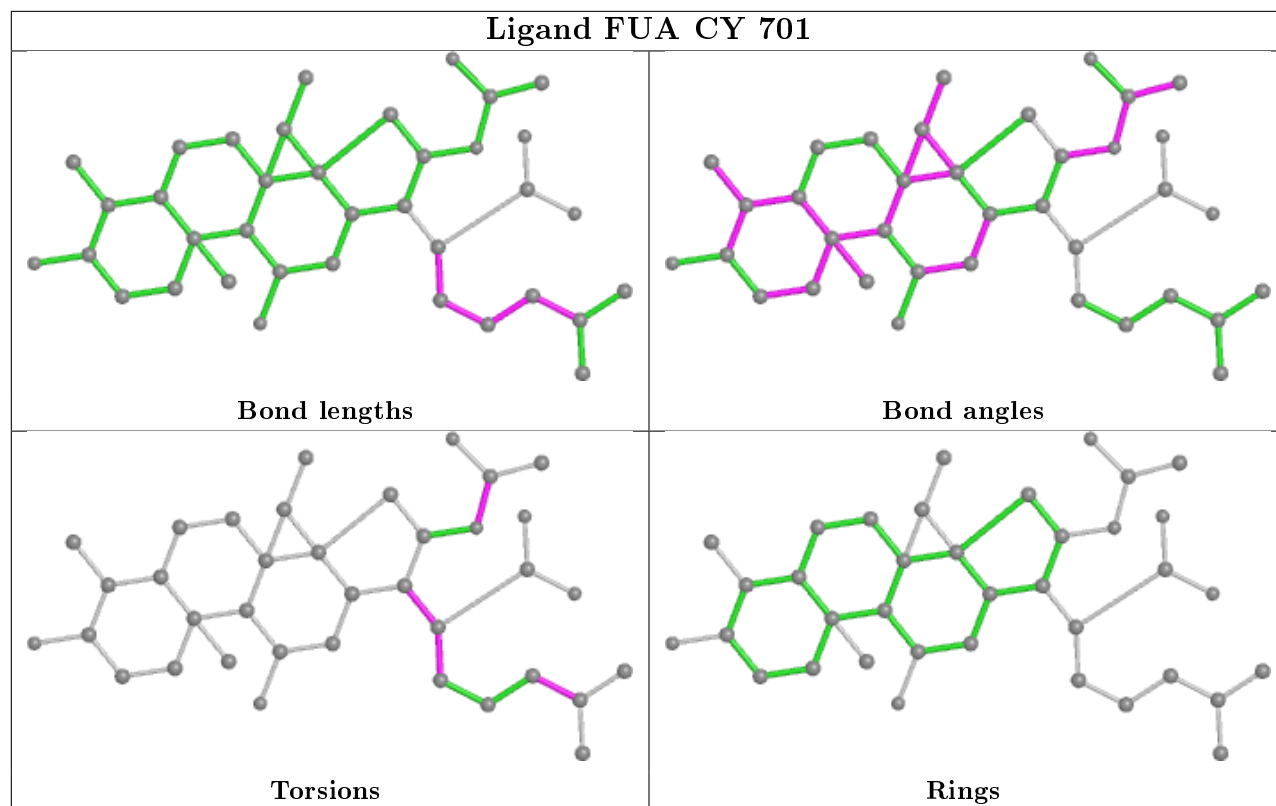
4 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	CY	702	GDP	6	0
60	CY	701	FUA	10	0
60	AY	701	FUA	13	0
61	AY	702	GDP	6	0

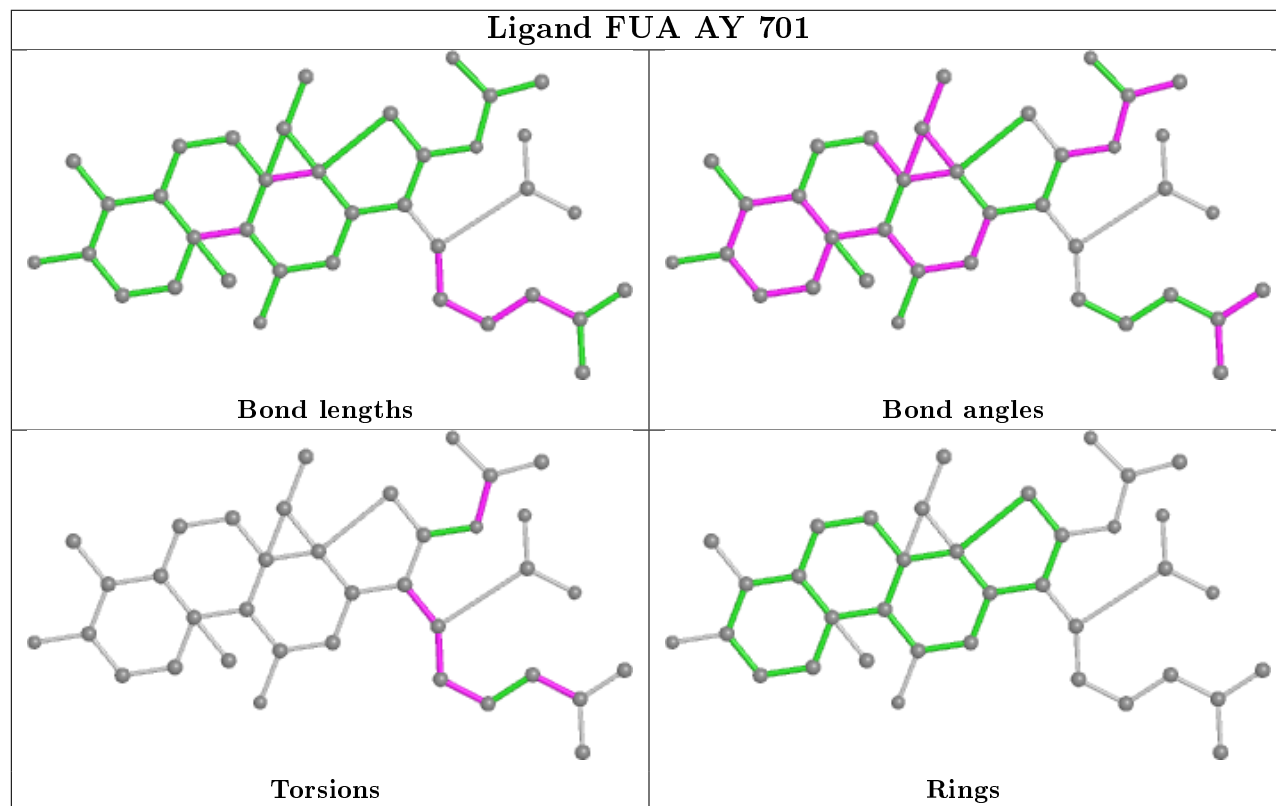
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

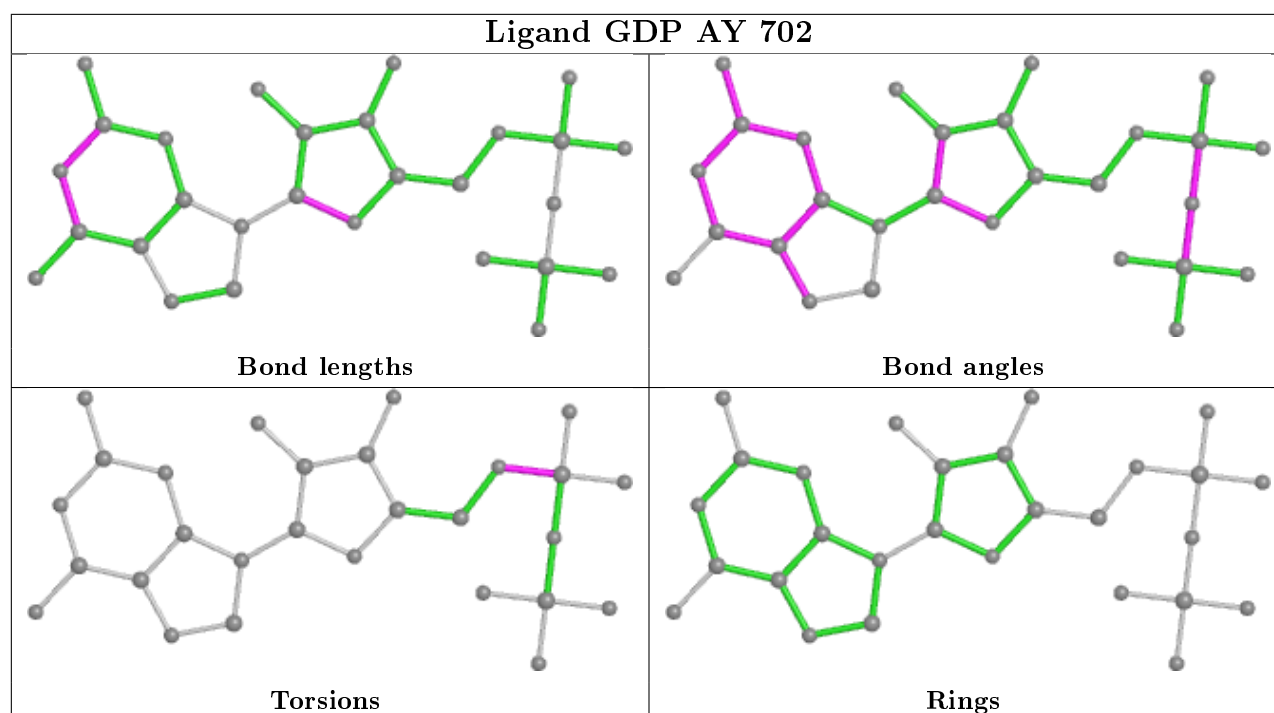


Ligand FUA CY 701



Ligand FUA AY 701





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
53	Be	1
53	De	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	De	30:UNK	C	51:ALA	N	37.61
1	Be	30:UNK	C	51:ALA	N	36.82

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%)	-0.59	0 100 100	41, 81, 119, 159	0
1	CB	235/235 (100%)	-0.50	2 (0%) 84 77	38, 80, 117, 178	0
2	AC	207/207 (100%)	0.23	24 (11%) 4 5	34, 76, 116, 152	0
2	CC	207/207 (100%)	0.25	27 (13%) 3 4	44, 78, 121, 158	0
3	AD	208/208 (100%)	-0.57	3 (1%) 75 65	37, 71, 125, 178	0
3	CD	208/208 (100%)	-0.47	4 (1%) 66 58	51, 83, 120, 165	0
4	AE	151/151 (100%)	0.68	29 (19%) 1 1	30, 57, 93, 133	0
4	CE	151/151 (100%)	0.62	33 (21%) 0 1	31, 61, 99, 185	0
5	AF	101/101 (100%)	-0.74	0 100 100	31, 52, 87, 115	0
5	CF	101/101 (100%)	-0.81	0 100 100	25, 52, 78, 129	0
6	AG	155/155 (100%)	0.23	13 (8%) 11 10	54, 100, 147, 205	0
6	CG	155/155 (100%)	0.62	20 (12%) 3 4	57, 99, 155, 218	0
7	AH	138/138 (100%)	-0.09	2 (1%) 75 65	28, 49, 83, 117	0
7	CH	138/138 (100%)	0.24	9 (6%) 18 15	29, 57, 101, 142	0
8	AI	127/127 (100%)	0.37	3 (2%) 59 49	48, 87, 128, 163	0
8	CI	127/127 (100%)	0.25	10 (7%) 12 11	51, 91, 136, 195	0
9	AJ	99/99 (100%)	0.05	8 (8%) 12 11	46, 74, 108, 114	0
9	CJ	99/99 (100%)	-0.09	11 (11%) 5 5	37, 82, 121, 145	0
10	AK	119/119 (100%)	0.07	5 (4%) 36 29	41, 71, 114, 157	0
10	CK	119/119 (100%)	-0.14	5 (4%) 36 29	22, 59, 106, 135	0
11	AL	125/125 (100%)	0.39	14 (11%) 5 5	31, 63, 97, 178	0
11	CL	125/125 (100%)	0.28	12 (9%) 8 7	29, 68, 109, 136	0
12	AM	125/125 (100%)	0.25	11 (8%) 10 9	61, 101, 139, 150	0
12	CM	125/125 (100%)	0.80	21 (16%) 1 2	52, 106, 160, 199	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AN	60/60 (100%)	0.78	7 (11%) 4 5	42, 64, 97, 106	0
13	CN	60/60 (100%)	0.19	1 (1%) 70 60	47, 67, 112, 156	0
14	AO	88/88 (100%)	-0.52	1 (1%) 80 72	32, 61, 102, 172	0
14	CO	88/88 (100%)	-0.51	0 100 100	29, 61, 108, 215	0
15	AP	84/84 (100%)	1.77	32 (38%) 0 0	47, 80, 118, 187	0
15	CP	84/84 (100%)	1.38	27 (32%) 0 0	53, 81, 118, 174	0
16	AQ	100/100 (100%)	0.40	15 (15%) 2 3	33, 56, 100, 124	0
16	CQ	100/100 (100%)	0.10	4 (4%) 38 30	30, 58, 89, 139	0
17	AR	70/70 (100%)	-0.13	2 (2%) 51 41	30, 55, 101, 156	0
17	CR	70/70 (100%)	-0.17	5 (7%) 16 13	32, 46, 123, 186	0
18	AS	79/79 (100%)	0.32	7 (8%) 9 8	68, 90, 148, 159	0
18	CS	79/79 (100%)	0.59	10 (12%) 3 4	59, 92, 146, 215	0
19	AT	99/99 (100%)	-0.13	4 (4%) 38 30	58, 86, 116, 146	0
19	CT	99/99 (100%)	0.13	3 (3%) 50 39	42, 81, 114, 147	0
20	AA	1511/1511 (100%)	0.05	79 (5%) 27 24	25, 78, 180, 324	0
20	CA	1511/1511 (100%)	0.01	64 (4%) 36 29	19, 82, 182, 332	0
21	AW	77/77 (100%)	-0.32	1 (1%) 77 68	55, 121, 189, 218	0
21	CW	77/77 (100%)	-0.48	0 100 100	58, 118, 230, 278	0
22	AV	23/23 (100%)	1.57	9 (39%) 0 0	70, 138, 188, 222	0
22	CV	23/23 (100%)	2.77	11 (47%) 0 0	88, 142, 211, 231	0
23	AY	667/687 (97%)	-0.26	25 (3%) 41 32	29, 79, 132, 191	0
23	CY	667/687 (97%)	-0.31	20 (2%) 50 39	32, 84, 131, 188	0
24	BC	228/228 (100%)	0.41	22 (9%) 8 7	91, 147, 211, 238	0
24	DC	228/228 (100%)	0.18	15 (6%) 18 14	89, 175, 227, 263	0
25	BD	275/275 (100%)	0.25	26 (9%) 8 7	24, 52, 90, 160	0
25	DD	275/275 (100%)	0.08	17 (6%) 20 17	23, 50, 94, 155	0
26	BE	205/205 (100%)	-0.15	2 (0%) 82 74	25, 52, 97, 202	0
26	DE	205/205 (100%)	-0.11	5 (2%) 59 49	28, 60, 135, 173	0
27	BF	208/208 (100%)	0.17	21 (10%) 7 7	32, 67, 126, 195	0
27	DF	208/208 (100%)	0.42	26 (12%) 3 5	34, 86, 165, 230	0
28	BG	181/181 (100%)	0.78	26 (14%) 2 3	52, 103, 150, 206	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DG	181/181 (100%)	0.70	26 (14%) 2 3	73, 110, 158, 205	0
29	BH	167/167 (100%)	-0.04	5 (2%) 50 39	38, 64, 111, 161	0
29	DH	167/167 (100%)	-0.09	11 (6%) 18 14	40, 74, 130, 167	0
30	BJ	0/170	-	-	-	-
30	DJ	0/170	-	-	-	-
31	BK	140/140 (100%)	0.04	13 (9%) 8 8	67, 118, 175, 206	0
31	DK	140/140 (100%)	0.01	9 (6%) 19 15	66, 132, 200, 220	0
32	BN	138/138 (100%)	0.21	12 (8%) 10 9	58, 85, 106, 118	0
32	DN	138/138 (100%)	0.10	6 (4%) 35 29	63, 87, 111, 121	0
33	BO	122/122 (100%)	-0.10	2 (1%) 72 62	24, 49, 67, 114	0
33	DO	122/122 (100%)	-0.02	4 (3%) 46 37	30, 56, 88, 125	0
34	BP	146/146 (100%)	-0.18	6 (4%) 37 30	28, 73, 113, 171	0
34	DP	146/146 (100%)	-0.34	4 (2%) 54 44	31, 84, 130, 202	0
35	BQ	141/141 (100%)	-0.56	2 (1%) 75 65	40, 66, 100, 164	0
35	DQ	141/141 (100%)	-0.42	5 (3%) 44 35	36, 64, 104, 161	0
36	BR	117/117 (100%)	-0.67	0 100 100	29, 53, 85, 105	0
36	DR	117/117 (100%)	-0.64	0 100 100	21, 53, 88, 156	0
37	BS	99/99 (100%)	0.07	6 (6%) 21 17	60, 111, 172, 189	0
37	DS	99/99 (100%)	0.90	21 (21%) 0 1	38, 128, 194, 220	0
38	BT	138/138 (100%)	-0.39	3 (2%) 62 52	36, 64, 106, 201	0
38	DT	138/138 (100%)	-0.28	3 (2%) 62 52	32, 71, 115, 216	0
39	BU	117/117 (100%)	-0.30	3 (2%) 56 46	26, 44, 83, 132	0
39	DU	117/117 (100%)	-0.26	3 (2%) 56 46	6, 45, 90, 155	0
40	BV	101/101 (100%)	0.35	11 (10%) 5 5	31, 51, 79, 104	0
40	DV	101/101 (100%)	-0.18	0 100 100	38, 70, 111, 124	0
41	BW	113/113 (100%)	0.15	8 (7%) 16 13	22, 51, 104, 120	0
41	DW	113/113 (100%)	0.41	7 (6%) 20 17	30, 49, 105, 202	0
42	BX	93/93 (100%)	0.13	1 (1%) 80 72	31, 59, 93, 113	0
42	DX	93/93 (100%)	-0.05	1 (1%) 80 72	29, 63, 111, 175	0
43	BY	107/107 (100%)	-0.50	3 (2%) 53 42	35, 71, 133, 156	0
43	DY	107/107 (100%)	-0.50	4 (3%) 41 32	55, 87, 133, 209	0
44	BZ	185/185 (100%)	-0.49	2 (1%) 80 72	42, 78, 126, 158	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	DZ	185/185 (100%)	-0.36	4 (2%) 62 52	36, 75, 123, 161	0
45	B0	84/84 (100%)	-0.11	2 (2%) 59 49	38, 70, 99, 162	0
45	D0	84/84 (100%)	0.15	2 (2%) 59 49	33, 67, 139, 212	0
46	B2	71/71 (100%)	-0.48	1 (1%) 75 65	44, 71, 114, 167	0
46	D2	71/71 (100%)	-0.53	0 100 100	53, 76, 129, 183	0
47	B3	60/60 (100%)	-0.61	0 100 100	26, 43, 74, 113	0
47	D3	60/60 (100%)	-0.23	1 (1%) 70 60	27, 57, 99, 111	0
48	B5	59/59 (100%)	-0.39	0 100 100	22, 56, 142, 156	0
48	D5	59/59 (100%)	-0.22	1 (1%) 70 60	18, 67, 175, 198	0
49	B6	50/50 (100%)	-0.20	0 100 100	65, 91, 124, 176	0
49	D6	50/50 (100%)	0.48	8 (16%) 1 2	66, 106, 136, 139	0
50	B7	49/49 (100%)	1.55	12 (24%) 0 0	30, 48, 107, 132	0
50	D7	49/49 (100%)	2.05	17 (34%) 0 0	38, 51, 125, 168	0
51	B8	64/64 (100%)	0.26	1 (1%) 72 62	30, 62, 80, 89	0
51	D8	64/64 (100%)	0.52	3 (4%) 31 26	38, 70, 114, 148	0
52	B9	37/37 (100%)	1.35	14 (37%) 0 0	41, 63, 116, 166	0
52	D9	37/37 (100%)	0.28	1 (2%) 54 44	36, 55, 111, 148	0
53	Be	72/102 (70%)	1.44	23 (31%) 0 0	69, 117, 170, 201	0
53	De	72/102 (70%)	1.21	16 (22%) 0 1	82, 121, 212, 249	0
54	Bf	0/31	-	-	-	-
54	Bg	0/31	-	-	-	-
54	Df	0/31	-	-	-	-
54	Dg	0/31	-	-	-	-
55	Bh	0/30	-	-	-	-
55	Dh	0/30	-	-	-	-
56	B1	93/93 (100%)	1.16	26 (27%) 0 0	40, 87, 151, 208	0
56	D1	93/93 (100%)	1.43	26 (27%) 0 0	42, 84, 174, 216	0
57	B4	35/35 (100%)	0.93	7 (20%) 1 1	96, 160, 227, 248	0
57	D4	35/35 (100%)	1.88	16 (45%) 0 0	116, 170, 265, 282	0
58	BA	2879/2879 (100%)	-0.24	21 (0%) 87 82	17, 60, 166, 304	0
58	DA	2879/2879 (100%)	-0.27	18 (0%) 89 84	17, 62, 182, 341	0
59	BB	119/119 (100%)	-0.24	0 100 100	32, 114, 187, 214	0
59	DB	119/119 (100%)	0.20	8 (6%) 17 14	53, 104, 162, 246	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	22682/23306 (97%)	-0.03	1162 (5%) 28 24	6, 73, 161, 341	0

The worst 5 of 1162 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
50	D7	48	LYS	10.1
56	D1	42	GLN	10.0
6	CG	82	GLY	9.2
53	Be	122	VAL	9.2
24	DC	227	PRO	9.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

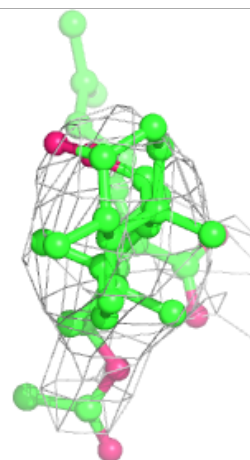
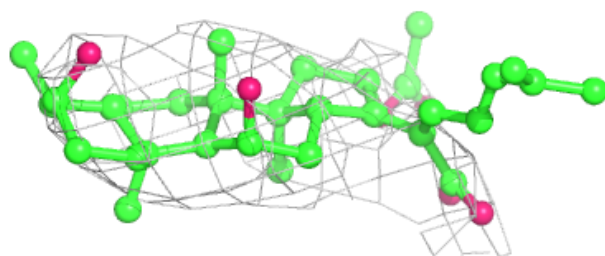
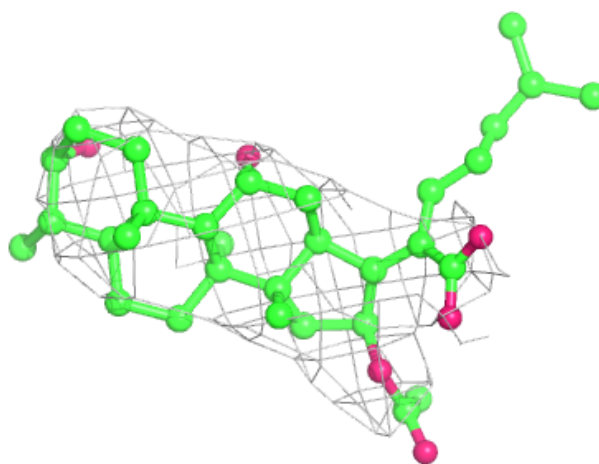
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
60	FUA	AY	701	37/37	0.85	0.62	119,146,161,162	0
60	FUA	CY	701	37/37	0.92	0.22	125,150,161,166	0
61	GDP	AY	702	28/28	0.93	0.23	58,89,106,121	0
61	GDP	CY	702	28/28	0.96	0.15	58,90,102,118	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.

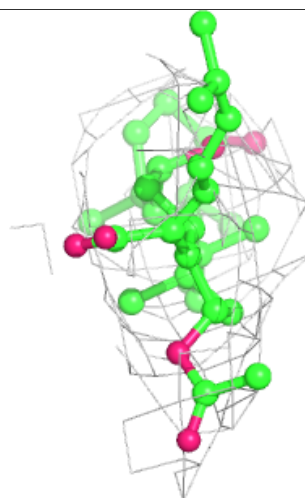
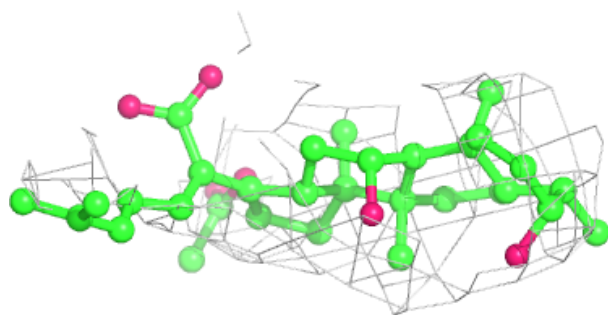
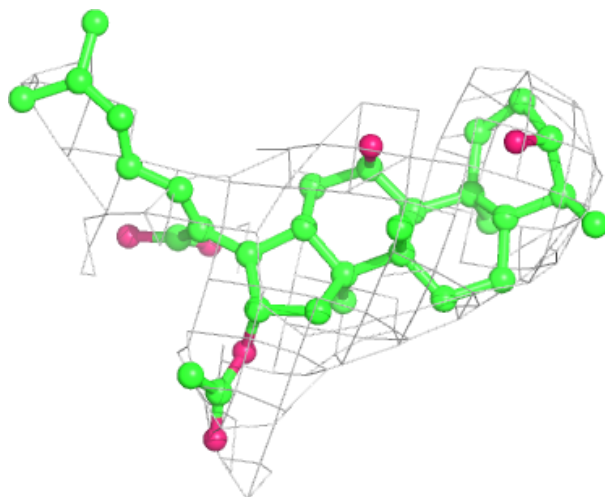
Electron density around FUA AY 701:

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



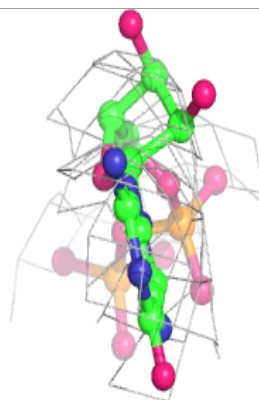
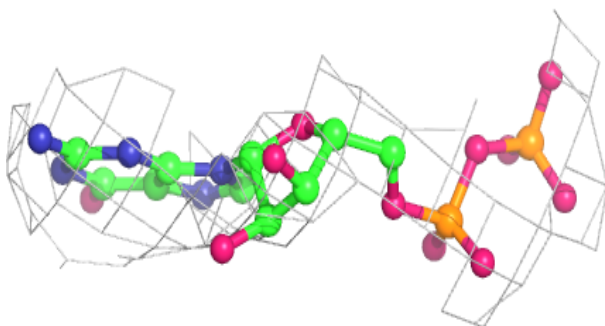
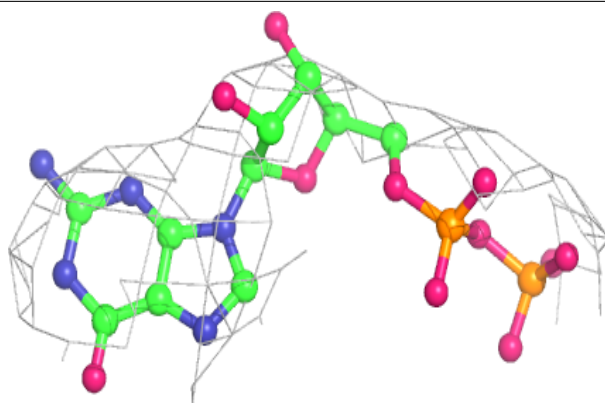
Electron density around FUA CY 701:

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

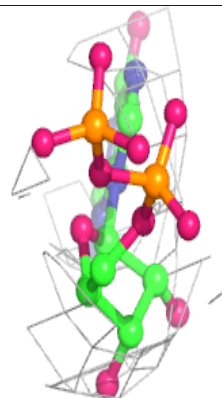
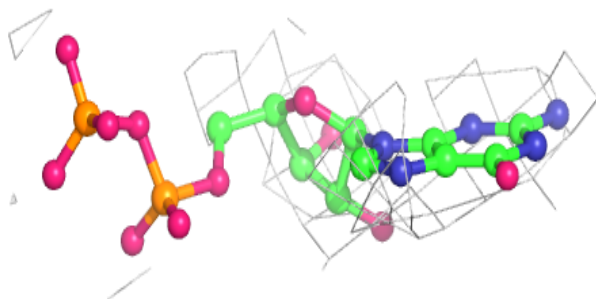
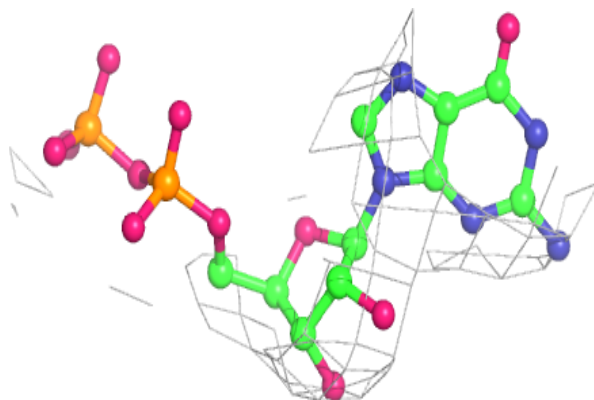


Electron density around GDP AY 702:

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

**Electron density around GDP 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.