



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 04:17 AM UTC

PDB ID : 4V9K / pdb_00004v9k
Title : 70S ribosome translocation intermediate GDPNP-I containing elongation factor EFG/GDPNP, mRNA, and tRNA bound in the pe*/E state.
Authors : Zhou, J.; Lancaster, L.; Donohue, J.P.; Noller, H.F.
Deposited on : 2013-04-24
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

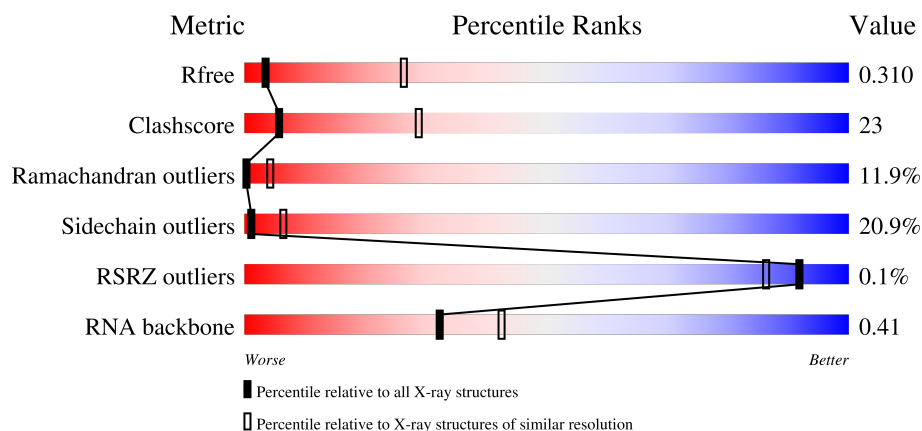
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

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



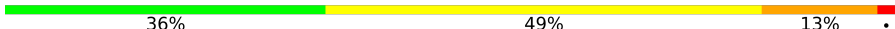
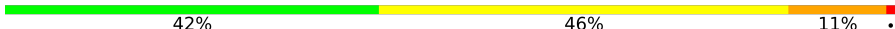
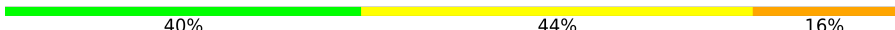
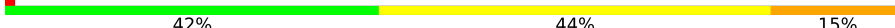
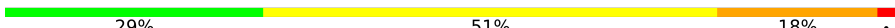
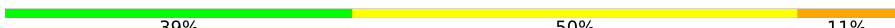
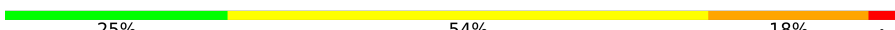
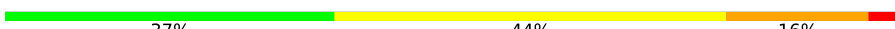
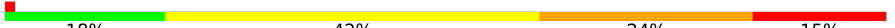
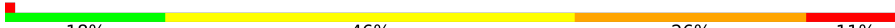
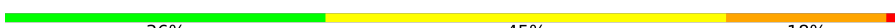
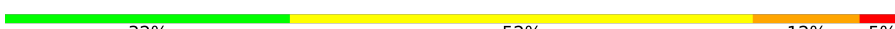
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)
RNA backbone	3983	1010 (3.98-3.02)

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

Mol	Chain	Length	Quality of chain
1	AB	235	35% 44% 17% •
1	CB	235	37% 46% 15% •
2	AC	207	38% 40% 20% •
2	CC	207	44% 42% 14%

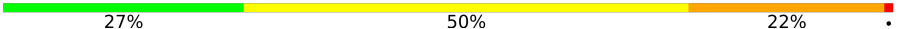
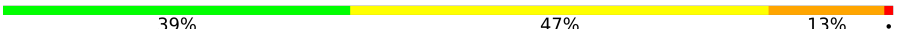
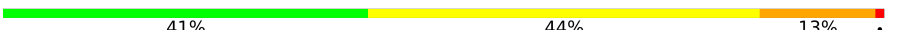
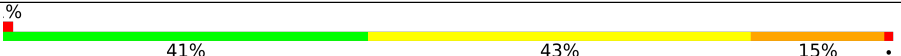
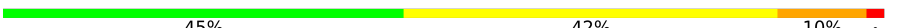
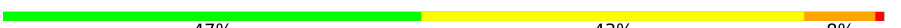
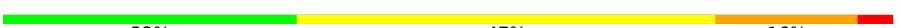
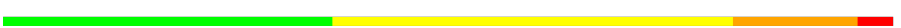
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Mol	Chain	Length	Quality of chain
3	AD	208	
3	CD	208	
4	AE	151	
4	CE	151	
5	AF	101	
5	CF	101	
6	AG	155	
6	CG	155	
7	AH	138	
7	CH	138	
8	AI	127	
8	CI	127	
9	AJ	99	
9	CJ	99	
10	AK	119	
10	CK	119	
11	AL	125	
11	CL	125	
12	AM	125	
12	CM	125	
13	AN	60	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

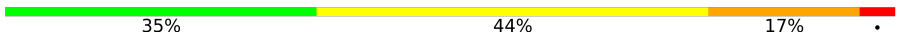
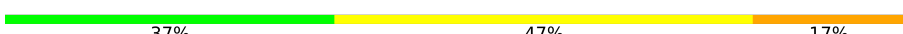
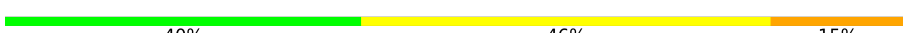
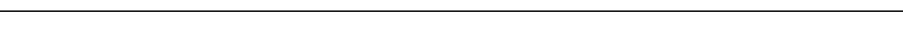
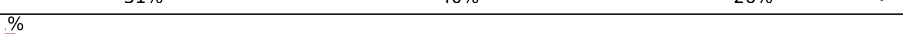
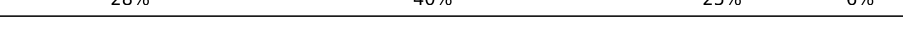
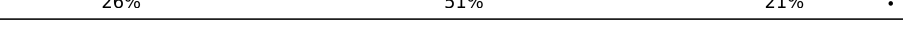
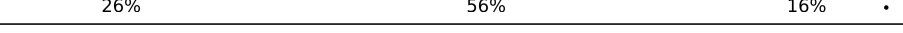
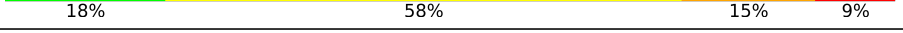
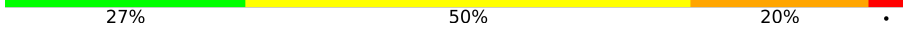
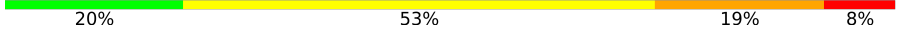
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Mol	Chain	Length	Quality of chain
15	CP	84	
16	AQ	100	
16	CQ	100	
17	AR	70	
17	CR	70	
18	AS	79	
18	CS	79	
19	AT	99	
19	CT	99	
20	AY	687	
20	CY	687	
21	AA	1511	
21	CA	1511	
22	AW	77	
22	CW	77	
23	AV	23	
23	CV	23	
24	AU	6	
24	CU	6	
25	BC	228	
25	DC	228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

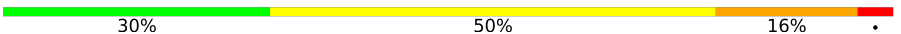
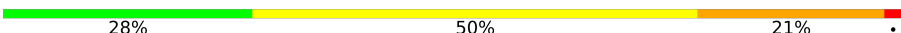
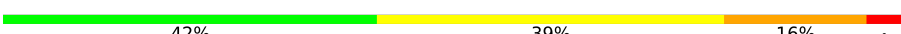
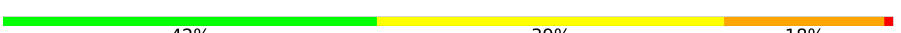
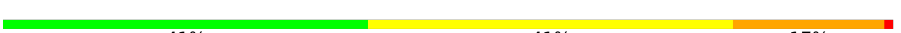
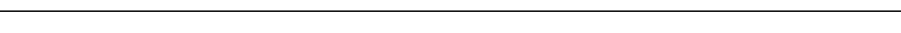
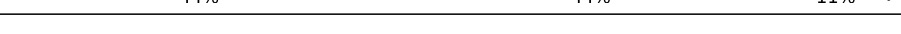
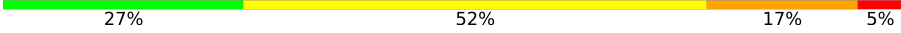
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Mol	Chain	Length	Quality of chain
28	BF	208	
28	DF	208	
29	BG	181	
29	DG	181	
30	BH	167	
30	DH	167	
31	BJ	170	
31	DJ	170	
32	BK	140	
32	DK	140	
33	BN	138	
33	DN	138	
34	BO	122	
34	DO	122	
35	BP	146	
35	DP	146	
36	BQ	141	
36	DQ	141	
37	BR	117	
37	DR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

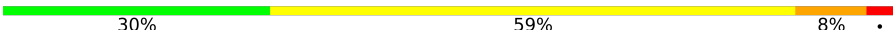
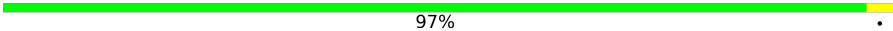
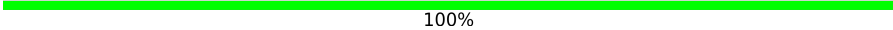
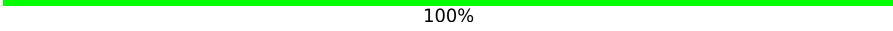
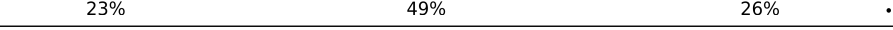
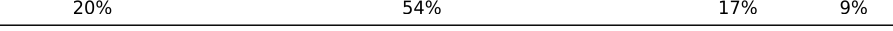
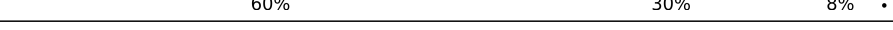
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Mol	Chain	Length	Quality of chain
40	DU	117	
41	BV	101	
41	DV	101	
42	BW	113	
42	DW	113	
43	BX	93	
43	DX	93	
44	BY	107	
44	DY	107	
45	BZ	185	
45	DZ	185	
46	B0	84	
46	D0	84	
47	B2	71	
47	D2	71	
48	B3	60	
48	D3	60	
49	B5	59	
49	D5	59	
50	B6	50	
50	D6	50	
51	B7	49	
51	D7	49	
52	B8	64	
52	D8	64	

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Mol	Chain	Length	Quality of chain
53	B9	37	
53	D9	37	
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	Be	102	
58	De	102	
59	BA	2879	
59	DA	2879	
60	BB	119	
60	DB	119	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	5OH	CU	6	-	-	X	-
61	GNP	AY	701	-	-	X	-
61	GNP	CY	701	-	-	X	-

2 Entry composition [i](#)

There are 62 unique types of molecules in this entry. The entry contains 308422 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 20 is a protein called Elongation factor G.

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

- Molecule 21 is a RNA chain called ribosomal RNA 16S.

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

- Molecule 22 is a RNA chain called transfer RNA.

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

- Molecule 23 is a RNA chain called messenger RNA.

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

- Molecule 24 is a protein called VIOMYCIN.

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

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

There are 10 discrepancies between the modelled and reference sequences:

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L10.

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

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

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

- Molecule 33 is a protein called 50S ribosomal protein L13.

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

- Molecule 34 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
34	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 35 is a protein called 50S ribosomal protein L15.

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

- Molecule 36 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
36	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 37 is a protein called 50S ribosomal protein L17.

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

- Molecule 38 is a protein called 50S ribosomal protein L18.

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

- Molecule 39 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BT	138	Total	C	N	O	S	0	0	0
			1147	713	235	198	1			
39	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 40 is a protein called 50S ribosomal protein L20.

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

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

- Molecule 41 is a protein called 50S ribosomal protein L21.

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

- Molecule 42 is a protein called 50S ribosomal protein L22.

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

- Molecule 43 is a protein called 50S ribosomal protein L23.

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

- Molecule 44 is a protein called 50S ribosomal protein L24.

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

- Molecule 45 is a protein called 50S ribosomal protein L25.

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

- Molecule 46 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	B0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			
46	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 47 is a protein called 50S ribosomal protein L29.

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

- Molecule 48 is a protein called 50S ribosomal protein L30.

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

- Molecule 49 is a protein called 50S ribosomal protein L32.

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

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

- Molecule 51 is a protein called 50S ribosomal protein L34.

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

- Molecule 52 is a protein called 50S ribosomal protein L35.

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

- Molecule 53 is a protein called 50S ribosomal protein L36.

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

- 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 protein called 50S ribosomal protein L7/L12.

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

- Molecule 59 is a RNA chain called 23S ribosomal RNA.

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

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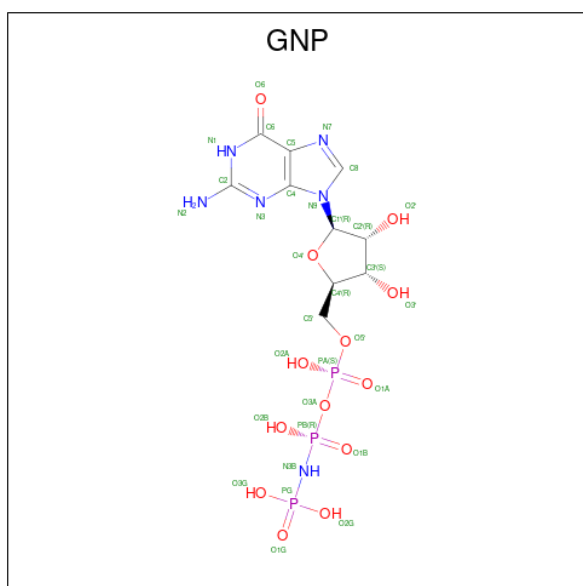
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	DA	2879	Total	C	N	O	P	0	0	0
			61997	27594	11582	19943	2878			

- Molecule 60 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 61 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



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

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

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

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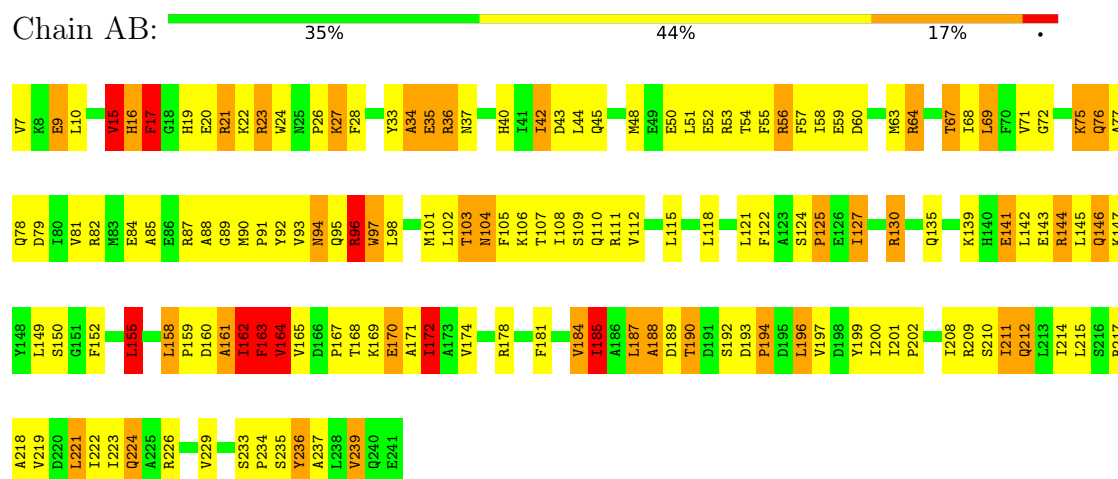
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	CY	1	Total	Mg	0	0
			1	1		

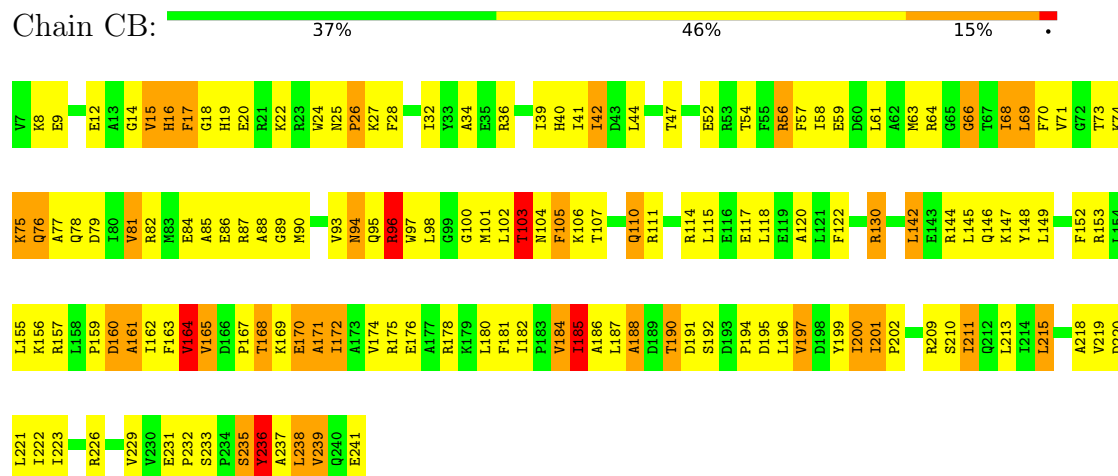
3 Residue-property plots

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

• Molecule 1: 30S ribosomal protein S2

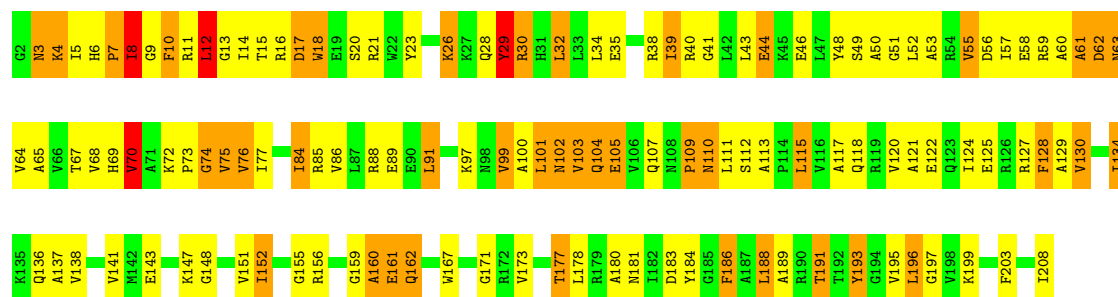


• Molecule 1: 30S ribosomal protein S2



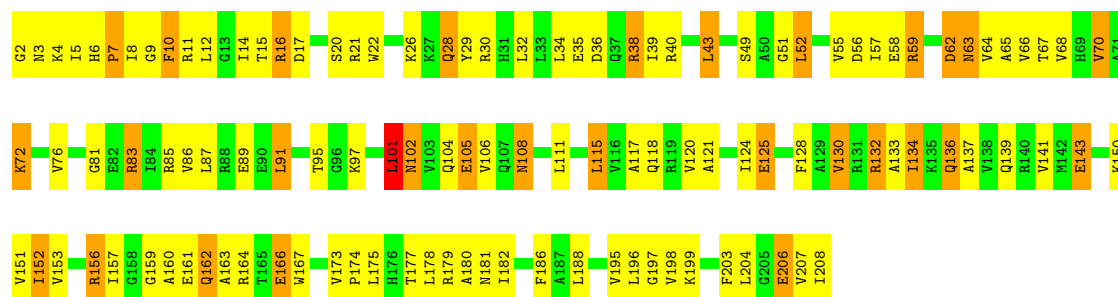
• Molecule 2: 30S ribosomal protein S3





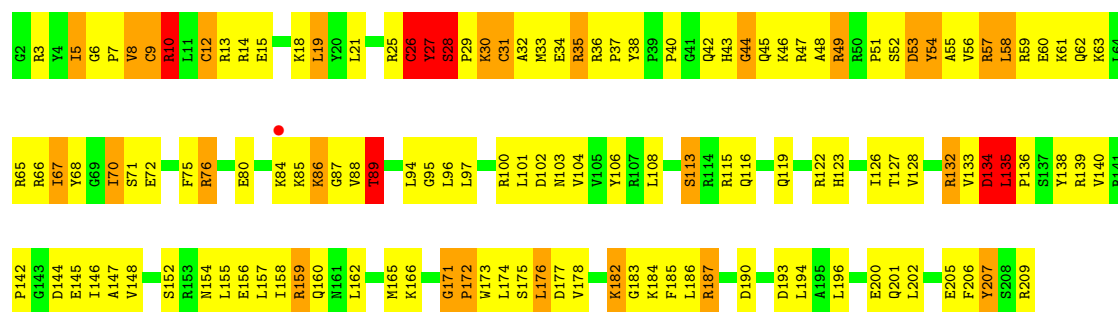
• Molecule 2: 30S ribosomal protein S3

Chain CC: 44% 42% 14%



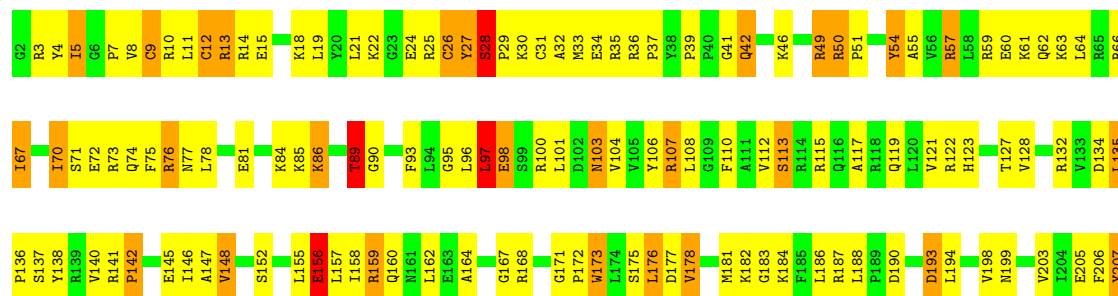
• Molecule 3: 30S ribosomal protein S4

Chain AD: 35% 49% 13%



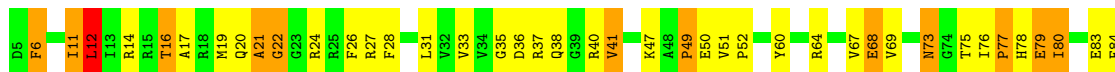
• Molecule 3: 30S ribosomal protein S4

Chain CD: 36% 49% 13%



S208
R209

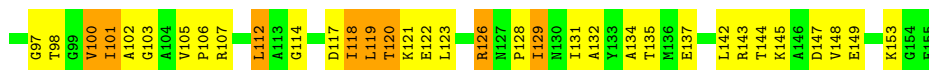
- Molecule 4: 30S ribosomal protein S5

Chain AE:  42% 46% 11%


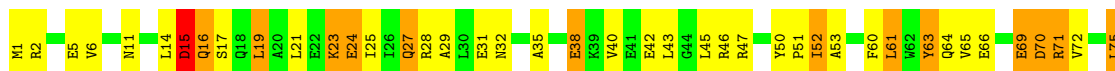
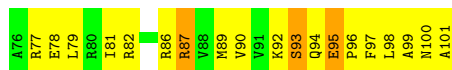
R152
K153
G154
E155

- Molecule 4: 30S ribosomal protein S5

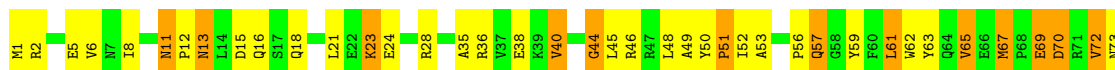
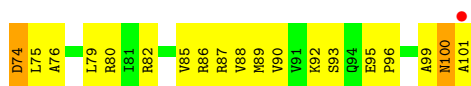
Chain CE:  52% 34% 15%



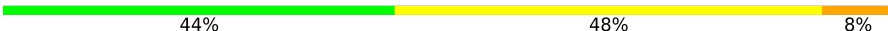
- Molecule 5: 30S ribosomal protein S6

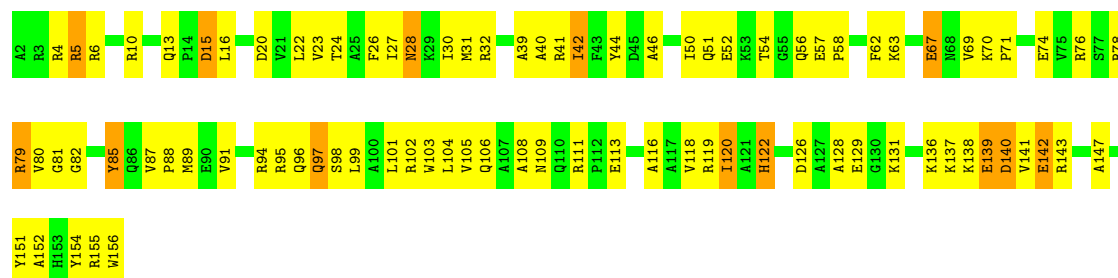
Chain AF:  40% 44% 16%



- Molecule 5: 30S ribosomal protein S6

Chain CF:  42% 44% 15%



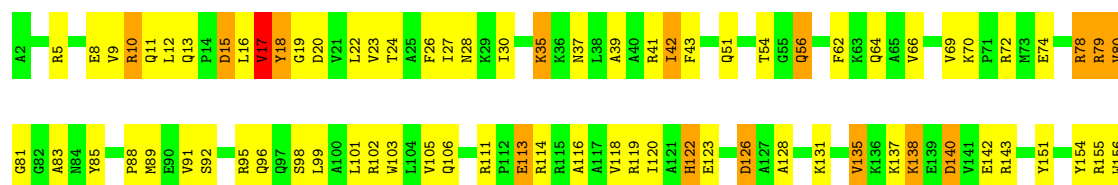
- Molecule 6: 30S ribosomal protein S7

Chain AG:  44% 48% 8%



- Molecule 6: 30S ribosomal protein S7

Chain CG: 50% 39% 10% .



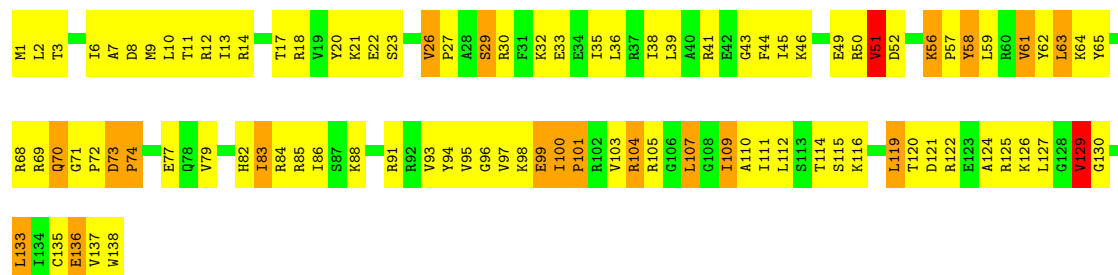
- Molecule 7: 30S ribosomal protein S8

Chain AH: 29% 51% 18% .



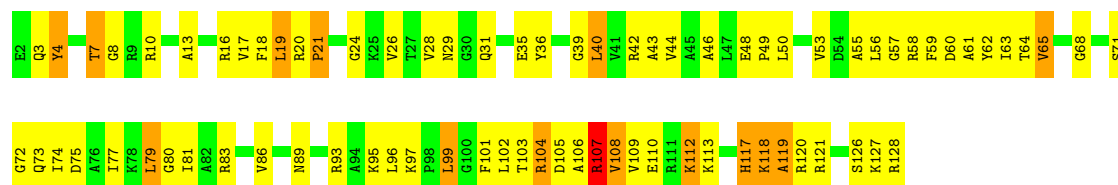
- Molecule 7: 30S ribosomal protein S8

Chain CH: 30% 55% 14% .

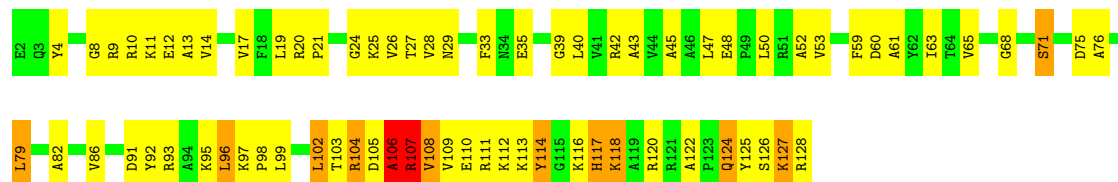


- Molecule 8: 30S ribosomal protein S9

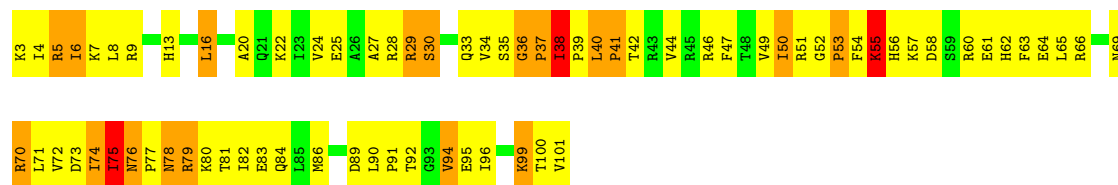
Chain AI: 39% 50% 11% .



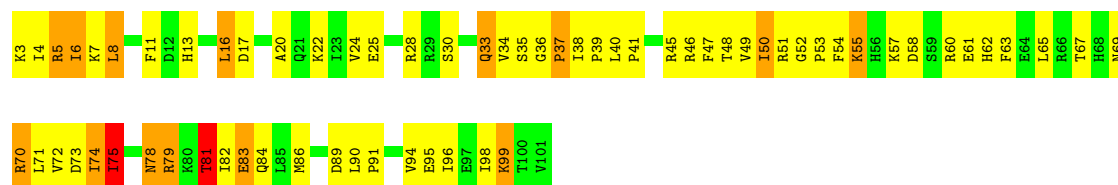
• Molecule 8: 30S ribosomal protein S9



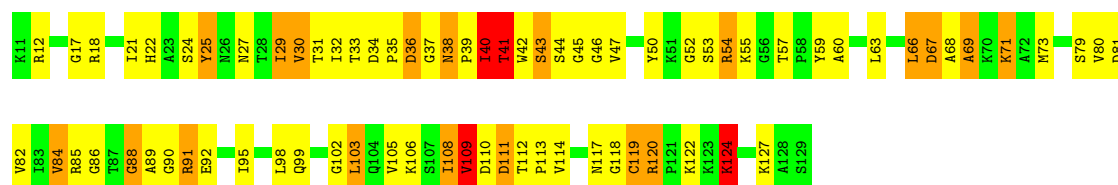
• Molecule 9: 30S ribosomal protein S10



• Molecule 9: 30S ribosomal protein S10



• Molecule 10: 30S ribosomal protein S11

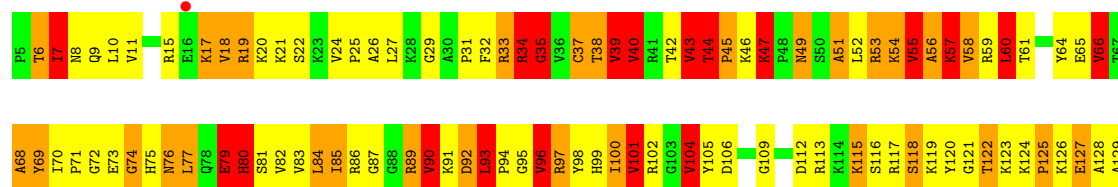
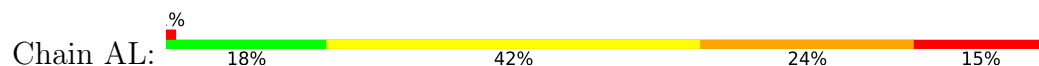


• Molecule 10: 30S ribosomal protein S11

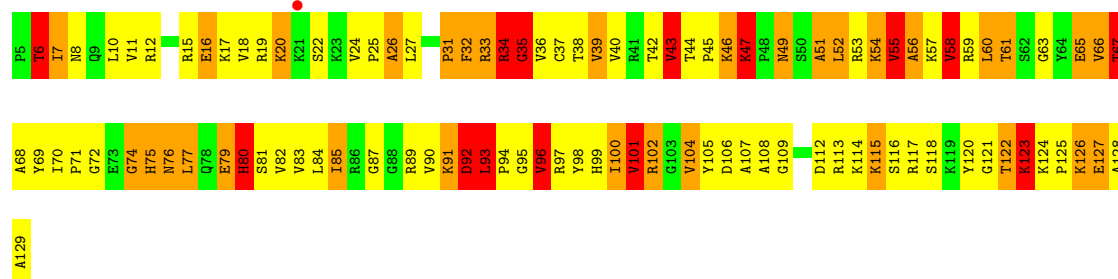
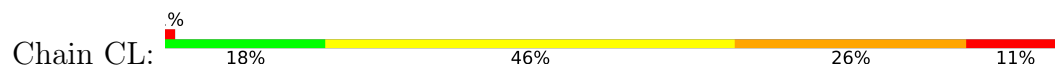




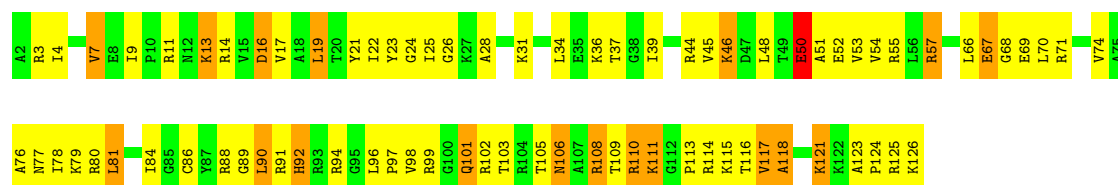
• Molecule 11: 30S ribosomal protein S12



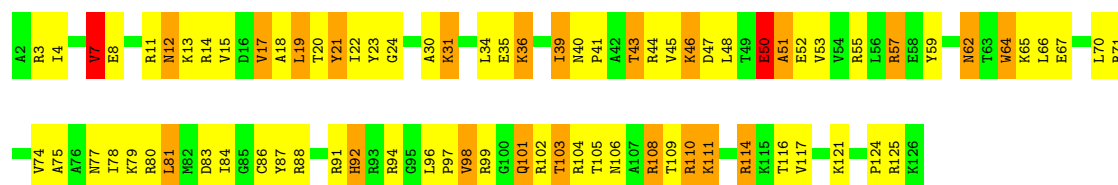
• Molecule 11: 30S ribosomal protein S12



• Molecule 12: 30S ribosomal protein S13

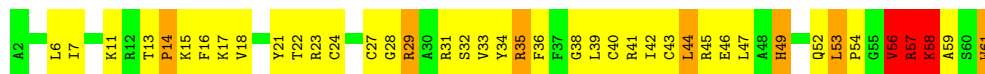


• Molecule 12: 30S ribosomal protein S13



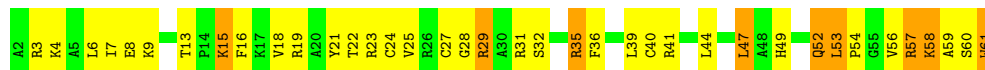
- Molecule 13: 30S ribosomal protein S14 type Z

Chain AN:  32% 52% 12% 5%



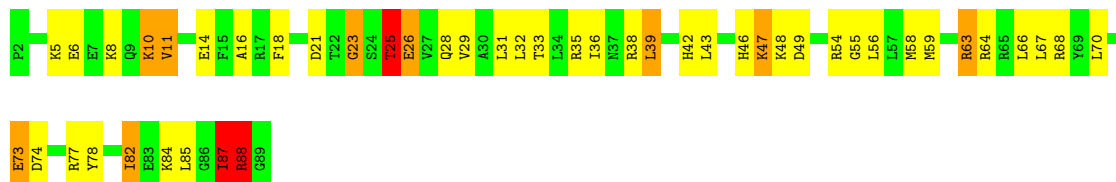
- Molecule 13: 30S ribosomal protein S14 type Z

Chain CN:  37% 48% 15%



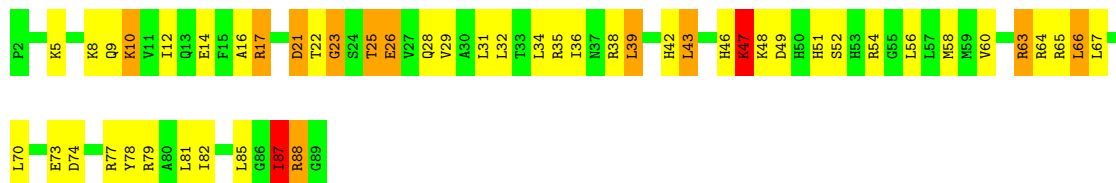
- Molecule 14: 30S ribosomal protein S15

Chain AO:  47% 40% 10% 3%



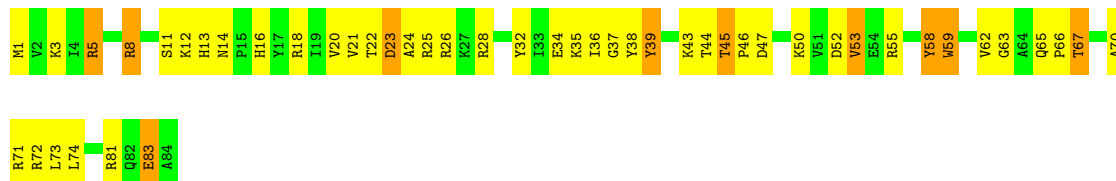
- Molecule 14: 30S ribosomal protein S15

Chain CO:  43% 42% 13% 2%



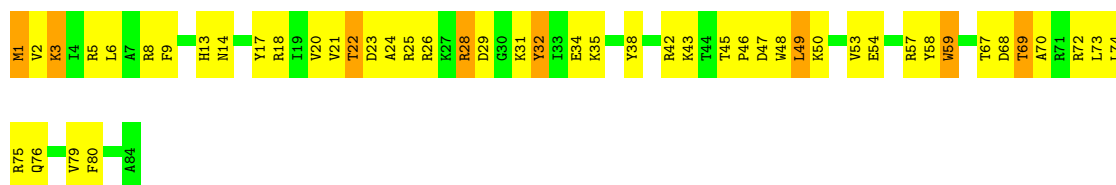
- Molecule 15: 30S ribosomal protein S16

Chain AP:  43% 45% 12%

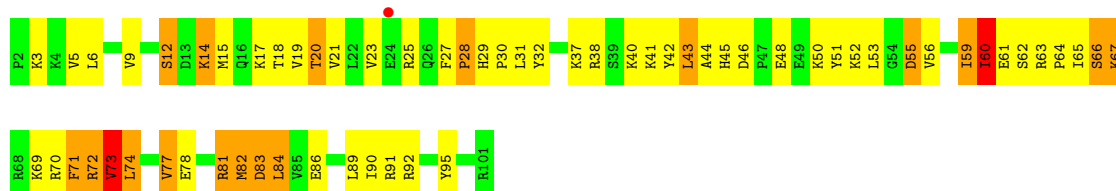


- Molecule 15: 30S ribosomal protein S16

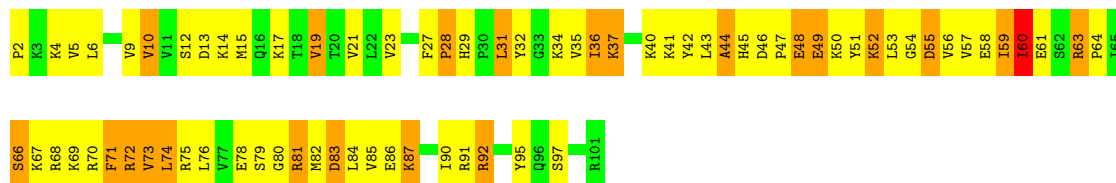
Chain CP:  42% 49% 10%



- Molecule 16: 30S ribosomal protein S17



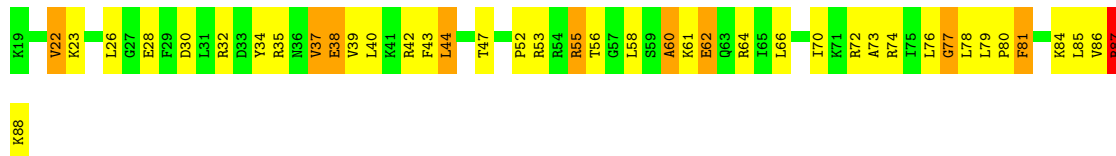
- Molecule 16: 30S ribosomal protein S17



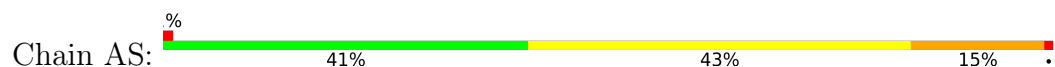
- Molecule 17: 30S ribosomal protein S18

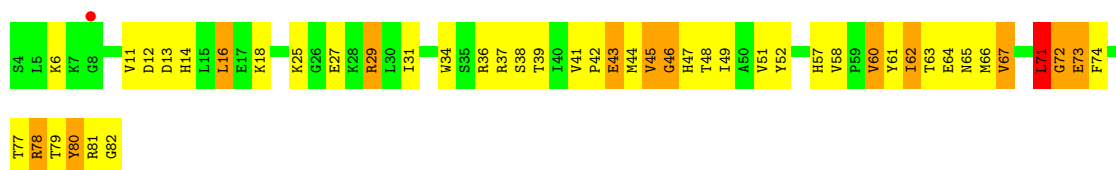


- Molecule 17: 30S ribosomal protein S18



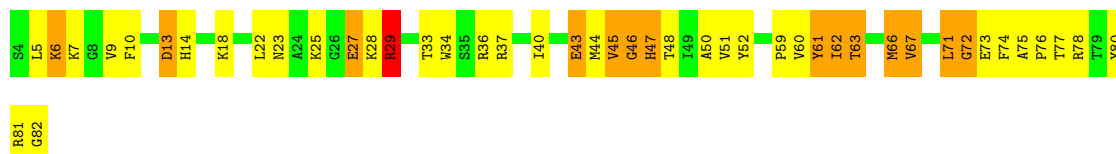
- Molecule 18: 30S ribosomal protein S19





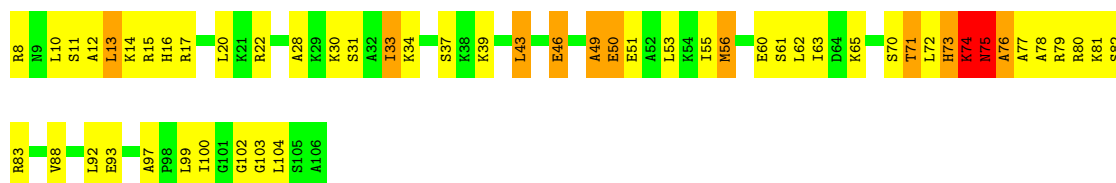
• Molecule 18: 30S ribosomal protein S19

Chain CS: 42% 39% 18%



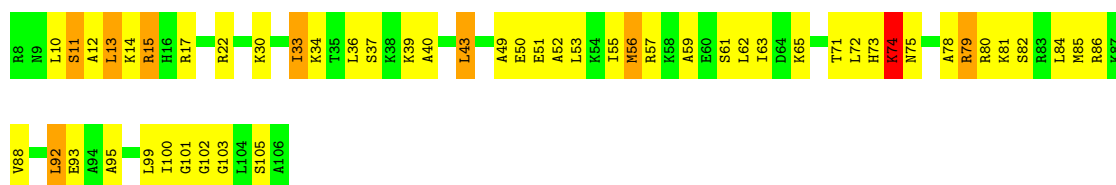
• Molecule 19: 30S ribosomal protein S20

Chain AT: 45% 42% 10%



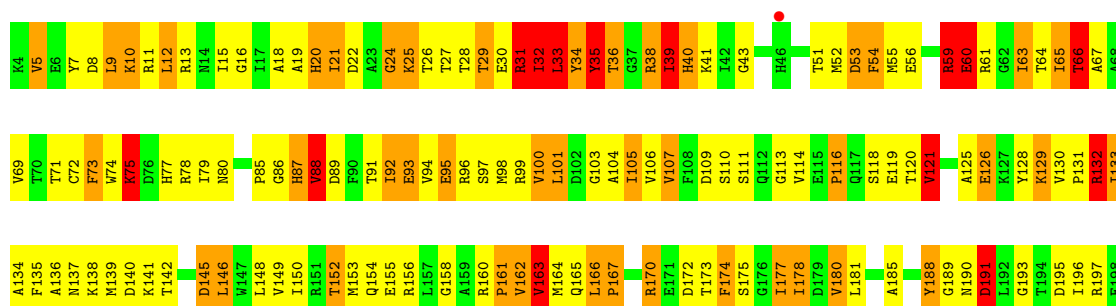
• Molecule 19: 30S ribosomal protein S20

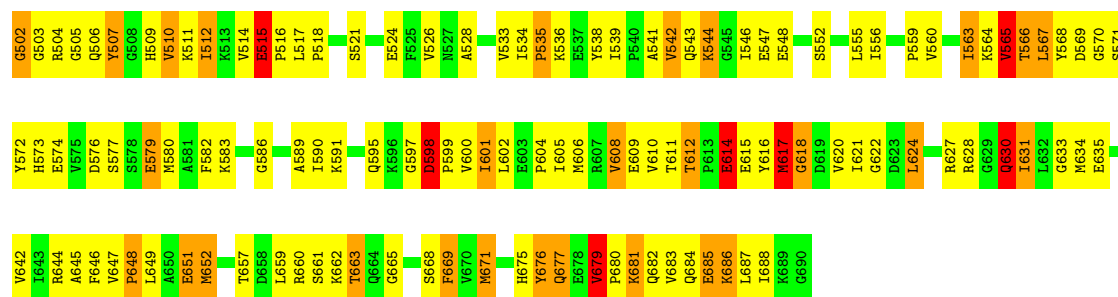
Chain CT: 47% 43% 8%



• Molecule 20: Elongation factor G

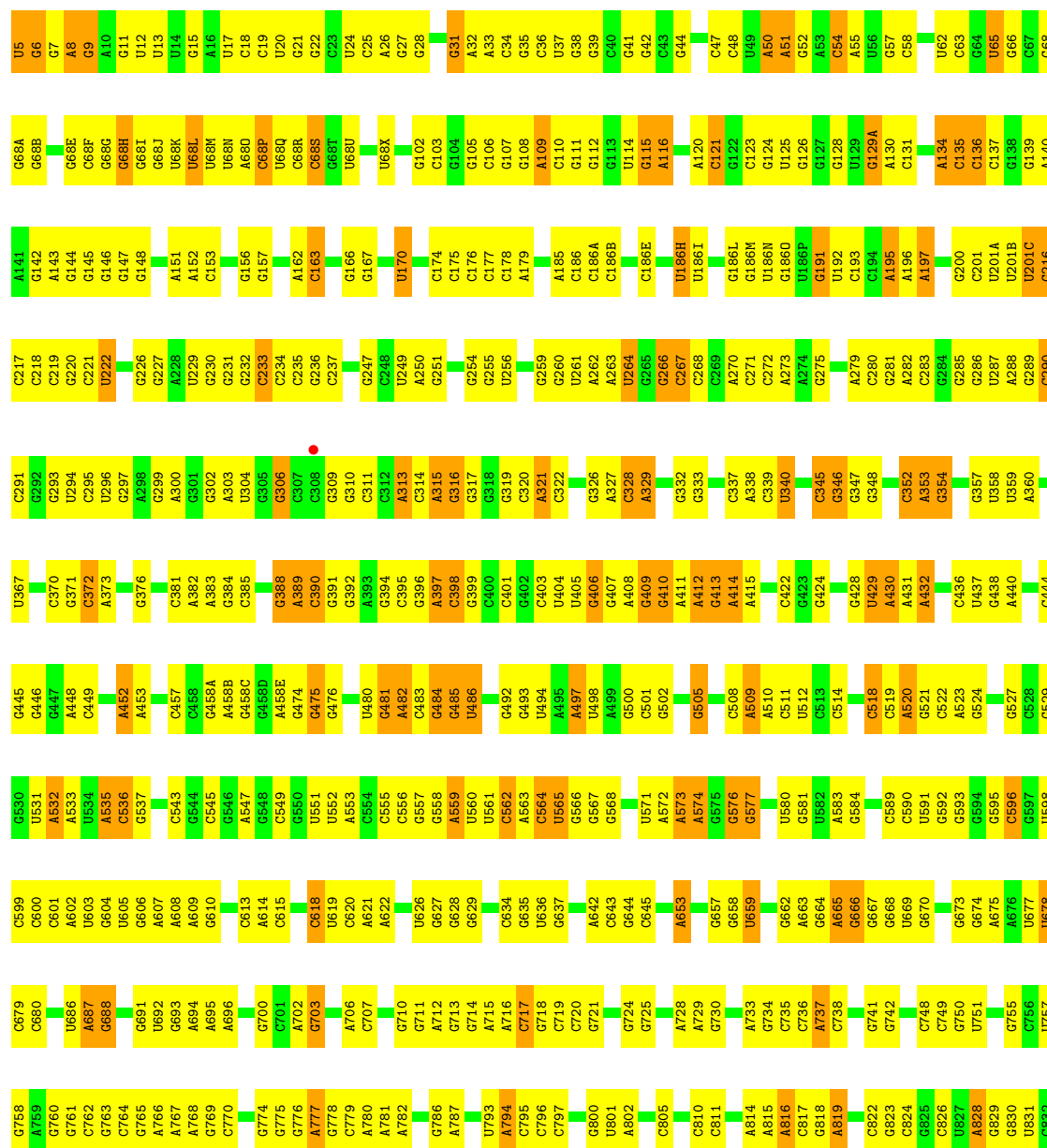
Chain AY: 33% 47% 16%

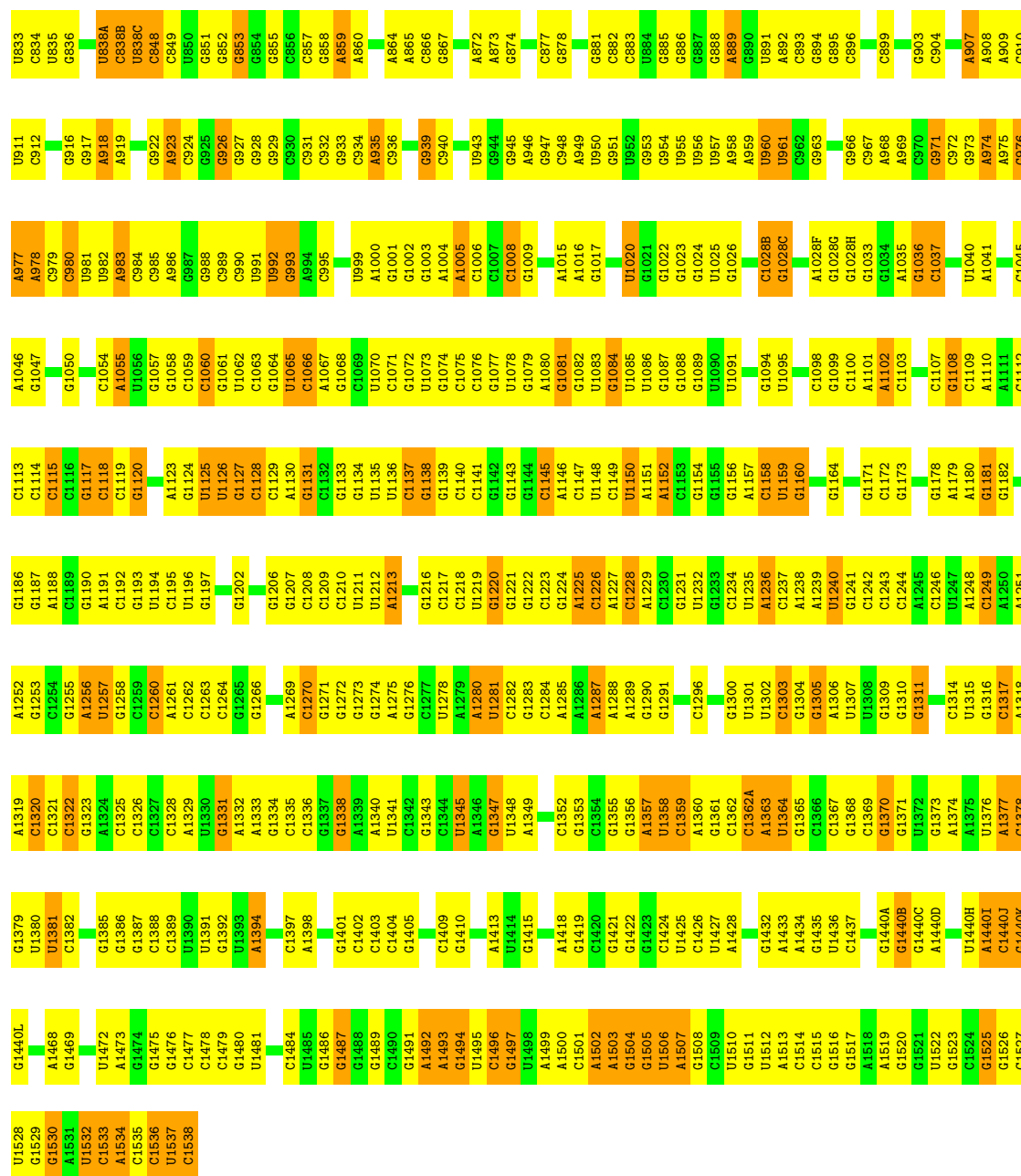




• Molecule 21: ribosomal RNA 16S

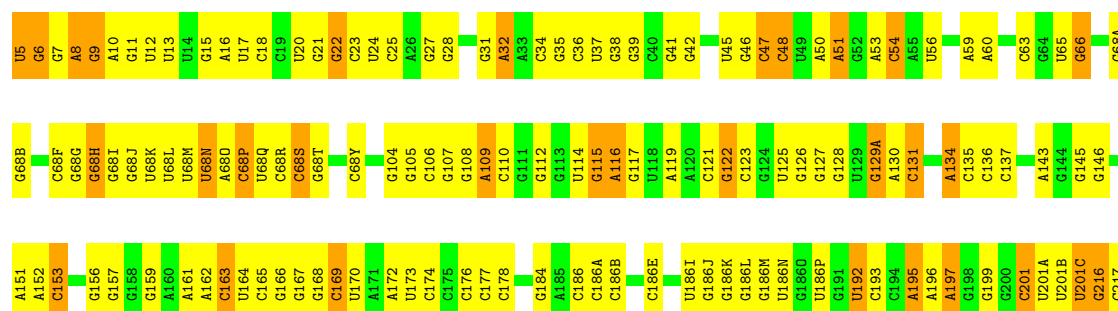
Chain AA: 33% 52% 15%



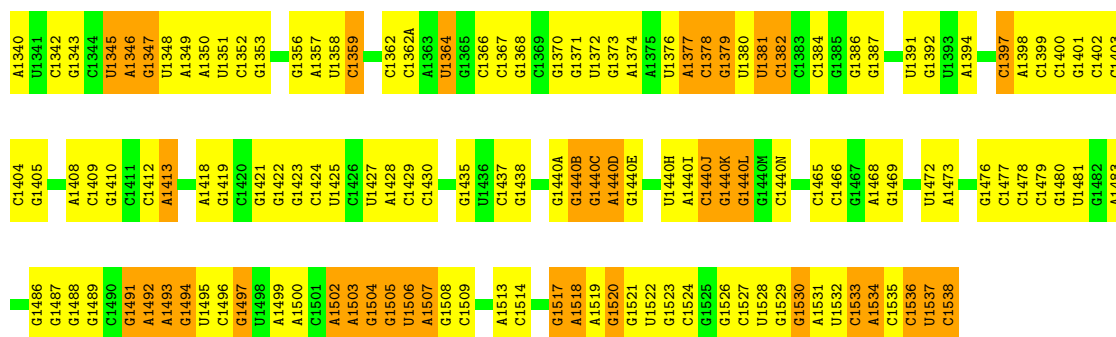


• Molecule 21: ribosomal RNA 16S

Chain CA:

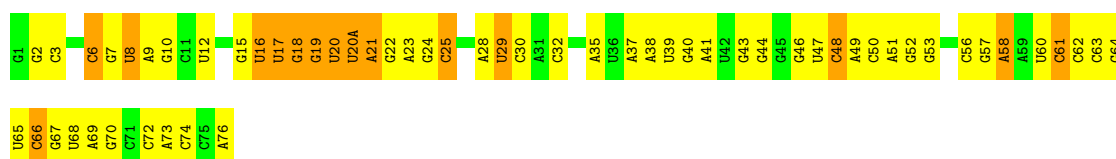


G1274	U1211	A1130	A975	G906	A828	C756	U677	C600	U531	A443	U865	U294	C218
U1212	A1213	G1131	G976	A907	G829	U757	C680	U603	A532	C442	U366	C295	C219
C1214	A1214	G1134	A977	A908	U833	G758	C680	U604	A533	C443	U367	U296	G220
G1215	A1215	U1135	A978	A909	U834	C762	A687	G604	U534	C444	U368	G297	C221
G1216	U1136	G1053	C979	C910	U835	G763	G688	U605	A535	G445	A298	G298	G226
C1217	C1054	C1054	C980	U911	G836	G764	C689	G606	C536	G446	G299	A300	G226
C1218	A1055	A1055	U981	C912	G837	G765	C690	A607	G537	G447	C372	A300	G226
G1138	U1056	U1056	C985	G916	G838	A766	G690	A608	G538	A448	A373	G301	U229
G1139	G1057	G1057	A986	G917	G839	A767	G691	A609	G539	A449	A374	G302	G230
C1140	U1058	U1058	A987	G918	U838A	A768	U692	G610	U534	A452	U375	A303	G231
C1141	C1059	A918	U982	A918	C838B	G769	G693	A611	G542	A453	G376	U304	G232
G1142	U1060	U1060	U992	A919	U838C	C770	A694	C612	C543	C457	G306	G305	C233
G1143	G983	G983	A994	U920	C848	C770	A695	C613	C544	C458	C307	G306	G236
G1144	U1062	U1062	C995	U921	C849	C771	A696	A614	C545	C459	C308	G307	G236
C1145	C1063	C1063	C995	G922	U850	G774	A697	C615	C546	C460	G309	G308	G236
C1146	G1064	G1064	C995	A923	G851	G775	C697	G616	A547	A458	C385	G310	C240
A1227	U1065	U1065	U999	C924	G852	G776	A701	G617	C548	G459	U387	C311	A243
C1228	C1068	C1068	A1000	G925	G853	A777	A702	C620	C549	G475	U388	C312	U244
A1229	G1069	G1069	G1001	G926	A859	A778	G703	C621	C550	G483	A389	C313	C245
G1149	U1070	U1070	G1002	G927	A860	C778	A704	A621	U551	A482	A390	C314	A246
U1150	G1071	G1071	G1003	G928	G861	C779	U705	G628	C552	G484	G391	A315	G247
C1151	A1004	A1004	A1004	G929	U863	A781	A706	G628	C553	A482	G392	A316	G247
A1152	C1005	C1005	C1005	G933	U864	C784	C707	C634	C554	G483	G392	G316	G251
A1157	A1006	A1006	A1006	C934	A865	G785	G710	G635	C555	G484	G396	A321	G254
C1158	C1007	C1007	C1007	A935	C866	G786	G711	U636	C556	G485	A397	G322	G254
U1159	U1009	U1009	G1009	C936	C867	G787	A712	G637	A559	G490	C398	U323	U256
C1160	G1087	G1087	C1087	C937	C868	G788	G713	A640	C562	G491	C401	G324	U256
C1161	U1088	U1088	G1011	A938	C869	U788	G714	U641	A563	G492	A325	G326	G257
C1162	G1089	G1089	G1012	U939	U870	U789	A715	A642	C564	G493	G326	G326	G258
G1171	U1013	U1013	C940	C940	U871	A790	A716	C643	C565	U494	C403	A327	G259
C1172	A1014	A1014	G941	G941	A872	G791	C717	C644	G566	A495	G406	C328	A262
G1173	A1015	A1015	G942	G942	A873	A792	G721	G645	C567	A497	A407	A329	A263
C1178	C1096	C1096	U943	U943	G874	U793	G721	U646	C568	U498	A408	G331	U264
A1179	G1017	G1017	G944	G944	C875	A794	G724	C647	C569	G501	G409	G332	G265
A1180	C1018	C1018	C945	C945	G876	A794	G725	A648	C570	C501	G410	G333	G266
G1181	U1020	U1020	G947	G947	C877	A802	G725	G649	A572	G505	A411	C334	G267
C1182	G1021	G1021	G1021	G1021	C878	G803	A728	G650	A573	G506	A412	A338	C268
G1186	G1022	G1022	U950	U950	C879	U804	A729	A853	A574	C508	A413	C339	C269
C1187	G1023	G1023	G951	G951	C880	C805	G730	G657	C575	A509	U340	G341	A270
A1188	U1024	U1024	U952	U952	G881	C806	G730	G658	C576	A510	U421	C345	C272
G1189	G1025	G1025	G953	G953	C882	G809	C735	U659	C577	C511	C422	G346	A273
C1190	U1026	U1026	G954	G954	C883	C810	C736	G660	C578	U512	G423	G347	C277
G1192	G1027	G1027	U955	U955	C884	C811	A737	G661	C579	C513	G424	G348	C277
C1193	C1028	C1028	U956	U956	C885	C812	C738	A663	C580	C514	U427	G351	C280
U1194	G1028A	G1028A	U960	U960	A889	U813	G741	G664	A583	C518	G428	C352	G281
C1195	G1028B	G1028B	U961	U961	C890	A814	G742	A665	C584	G521	U429	A353	G285
U1196	G1028C	G1028C	C962	C962	A892	A816	U743	G666	C585	A523	U430	G354	G286
C1197	A1028F	A1028F	G963	G963	C893	C817	C744	G667	C586	G524	A431	A356	U287
G1198	G1028G	G1028G	G966	G966	C894	G818	C745	G668	C587	G525	U434	G357	A288
C1199	G1028H	G1028H	C967	C967	C895	U819	C745	G669	C588	G526	U435	U358	G289
G1124	A1035	A1035	A968	A968	C896	U820	C745	U669	C589	G527	U436	U359	C290
U1125	U1036	U1036	A969	A969	C897	U821	C745	G670	C590	C522	A437	A360	C291
U1126	G1037	G1037	G971	G971	A900	G821	G750	U671	C591	A523	U438	G361	G292
C1127	C1037	C1037	C972	C972	A901	C824	A753	G672	C592	G524	U439	G362	G293
C1128	U1040	U1040	G973	G973	G902	G825	C754	A674	C593	G525	U440	G363	G293
C1129	A1041	A1041	G974	G974	G903	U827	G755	A676	C594	G530			



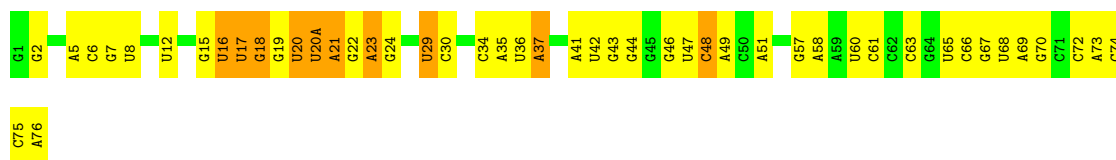
- Molecule 22: transfer RNA

Chain AW: 25% 56% 19%



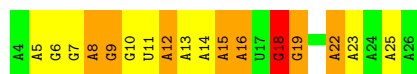
- Molecule 22: transfer RNA

Chain CW: 38% 49% 13%



- Molecule 23: messenger RNA

Chain AV: 26% 39% 30%



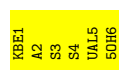
- Molecule 23: messenger RNA

Chain CV: 22% 57% 13% 9%

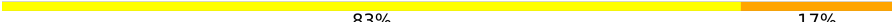


- Molecule 24: VIOMYCIN

Chain AU: 100%

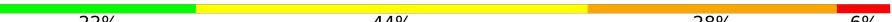


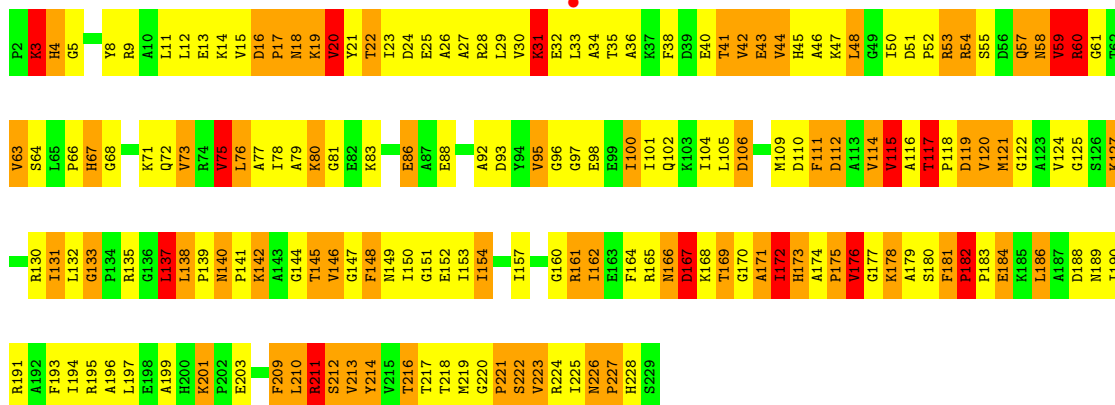
- Molecule 24: VIOMYCIN

Chain CU:  83% 17%

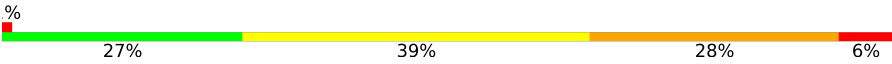
KBE1
A2
S3
S4
UAL5
50H6

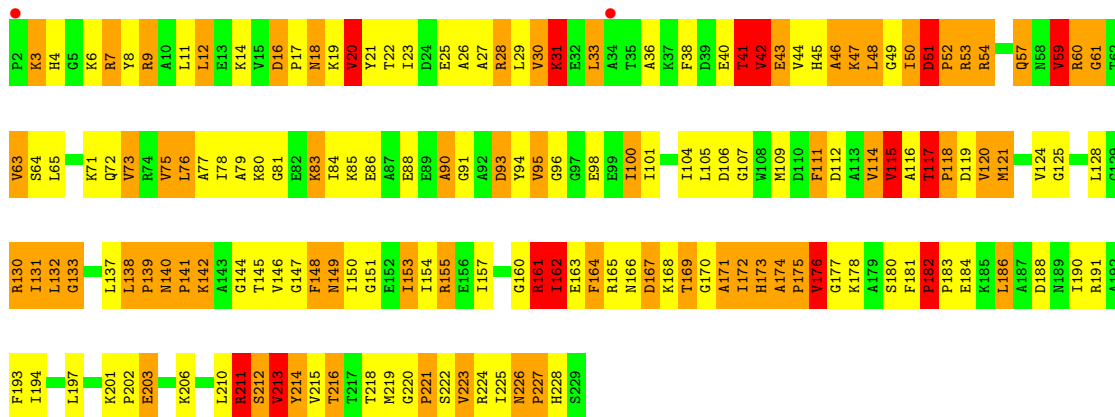
• Molecule 25: 50S ribosomal protein L1

Chain BC:  22% 44% 28% 6%

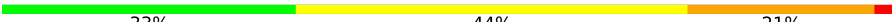


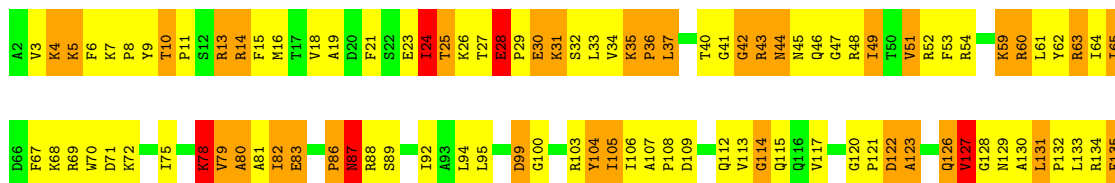
• Molecule 25: 50S ribosomal protein L1

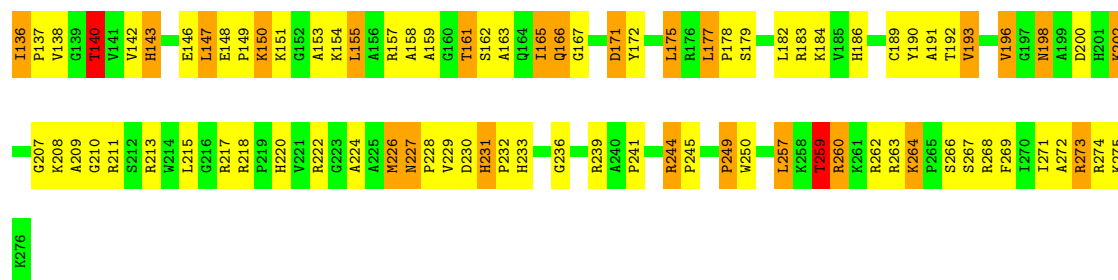
Chain DC:  27% 39% 28% 6%



• Molecule 26: 50S ribosomal protein L2

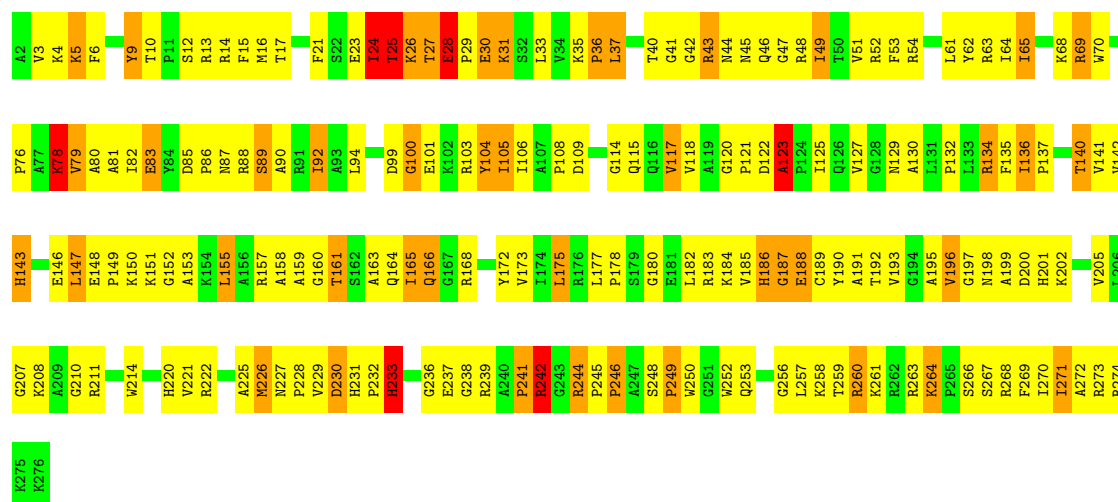
Chain BD:  33% 44% 21% 0%





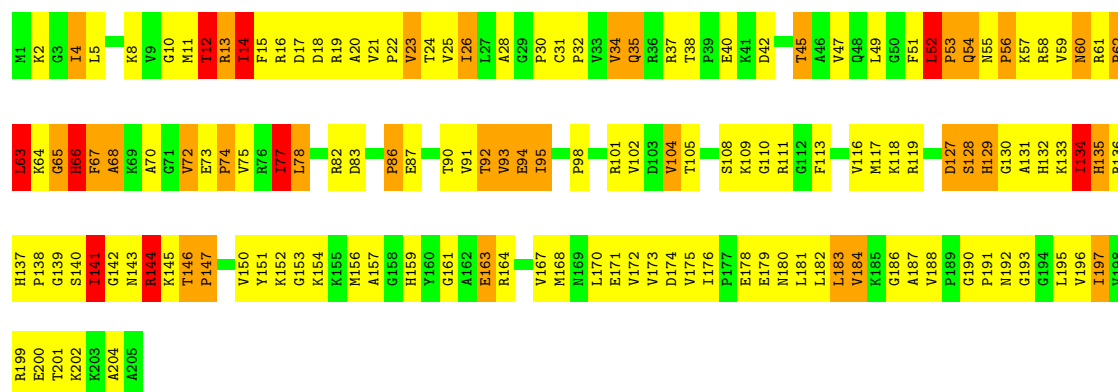
• Molecule 26: 50S ribosomal protein L2

Chain DD: 32% 50% 16% .



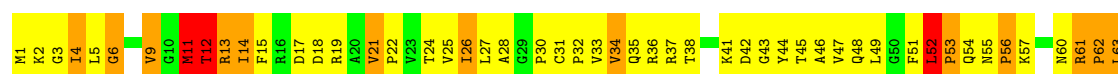
• Molecule 27: 50S ribosomal protein L3

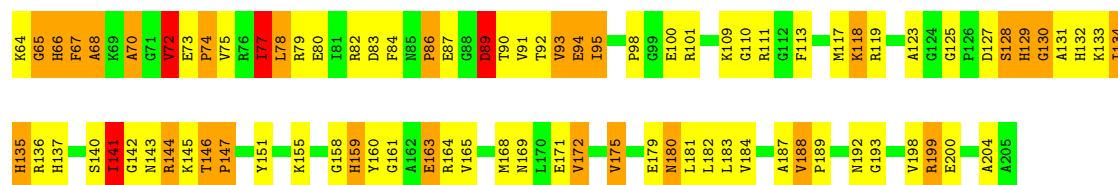
Chain BE: 29% 50% 17% .



• Molecule 27: 50S ribosomal protein L3

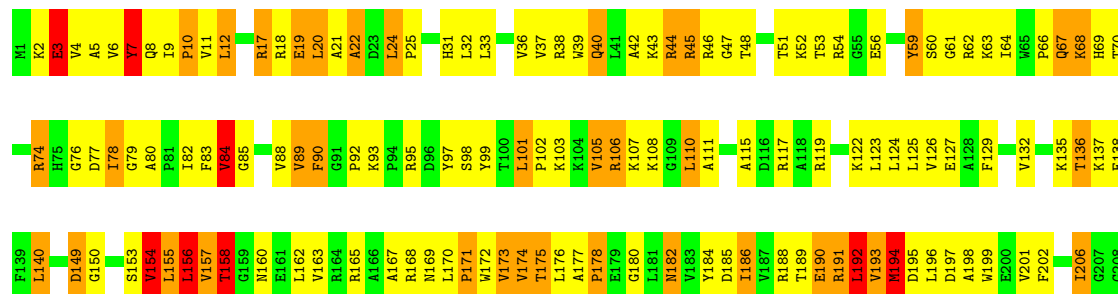
Chain DE: 33% 44% 20% .





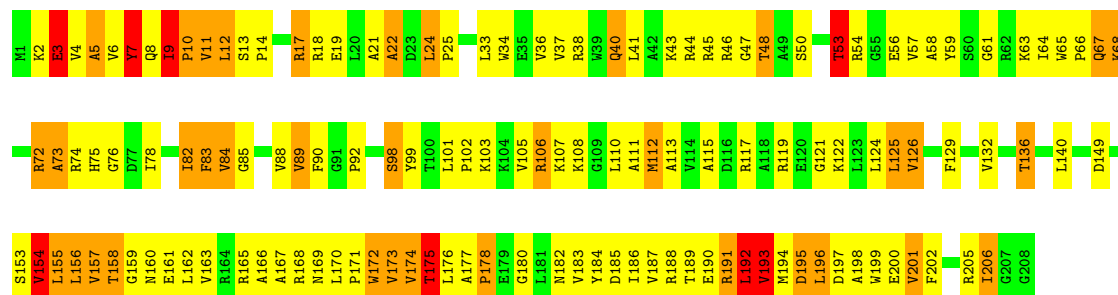
- Molecule 28: 50S ribosomal protein L4

Chain BF: 34% 45% 18% .



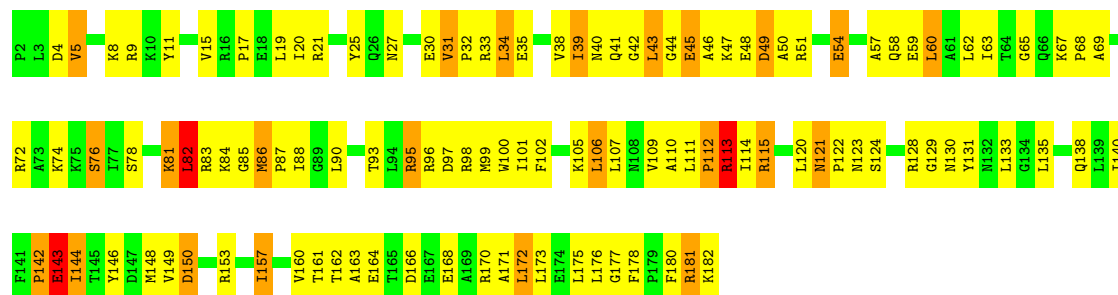
- Molecule 28: 50S ribosomal protein L4

Chain DF: 35% 44% 17% .



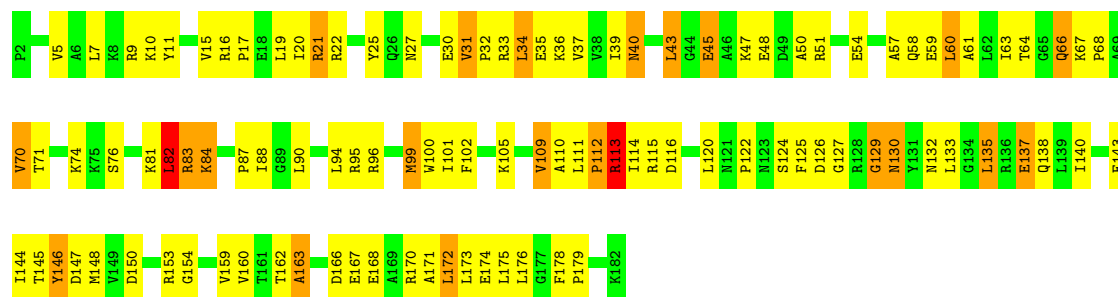
- Molecule 29: 50S ribosomal protein L5

Chain BG: 36% 49% 13% .

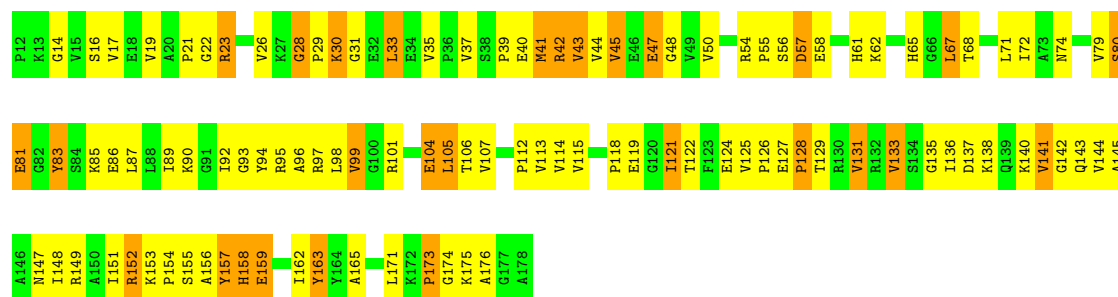


- Molecule 29: 50S ribosomal protein L5

Chain DG: 41% 46% 12% .



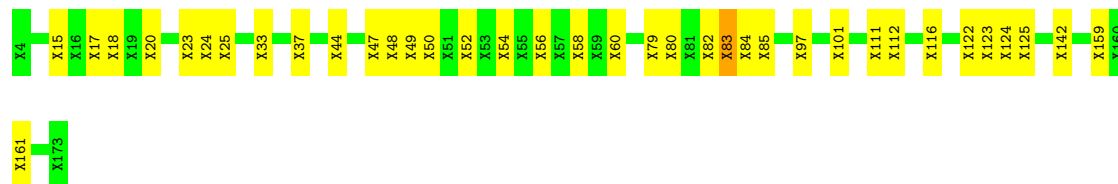
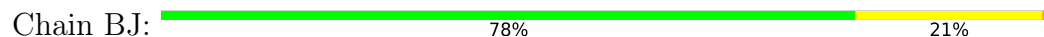
- Molecule 30: 50S ribosomal protein L6



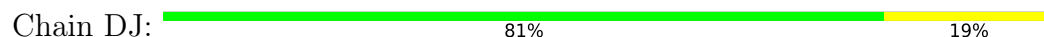
- Molecule 30: 50S ribosomal protein L6



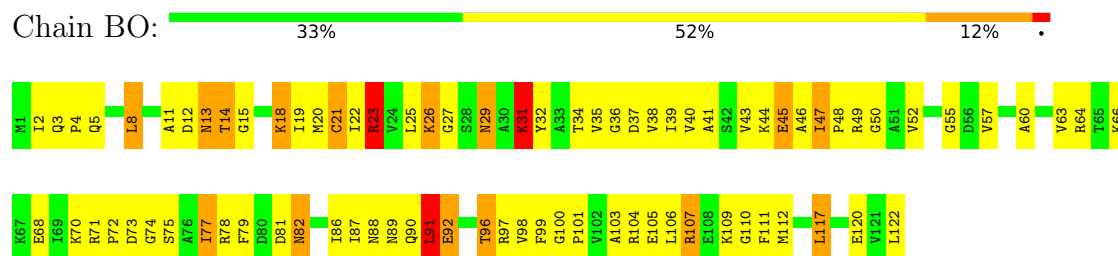
- Molecule 31: 50S RIBOSOMAL PROTEIN L10



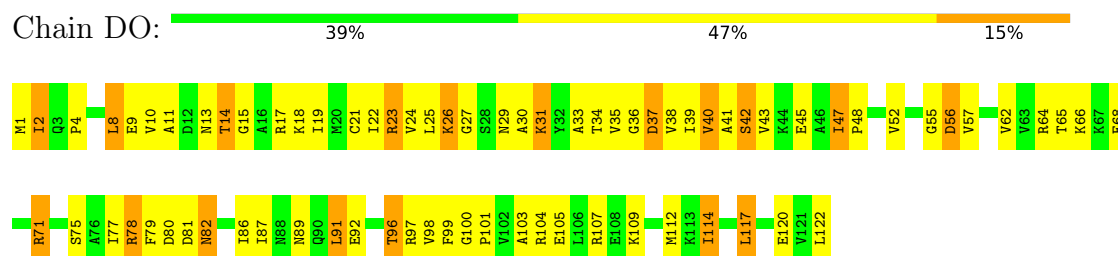
- Molecule 31: 50S RIBOSOMAL PROTEIN L10



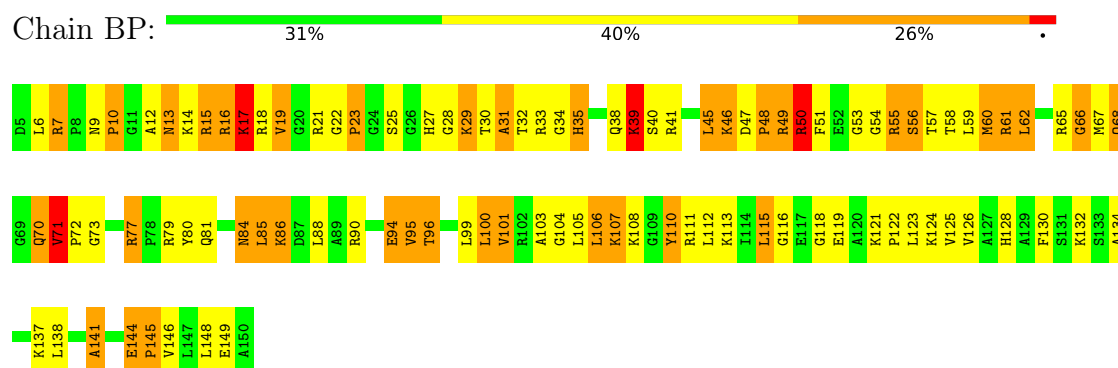
- Molecule 34: 50S ribosomal protein L14



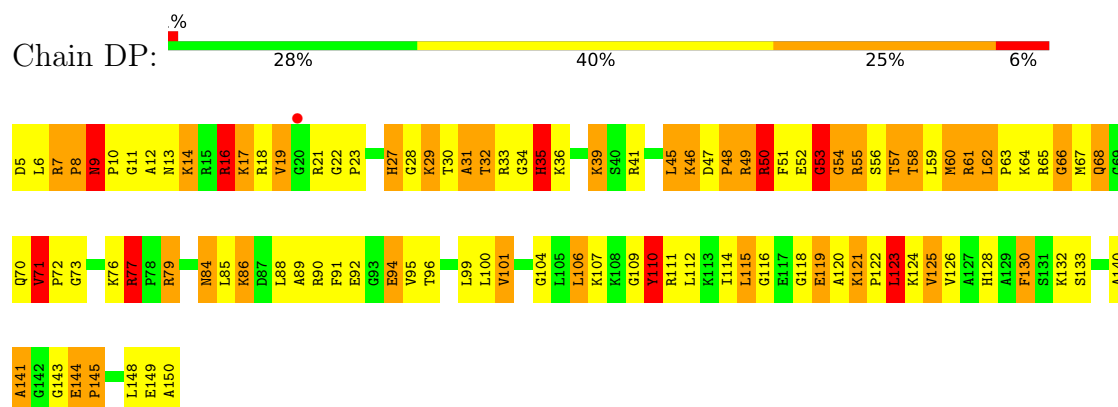
- Molecule 34: 50S ribosomal protein L14



- Molecule 35: 50S ribosomal protein L15



- Molecule 35: 50S ribosomal protein L15

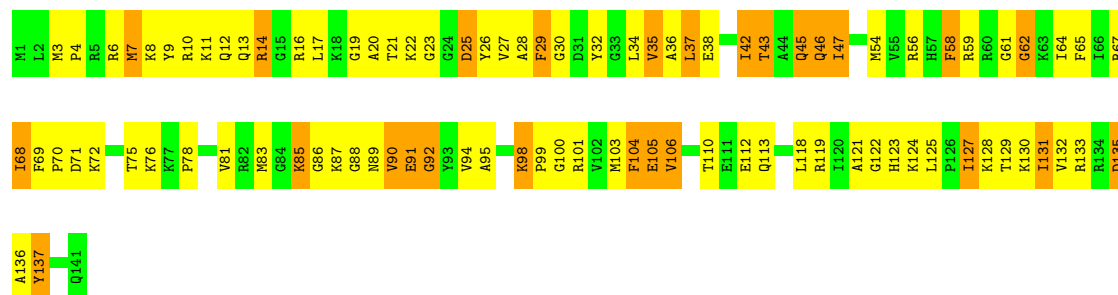
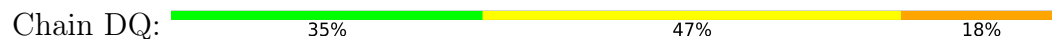


- Molecule 36: 50S ribosomal protein L16

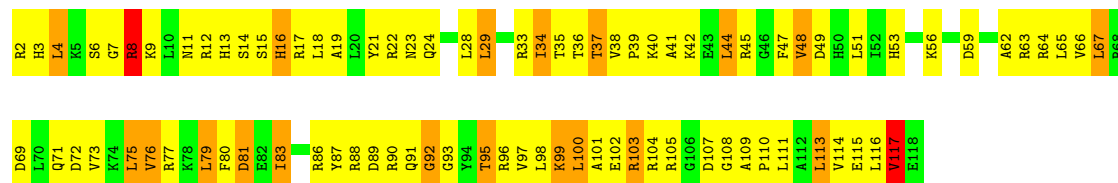




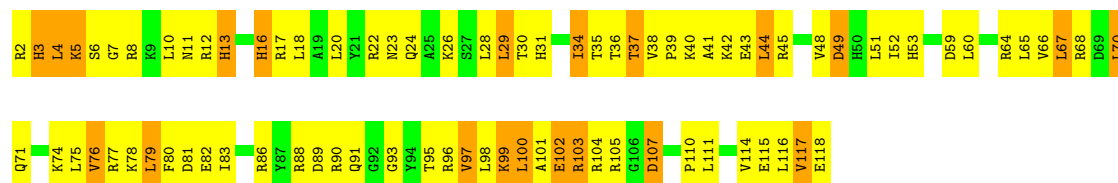
• Molecule 36: 50S ribosomal protein L16



• Molecule 37: 50S ribosomal protein L17

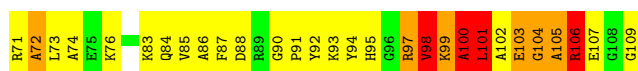


• Molecule 37: 50S ribosomal protein L17



• Molecule 38: 50S ribosomal protein L18

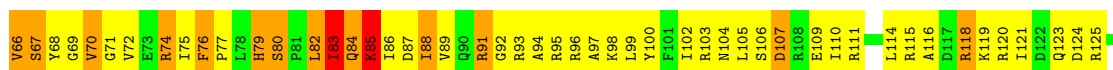
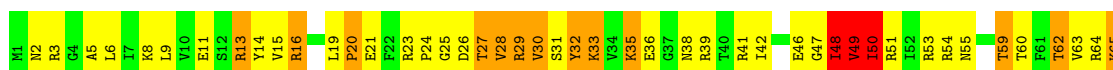




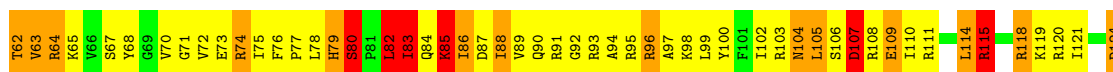
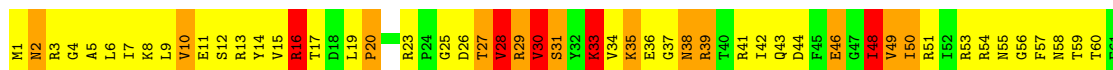
• Molecule 38: 50S ribosomal protein L18



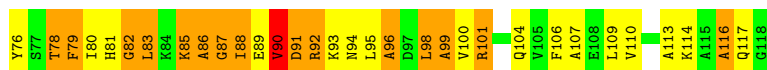
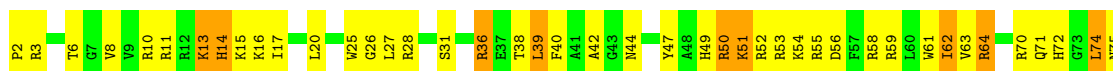
• Molecule 39: 50S ribosomal protein L19



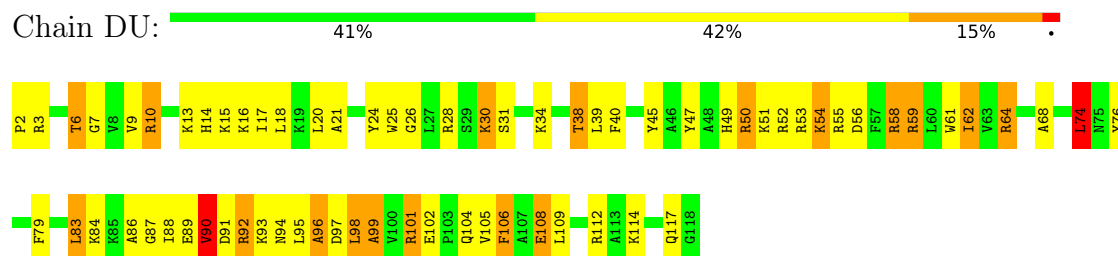
• Molecule 39: 50S ribosomal protein L19



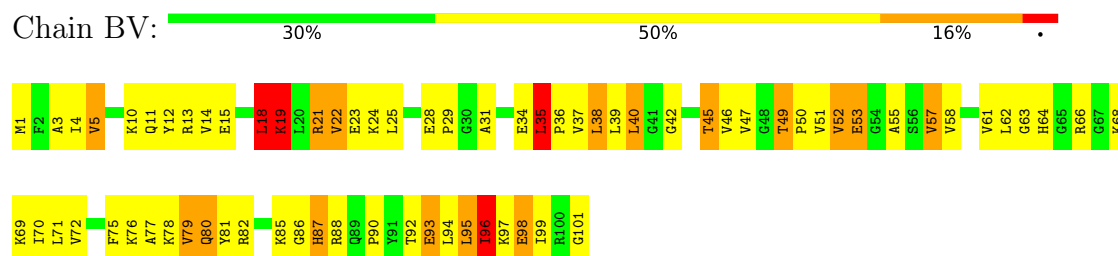
• Molecule 40: 50S ribosomal protein L20



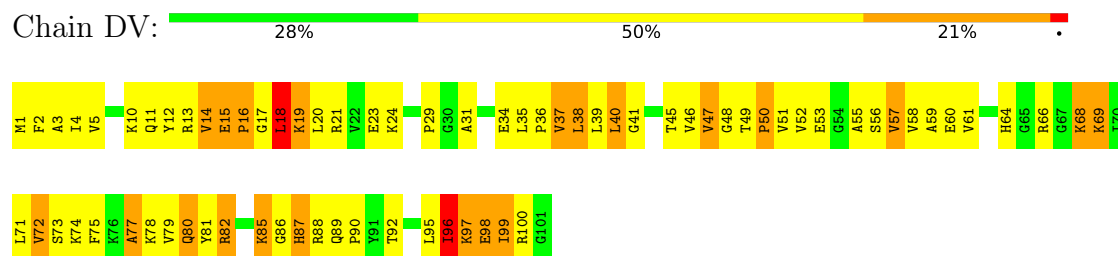
- Molecule 40: 50S ribosomal protein L20



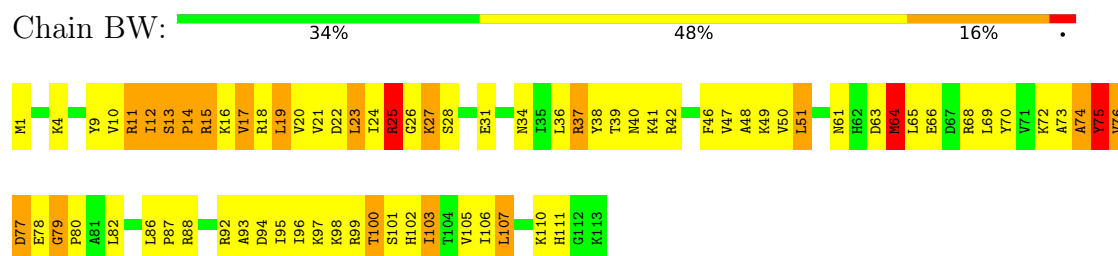
- Molecule 41: 50S ribosomal protein L21



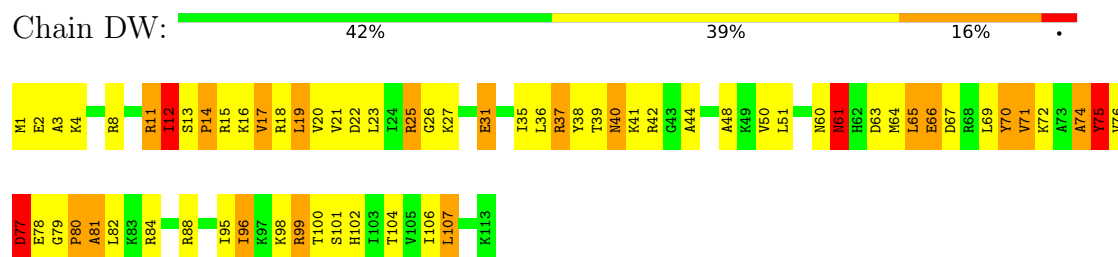
- Molecule 41: 50S ribosomal protein L21



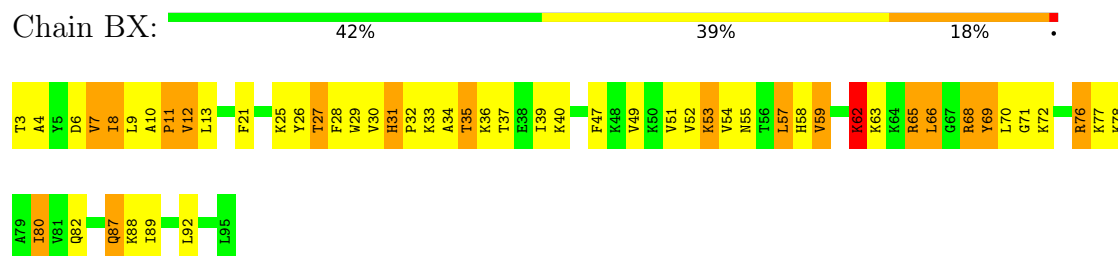
- Molecule 42: 50S ribosomal protein L22



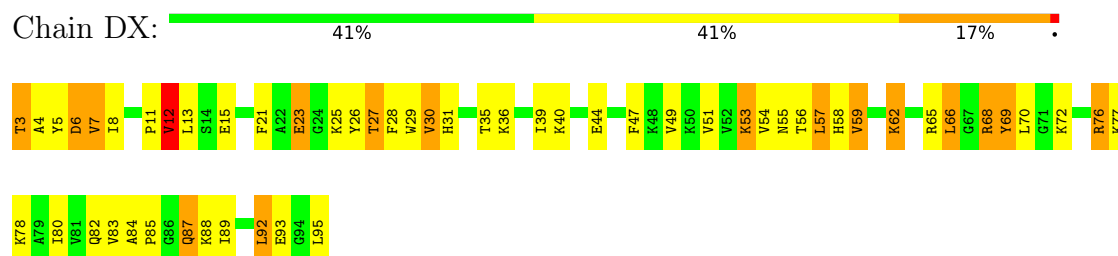
- Molecule 42: 50S ribosomal protein L22



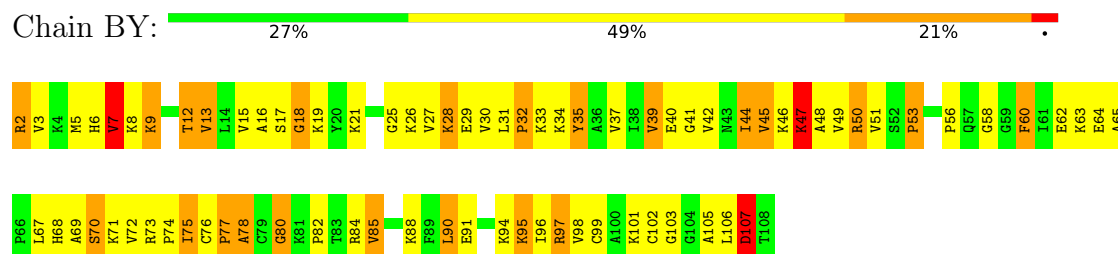
- Molecule 43: 50S ribosomal protein L23



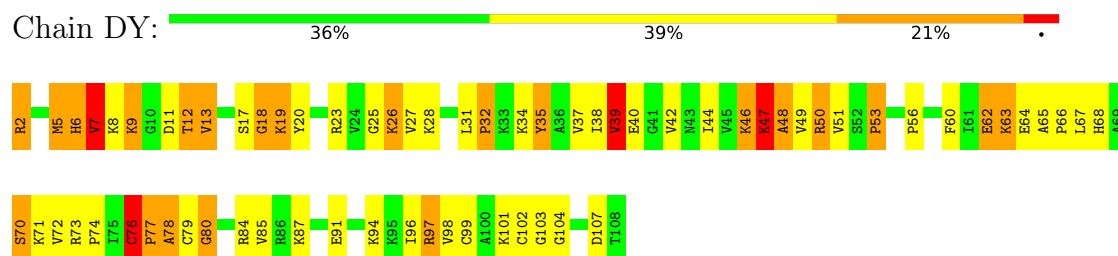
- Molecule 43: 50S ribosomal protein L23



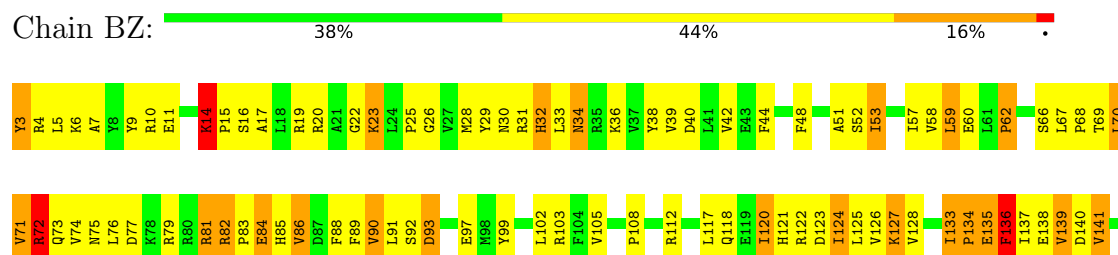
- Molecule 44: 50S ribosomal protein L24



- Molecule 44: 50S ribosomal protein L24



- Molecule 45: 50S ribosomal protein L25

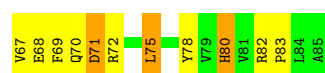
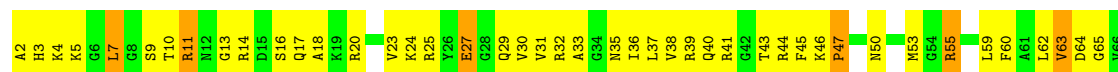




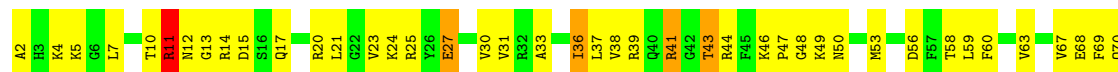
- Molecule 45: 50S ribosomal protein L25



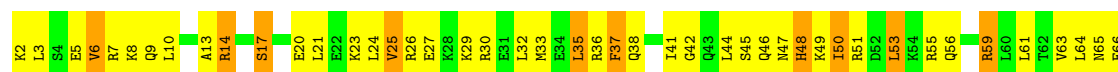
- Molecule 46: 50S ribosomal protein L27



- Molecule 46: 50S ribosomal protein L27

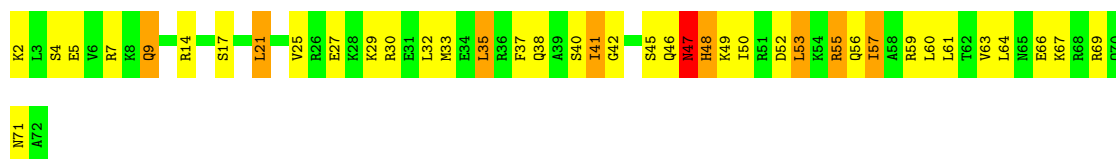


- Molecule 47: 50S ribosomal protein L29

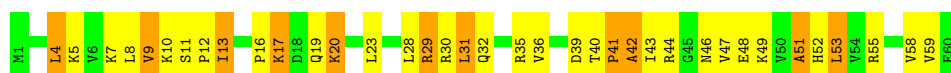


- Molecule 47: 50S ribosomal protein L29

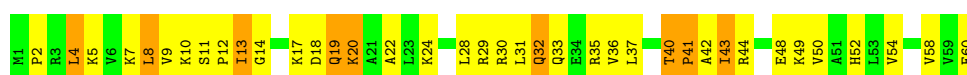




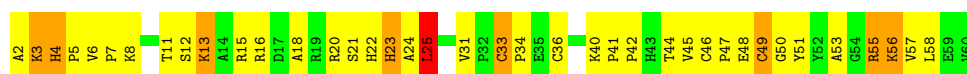
- Molecule 48: 50S ribosomal protein L30



- Molecule 48: 50S ribosomal protein L30



- Molecule 49: 50S ribosomal protein L32



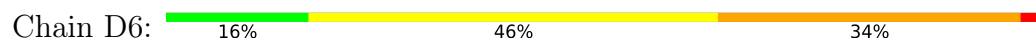
- Molecule 49: 50S ribosomal protein L32



- Molecule 50: 50S ribosomal protein L33

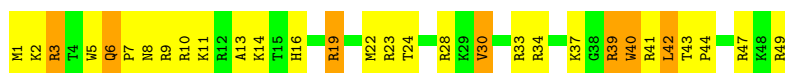


- Molecule 50: 50S ribosomal protein L33



- Molecule 51: 50S ribosomal protein L34

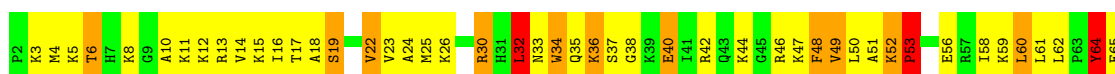




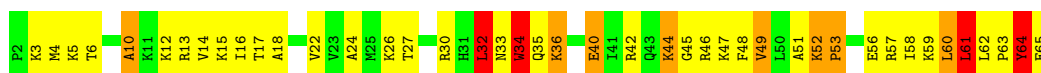
- Molecule 51: 50S ribosomal protein L34



- Molecule 52: 50S ribosomal protein L35



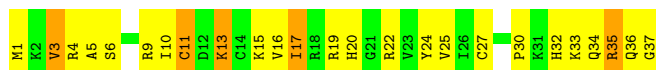
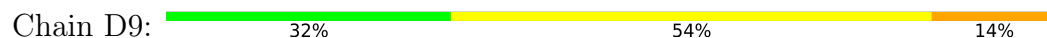
- Molecule 52: 50S ribosomal protein L35



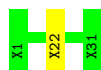
- Molecule 53: 50S ribosomal protein L36



- Molecule 53: 50S ribosomal protein L36



- Molecule 54: 50S RIBOSOMAL PROTEIN L7/L12



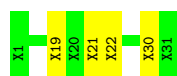
- Molecule 54: 50S RIBOSOMAL PROTEIN L7/L12



There are no outlier residues recorded for this chain.

- Molecule 54: 50S RIBOSOMAL PROTEIN L7/L12

Chain Df:  87% 13%



- Molecule 54: 50S RIBOSOMAL PROTEIN L7/L12

Chain Dg:  100%

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:  90% 10%

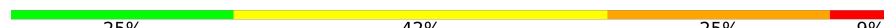


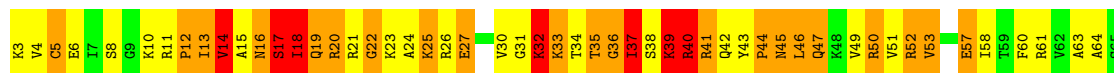
- Molecule 56: 50S ribosomal protein L28

Chain B1:  28% 35% 26% 11%

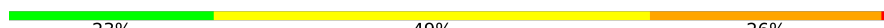


- Molecule 56: 50S ribosomal protein L28

Chain D1:  25% 42% 25% 9%

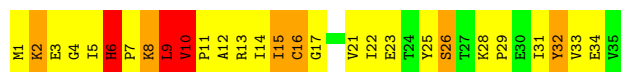


- Molecule 57: 50S ribosomal protein L31

Chain B4:  23% 49% 26% 2%



- Molecule 57: 50S ribosomal protein L31



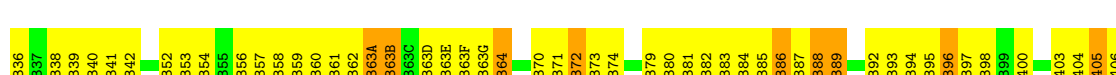
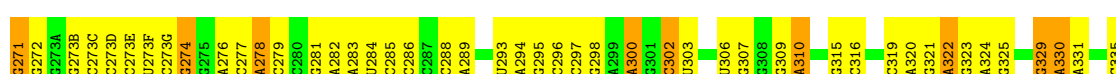
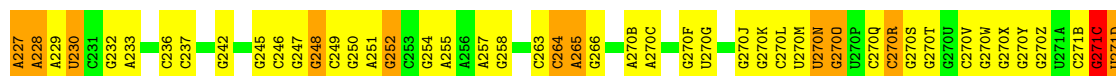
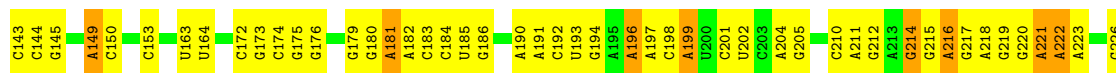
- Molecule 58: 50S ribosomal protein L7/L12



- Molecule 58: 50S ribosomal protein L7/L12

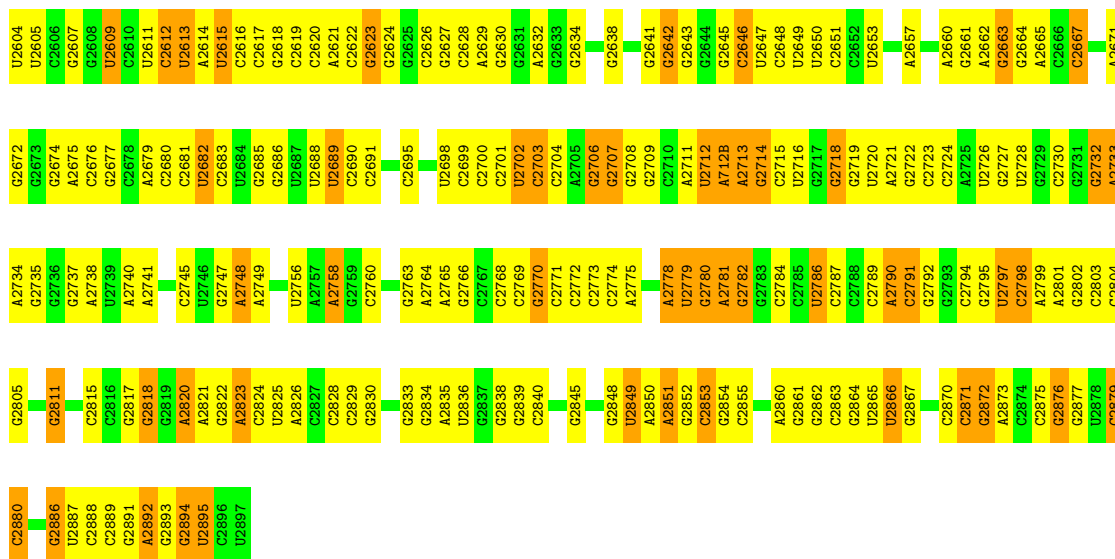


- Molecule 59: 23S ribosomal RNA



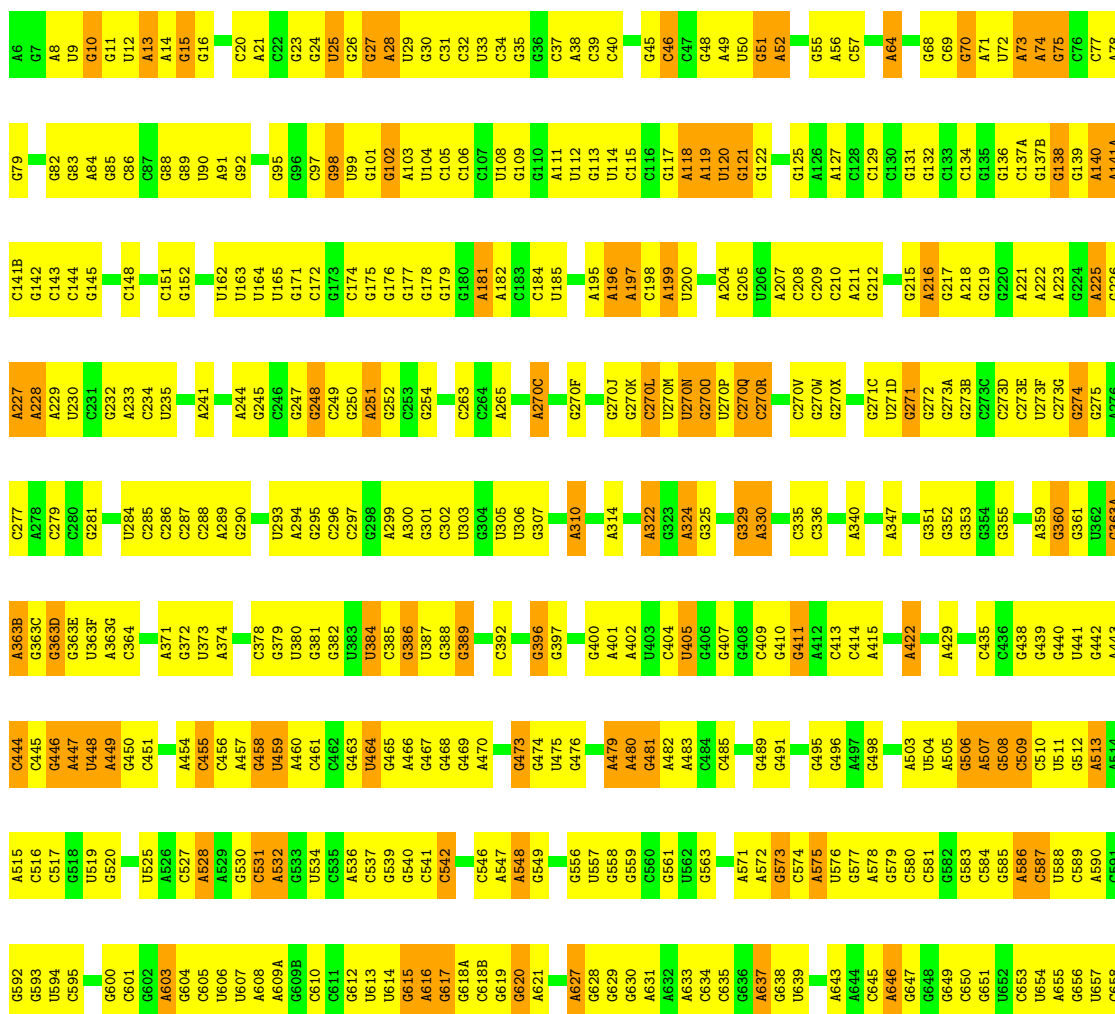
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G2096	G2097	G2098	G2099	G2100	G2101	G2102	G2103	G2104	G2105	G2106	G2107	G2108	G2109	G2110	G2111	G2112	G2113	G2114	G2115	G2116	G2117	G2118	G2119	G2120	G2121	G2122	G2123	G2124	G2125	G2126
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G1959	G1960	G1961	G1962	G1963	G1964	G1965	G1966	G1967	G1968	G1969	G1970	G1971	G1972	G1973	G1974	G1975	G1976	G1977	G1978	G1979	G1980	G1981	G1982	G1983	G1984	G1985	G1986	G1987	G1988	G1989
A1884	A1885	A1886	A1887	A1888	A1889	A1890	A1891	A1892	A1893	A1894	A1895	A1896	A1897	A1898	A1899	A1900	A1901	A1902	A1903	A1904	A1905	A1906	A1907	A1908	A1909	A1910	A1911	A1912	A1913	A1914
U1798	U1799	U1800	U1801	U1802	U1803	U1804	U1805	U1806	U1807	U1808	U1809	U1810	U1811	U1812	U1813	U1814	U1815	U1816	U1817	U1818	U1819	U1820	U1821	U1822	U1823	U1824	U1825	U1826	U1827	U1828
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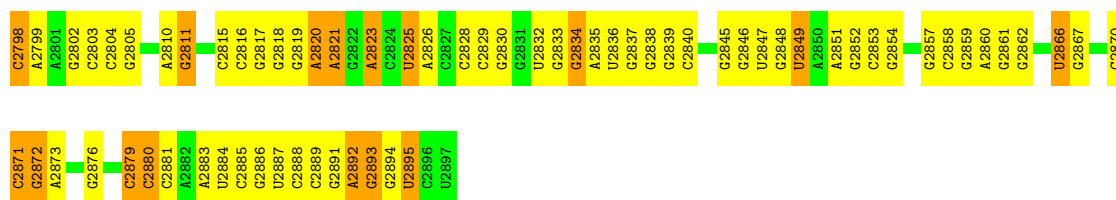
• Molecule 59: 23S ribosomal RNA

Chain DA: 34% 53% 13%



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A1634	G1487	U1420	U1352	G1279	A1214	A1148	C1076	A1001	G939	U871	A804	G726	G660
G1635	G1488	G1421	U1353	A1286	G1215	G1143	C1077	G1002	G940	A872	A805	G729	G661
C1636	A1558	A1637	A1354	U1287	G1216	A1144	A1077	C1005	G942	G873	C806	G731	G662
C1638	G1492	G1423	G1355	U1288	C1217	A1148	C1078	C1006	U943	G874	U807	G732	G663
U1639	C1493	G1424	G1356	C1291	C1221	G1149	C1080	C1007	G944	U877	G808	G733	G665
C1640	A1494	A1427	U1357	C1292	C1222	C1152	U1081	C1008	A945	A878	G809	A734	G666
A1641	A1495	C1428	G1358	U1292	C1224	C1153	U1082	A1009	G946	G879	C812	A670	A670
G1642	A1496	C1429	A1359	C1293	G1225	C1154	U1083	A1010	G947	G880	C813	A671	A671
A1643	U1497	C1430	A1360	U1294	A1226	A1154	A1084	G1011	G948	G881	C814	G738	G670
C1644	C1498	U1431	G1361	C1295	G1227	A1155	A1085	U1012	G949	G882	C815	G739	G672
G1645	C1499	U1432	C1362	G1296	C1230	A1156	A1086	G1013	G950	G883	C816	U740	G673
C1646	G1500	U1433	C1363	C1297	G1231	A1157	G1087	U1014	C951	C884	C817	G741	G674
G1647	C1501	A1434	G1364	U1300	G1232	C1158	A1088	G1015	G952	C885	C818	G742	A675
C1648	G1502	G1435	A1365	A1301	G1233	U1159	G1089	G1016	A953	C886	G819	G743	A676
G1651	C1505	G1436	G1366	A1302	C1234	C1161	U1090	G1017	G954	A887	A820	U747	A677
A1652	C1506	U1437	G1367	G1303	U1235	G1162	G1091	C1018	C955	C888	A821	G748	C678
G1653	U1510	A1438	U1372	C1306	G1236	G1163	U1094	U1019	G956	C889	A822	C749	C679
A1654	A1511	G1440	U1373	G1309	A1237	C1164	A1095	A1020	A957	A890	U822	C749	G680
C1655	G1512	G1441	A1374	G1310	G1238	U1165	A1096	A1021	U958	G892	U826	U757	G681
G1656	G1513	G1442	G1375	G1311	G1239	C1166	U1097	G1022	A959	C893	U827	C758	G682
C1657	C1514	A1448	C1376	U1312	U1240	U1167	C1101	G1024	C961	U895	U828	C758	A685
C1658	C1515	C1445	G1377	U1313	A1241	G1170	C1102	G1025	C964	A896	A829	A761	G686
G1659	U1516	C1446	A1378	C1314	G1242	G1171	C1103	U1026	C965	C897	G830	U762	G687
C1660	G1517	G1447	A1379	C1315	G1243	G1172	C1104	A1027	C966	A900	G831	G763	U688
G1661	G1518	G1448	G1380	U1316	G1244	A1173	U1105	A1028	A967	A901	U836	A764	U689
A1662	G1522	A1449	G1381	U1317	G1245	U1174	G1106	A1029	C967	G902	G837	G765	G690
G1663	U1523	C1448	A1382	A1317	A1246	U1175	G1107	G1030	C968	C903	C838	G766	C691
A1664	G1524	C1449	U1383	G1320	U1247	G1176	U1108	U1033	U969	G904	U839	G767	C692
G1665	G1525	A1453	G1384	A1321	G1248	A1177	U1109	U1036	C970	U905	C840	G768	G695
C1666	U1526	G1454	C1385	A1322	U1249	C1178	C1110	G1037	G972	G906	A841	G771	G696
G1667	G1527	G1455	C1386	G1323	C1251	C1179	A1111	G1038	A973	C907	G842	G772	C697
A1668	A1528	U1458	U1394	G1324	G1252	G1184	U1112	A1045	G974A	C908	G843	A774	A698
C1669	C1530	C1459	A1395	U1325	A1253	C1185	U1113	A1046	C974B	A909	C846	G775	A699
G1670	C1531	A1460	U1396	U1326	A1254	G1186	G1114	A1047	G975	A910	U847	G776	G700
C1671	G1532	G1461	U1397	C1327	U1255	G1187	G1115	G1048	C976	A911	C848	A777	G701
A1672	C1533	C1462	C1398	G1328	G1256	U1188	C1116	U1049	G977	C912	G849	G778	G702
G1673	G1534	A1463	C1399	U1329	C1257	G1190	C1117	A1050	G978	U913	G852	G779	U703
C1674	U1535	C1464	G1400	C1330	C1258	G1191	C1118	G1051	G979	C914	G853	G780	G704
A1675	G1536	G1465	G1401	A1331	G1259	G1192	G1119	A1055	A980	C915	C854	A781	A705
G1676	C1537	G1466	C1402	G1332	G1260	C1193	C1120	G1056	A983	G916	G855	A782	G706
C1677	G1538	A1467	C1403	C1333	C1261	U1194	G1121	G1057	A984	A917	G856	A783	G707
G1681	G1539	C1468	C1404	G1334	A1262	U1195	G1122	A1058	C985	A918	C857	A784	G710
A1682	G1540	C1469	U1405	U1335	U1263	G1196	C1123	G1059	C986	G919	U858	G785	G711
C1683	U1541	A1470	A1406	A1336	G1264	U1199	C1124	U1060	G987	G920	U859	G786	G712
G1689	G1542	G1471	C1407	G1337	A1265	C1200	A1125	G1061	A990	U922	U860	A787	G713
A1690	C1543	A1472	C1408	G1338	G1266	C1201	C1127	U1062	C991	U923	U861	A788	U714
C1691	G1544	C1473	G1409	G1339	U1267	C1202	A1132	G1063	C992	C924	A862	C790	G717
U1692	A1545	A1474	C1410	U1340	A1268	U1203	U1133	G1064	C993	G925	G863	G791	A718
G1693	C1546	G1475	C1411	A1341	A1269	U1204	C1135	C1065	C994	C926	A864	G792	A719
C1694	U1547	G1476	A1412	A1342	U1270	G1205	G1136	U1066	C995	G927	C865	A793	C720
A1695	G1548	G1477	G1413	G1343	A1271	C1206	G1137	A1067	C996	U928	A866	G794	C721
G1696	C1549	A1478	C1414	G1344	G1272	C1207	G1138	A1070	G997	G931	C867	C795	G722
C1697	U1550	U1481	U1415	C1345	A1275	U1210	C1139	G1071	C998	A932	U868	C796	A723
A1698	G1551	G1483	G1416	G1346	A1276	U1211	G1140	U1071	U999	A933	G869	G799	U724
G1707	C1552	G1484	G1417	G1347	G1277	G1212	U1141						
C1708	A1632	G1485	G1418	G1348									

C2730	A2665	G2564	A2598	G2529	U2462	G2394	A2322	G2250	A2173	C2105	C2039	G1894	A1810	U1709
G2731	A2666	G2395	G2323	A2530	C2466	G2396	G2323	C2254	C2174	G2106	C2040	C1895	G1811	C1710
G2732	C2667	G2396	C2324	A2531	C2467	G2397	G2324	G2255	C2175	C2107	U2041	G1896	G1812	C1711
A2733	G2668	G2397	G2325	G2532	G2468	U2398	C2326	C2261	A2176	U2109	A2042	G1899	G1813	C1712
G2737	G2669	G2603	A2327	G2533	G2469	G2399	A2328	U2262	C2177	G2110	C2044	C1900	A1815	U1727
A2738	A2670	G2604	A2328	G2400	G2470	G2400	A2329	U2263	C2178	G2111	C2045	A1901	G1728	G1728
G2739	A2671	U2401	G2330	U2401	C2471	G2402	G2331	C2264	C2179	G2112	G2046	C1902	G1816	A1729
A2740	G2672	G2403	G2331	G2403	G2472	C2404	G2331	U2265	G2184	G2113	U2047	G1903	G1817	
A2741	G2673	G2404	G2332	G2404	C2473	C2404	G2332	U2266	C2185	G2114	G2048	G1906	A1819	A1732
C2742	G2674	C2405	G2333	C2405	U2474	G2406	G2334	A2267	G2190	G2115	G2049	C1907	U1820	G1733
C2743	A2675	G2406	G2334	G2406	C2475	U2406	A2335	A2268	G2191	G2116	C2050	G1908	A1821	
G2744	A2476	G2407	A2335	G2407	A2476	G2407	A2336	A2269	G2192	U2118	G2052	C1909	G1750	C1751
G2745	A2477	G2408	A2336	G2408	C2477	G2408	A2337	A2270	G2193	G2119	G2053	G1910	A1825	
U2746	A2478	G2409	A2337	G2409	A2478	G2409	A2338	G2271	G2194	U2120	G2054	G1911	G1826	A1755
G2747	A2479	G2410	G2339	G2410	C2479	G2410	G2340	U2272	G2195	G2121	C2055	U1912	G1827	
A2748	G2480	A2411	G2340	A2411	G2480	A2411	G2341	U2273	C2196	G2122	G2056	U1913	A1828	U1757
	G2481	A2412	U2344	G2412	G2481	A2412	U2345	A2274	C2197	G2123	C2057	C1914	A1829	
G2751	G2482	G2413	U2346	G2413	G2482	A2413	U2347	C2275	C1994	G2124	A2060	U1915	A1830	A1762
	G2483	G2414	G2347	G2414	G2483	A2414	G2348	C2276	U1995	G2125	G2061	U1916	U1833	A1763
G2756	G2484	G2415	U2348	G2415	G2484	A2415	U2349	C2277	C1996	G1997	A1917	U1917	U1834	G1764
A2757	G2485	G2416	U2349	G2416	G2485	A2416	U2350	C2278	G1998	G1998	C1920	C1920	G1837	G1770
G2758	G2486	G2417	U2350	G2417	G2486	A2417	U2351	C2279	C1999	G1999	C1921	C1921	C1838	C1771
A2759	G2487	G2418	G2350	G2418	G2487	A2418	U2352	C2280	G2000	G2000	G2000	C1922	G1839	G1772
C2760	G2488	G2419	G2351	G2419	G2488	A2419	U2353	C2281	A2001	G2001	G2001	C1923	G1840	A1773
	G2489	G2420	G2352	G2420	G2489	A2420	U2354	C2282	G2002	G2002	G2002	C1924	G1841	C1774
G2763	G2490	G2421	G2353	G2421	G2490	A2421	U2355	C2283	G2003	G2003	G2003	C1925	G1842	G1775
G2765	G2491	G2422	G2354	G2422	G2491	A2422	U2356	C2284	G2004	G2004	G2004	C1926	G1843	U1776
	G2492	G2423	G2355	G2423	G2492	A2423	U2357	C2285	A2005	G2005	G2005	C1927	G1844	
G2767	G2493	G2424	G2356	G2424	G2493	A2424	U2358	C2286	C2006	G2006	G2006	C1928	G1845	U1779
G2768	G2494	G2425	G2357	G2425	G2494	A2425	U2359	C2287	C2007	G2007	G2007	C1929	G1846	A1760
G2769	G2495	G2426	G2358	G2426	G2495	A2426	U2360	C2288	G2008	G2008	G2008	C1930	G1847	U1781
G2770	G2496	G2427	G2359	G2427	G2496	A2427	U2361	C2289	G2009	G2009	G2009	C1931	A1854	A1783
G2771	G2497	G2428	G2360	G2428	G2497	A2428	U2362	C2290	G2010	G2010	G2010	C1932	G1858	A1784
C2772	G2498	G2429	G2361	G2429	G2498	A2429	U2363	C2291	G2011	G2011	G2011	C1933	G1859	A1785
G2773	G2499	G2430	G2362	G2430	G2499	A2430	U2364	C2292	G2012	G2012	G2012	C1934	G1860	A1786
C2774	G2500	G2431	G2363	G2431	G2500	A2431	U2365	C2293	G2013	G2013	G2013	C1935	G1861	C1788
	G2501	G2432	G2364	G2432	G2501	A2432	U2366	C2294	A2013	G2014	G2014	C1936	G1862	A1789
G2777	G2502	G2433	G2365	G2433	G2502	A2433	U2367	C2295	G2015	G2015	G2015	C1937	G1863	C1790
U2778	G2503	G2434	G2366	G2434	G2503	A2434	U2368	C2296	G2016	G2016	G2016	C1938	G1864	U1791
G2779	G2504	G2435	G2367	G2435	G2504	A2435	U2369	C2297	G2017	G2017	G2017	C1939	G1865	G1792
U2780	G2505	G2436	G2368	G2436	G2505	A2436	U2370	C2298	G2018	G2018	G2018	C1940	G1866	C1793
G2781	G2506	G2437	G2369	G2437	G2506	A2437	U2371	C2299	G2019	G2019	G2019	C1941	G1867	U1794
G2782	G2507	G2438	G2370	G2438	G2507	A2438	U2372	C2300	G2020	G2020	G2020	C1942	G1868	C1795
G2783	G2508	G2439	G2371	G2439	G2508	A2439	U2373	C2301	G2021	G2021	G2021	C1943	G1869	U1796
G2784	G2509	G2440	G2372	G2440	G2509	A2440	U2374	C2302	G2022	G2022	G2022	C1944	G1870	C1797
C2785	G2510	G2441	G2373	G2441	G2510	A2441	U2375	C2303	G2023	G2023	G2023	C1945	G1871	U1798
U2786	G2511	G2442	G2374	G2442	G2511	A2442	U2376	C2304	G2024	G2024	G2024	C1946	G1882	U1799
G2787	G2512	G2443	G2375	G2443	G2512	A2443	U2377	C2305	G2025	G2025	G2025	C1947	G1883	A1800
G2788	G2513	G2444	G2376	G2444	G2513	A2444	U2378	C2306	G2026	G2026	G2026	C1948	G1884	C1800
C2789	G2514	G2445	G2377	G2445	G2514	A2445	U2379	C2307	G2027	G2027	G2027	C1949	G1885	G1801
U2790	G2515	G2446	G2378	G2446	G2515	A2446	U2380	C2308	G2028	G2028	G2028	C1950	G1886	C1795
G2791	G2516	G2447	G2379	G2447	G2516	A2447	U2381	G2309	G2029	G2029	G2029	C1951	G1887	A1802
A2792	G2517	G2448	G2380	G2448	G2517	A2448	U2382	G2310	G2030	G2030	G2030	C1952	G1888	A1803
G2793	G2518	G2449	G2381	G2449	G2518	A2449	U2383	G2311	G2031	G2031	G2031	C1953	G1889	C1804
G2794	G2519	G2450	G2382	G2450	G2519	A2450	U2384	G2312	G2032	G2032	G2032	C1954	U1805	U1806
U2797	G2520	G2451	G2383	G2451	G2520	A2451	U2385	G2313	G2033	G2033	G2033	C1955	G1893	
	G2521	G2452	G2384	G2452	G2521	A2452	U2386	G2314	G2034	G2034	G2034	C1956	G1894	
G2798	G2522	G2453	G2385	G2453	G2522	A2453	U2387	G2315	G2035	G2035	G2035	C1957	G1895	
G2799	G2523	G2454	G2386	G2454	G2523	A2454	U2388	G2316	G2036	G2036	G2036	C1958	G1896	
G2800	G2524	G2455	G2387	G2455	G2524	A2455	U2389	G2317	G2037	G2037	G2037	C1959	G1897	
G2801	G2525	G2456	G2388	G2456	G2525									



• Molecule 60: 5S ribosomal RNA



• Molecule 60: 5S ribosomal RNA



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	306.01Å 673.49Å 351.98Å 90.00° 92.69° 90.00°	Depositor
Resolution (Å)	40.00 – 3.50 40.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.50) 75.0 (40.00-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 3.49Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.262 , 0.309 0.270 , 0.310	Depositor DCC
R_{free} test set	38188 reflections (4.29%)	wwPDB-VP
Wilson B-factor (Å ²)	80.5	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 362.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.26$, $\langle L^2 \rangle = 0.11$	Xtriage
Estimated twinning fraction	0.247 for h,-k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	308422	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% 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: UAL, DPP, 5OH, GNP, KBE, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AB	0.58	0/1945	1.14	18/2621 (0.7%)
1	CB	0.53	0/1945	1.10	18/2621 (0.7%)
2	AC	0.45	0/1645	0.94	4/2216 (0.2%)
2	CC	0.44	0/1645	0.94	6/2216 (0.3%)
3	AD	0.44	0/1733	0.99	8/2318 (0.3%)
3	CD	0.41	0/1733	0.97	5/2318 (0.2%)
4	AE	0.48	0/1172	0.96	0/1576
4	CE	0.44	0/1172	0.99	1/1576 (0.1%)
5	AF	0.48	0/856	0.99	4/1154 (0.3%)
5	CF	0.42	0/856	0.92	1/1154 (0.1%)
6	AG	0.43	0/1276	0.93	1/1709 (0.1%)
6	CG	0.44	0/1276	0.92	0/1709
7	AH	0.42	0/1136	0.91	2/1527 (0.1%)
7	CH	0.42	0/1136	0.96	3/1527 (0.2%)
8	AI	0.45	0/1029	0.91	1/1378 (0.1%)
8	CI	0.43	0/1029	0.90	3/1378 (0.2%)
9	AJ	0.47	0/815	1.08	9/1095 (0.8%)
9	CJ	0.44	0/815	0.97	1/1095 (0.1%)
10	AK	0.55	1/900 (0.1%)	1.00	4/1213 (0.3%)
10	CK	0.50	0/900	0.96	3/1213 (0.2%)
11	AL	0.64	0/992	1.28	16/1327 (1.2%)
11	CL	0.66	0/992	1.22	7/1327 (0.5%)
12	AM	0.45	0/1008	0.93	1/1347 (0.1%)
12	CM	0.44	0/1008	0.92	2/1347 (0.1%)
13	AN	0.44	0/501	0.84	0/664
13	CN	0.40	0/501	0.87	0/664
14	AO	0.55	0/745	0.94	2/992 (0.2%)
14	CO	0.45	0/745	0.87	0/992
15	AP	0.43	0/722	0.91	2/970 (0.2%)
15	CP	0.40	0/722	0.85	0/970
16	AQ	0.55	0/848	1.20	8/1131 (0.7%)
16	CQ	0.54	0/848	1.13	6/1131 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AR	0.45	0/579	0.98	2/768 (0.3%)
17	CR	0.38	0/579	0.89	1/768 (0.1%)
18	AS	0.42	0/647	0.98	1/870 (0.1%)
18	CS	0.40	0/647	0.96	1/870 (0.1%)
19	AT	0.48	0/764	0.87	0/1006
19	CT	0.49	0/764	0.94	0/1006
20	AY	0.67	9/5481 (0.2%)	1.12	41/7418 (0.6%)
20	CY	0.73	10/5481 (0.2%)	1.14	41/7418 (0.6%)
21	AA	0.22	0/36351	0.43	0/56736
21	CA	0.21	0/36351	0.42	0/56736
22	AW	0.22	0/1827	0.46	0/2845
22	CW	0.26	1/1827 (0.1%)	0.52	1/2845 (0.0%)
23	AV	0.40	0/568	0.79	2/886 (0.2%)
23	CV	0.55	1/568 (0.2%)	1.07	6/886 (0.7%)
24	AU	0.98	0/11	1.41	0/13
24	CU	0.98	0/11	1.41	0/13
25	BC	0.63	0/1774	1.19	25/2391 (1.0%)
25	DC	0.72	3/1774 (0.2%)	1.27	28/2391 (1.2%)
26	BD	0.52	0/2195	1.00	5/2955 (0.2%)
26	DD	0.52	0/2195	1.02	6/2955 (0.2%)
27	BE	0.53	0/1602	1.13	8/2160 (0.4%)
27	DE	0.46	0/1602	1.08	13/2160 (0.6%)
28	BF	0.55	0/1663	1.17	14/2249 (0.6%)
28	DF	0.55	0/1663	1.21	16/2249 (0.7%)
29	BG	0.80	3/1499 (0.2%)	0.95	5/2016 (0.2%)
29	DG	0.83	4/1499 (0.3%)	1.04	8/2016 (0.4%)
30	BH	0.45	0/1298	0.96	7/1751 (0.4%)
30	DH	0.46	0/1298	0.98	6/1751 (0.3%)
32	BK	0.53	0/1054	1.02	5/1427 (0.4%)
32	DK	0.52	0/1054	1.01	7/1427 (0.5%)
33	BN	0.76	0/1131	1.29	13/1525 (0.9%)
33	DN	0.68	0/1131	1.15	4/1525 (0.3%)
34	BO	0.45	0/943	1.14	11/1269 (0.9%)
34	DO	0.46	0/943	1.06	4/1269 (0.3%)
35	BP	0.45	0/1131	1.07	3/1504 (0.2%)
35	DP	0.45	0/1131	1.11	12/1504 (0.8%)
36	BQ	0.49	0/1143	1.03	7/1527 (0.5%)
36	DQ	0.44	0/1143	0.99	2/1527 (0.1%)
37	BR	0.48	0/974	1.00	3/1302 (0.2%)
37	DR	0.47	0/974	0.94	1/1302 (0.1%)
38	BS	0.57	0/783	1.21	9/1041 (0.9%)
38	DS	0.57	0/783	1.20	6/1041 (0.6%)
39	BT	0.55	0/1161	1.15	9/1549 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	DT	0.51	0/1161	1.07	6/1549 (0.4%)
40	BU	0.52	0/982	0.95	2/1306 (0.2%)
40	DU	0.56	0/982	0.99	3/1306 (0.2%)
41	BV	0.50	0/790	1.00	5/1057 (0.5%)
41	DV	0.51	0/790	1.06	3/1057 (0.3%)
42	BW	0.51	0/911	1.06	5/1220 (0.4%)
42	DW	0.51	0/911	1.06	5/1220 (0.4%)
43	BX	0.43	0/748	1.01	3/1004 (0.3%)
43	DX	0.44	0/748	1.02	7/1004 (0.7%)
44	BY	0.49	0/831	1.00	1/1108 (0.1%)
44	DY	0.46	0/831	0.95	3/1108 (0.3%)
45	BZ	0.45	0/1505	1.01	3/2042 (0.1%)
45	DZ	0.41	0/1505	0.99	8/2042 (0.4%)
46	B0	0.40	0/671	0.87	0/892
46	D0	0.40	0/671	0.95	3/892 (0.3%)
47	B2	0.45	0/600	0.92	3/793 (0.4%)
47	D2	0.40	0/600	0.88	0/793
48	B3	0.46	0/482	1.12	2/646 (0.3%)
48	D3	0.41	0/482	1.07	2/646 (0.3%)
49	B5	0.46	0/473	0.93	3/639 (0.5%)
49	D5	0.50	0/473	0.96	1/639 (0.2%)
50	B6	0.51	0/440	1.14	3/586 (0.5%)
50	D6	0.48	0/440	1.18	5/586 (0.9%)
51	B7	0.46	0/438	1.00	1/575 (0.2%)
51	D7	0.55	0/438	1.04	2/575 (0.3%)
52	B8	0.53	0/525	1.03	1/691 (0.1%)
52	D8	0.48	0/525	1.03	3/691 (0.4%)
53	B9	0.42	0/310	0.86	1/407 (0.2%)
53	D9	0.37	0/310	0.92	1/407 (0.2%)
56	B1	0.82	3/739 (0.4%)	1.41	14/981 (1.4%)
56	D1	0.83	6/739 (0.8%)	1.36	9/981 (0.9%)
57	B4	0.65	0/276	1.16	2/372 (0.5%)
57	D4	0.72	0/276	1.13	2/372 (0.5%)
58	Be	0.44	0/538	0.93	1/715 (0.1%)
58	De	0.44	0/538	0.95	2/715 (0.3%)
59	BA	0.22	0/69437	0.44	3/108401 (0.0%)
59	DA	0.22	0/69437	0.42	1/108401 (0.0%)
60	BB	0.19	0/2853	0.40	0/4451
60	DB	0.19	0/2853	0.37	0/4451
All	All	0.36	41/330902 (0.0%)	0.68	588/492664 (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	1
10	AK	0	1
11	AL	0	1
11	CL	0	1
20	AY	0	3
20	CY	0	8
25	BC	0	3
25	DC	0	2
26	DD	0	1
28	BF	0	2
28	DF	0	2
29	BG	0	1
29	DG	0	1
31	BJ	0	1
31	DJ	0	1
38	BS	0	2
38	DS	0	2
39	BT	0	2
39	DT	0	1
42	DW	0	1
56	B1	0	2
56	D1	0	3
All	All	0	44

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	CY	502	GLY	C-O	25.88	1.53	1.23
29	DG	112	PRO	CA-C	25.09	1.88	1.52
29	BG	112	PRO	CA-C	25.02	1.88	1.52
20	AY	499	ARG	C-N	15.12	1.56	1.33
20	CY	499	ARG	C-N	10.64	1.48	1.33

The worst 5 of 588 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	DF	193	VAL	N-CA-C	-18.82	83.28	109.45
22	CW	37	A	P-O3'-C3'	15.26	143.09	120.20
23	CV	16	A	P-O3'-C3'	14.81	142.41	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	CY	502	GLY	O-C-N	-14.78	101.35	122.19
23	CV	16	A	O3'-P-O5'	-13.63	83.56	104.00

There are no chirality outliers.

5 of 44 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AB	162	ILE	Peptide
1	AB	163	PHE	Peptide
10	AK	109	VAL	Peptide
11	AL	57	LYS	Peptide
20	AY	31	ARG	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AB	1910	0	1957	136	0
1	CB	1910	0	1957	103	0
2	AC	1621	0	1688	93	0
2	CC	1621	0	1688	68	0
3	AD	1703	0	1763	121	0
3	CD	1703	0	1763	124	0
4	AE	1156	0	1213	74	0
4	CE	1156	0	1213	56	0
5	AF	843	0	857	41	0
5	CF	843	0	857	42	0
6	AG	1257	0	1296	62	0
6	CG	1257	0	1296	62	0
7	AH	1116	0	1177	83	0
7	CH	1116	0	1177	74	0
8	AI	1011	0	1043	78	5
8	CI	1011	0	1043	56	0
9	AJ	802	0	849	72	0
9	CJ	802	0	849	61	0
10	AK	885	0	904	64	0
10	CK	885	0	904	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	AL	976	0	1062	112	0
11	CL	976	0	1062	118	0
12	AM	997	0	1072	77	0
12	CM	997	0	1072	72	5
13	AN	492	0	529	39	0
13	CN	492	0	529	35	0
14	AO	734	0	771	44	0
14	CO	734	0	771	44	0
15	AP	706	0	725	38	0
15	CP	706	0	725	41	0
16	AQ	835	0	906	63	0
16	CQ	835	0	906	65	0
17	AR	574	0	644	46	0
17	CR	574	0	644	37	0
18	AS	634	0	655	40	0
18	CS	634	0	655	34	0
19	AT	762	0	859	52	0
19	CT	762	0	859	32	0
20	AY	5380	0	5434	380	0
20	CY	5380	0	5435	365	0
21	AA	32474	0	16393	916	0
21	CA	32474	0	16393	849	0
22	AW	1635	0	831	64	0
22	CW	1635	0	831	55	0
23	AV	503	0	252	24	0
23	CV	503	0	252	34	0
24	AU	48	0	39	9	0
24	CU	48	0	39	9	0
25	BC	1742	0	1798	168	0
25	DC	1742	0	1798	149	0
26	BD	2145	0	2234	180	0
26	DD	2145	0	2234	169	0
27	BE	1569	0	1634	146	0
27	DE	1569	0	1634	123	0
28	BF	1628	0	1680	148	0
28	DF	1628	0	1680	142	0
29	BG	1474	0	1535	105	0
29	DG	1474	0	1535	86	0
30	BH	1274	0	1342	77	0
30	DH	1274	0	1342	75	0
31	BJ	851	0	197	30	0
31	DJ	851	0	196	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	BK	1035	0	1082	62	0
32	DK	1035	0	1082	62	0
33	BN	1104	0	1180	120	0
33	DN	1104	0	1180	121	0
34	BO	933	0	996	61	0
34	DO	933	0	996	72	0
35	BP	1114	0	1187	98	0
35	DP	1114	0	1187	112	0
36	BQ	1122	0	1179	85	0
36	DQ	1122	0	1179	66	0
37	BR	960	0	1021	78	0
37	DR	960	0	1021	71	0
38	BS	775	0	835	78	0
38	DS	775	0	835	79	0
39	BT	1147	0	1207	92	0
39	DT	1147	0	1207	113	0
40	BU	964	0	1022	85	0
40	DU	964	0	1022	78	0
41	BV	779	0	852	49	0
41	DV	779	0	852	63	0
42	BW	900	0	964	64	0
42	DW	900	0	964	58	0
43	BX	734	0	789	42	0
43	DX	734	0	789	46	0
44	BY	818	0	908	66	0
44	DY	818	0	908	62	0
45	BZ	1473	0	1497	90	0
45	DZ	1473	0	1497	86	0
46	B0	662	0	688	43	0
46	D0	662	0	688	40	0
47	B2	598	0	653	38	0
47	D2	598	0	653	28	0
48	B3	477	0	529	25	0
48	D3	477	0	529	25	0
49	B5	459	0	477	37	0
49	D5	459	0	477	34	0
50	B6	433	0	461	35	0
50	D6	433	0	461	38	0
51	B7	430	0	480	45	0
51	D7	430	0	480	32	0
52	B8	517	0	582	51	0
52	D8	517	0	582	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	B9	307	0	336	23	0
53	D9	307	0	335	21	0
54	Bf	156	0	41	1	0
54	Bg	156	0	39	0	0
54	Df	156	0	41	3	0
54	Dg	156	0	39	0	0
55	Bh	151	0	39	0	0
55	Dh	151	0	37	2	0
56	B1	732	0	808	88	0
56	D1	732	0	808	77	0
57	B4	271	0	284	31	0
57	D4	271	0	284	20	0
58	Be	686	0	620	21	0
58	De	686	0	619	23	0
59	BA	61997	0	31250	1821	0
59	DA	61997	0	31250	1734	0
60	BB	2551	0	1295	76	0
60	DB	2551	0	1295	70	0
61	AY	32	0	13	18	0
61	CY	32	0	13	33	0
62	AY	1	0	0	0	0
62	CY	1	0	0	0	0
All	All	308422	0	213302	12013	5

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 23.

The worst 5 of 12013 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)
22:CW:37:A:C2	23:CV:16:A:C2	1.85	1.57
20:AY:33:LEU:HD21	20:AY:34:TYR:CE2	1.42	1.54
29:DG:112:PRO:CA	29:DG:112:PRO:C	1.88	1.45
29:BG:112:PRO:CA	29:BG:112:PRO:C	1.87	1.45
20:AY:33:LEU:HD21	20:AY:34:TYR:CD2	1.54	1.43

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AI:58:ARG:CZ	12:CM:46:LYS:CG[2_555]	1.66	0.54
8:AI:58:ARG:CD	12:CM:47:ASP:OD1[2_555]	1.74	0.46
8:AI:58:ARG:NH2	12:CM:46:LYS:CG[2_555]	1.88	0.32
8:AI:58:ARG:NE	12:CM:46:LYS:CG[2_555]	2.01	0.19
8:AI:58:ARG:NH2	12:CM:46:LYS:CD[2_555]	2.04	0.16

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%)	173 (74%)	40 (17%)	20 (9%)	0	7
1	CB	233/235 (99%)	174 (75%)	36 (16%)	23 (10%)	0	6
2	AC	205/207 (99%)	137 (67%)	44 (22%)	24 (12%)	0	4
2	CC	205/207 (99%)	152 (74%)	34 (17%)	19 (9%)	0	6
3	AD	206/208 (99%)	146 (71%)	42 (20%)	18 (9%)	0	7
3	CD	206/208 (99%)	149 (72%)	46 (22%)	11 (5%)	1	14
4	AE	149/151 (99%)	107 (72%)	31 (21%)	11 (7%)	1	9
4	CE	149/151 (99%)	116 (78%)	24 (16%)	9 (6%)	1	12
5	AF	99/101 (98%)	75 (76%)	17 (17%)	7 (7%)	1	10
5	CF	99/101 (98%)	81 (82%)	7 (7%)	11 (11%)	0	5
6	AG	153/155 (99%)	120 (78%)	27 (18%)	6 (4%)	2	20
6	CG	153/155 (99%)	119 (78%)	27 (18%)	7 (5%)	2	17
7	AH	136/138 (99%)	98 (72%)	22 (16%)	16 (12%)	0	4
7	CH	136/138 (99%)	102 (75%)	21 (15%)	13 (10%)	0	6
8	AI	125/127 (98%)	88 (70%)	26 (21%)	11 (9%)	0	7
8	CI	125/127 (98%)	92 (74%)	25 (20%)	8 (6%)	1	11
9	AJ	97/99 (98%)	71 (73%)	17 (18%)	9 (9%)	0	6
9	CJ	97/99 (98%)	71 (73%)	16 (16%)	10 (10%)	0	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	AK	117/119 (98%)	74 (63%)	25 (21%)	18 (15%)	0	2
10	CK	117/119 (98%)	78 (67%)	26 (22%)	13 (11%)	0	5
11	AL	123/125 (98%)	42 (34%)	46 (37%)	35 (28%)	0	0
11	CL	123/125 (98%)	39 (32%)	44 (36%)	40 (32%)	0	0
12	AM	123/125 (98%)	86 (70%)	24 (20%)	13 (11%)	0	5
12	CM	123/125 (98%)	91 (74%)	18 (15%)	14 (11%)	0	5
13	AN	58/60 (97%)	40 (69%)	11 (19%)	7 (12%)	0	4
13	CN	58/60 (97%)	40 (69%)	14 (24%)	4 (7%)	1	10
14	AO	86/88 (98%)	65 (76%)	14 (16%)	7 (8%)	1	8
14	CO	86/88 (98%)	66 (77%)	15 (17%)	5 (6%)	1	13
15	AP	82/84 (98%)	55 (67%)	18 (22%)	9 (11%)	0	5
15	CP	82/84 (98%)	59 (72%)	18 (22%)	5 (6%)	1	12
16	AQ	98/100 (98%)	68 (69%)	18 (18%)	12 (12%)	0	4
16	CQ	98/100 (98%)	68 (69%)	20 (20%)	10 (10%)	0	6
17	AR	68/70 (97%)	50 (74%)	12 (18%)	6 (9%)	0	7
17	CR	68/70 (97%)	52 (76%)	10 (15%)	6 (9%)	0	7
18	AS	77/79 (98%)	51 (66%)	18 (23%)	8 (10%)	0	5
18	CS	77/79 (98%)	56 (73%)	12 (16%)	9 (12%)	0	4
19	AT	97/99 (98%)	72 (74%)	17 (18%)	8 (8%)	0	8
19	CT	97/99 (98%)	75 (77%)	14 (14%)	8 (8%)	0	8
20	AY	685/687 (100%)	431 (63%)	168 (24%)	86 (13%)	0	4
20	CY	685/687 (100%)	457 (67%)	156 (23%)	72 (10%)	0	5
24	AU	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
24	CU	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
25	BC	226/228 (99%)	108 (48%)	70 (31%)	48 (21%)	0	1
25	DC	226/228 (99%)	105 (46%)	75 (33%)	46 (20%)	0	1
26	BD	273/275 (99%)	180 (66%)	54 (20%)	39 (14%)	0	3
26	DD	273/275 (99%)	188 (69%)	47 (17%)	38 (14%)	0	3
27	BE	203/205 (99%)	130 (64%)	43 (21%)	30 (15%)	0	2
27	DE	203/205 (99%)	133 (66%)	36 (18%)	34 (17%)	0	2
28	BF	206/208 (99%)	126 (61%)	54 (26%)	26 (13%)	0	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	DF	206/208 (99%)	137 (66%)	47 (23%)	22 (11%)	0	5
29	BG	179/181 (99%)	120 (67%)	46 (26%)	13 (7%)	1	9
29	DG	179/181 (99%)	127 (71%)	44 (25%)	8 (4%)	2	17
30	BH	165/167 (99%)	118 (72%)	29 (18%)	18 (11%)	0	5
30	DH	165/167 (99%)	118 (72%)	32 (19%)	15 (9%)	0	7
32	BK	138/140 (99%)	88 (64%)	33 (24%)	17 (12%)	0	4
32	DK	138/140 (99%)	86 (62%)	33 (24%)	19 (14%)	0	3
33	BN	136/138 (99%)	93 (68%)	24 (18%)	19 (14%)	0	3
33	DN	136/138 (99%)	91 (67%)	27 (20%)	18 (13%)	0	3
34	BO	120/122 (98%)	92 (77%)	20 (17%)	8 (7%)	1	11
34	DO	120/122 (98%)	95 (79%)	20 (17%)	5 (4%)	2	19
35	BP	144/146 (99%)	81 (56%)	36 (25%)	27 (19%)	0	1
35	DP	144/146 (99%)	76 (53%)	35 (24%)	33 (23%)	0	1
36	BQ	139/141 (99%)	87 (63%)	32 (23%)	20 (14%)	0	3
36	DQ	139/141 (99%)	91 (66%)	31 (22%)	17 (12%)	0	4
37	BR	115/117 (98%)	83 (72%)	21 (18%)	11 (10%)	0	6
37	DR	115/117 (98%)	91 (79%)	17 (15%)	7 (6%)	1	12
38	BS	97/99 (98%)	56 (58%)	25 (26%)	16 (16%)	0	2
38	DS	97/99 (98%)	57 (59%)	25 (26%)	15 (16%)	0	2
39	BT	136/138 (99%)	76 (56%)	41 (30%)	19 (14%)	0	3
39	DT	136/138 (99%)	82 (60%)	28 (21%)	26 (19%)	0	1
40	BU	115/117 (98%)	79 (69%)	25 (22%)	11 (10%)	0	6
40	DU	115/117 (98%)	80 (70%)	23 (20%)	12 (10%)	0	5
41	BV	99/101 (98%)	57 (58%)	28 (28%)	14 (14%)	0	3
41	DV	99/101 (98%)	64 (65%)	22 (22%)	13 (13%)	0	3
42	BW	111/113 (98%)	82 (74%)	14 (13%)	15 (14%)	0	3
42	DW	111/113 (98%)	81 (73%)	16 (14%)	14 (13%)	0	4
43	BX	91/93 (98%)	73 (80%)	12 (13%)	6 (7%)	1	11
43	DX	91/93 (98%)	70 (77%)	16 (18%)	5 (6%)	1	13
44	BY	105/107 (98%)	50 (48%)	30 (29%)	25 (24%)	0	0
44	DY	105/107 (98%)	50 (48%)	34 (32%)	21 (20%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	BZ	183/185 (99%)	116 (63%)	46 (25%)	21 (12%)	0	5
45	DZ	183/185 (99%)	121 (66%)	44 (24%)	18 (10%)	0	6
46	B0	82/84 (98%)	59 (72%)	16 (20%)	7 (8%)	0	7
46	D0	82/84 (98%)	65 (79%)	13 (16%)	4 (5%)	1	16
47	B2	69/71 (97%)	49 (71%)	14 (20%)	6 (9%)	0	7
47	D2	69/71 (97%)	50 (72%)	17 (25%)	2 (3%)	3	26
48	B3	58/60 (97%)	46 (79%)	7 (12%)	5 (9%)	0	7
48	D3	58/60 (97%)	44 (76%)	9 (16%)	5 (9%)	0	7
49	B5	57/59 (97%)	44 (77%)	4 (7%)	9 (16%)	0	2
49	D5	57/59 (97%)	42 (74%)	11 (19%)	4 (7%)	1	10
50	B6	48/50 (96%)	28 (58%)	9 (19%)	11 (23%)	0	1
50	D6	48/50 (96%)	27 (56%)	8 (17%)	13 (27%)	0	0
51	B7	47/49 (96%)	30 (64%)	13 (28%)	4 (8%)	0	7
51	D7	47/49 (96%)	34 (72%)	11 (23%)	2 (4%)	2	18
52	B8	62/64 (97%)	42 (68%)	7 (11%)	13 (21%)	0	1
52	D8	62/64 (97%)	40 (64%)	11 (18%)	11 (18%)	0	1
53	B9	35/37 (95%)	28 (80%)	5 (14%)	2 (6%)	1	13
53	D9	35/37 (95%)	29 (83%)	4 (11%)	2 (6%)	1	13
56	B1	91/93 (98%)	56 (62%)	17 (19%)	18 (20%)	0	1
56	D1	91/93 (98%)	59 (65%)	18 (20%)	14 (15%)	0	2
57	B4	33/35 (94%)	15 (46%)	11 (33%)	7 (21%)	0	1
57	D4	33/35 (94%)	15 (46%)	9 (27%)	9 (27%)	0	0
58	Be	70/102 (69%)	36 (51%)	29 (41%)	5 (7%)	1	10
58	De	70/102 (69%)	40 (57%)	22 (31%)	8 (11%)	0	5
All	All	13304/13576 (98%)	8904 (67%)	2822 (21%)	1578 (12%)	0	4

5 of 1578 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AB	17	PHE
1	AB	22	LYS
1	AB	35	GLU
1	AB	75	LYS
1	AB	76	GLN

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%)	170 (84%)	33 (16%)	2	14
2	AC	161/161 (100%)	119 (74%)	42 (26%)	0	3
2	CC	161/161 (100%)	123 (76%)	38 (24%)	1	4
3	AD	180/180 (100%)	147 (82%)	33 (18%)	2	10
3	CD	180/180 (100%)	147 (82%)	33 (18%)	2	10
4	AE	116/116 (100%)	100 (86%)	16 (14%)	3	19
4	CE	116/116 (100%)	92 (79%)	24 (21%)	1	6
5	AF	90/90 (100%)	74 (82%)	16 (18%)	2	10
5	CF	90/90 (100%)	76 (84%)	14 (16%)	2	15
6	AG	126/126 (100%)	107 (85%)	19 (15%)	3	16
6	CG	126/126 (100%)	109 (86%)	17 (14%)	4	20
7	AH	119/119 (100%)	96 (81%)	23 (19%)	1	8
7	CH	119/119 (100%)	92 (77%)	27 (23%)	1	5
8	AI	98/98 (100%)	84 (86%)	14 (14%)	3	18
8	CI	98/98 (100%)	80 (82%)	18 (18%)	1	9
9	AJ	89/89 (100%)	68 (76%)	21 (24%)	1	4
9	CJ	89/89 (100%)	67 (75%)	22 (25%)	1	4
10	AK	90/90 (100%)	72 (80%)	18 (20%)	1	7
10	CK	90/90 (100%)	74 (82%)	16 (18%)	2	10
11	AL	104/104 (100%)	71 (68%)	33 (32%)	0	2
11	CL	104/104 (100%)	76 (73%)	28 (27%)	0	3
12	AM	100/100 (100%)	85 (85%)	15 (15%)	3	17
12	CM	100/100 (100%)	83 (83%)	17 (17%)	2	12
13	AN	49/49 (100%)	39 (80%)	10 (20%)	1	7
13	CN	49/49 (100%)	37 (76%)	12 (24%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	AO	79/79 (100%)	68 (86%)	11 (14%)	3	19
14	CO	79/79 (100%)	64 (81%)	15 (19%)	1	8
15	AP	72/72 (100%)	61 (85%)	11 (15%)	3	16
15	CP	72/72 (100%)	62 (86%)	10 (14%)	3	19
16	AQ	95/95 (100%)	80 (84%)	15 (16%)	2	15
16	CQ	95/95 (100%)	79 (83%)	16 (17%)	2	13
17	AR	61/61 (100%)	54 (88%)	7 (12%)	5	24
17	CR	61/61 (100%)	50 (82%)	11 (18%)	2	10
18	AS	69/69 (100%)	55 (80%)	14 (20%)	1	7
18	CS	69/69 (100%)	50 (72%)	19 (28%)	0	3
19	AT	76/76 (100%)	65 (86%)	11 (14%)	3	17
19	CT	76/76 (100%)	65 (86%)	11 (14%)	3	17
20	AY	579/579 (100%)	447 (77%)	132 (23%)	1	5
20	CY	579/579 (100%)	468 (81%)	111 (19%)	1	8
24	AU	2/2 (100%)	2 (100%)	0	100	100
24	CU	2/2 (100%)	2 (100%)	0	100	100
25	BC	180/180 (100%)	127 (71%)	53 (29%)	0	2
25	DC	180/180 (100%)	126 (70%)	54 (30%)	0	2
26	BD	217/217 (100%)	162 (75%)	55 (25%)	0	3
26	DD	217/217 (100%)	172 (79%)	45 (21%)	1	6
27	BE	165/165 (100%)	133 (81%)	32 (19%)	1	8
27	DE	165/165 (100%)	135 (82%)	30 (18%)	2	10
28	BF	165/165 (100%)	131 (79%)	34 (21%)	1	7
28	DF	165/165 (100%)	132 (80%)	33 (20%)	1	7
29	BG	155/155 (100%)	130 (84%)	25 (16%)	2	14
29	DG	155/155 (100%)	129 (83%)	26 (17%)	2	13
30	BH	136/136 (100%)	111 (82%)	25 (18%)	1	9
30	DH	136/136 (100%)	113 (83%)	23 (17%)	2	13
32	BK	105/105 (100%)	70 (67%)	35 (33%)	0	2
32	DK	105/105 (100%)	73 (70%)	32 (30%)	0	2
33	BN	117/117 (100%)	92 (79%)	25 (21%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	DN	117/117 (100%)	87 (74%)	30 (26%)	0	3
34	BO	100/100 (100%)	83 (83%)	17 (17%)	2	12
34	DO	100/100 (100%)	85 (85%)	15 (15%)	3	17
35	BP	112/112 (100%)	84 (75%)	28 (25%)	0	4
35	DP	112/112 (100%)	86 (77%)	26 (23%)	1	5
36	BQ	111/111 (100%)	81 (73%)	30 (27%)	0	3
36	DQ	111/111 (100%)	84 (76%)	27 (24%)	1	4
37	BR	100/100 (100%)	77 (77%)	23 (23%)	1	5
37	DR	100/100 (100%)	76 (76%)	24 (24%)	1	4
38	BS	77/77 (100%)	60 (78%)	17 (22%)	1	5
38	DS	77/77 (100%)	60 (78%)	17 (22%)	1	5
39	BT	120/120 (100%)	94 (78%)	26 (22%)	1	6
39	DT	120/120 (100%)	92 (77%)	28 (23%)	1	5
40	BU	93/93 (100%)	74 (80%)	19 (20%)	1	7
40	DU	93/93 (100%)	71 (76%)	22 (24%)	1	4
41	BV	82/82 (100%)	59 (72%)	23 (28%)	0	3
41	DV	82/82 (100%)	63 (77%)	19 (23%)	1	5
42	BW	92/92 (100%)	69 (75%)	23 (25%)	0	4
42	DW	92/92 (100%)	73 (79%)	19 (21%)	1	6
43	BX	75/75 (100%)	53 (71%)	22 (29%)	0	2
43	DX	75/75 (100%)	57 (76%)	18 (24%)	1	4
44	BY	88/88 (100%)	68 (77%)	20 (23%)	1	5
44	DY	88/88 (100%)	71 (81%)	17 (19%)	1	8
45	BZ	162/162 (100%)	129 (80%)	33 (20%)	1	7
45	DZ	162/162 (100%)	122 (75%)	40 (25%)	1	4
46	B0	66/66 (100%)	54 (82%)	12 (18%)	2	10
46	D0	66/66 (100%)	58 (88%)	8 (12%)	5	22
47	B2	66/66 (100%)	57 (86%)	9 (14%)	3	19
47	D2	66/66 (100%)	55 (83%)	11 (17%)	2	13
48	B3	52/52 (100%)	42 (81%)	10 (19%)	1	8
48	D3	52/52 (100%)	43 (83%)	9 (17%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	B5	51/51 (100%)	39 (76%)	12 (24%)	1	4
49	D5	51/51 (100%)	42 (82%)	9 (18%)	2	11
50	B6	49/49 (100%)	37 (76%)	12 (24%)	1	4
50	D6	49/49 (100%)	34 (69%)	15 (31%)	0	2
51	B7	42/42 (100%)	34 (81%)	8 (19%)	1	8
51	D7	42/42 (100%)	37 (88%)	5 (12%)	5	23
52	B8	54/54 (100%)	43 (80%)	11 (20%)	1	7
52	D8	54/54 (100%)	43 (80%)	11 (20%)	1	7
53	B9	34/34 (100%)	30 (88%)	4 (12%)	5	23
53	D9	34/34 (100%)	30 (88%)	4 (12%)	5	23
56	B1	78/78 (100%)	58 (74%)	20 (26%)	0	3
56	D1	78/78 (100%)	58 (74%)	20 (26%)	0	3
57	B4	31/31 (100%)	24 (77%)	7 (23%)	1	5
57	D4	31/31 (100%)	21 (68%)	10 (32%)	0	2
58	Be	54/54 (100%)	45 (83%)	9 (17%)	2	13
58	De	54/54 (100%)	44 (82%)	10 (18%)	1	9
All	All	11174/11174 (100%)	8843 (79%)	2331 (21%)	1	6

5 of 2331 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
29	DG	99	MET
56	D1	14	VAL
32	DK	110	GLN
29	DG	82	LEU
39	DT	114	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 143 such sidechains are listed below:

Mol	Chain	Res	Type
29	DG	27	ASN
35	DP	9	ASN
40	DU	66	ASN
34	BO	90	GLN
32	BK	30	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1511/1511 (100%)	327 (21%)	19 (1%)
21	CA	1511/1511 (100%)	310 (20%)	16 (1%)
22	AW	76/77 (98%)	22 (28%)	1 (1%)
22	CW	76/77 (98%)	19 (25%)	1 (1%)
23	AV	22/23 (95%)	11 (50%)	2 (9%)
23	CV	22/23 (95%)	9 (40%)	3 (13%)
59	BA	2878/2879 (99%)	666 (23%)	21 (0%)
59	DA	2878/2879 (99%)	629 (21%)	17 (0%)
60	BB	118/119 (99%)	20 (16%)	4 (3%)
60	DB	118/119 (99%)	19 (16%)	3 (2%)
All	All	9210/9218 (99%)	2032 (22%)	87 (0%)

5 of 2032 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	6	G
21	AA	7	G
21	AA	8	A
21	AA	9	G
21	AA	13	U

5 of 87 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
21	CA	1064	G
59	DA	586	A
21	CA	1324	A
23	CV	16	A
59	DA	1240	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	5OH	CU	6	24	7,12,13	0.76	0	4,16,18	0.95	0
24	DPP	AU	2	24	4,5,6	0.54	0	1,5,7	1.04	0
24	UAL	AU	5	24	6,8,9	2.49	3 (50%)	4,9,11	1.32	1 (25%)
24	DPP	CU	2	24	4,5,6	0.54	0	1,5,7	1.03	0
24	5OH	AU	6	24	7,12,13	0.75	0	4,16,18	0.95	0
24	KBE	AU	1	24	8,8,9	0.63	0	6,8,10	1.45	1 (16%)
24	UAL	CU	5	24	6,8,9	2.49	3 (50%)	4,9,11	1.32	1 (25%)
24	KBE	CU	1	24	8,8,9	0.63	0	6,8,10	1.46	1 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	5OH	CU	6	24	-	0/2/18/20	0/1/1/1
24	DPP	AU	2	24	-	0/2/4/6	-
24	UAL	AU	5	24	-	0/3/7/9	-
24	DPP	CU	2	24	-	0/2/4/6	-
24	5OH	AU	6	24	-	0/2/18/20	0/1/1/1
24	KBE	AU	1	24	-	1/7/7/8	-
24	UAL	CU	5	24	-	0/3/7/9	-
24	KBE	CU	1	24	-	1/7/7/8	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	CU	5	UAL	C-CA	4.52	1.52	1.45
24	AU	5	UAL	C-CA	4.51	1.52	1.45
24	AU	5	UAL	C1-N1	-3.39	1.35	1.40
24	CU	5	UAL	C1-N1	-3.37	1.35	1.40
24	AU	5	UAL	CB-N1	-2.20	1.30	1.35

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	CU	1	KBE	CB-CA-C	3.08	117.15	112.17
24	AU	1	KBE	CB-CA-C	3.06	117.11	112.17
24	AU	5	UAL	O-C-CA	-2.51	122.25	125.39
24	CU	5	UAL	O-C-CA	-2.51	122.25	125.39

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	AU	1	KBE	CG-CD-CE-NZ
24	CU	1	KBE	CG-CD-CE-NZ

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	CU	6	5OH	6	0
24	AU	2	DPP	1	0
24	CU	2	DPP	1	0
24	AU	6	5OH	4	0
24	CU	1	KBE	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
61	GNP	AY	701	62	34,34,34	1.48	5 (14%)	47,54,54	1.36	8 (17%)
61	GNP	CY	701	62	34,34,34	1.48	5 (14%)	47,54,54	1.36	8 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	GNP	AY	701	62	-	7/18/38/38	0/3/3/3
61	GNP	CY	701	62	-	7/18/38/38	0/3/3/3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	AY	701	GNP	PG-O1G	4.99	1.53	1.46
61	CY	701	GNP	PG-O1G	4.96	1.53	1.46
61	CY	701	GNP	PA-O3A	-4.30	1.54	1.59
61	AY	701	GNP	PA-O3A	-4.29	1.54	1.59
61	AY	701	GNP	PB-O3A	-2.43	1.56	1.59

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	CY	701	GNP	O2B-PB-O1B	3.43	117.23	109.87
61	AY	701	GNP	O2B-PB-O1B	3.43	117.22	109.87
61	AY	701	GNP	O2G-PG-O3G	3.30	116.46	107.59
61	CY	701	GNP	O2G-PG-O3G	3.29	116.43	107.59
61	AY	701	GNP	O3G-PG-O1G	-2.98	105.99	113.45

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

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

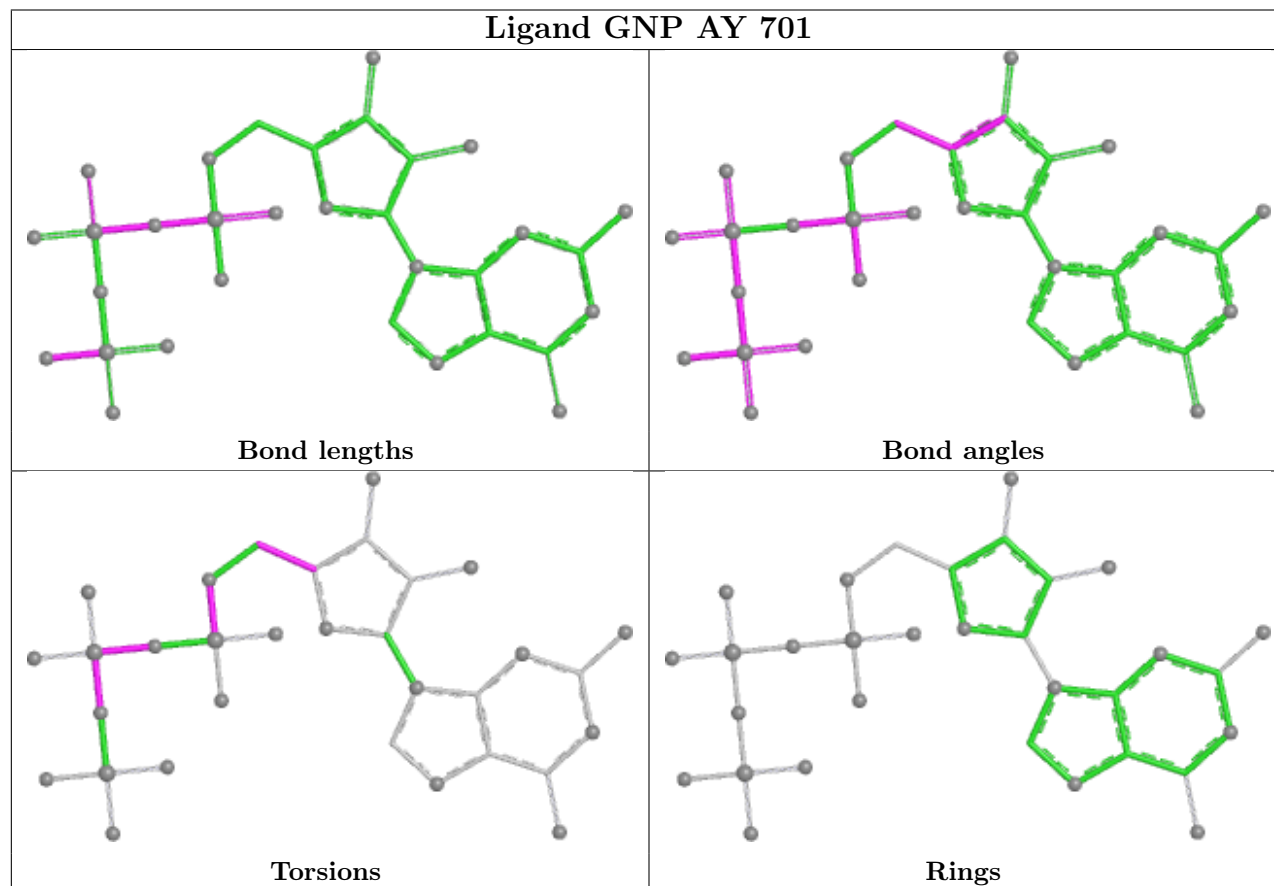
There are no ring outliers.

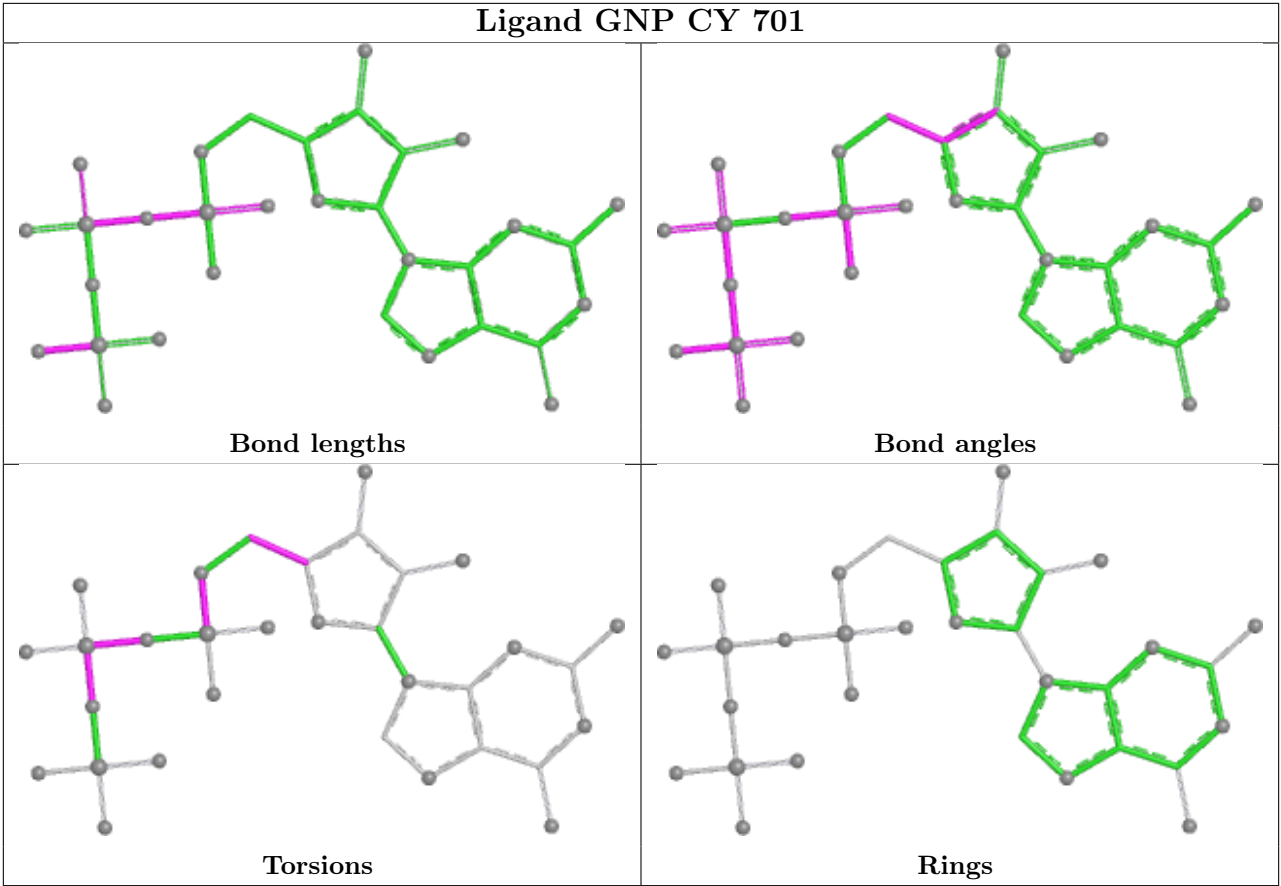
2 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	AY	701	GNP	18	0
61	CY	701	GNP	33	0

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

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





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
58	De	1
58	Be	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	36.11
1	Be	30:UNK	C	51:ALA	N	35.10

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%)	-1.34	0 100 100	30, 75, 127, 171	0
1	CB	235/235 (100%)	-1.26	0 100 100	34, 86, 153, 201	0
2	AC	207/207 (100%)	-1.24	0 100 100	27, 59, 115, 156	0
2	CC	207/207 (100%)	-1.30	0 100 100	23, 74, 130, 190	0
3	AD	208/208 (100%)	-1.24	1 (0%) 87 68	24, 72, 124, 159	0
3	CD	208/208 (100%)	-1.16	0 100 100	23, 85, 142, 184	0
4	AE	151/151 (100%)	-1.25	0 100 100	17, 48, 101, 156	0
4	CE	151/151 (100%)	-1.11	0 100 100	14, 58, 106, 151	0
5	AF	101/101 (100%)	-1.36	0 100 100	15, 50, 100, 133	0
5	CF	101/101 (100%)	-1.25	1 (0%) 79 56	29, 61, 123, 148	0
6	AG	155/155 (100%)	-1.22	0 100 100	30, 80, 139, 199	0
6	CG	155/155 (100%)	-1.08	0 100 100	38, 82, 137, 180	0
7	AH	138/138 (100%)	-1.25	0 100 100	28, 59, 103, 142	0
7	CH	138/138 (100%)	-1.20	0 100 100	25, 75, 121, 155	0
8	AI	127/127 (100%)	-1.22	0 100 100	0, 71, 117, 134	0
8	CI	127/127 (100%)	-1.03	0 100 100	0, 84, 149, 220	0
9	AJ	99/99 (100%)	-1.23	0 100 100	25, 62, 116, 159	0
9	CJ	99/99 (100%)	-1.18	0 100 100	31, 75, 127, 166	0
10	AK	119/119 (100%)	-1.15	0 100 100	31, 69, 116, 157	0
10	CK	119/119 (100%)	-1.05	2 (1%) 69 43	38, 72, 133, 151	0
11	AL	125/125 (100%)	-1.15	1 (0%) 82 60	10, 66, 120, 181	0
11	CL	125/125 (100%)	-0.96	1 (0%) 82 60	29, 69, 136, 170	0
12	AM	125/125 (100%)	-1.00	0 100 100	49, 86, 144, 212	0
12	CM	125/125 (100%)	-0.85	0 100 100	53, 100, 158, 223	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AN	60/60 (100%)	-1.17	0 100 100	28, 52, 87, 120	0
13	CN	60/60 (100%)	-1.25	0 100 100	39, 69, 117, 135	0
14	AO	88/88 (100%)	-1.37	0 100 100	22, 60, 114, 139	0
14	CO	88/88 (100%)	-1.32	0 100 100	25, 68, 119, 170	0
15	AP	84/84 (100%)	-1.23	0 100 100	26, 66, 109, 117	0
15	CP	84/84 (100%)	-1.12	0 100 100	52, 81, 127, 153	0
16	AQ	100/100 (100%)	-1.15	1 (1%) 79 56	0, 67, 117, 139	0
16	CQ	100/100 (100%)	-1.17	0 100 100	0, 68, 126, 150	0
17	AR	70/70 (100%)	-1.44	0 100 100	14, 54, 120, 154	0
17	CR	70/70 (100%)	-1.20	0 100 100	38, 63, 113, 155	0
18	AS	79/79 (100%)	-1.11	1 (1%) 75 50	47, 92, 136, 169	0
18	CS	79/79 (100%)	-1.15	0 100 100	44, 99, 145, 189	0
19	AT	99/99 (100%)	-1.25	0 100 100	0, 77, 128, 159	0
19	CT	99/99 (100%)	-1.07	0 100 100	0, 79, 131, 166	0
20	AY	687/687 (100%)	-1.16	1 (0%) 92 86	23, 84, 139, 174	0
20	CY	687/687 (100%)	-1.15	0 100 100	40, 92, 149, 204	0
21	AA	1511/1511 (100%)	-1.65	1 (0%) 92 86	15, 67, 145, 258	0
21	CA	1511/1511 (100%)	-1.61	0 100 100	18, 70, 157, 272	0
22	AW	77/77 (100%)	-1.69	0 100 100	32, 90, 174, 205	0
22	CW	77/77 (100%)	-1.68	0 100 100	39, 101, 193, 240	0
23	AV	23/23 (100%)	-1.20	0 100 100	41, 100, 156, 172	0
23	CV	23/23 (100%)	-0.87	0 100 100	41, 118, 186, 216	0
24	AU	2/6 (33%)	-1.17	0 100 100	114, 114, 114, 114	0
24	CU	2/6 (33%)	-1.10	0 100 100	119, 119, 119, 119	0
25	BC	228/228 (100%)	-1.20	1 (0%) 88 72	81, 124, 178, 222	0
25	DC	228/228 (100%)	-1.09	2 (0%) 81 58	102, 162, 214, 247	0
26	BD	275/275 (100%)	-1.15	0 100 100	11, 47, 102, 126	0
26	DD	275/275 (100%)	-1.12	0 100 100	23, 54, 107, 147	0
27	BE	205/205 (100%)	-1.18	0 100 100	19, 55, 101, 193	0
27	DE	205/205 (100%)	-1.11	0 100 100	12, 60, 120, 175	0
28	BF	208/208 (100%)	-1.13	0 100 100	16, 69, 131, 178	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
28	DF	208/208 (100%)	-1.02	0	100	100	34, 83, 176, 205	0
29	BG	181/181 (100%)	-1.18	0	100	100	41, 90, 132, 195	0
29	DG	181/181 (100%)	-1.22	0	100	100	44, 104, 159, 196	0
30	BH	167/167 (100%)	-1.31	0	100	100	21, 68, 123, 159	0
30	DH	167/167 (100%)	-1.29	0	100	100	36, 72, 140, 192	0
31	BJ	0/170	-	-			-	-
31	DJ	0/170	-	-			-	-
32	BK	140/140 (100%)	-1.12	1 (0%)	84	63	60, 114, 165, 206	0
32	DK	140/140 (100%)	-0.90	3 (2%)	63	38	72, 142, 197, 229	0
33	BN	138/138 (100%)	-1.02	0	100	100	59, 83, 108, 111	0
33	DN	138/138 (100%)	-0.99	0	100	100	61, 89, 110, 118	0
34	BO	122/122 (100%)	-1.32	0	100	100	23, 44, 90, 158	0
34	DO	122/122 (100%)	-1.29	0	100	100	26, 47, 96, 121	0
35	BP	146/146 (100%)	-1.07	0	100	100	23, 71, 132, 167	0
35	DP	146/146 (100%)	-0.89	1 (0%)	84	63	19, 88, 140, 212	0
36	BQ	141/141 (100%)	-1.15	0	100	100	32, 53, 103, 155	0
36	DQ	141/141 (100%)	-1.11	0	100	100	34, 58, 126, 178	0
37	BR	117/117 (100%)	-1.20	0	100	100	22, 57, 106, 123	0
37	DR	117/117 (100%)	-1.15	0	100	100	34, 67, 108, 138	0
38	BS	99/99 (100%)	-1.07	0	100	100	41, 104, 177, 190	0
38	DS	99/99 (100%)	-1.07	0	100	100	44, 114, 168, 203	0
39	BT	138/138 (100%)	-1.17	0	100	100	23, 68, 126, 162	0
39	DT	138/138 (100%)	-1.10	0	100	100	25, 71, 133, 177	0
40	BU	117/117 (100%)	-1.29	0	100	100	20, 45, 102, 140	0
40	DU	117/117 (100%)	-1.18	0	100	100	29, 54, 89, 222	0
41	BV	101/101 (100%)	-1.12	0	100	100	22, 58, 105, 172	0
41	DV	101/101 (100%)	-1.06	0	100	100	28, 60, 114, 177	0
42	BW	113/113 (100%)	-1.26	0	100	100	14, 43, 101, 135	0
42	DW	113/113 (100%)	-1.23	0	100	100	11, 60, 133, 215	0
43	BX	93/93 (100%)	-1.16	0	100	100	16, 55, 107, 137	0
43	DX	93/93 (100%)	-1.21	0	100	100	16, 66, 134, 180	0
44	BY	107/107 (100%)	-1.05	0	100	100	38, 88, 141, 193	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
44	DY	107/107 (100%)	-0.96	0	100	100	45, 96, 167, 200	0
45	BZ	185/185 (100%)	-1.32	0	100	100	36, 70, 124, 167	0
45	DZ	185/185 (100%)	-1.11	1 (0%)	87	68	48, 82, 136, 193	0
46	B0	84/84 (100%)	-1.00	0	100	100	24, 65, 112, 142	0
46	D0	84/84 (100%)	-1.06	0	100	100	47, 77, 140, 162	0
47	B2	71/71 (100%)	-1.40	0	100	100	34, 64, 118, 140	0
47	D2	71/71 (100%)	-1.21	0	100	100	33, 85, 127, 141	0
48	B3	60/60 (100%)	-1.25	0	100	100	28, 61, 116, 135	0
48	D3	60/60 (100%)	-1.10	0	100	100	32, 73, 137, 160	0
49	B5	59/59 (100%)	-1.31	0	100	100	22, 55, 125, 138	0
49	D5	59/59 (100%)	-1.15	0	100	100	29, 75, 130, 161	0
50	B6	50/50 (100%)	-1.15	0	100	100	36, 74, 120, 139	0
50	D6	50/50 (100%)	-1.04	0	100	100	49, 81, 143, 164	0
51	B7	49/49 (100%)	-0.99	0	100	100	43, 53, 102, 126	0
51	D7	49/49 (100%)	-1.13	0	100	100	34, 61, 112, 165	0
52	B8	64/64 (100%)	-1.01	0	100	100	22, 66, 108, 137	0
52	D8	64/64 (100%)	-1.08	0	100	100	33, 70, 118, 139	0
53	B9	37/37 (100%)	-1.01	0	100	100	39, 60, 122, 134	0
53	D9	37/37 (100%)	-1.10	0	100	100	46, 60, 134, 159	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%)	-1.05	0	100	100	22, 78, 160, 236	0
56	D1	93/93 (100%)	-0.90	0	100	100	41, 89, 159, 194	0
57	B4	35/35 (100%)	-1.32	0	100	100	67, 116, 167, 189	0
57	D4	35/35 (100%)	-1.19	0	100	100	73, 136, 168, 196	0
58	Be	72/102 (70%)	-1.22	0	100	100	77, 113, 160, 174	0
58	De	72/102 (70%)	-1.03	0	100	100	87, 141, 192, 236	0
59	BA	2879/2879 (100%)	-1.68	1 (0%)	100	100	9, 59, 146, 260	0
59	DA	2879/2879 (100%)	-1.61	0	100	100	5, 63, 160, 308	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
60	BB	119/119 (100%)	-1.58	0 100 100	36, 102, 157, 192	0
60	DB	119/119 (100%)	-1.71	0 100 100	33, 108, 159, 193	0
All	All	22726/23318 (97%)	-1.35	20 (0%) 92 86	0, 72, 150, 308	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
45	DZ	21	ALA	3.6
32	DK	61	ALA	3.4
32	DK	62	ASP	3.2
3	AD	84	LYS	3.0
25	DC	2	PRO	3.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
24	KBE	AU	1	9/10	0.98	0.11	114,114,114,114	0
24	UAL	AU	5	9/10	0.98	0.05	114,114,114,114	0
24	DPP	AU	2	6/7	0.99	0.06	114,114,114,114	0
24	DPP	CU	2	6/7	0.99	0.07	118,118,118,118	0
24	KBE	CU	1	9/10	0.99	0.09	118,118,118,118	0
24	UAL	CU	5	9/10	0.99	0.05	118,118,118,118	0
24	5OH	AU	6	12/13	0.99	0.07	99,101,102,102	0
24	5OH	CU	6	12/13	0.99	0.05	99,101,102,102	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column

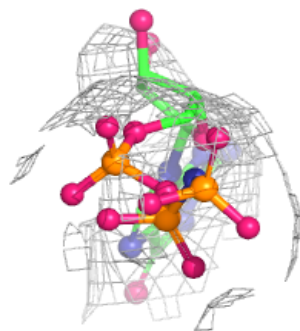
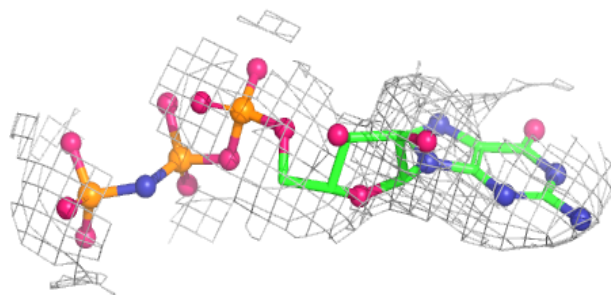
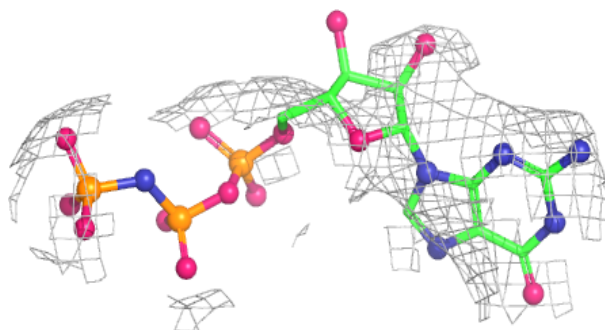
labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
61	GNP	AY	701	32/32	0.99	0.04	58,71,81,83	0
61	GNP	CY	701	32/32	0.99	0.05	58,71,81,83	0
62	MG	CY	702	1/1	0.99	0.03	135,135,135,135	0
62	MG	AY	702	1/1	1.00	0.05	88,88,88,88	0

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

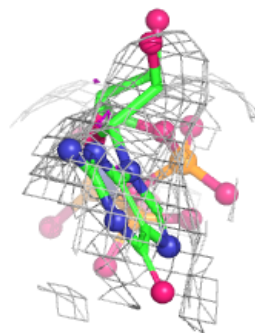
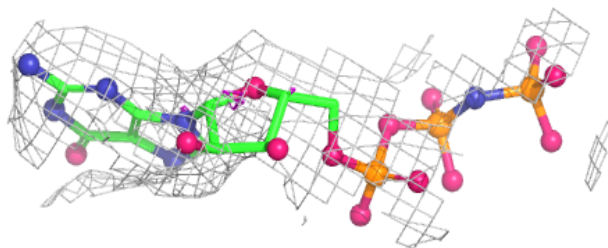
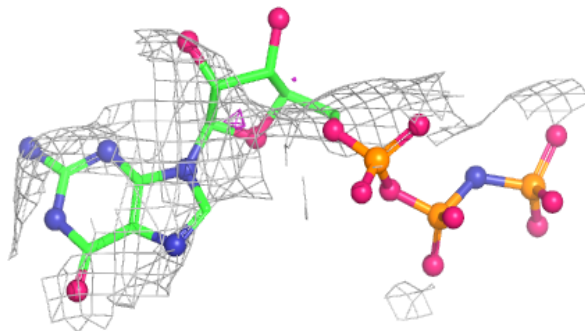
Electron density around GNP AY 701:

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



Electron density around GNP CY 701:

$2mF_o-DF_c$ (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.