



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 28, 2026 – 05:49 PM UTC

PDB ID : 4V9L / pdb_00004v9l
Title : 70S Ribosome translocation intermediate FA-3.6A containing elongation factor EFG/FUSIDIC ACID/GDP, mRNA, and tRNA bound in the pe^{*}/E state.
Authors : Zhou, J.; Lancaster, L.; Donohue, J.P.; Noller, H.F.
Deposited on : 2013-04-24
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

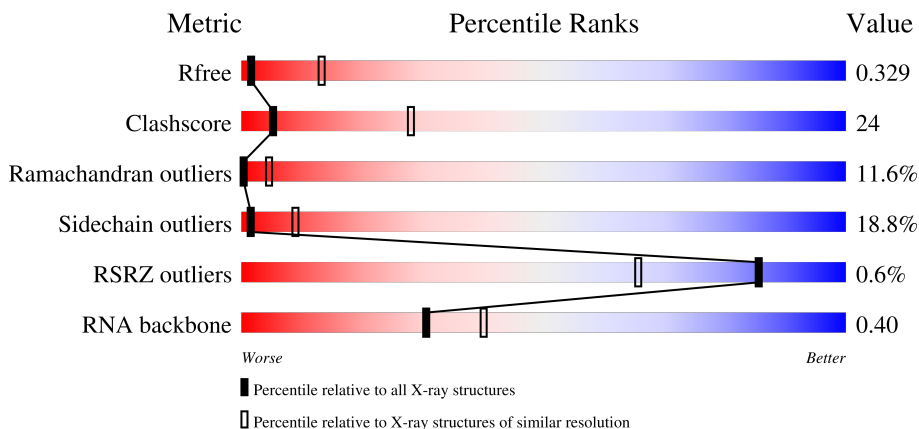
1 Overall quality at a glance

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.



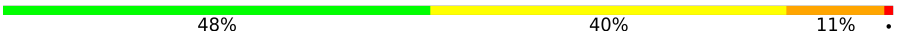
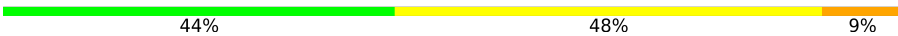
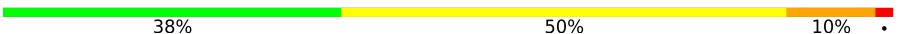
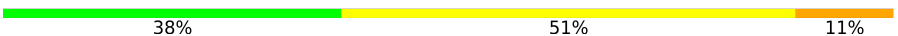
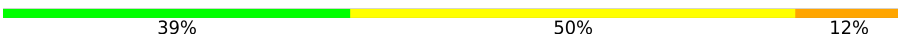
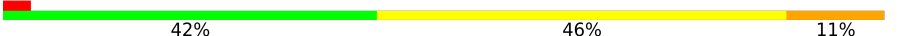
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)
RNA backbone	3983	1010 (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	32% 45% 19% .
1	CB	235	38% 42% 18% .
2	AC	207	37% 52% 10% .
2	CC	207	46% 46% 8%

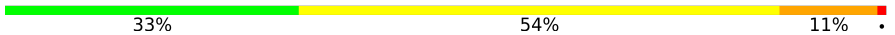
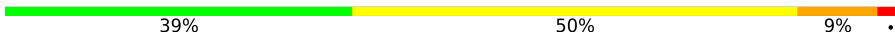
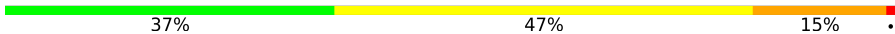
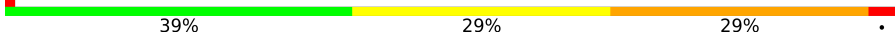
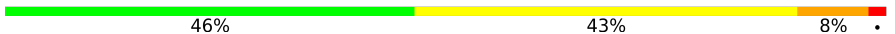
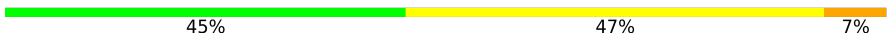
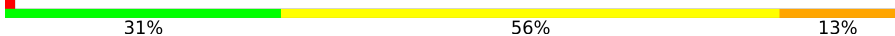
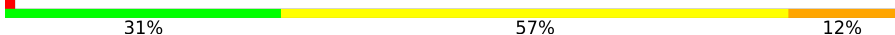
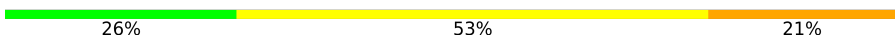
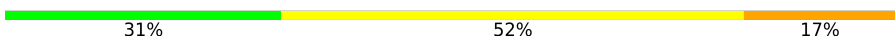
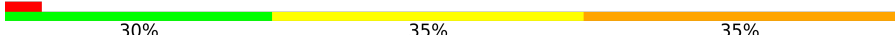
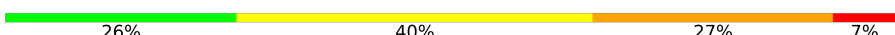
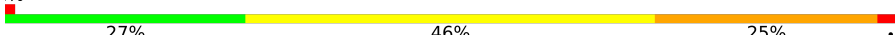
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Mol	Chain	Length	Quality of chain
3	AD	208	
3	CD	208	
4	AE	151	
4	CE	151	
5	AF	101	
5	CF	101	
6	AG	155	
6	CG	155	
7	AH	138	
7	CH	138	
8	AI	127	
8	CI	127	
9	AJ	99	
9	CJ	99	
10	AK	119	
10	CK	119	
11	AL	125	
11	CL	125	
12	AM	125	
12	CM	125	
13	AN	60	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

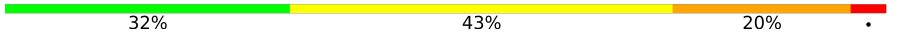
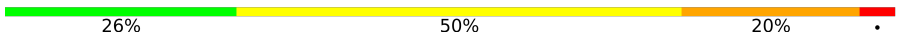
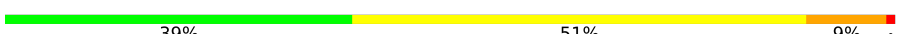
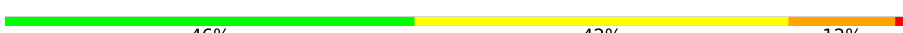
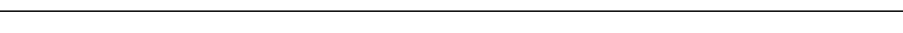
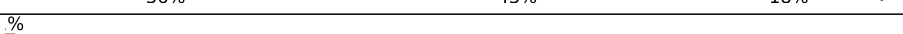
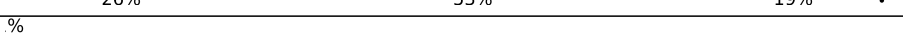
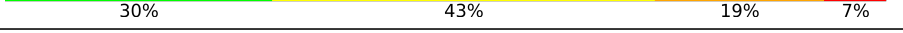
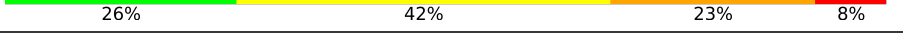
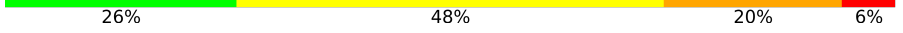
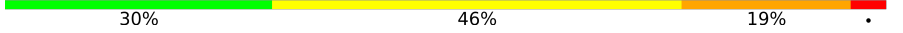
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Mol	Chain	Length	Quality of chain
15	CP	84	
16	AQ	100	
16	CQ	100	
17	AR	70	
17	CR	70	
18	AS	79	
18	CS	79	
19	AT	99	
19	CT	99	
20	AA	1511	
20	CA	1511	
21	AW	77	
21	CW	77	
22	AV	23	
22	CV	23	
23	AY	687	
23	CY	687	
24	AU	6	
24	CU	6	
25	BC	228	
25	DC	228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

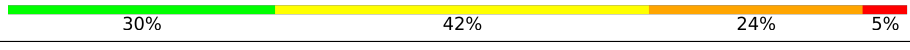
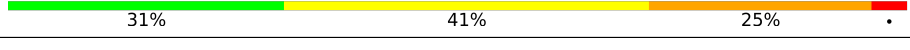
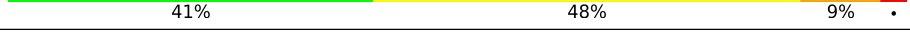
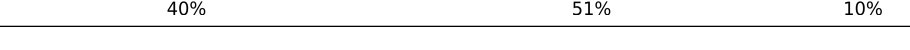
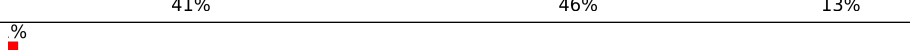
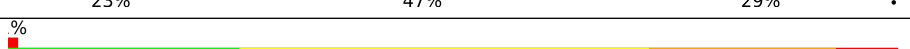
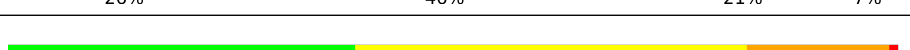
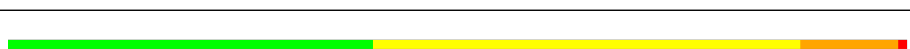
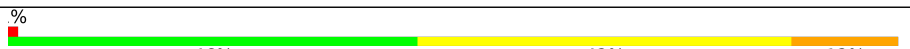
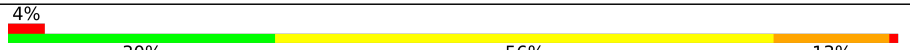
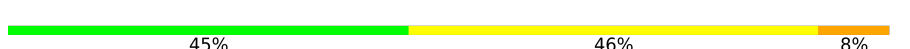
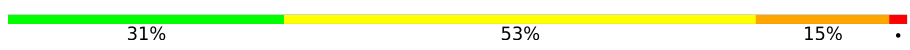
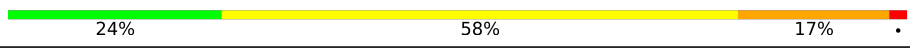
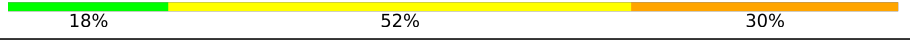
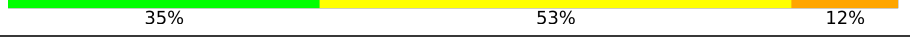
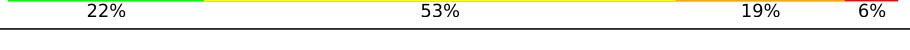
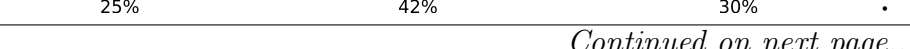
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Mol	Chain	Length	Quality of chain
28	BF	208	
28	DF	208	
29	BG	181	
29	DG	181	
30	BH	167	
30	DH	167	
31	BJ	170	
31	DJ	170	
32	BK	140	
32	DK	140	
33	BN	138	
33	DN	138	
34	BO	122	
34	DO	122	
35	BP	146	
35	DP	146	
36	BQ	141	
36	DQ	141	
37	BR	117	
37	DR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

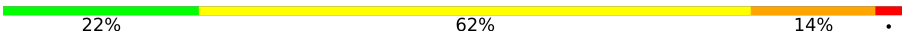
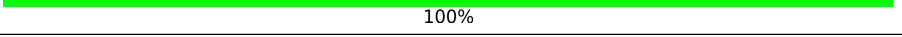
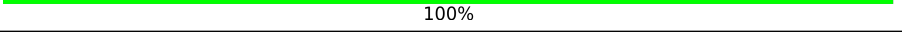
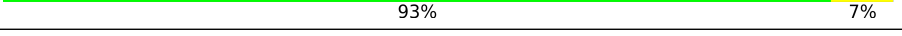
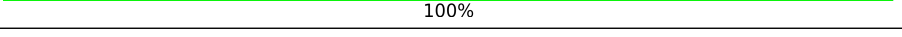
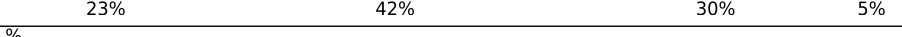
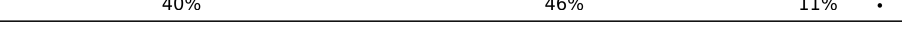
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Mol	Chain	Length	Quality of chain
40	DU	117	% 
41	BV	101	
41	DV	101	
42	BW	113	
42	DW	113	
43	BX	93	
43	DX	93	
44	BY	107	% 
44	DY	107	% 
45	BZ	185	
45	DZ	185	
46	B0	84	% 
46	D0	84	4% 
47	B2	71	
47	D2	71	
48	B3	60	
48	D3	60	
49	B5	59	
49	D5	59	
50	B6	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	Be	102	
54	De	102	
55	Bf	31	
55	Bg	31	
55	Df	31	
55	Dg	31	
56	Bh	30	
56	Dh	30	
57	B1	93	
57	D1	93	
58	B4	35	
58	D4	35	
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
62	GDP	AY	702	-	-	X	-
62	GDP	CY	702	-	-	X	-

2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 308166 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	AI	127	Total	C	N	O	0	0	0
			1010	639	197	174			
8	CI	127	Total	C	N	O	0	0	0
			1010	639	197	174			

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AQ	100	Total	C	N	O	S	0	0	0
			835	534	155	144	2			
16	CQ	100	Total	C	N	O	S	0	0	0
			835	534	155	144	2			

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			
19	CT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

- Molecule 21 is a RNA chain called transfer RNA.

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

- Molecule 22 is a RNA chain called messenger RNA.

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

- Molecule 23 is a protein called Elongation factor G.

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

- Molecule 24 is a protein called 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			
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
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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			
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			

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

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

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

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

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

- Molecule 57 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	B1	93	Total	C	N	O	S	0	0	0
			732	460	145	126	1			
57	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 58 is a protein called 50S ribosomal protein L31.

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

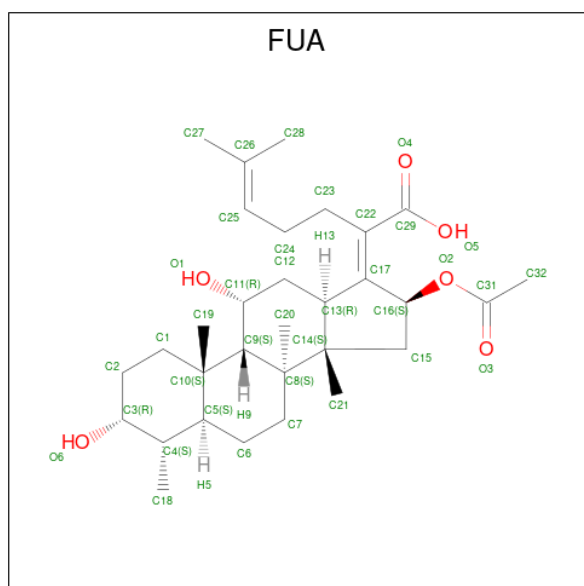
- Molecule 59 is a RNA chain called 23S ribosomal RNA.

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

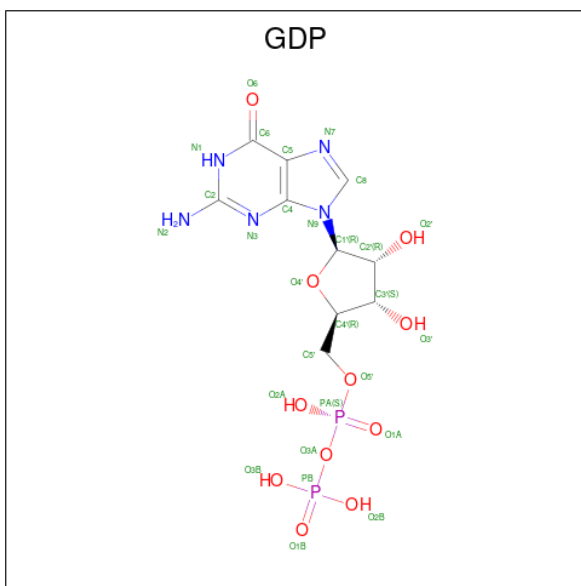
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
60	BB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			
60	DB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

- Molecule 61 is FUSIDIC ACID (CCD ID: FUA) (formula: $C_{31}H_{48}O_6$).



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

- Molecule 62 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
62	AY	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
62	CY	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

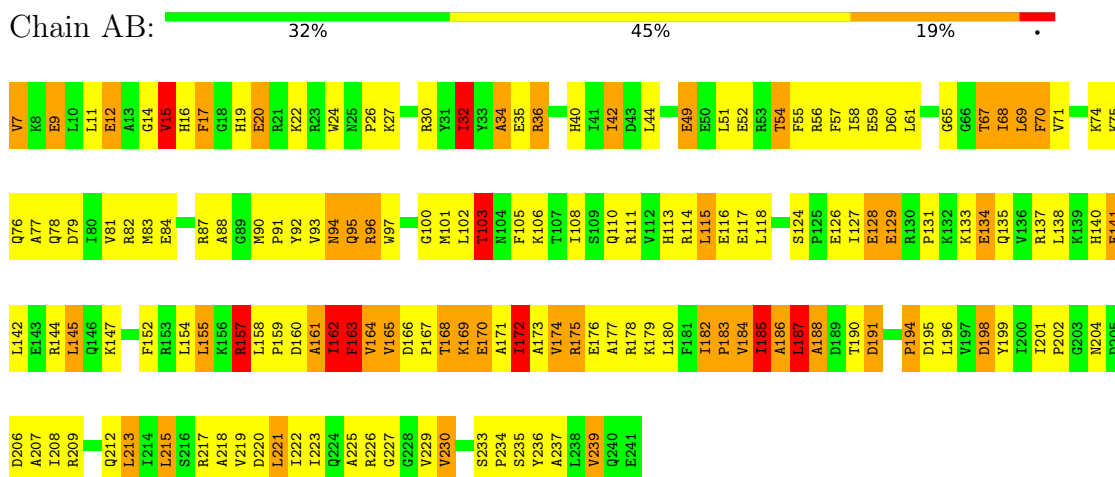
- Molecule 63 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	BA	1	Total	Mg	0	0
			1	1		
63	CY	1	Total	Mg	0	0
			1	1		

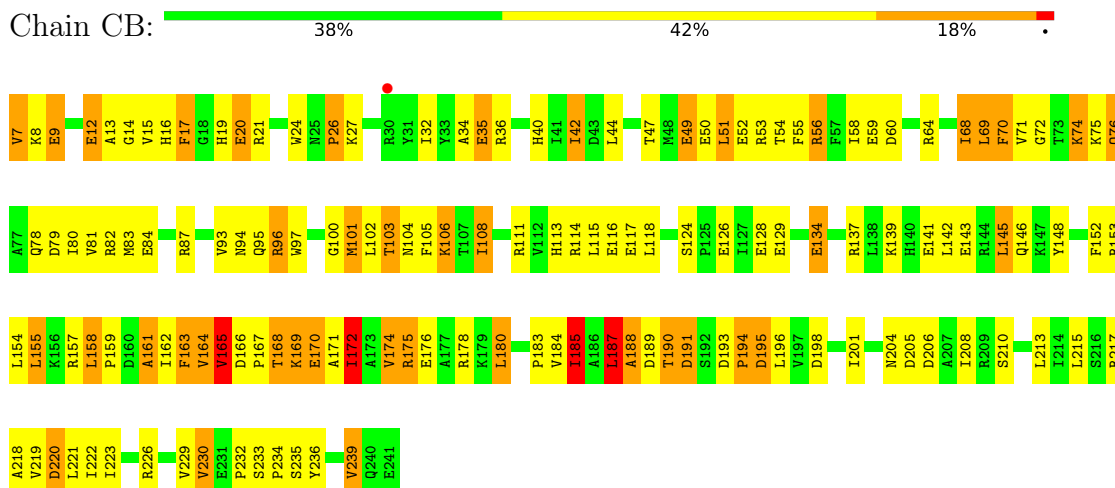
3 Residue-property plots

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

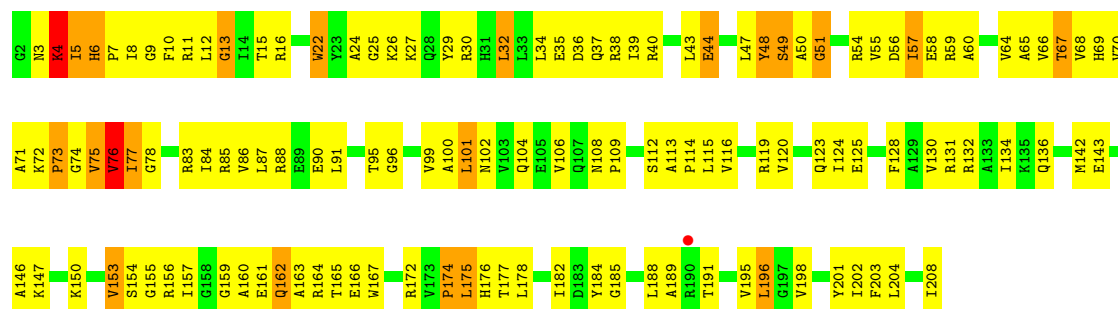


• Molecule 1: 30S ribosomal protein S2

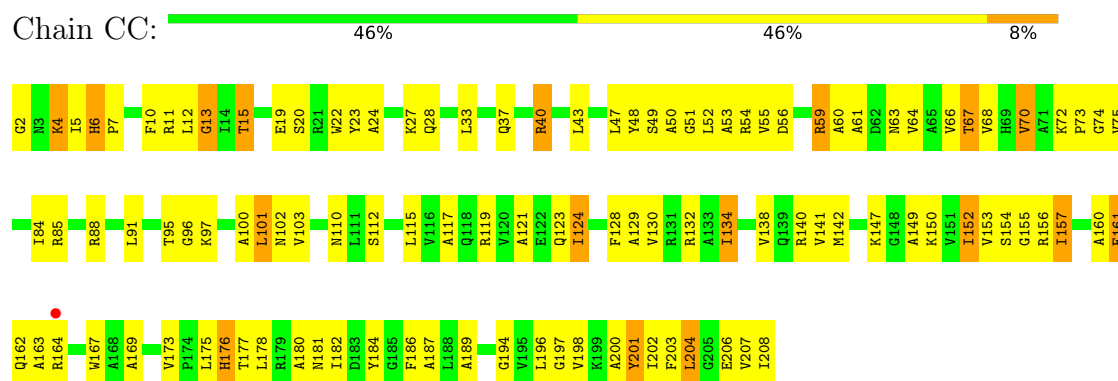


• Molecule 2: 30S ribosomal protein S3

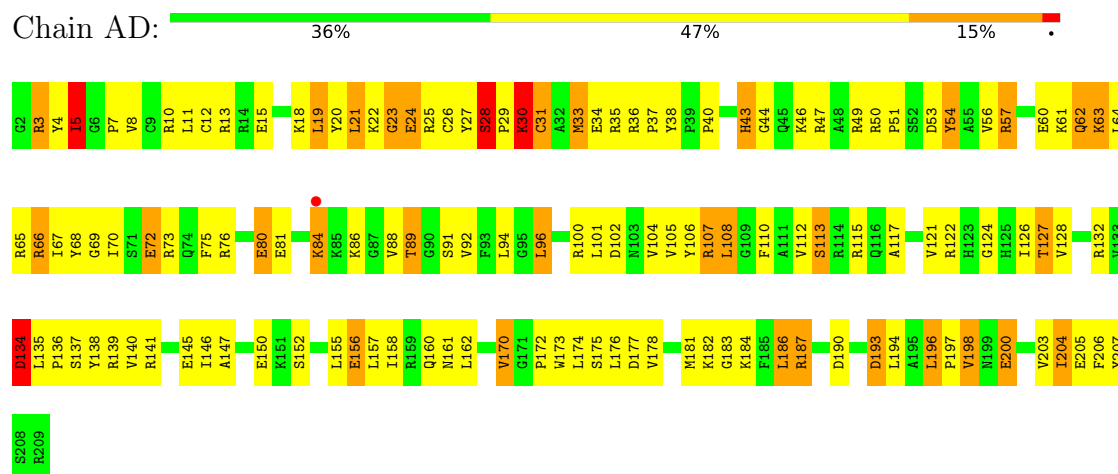




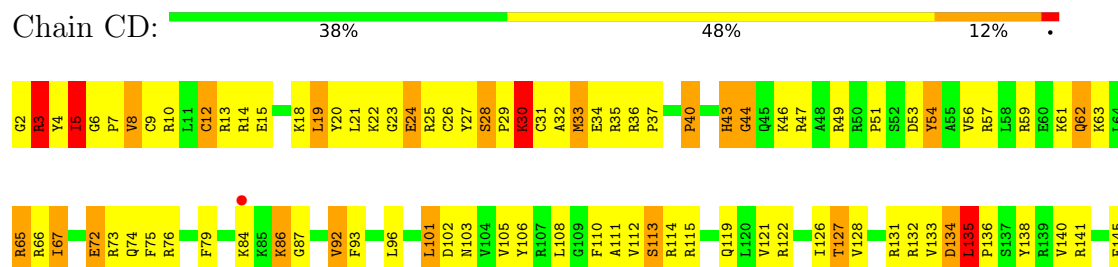
• Molecule 2: 30S ribosomal protein S3



• Molecule 3: 30S ribosomal protein S4

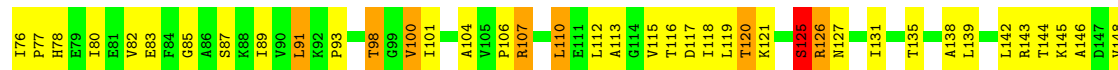


• Molecule 3: 30S ribosomal protein S4





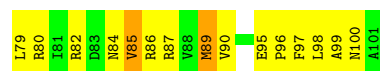
• Molecule 4: 30S ribosomal protein S5



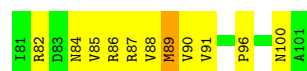
• Molecule 4: 30S ribosomal protein S5



• Molecule 5: 30S ribosomal protein S6

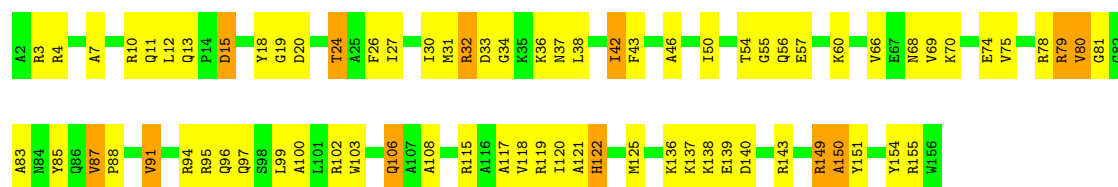


• Molecule 5: 30S ribosomal protein S6



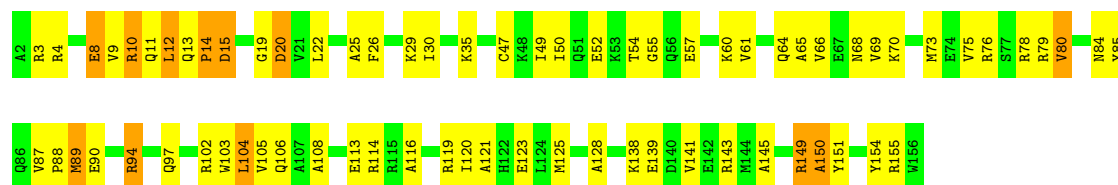
• Molecule 6: 30S ribosomal protein S7

Chain AG: 

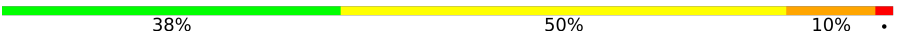


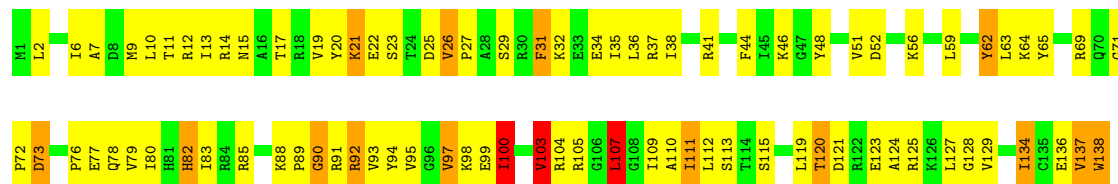
- Molecule 6: 30S ribosomal protein S7

Chain CG: 



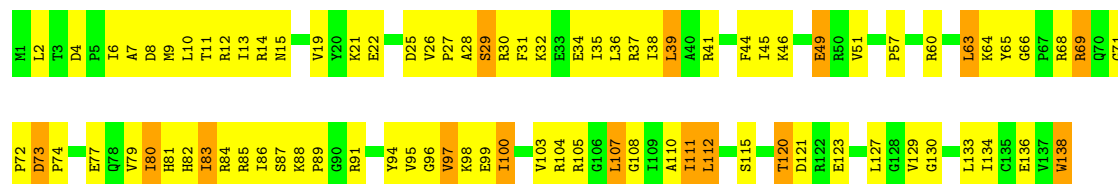
- Molecule 7: 30S ribosomal protein S8

Chain AH: 



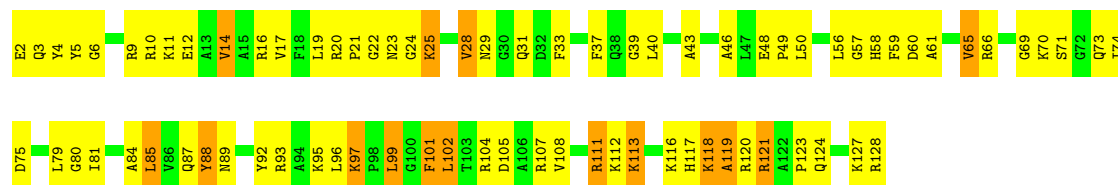
- Molecule 7: 30S ribosomal protein S8

Chain CH: 

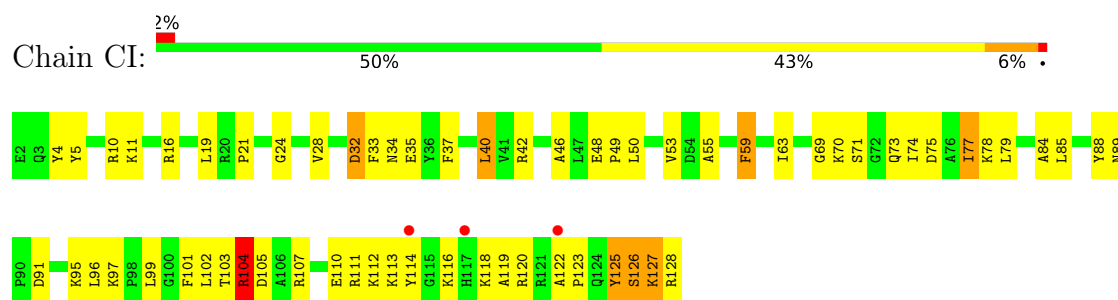


- Molecule 8: 30S ribosomal protein S9

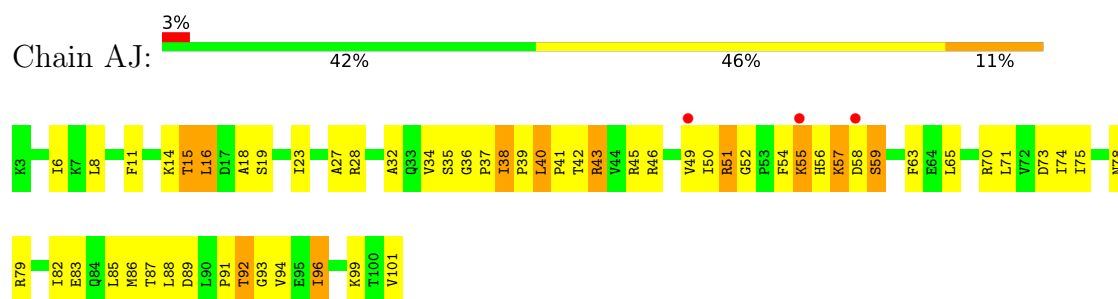
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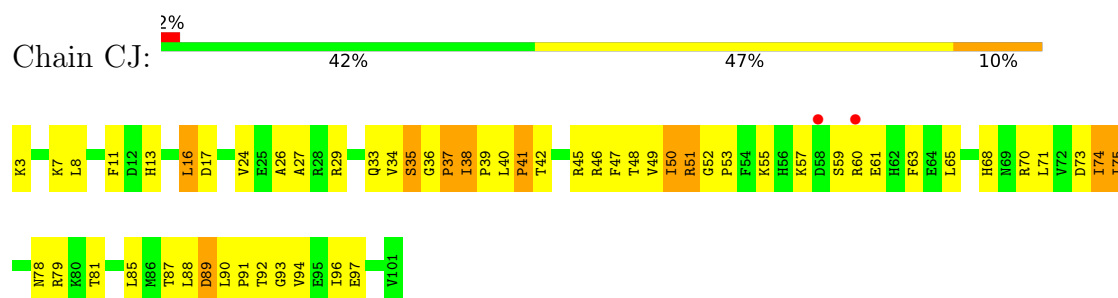
- Molecule 8: 30S ribosomal protein S9



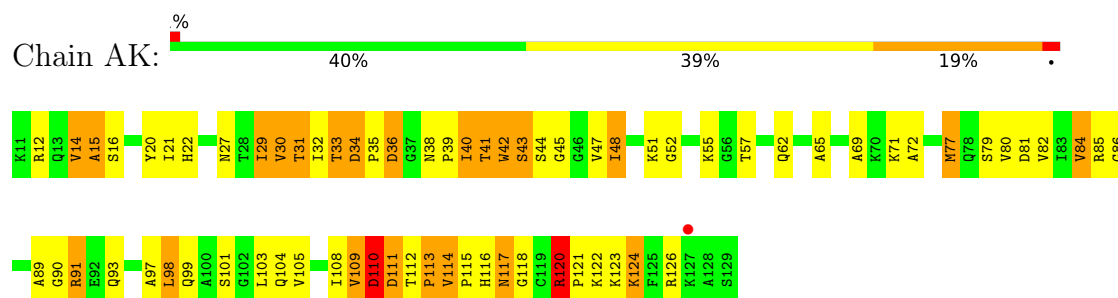
• Molecule 9: 30S ribosomal protein S10



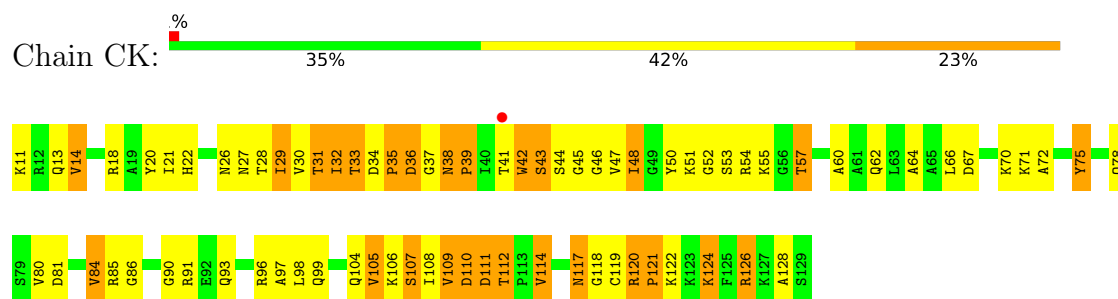
• Molecule 9: 30S ribosomal protein S10



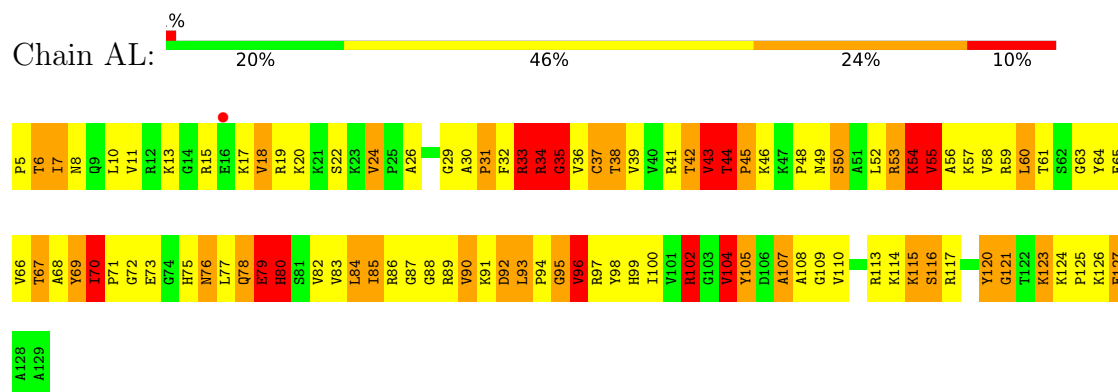
• Molecule 10: 30S ribosomal protein S11



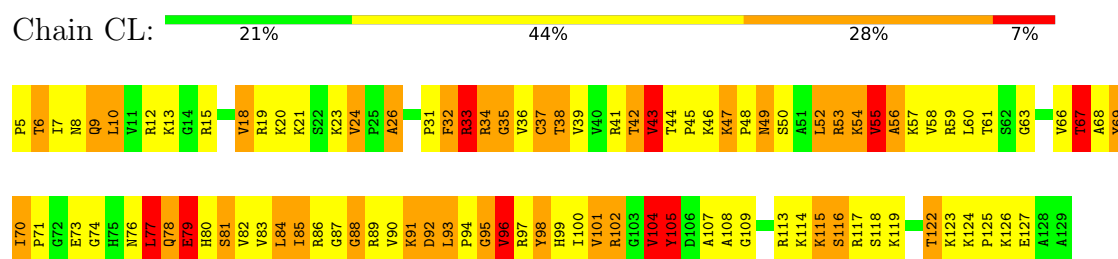
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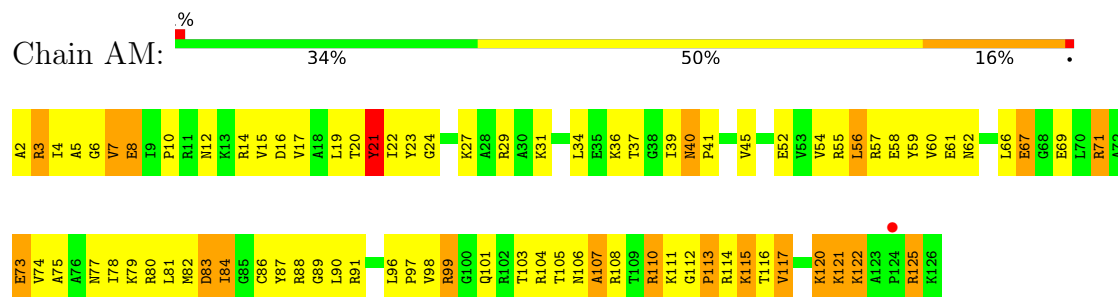
• Molecule 11: 30S ribosomal protein S12



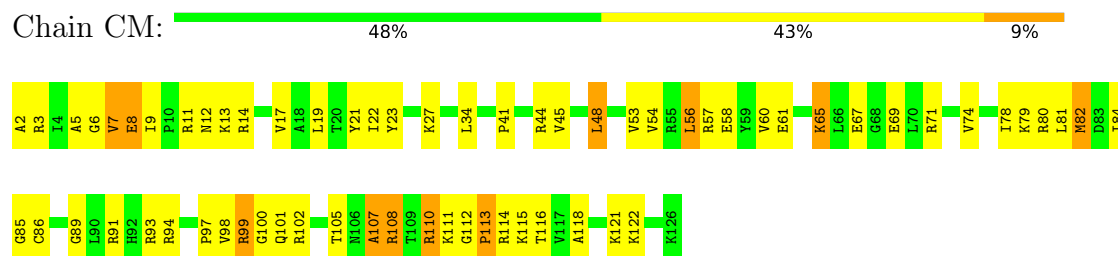
• Molecule 11: 30S ribosomal protein S12



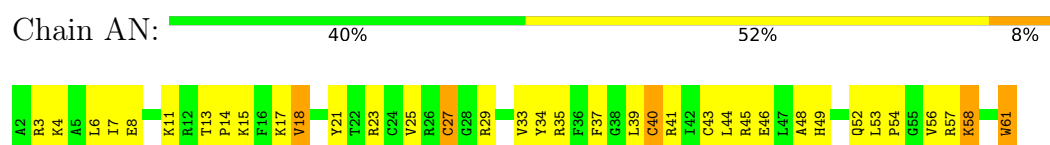
• Molecule 12: 30S ribosomal protein S13



• Molecule 12: 30S ribosomal protein S13

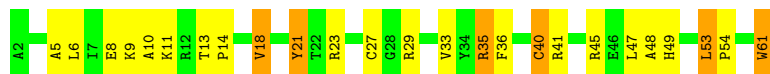


• Molecule 13: 30S ribosomal protein S14 type Z



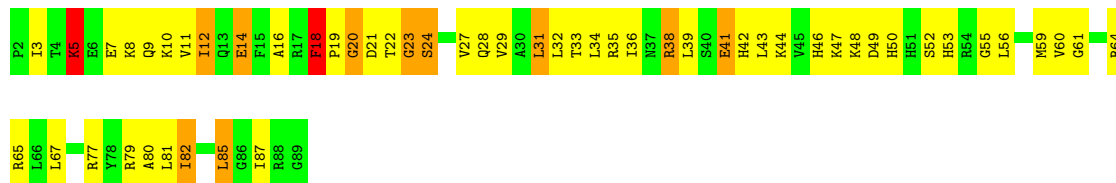
- Molecule 13: 30S ribosomal protein S14 type Z

Chain CN:  58% 32% 10%



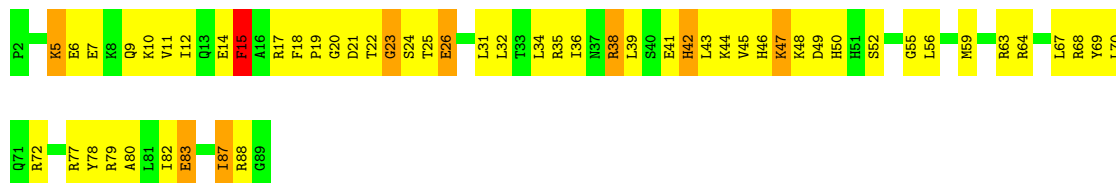
- Molecule 14: 30S ribosomal protein S15

Chain AO:  39% 48% 11%

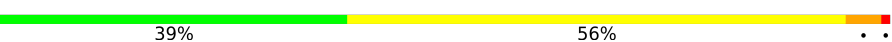


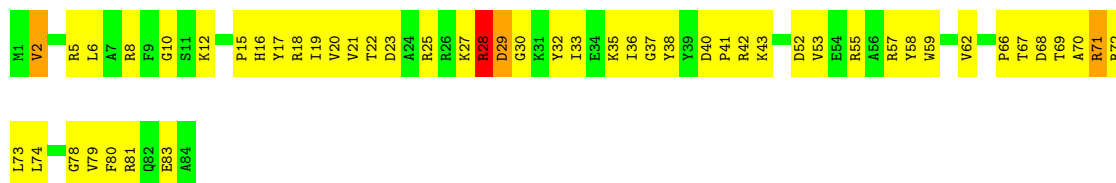
- Molecule 14: 30S ribosomal protein S15

Chain CO:  38% 52% 9%



- Molecule 15: 30S ribosomal protein S16

Chain AP:  39% 56%



- Molecule 15: 30S ribosomal protein S16

Chain CP:  52% 38% 10%

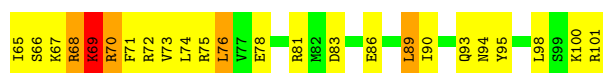
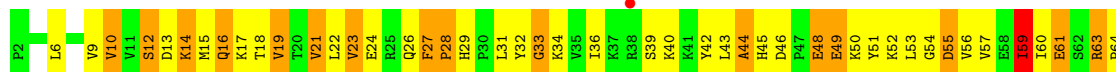


- Molecule 16: 30S ribosomal protein S17

Chain AQ:  32% 54% 12%



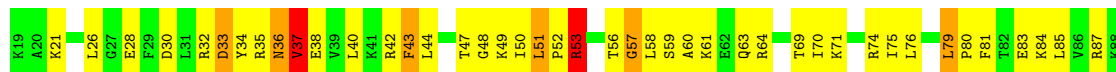
- Molecule 16: 30S ribosomal protein S17



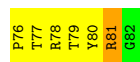
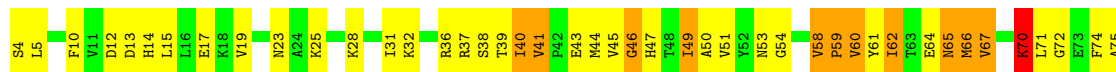
- Molecule 17: 30S ribosomal protein S18



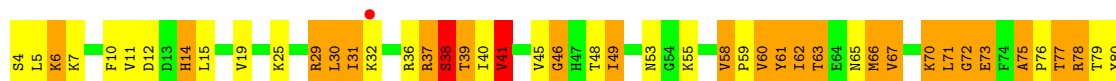
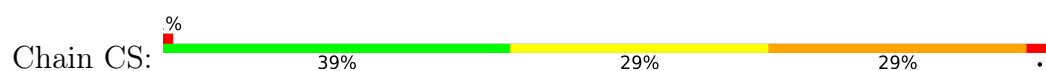
- Molecule 17: 30S ribosomal protein S18



- Molecule 18: 30S ribosomal protein S19



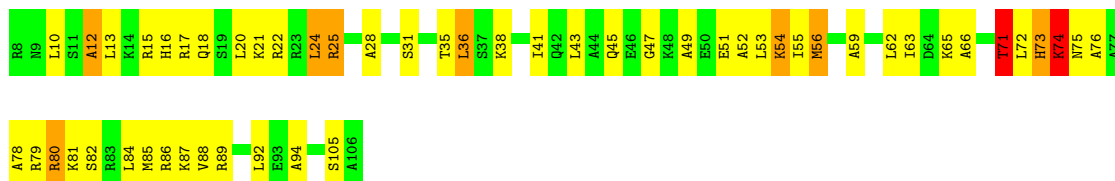
- Molecule 18: 30S ribosomal protein S19



R81
G82

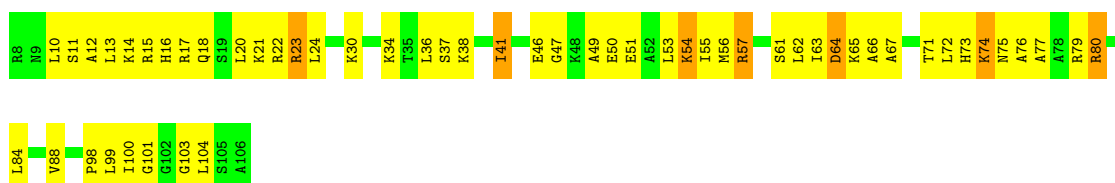
- Molecule 19: 30S ribosomal protein S20

Chain AT: 46% 43% 8%



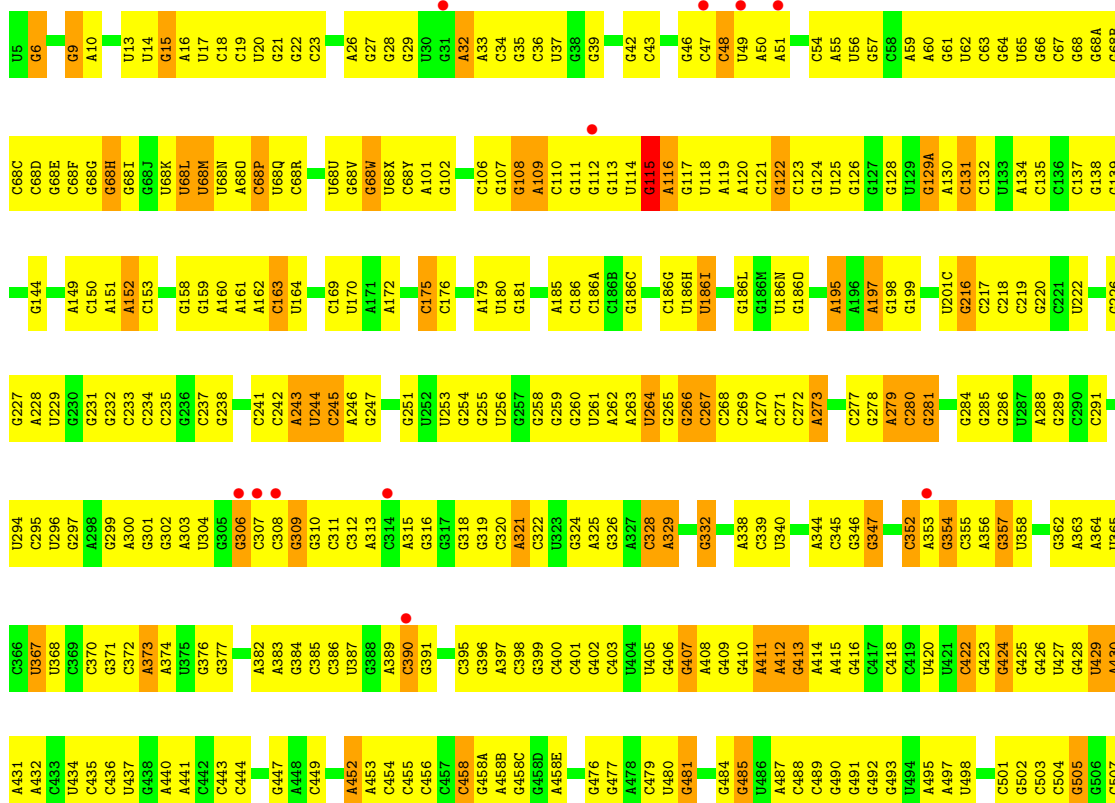
- Molecule 19: 30S ribosomal protein S20

Chain CT: 45% 47% 7%



- Molecule 20: ribosomal RNA 16S

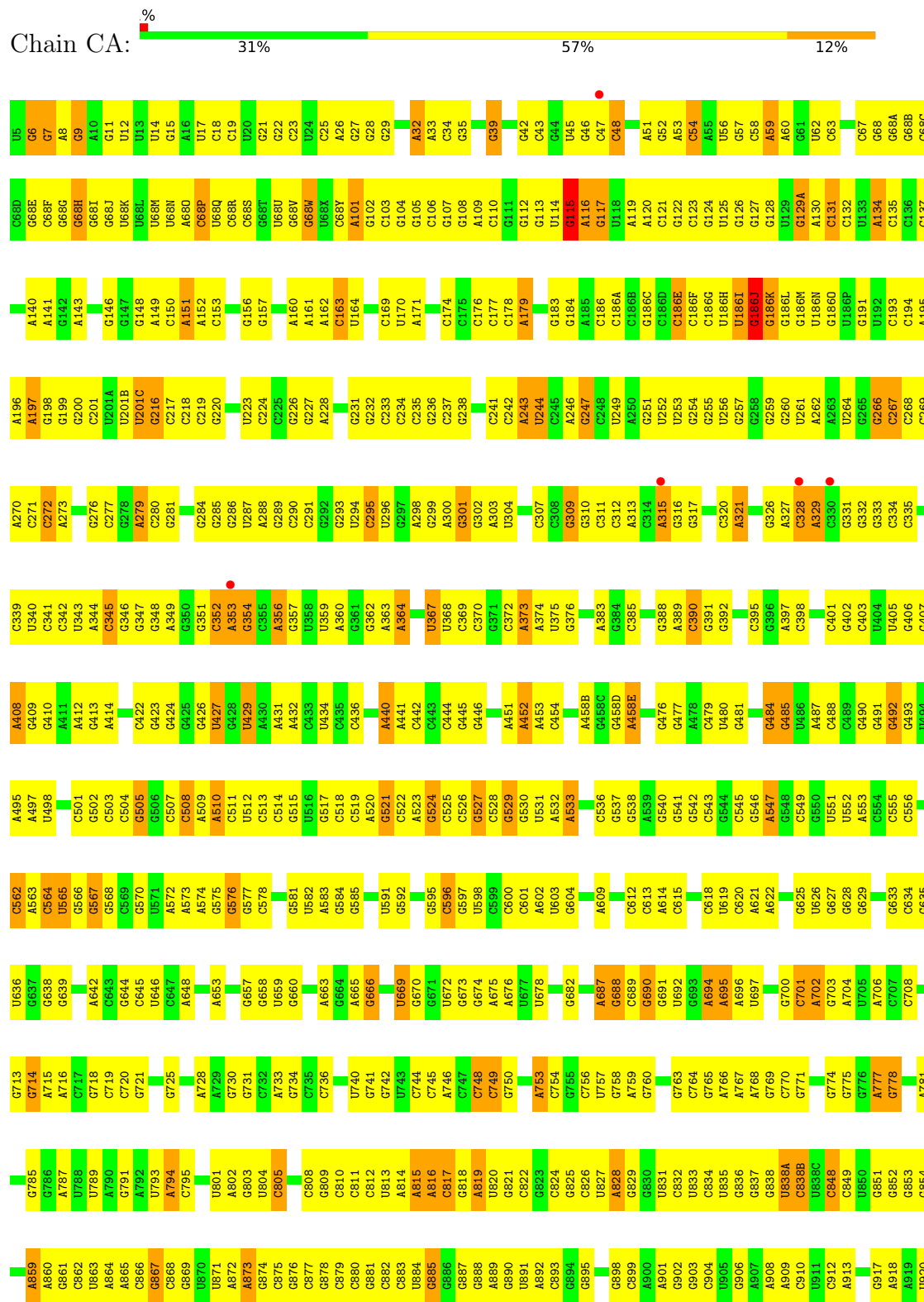
Chain AA: 31% 56% 13%

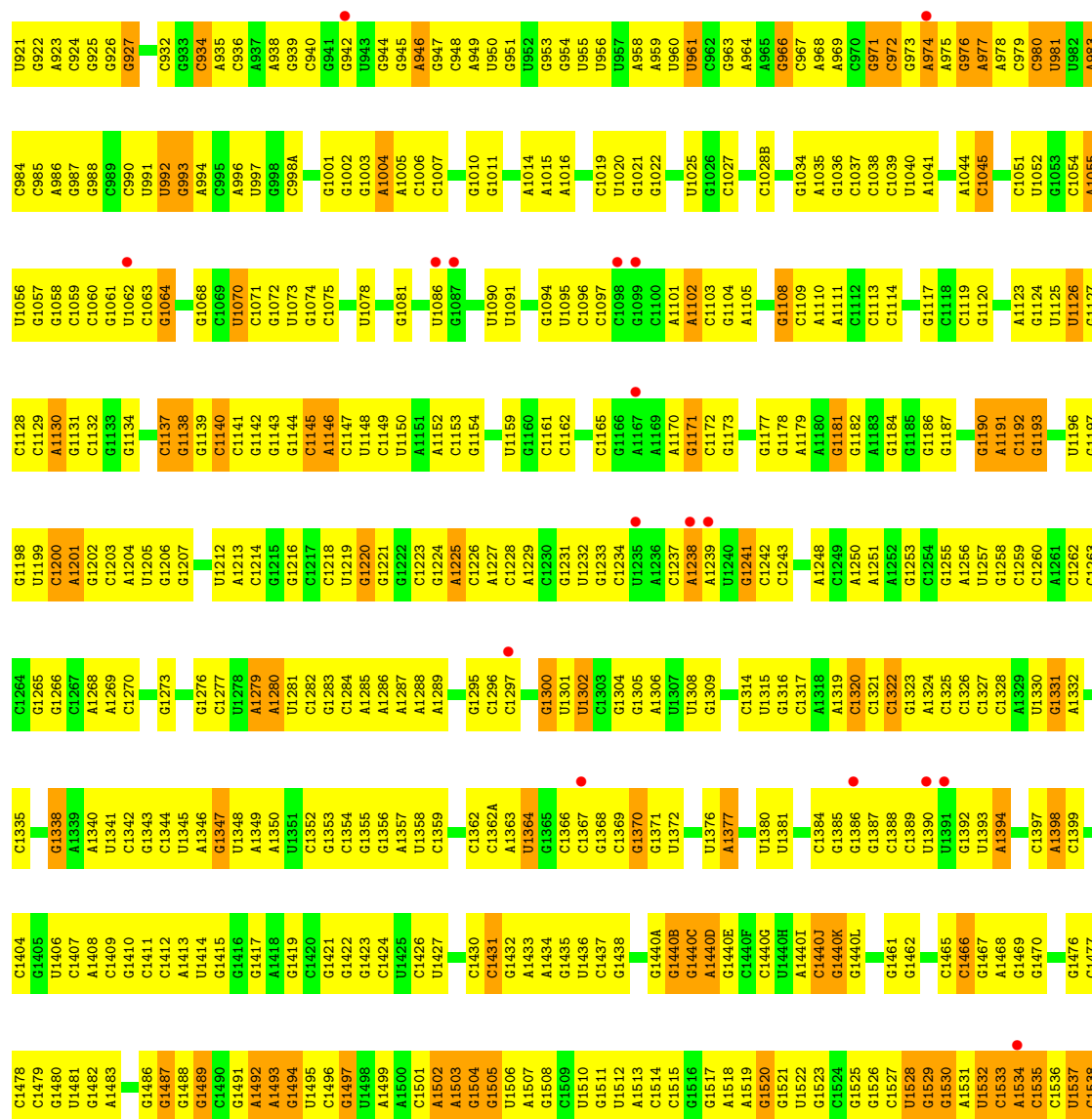


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G1353	G1354	G1355	G1356	G1357	G1358	G1359	G1359	G1295	A1226	A1151	G1082	U1012	G945	U870	C763	G713	C643	G574	C513
A1288	A1289	A1290	G1291	A1357	A1358	G1360	G1360	G1299	A1227	A1152	U1083	G1013	A946	A873	G714	G714	G644	G575	C514
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G1418	G1419	G1420	G1421	G1422	G1423	G1424	G1424	A1308	A1242	A1164	C1098	A1041	U960	A889	A728	G725	G664	G586	C525
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G1719	G1720	G1721	G1722	G1723	G1724	G1725	G1725	A1351	A1287	A1207	C1145	A1083	U1003	C850	C636	G770	G707	G635	C569
G1726	G1727	G1728	G1729	G1730	G1731	G1732	G1732	A1352	A1288	A1208	G1146	A1084	U1004	C851	C637	G771	G708	G636	C570
G1733	G1734	G1735	G1736	G1737	G1738	G1739	G1739	A1353	A1289	A1209	C1146	A1085	U1005	C852	C638	G772	G709	G637	C571
G1740	G1741	G1742	G1743	G1744	G1745	G1746	G1746	A1354	A1290	A1210	G1147	A1086	U1006	C853	C639	G773	G710	G638	C572
G1747	G1748	G1749	G1750	G1751	G1752	G1753	G1753	A1355	A1291	A1211	C1148	A1087	U1007	C854	C640	G774	G711	G639	C573
G1754	G1755	G1756	G1757	G1758	G1759	G1760	G1760	A1356	A1292	A1212	G1149	A1088	U1008	C855	C641	G775	G712	G640	C574
G1761	G1762	G1763	G1764	G1765	G1766	G1767	G1767	A1357	A1293	A1213	C1149	A1089	U1009	C856	C642	G776	G713	G641	C575
G1768	G1769	G1770	G1771	G1772	G1773	G1774	G1774	A1358	A1294	A1214	G1150	A1090	U1010	C857	C643	G777	G714	G642	C576
G1775	G1776	G1777	G1778	G1779	G1780	G1781	G1781	A1359	A1295	A1215	C1150	A1091	U1011	C858	C644	G778	G715	G643	C577
G1782	G1783	G1784	G1785	G1786	G1787	G1788	G1788	A1360	A1296	A1216	C1151	A1092	U1012	C859	C645	G779	G716	G644	C578
G1789	G1790	G1791	G1792	G1793	G1794	G1795	G1795	A1361	A1297	A1217	G1151	A1093	U1013	C860	C646	G780	G717	G645	C579
G1796	G1797	G1798	G1799	G1800	G1801	G1802	G1802	A1362	A1298	A1218	C1152	A1094	U1014	C861	C647	G781	G718	G646	C580
G1803	G1804	G1805	G1806	G1807	G1808	G1809	G1809	A1363	A1299	A1219	U1085	A1095	U1015	C862	C648	G782	G719	G647	A520
G1810	G1811	G1812	G1813	G1814	G1815	G1816	G1816	A1364	A1300	A1220	U1086	A1096	U1016	C863	C649	G783	G720	G648	A521
G1817	G1818	G1819	G1820	G1821	G182														



● Molecule 20: ribosomal RNA 16S





C75
A76

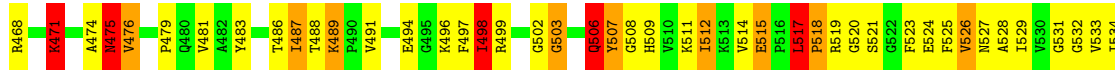
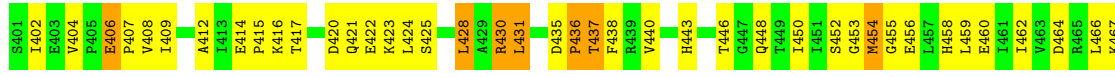
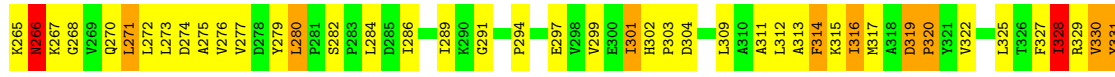
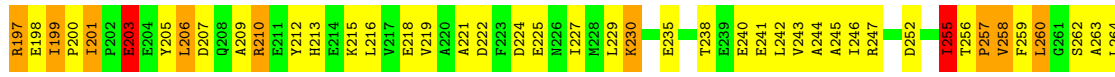
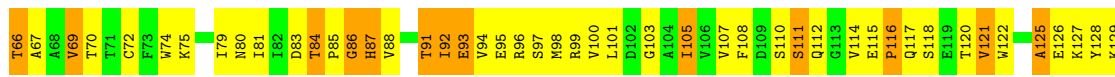
- Molecule 22: messenger RNA

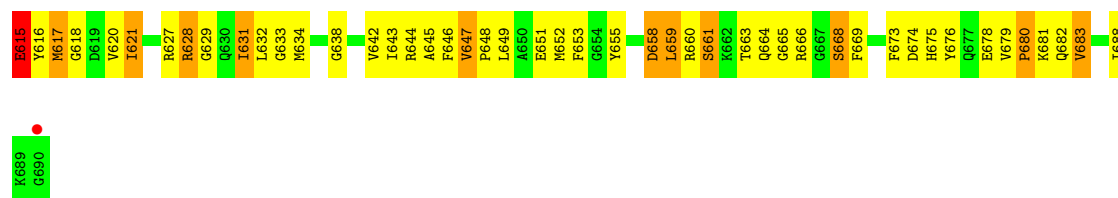


- Molecule 22: messenger RNA

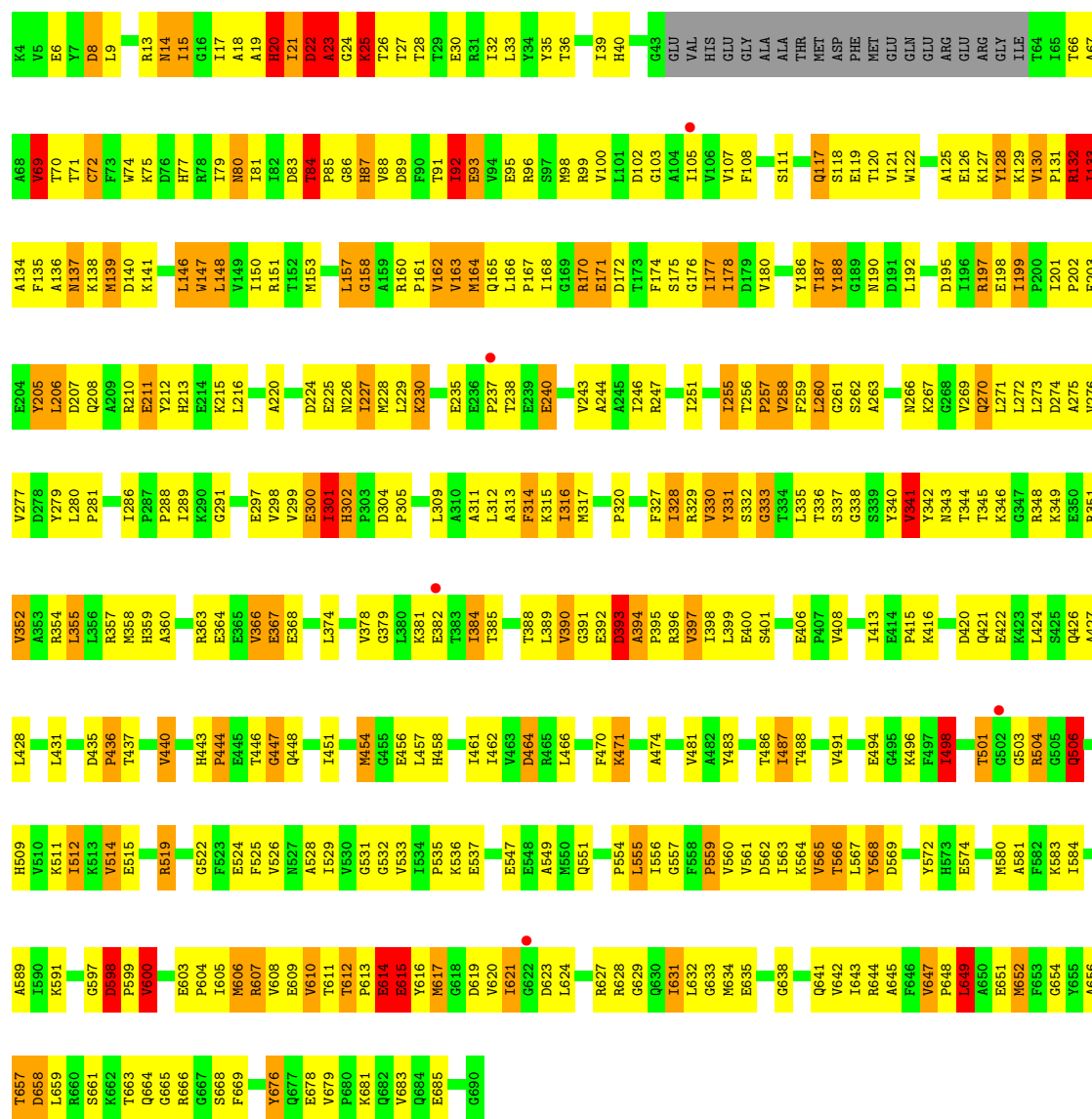
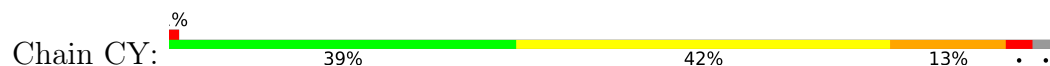


- Molecule 23: Elongation factor G





• Molecule 23: Elongation factor G

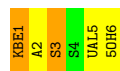


• Molecule 24: VIOMYCIN



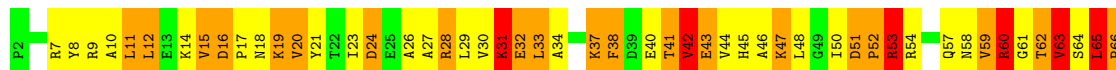
- Molecule 24: VIOMYCIN

Chain CU: 



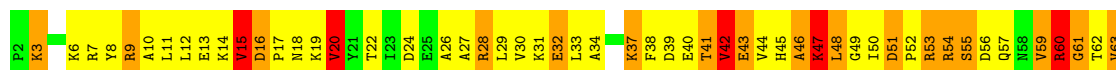
- Molecule 25: 50S ribosomal protein L1

Chain BC: 

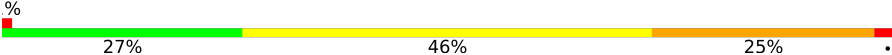


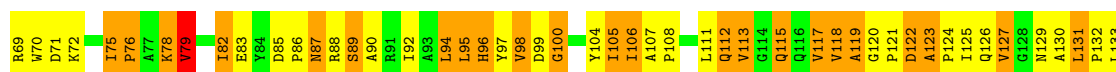
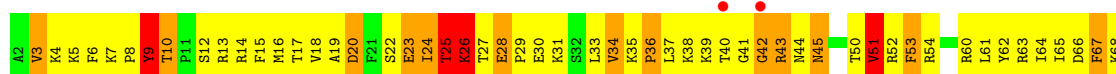
- Molecule 25: 50S ribosomal protein L1

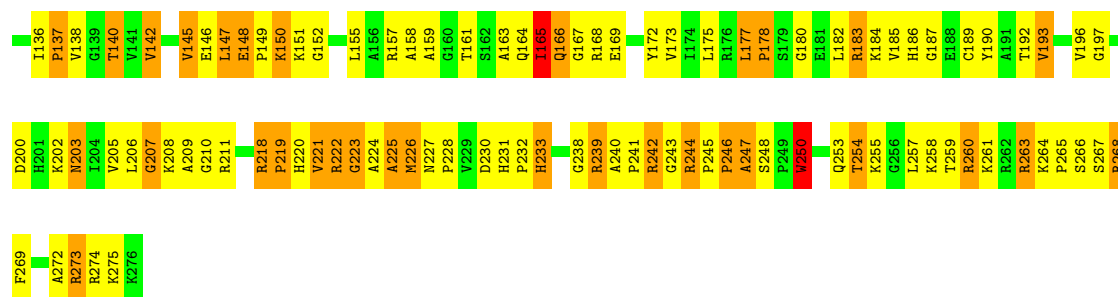
Chain DC: 



- Molecule 26: 50S ribosomal protein L2

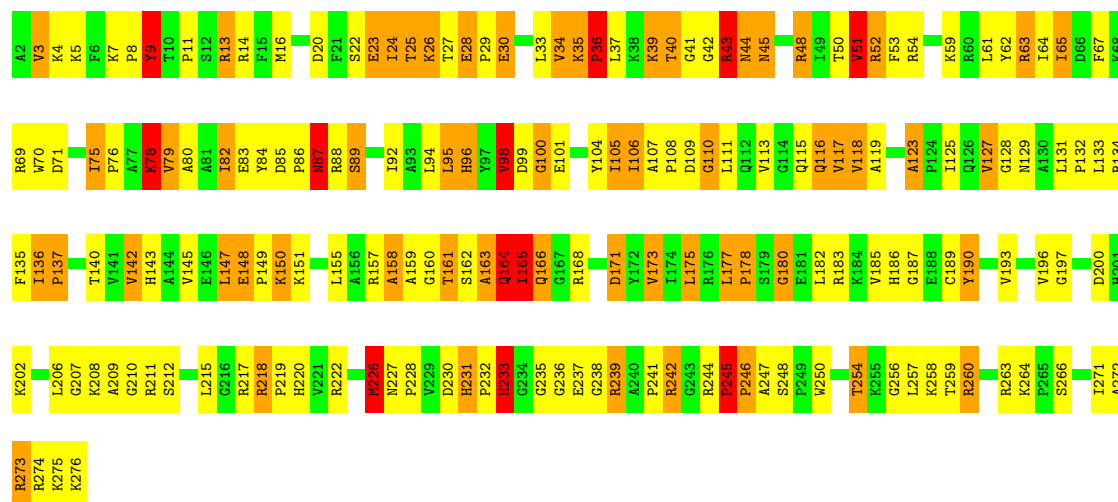
Chain BD: 





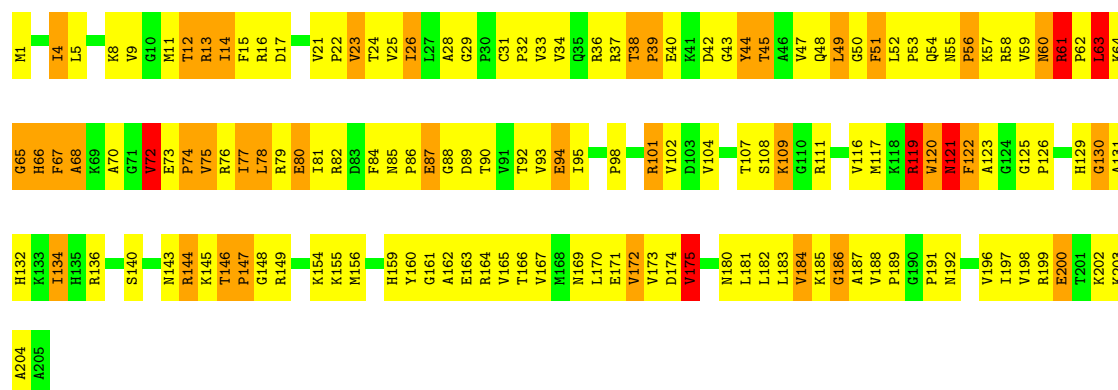
- Molecule 26: 50S ribosomal protein L2

Chain DD: 34% 41% 21% .



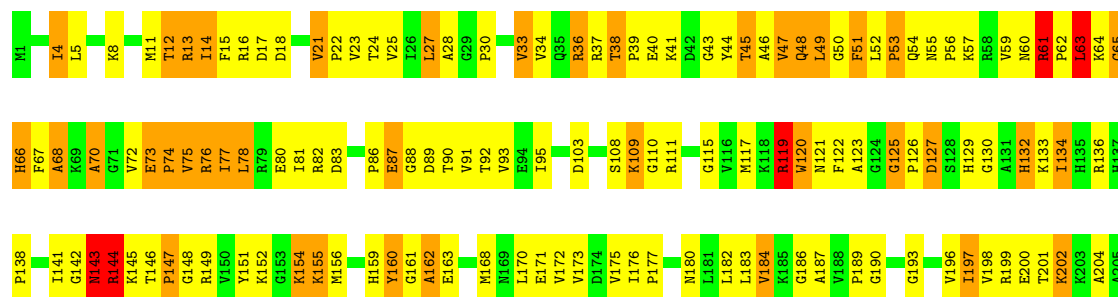
- Molecule 27: 50S ribosomal protein L3

Chain BE: 28% 51% 19% .

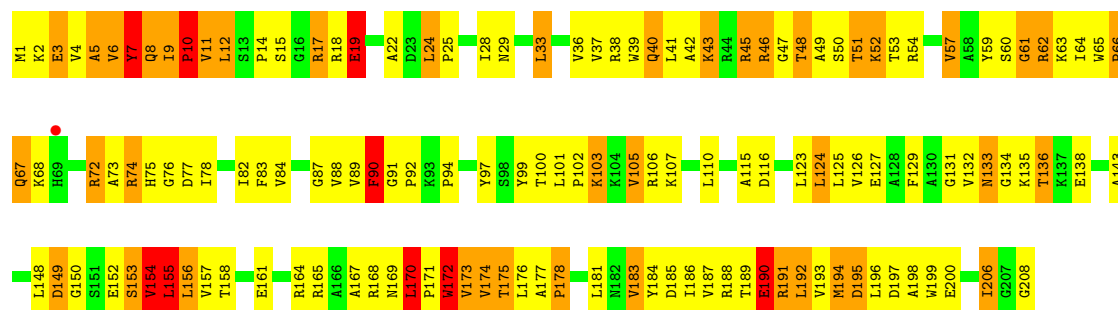


- Molecule 27: 50S ribosomal protein L3

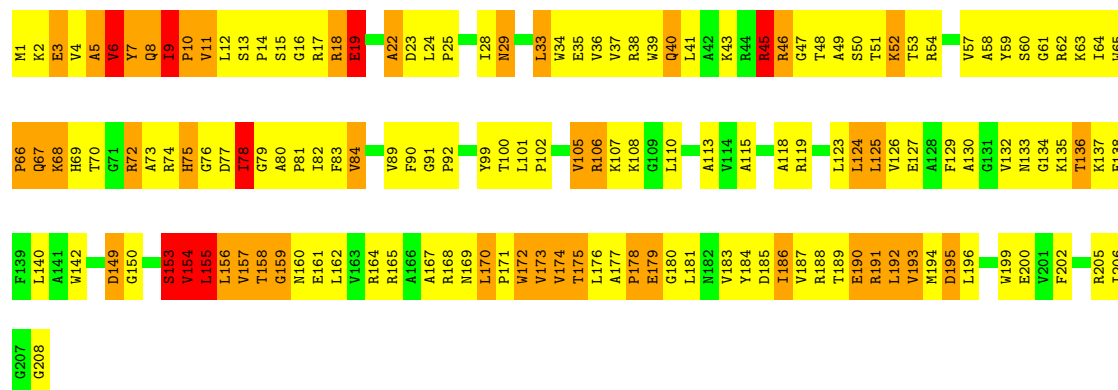
Chain DE: 32% 46% 20% .



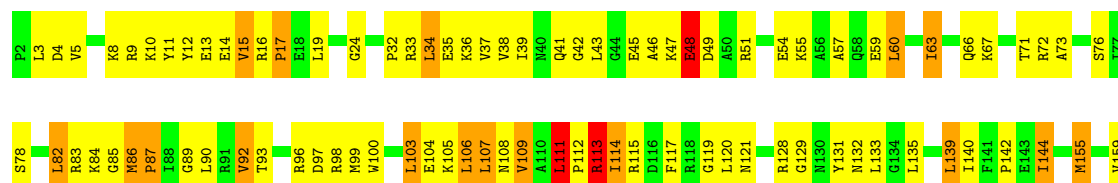
• Molecule 28: 50S ribosomal protein L4



• Molecule 28: 50S ribosomal protein L4

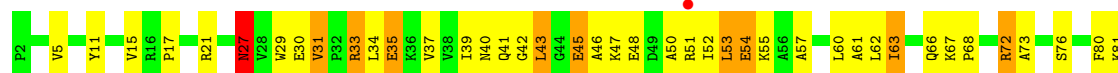


• Molecule 29: 50S ribosomal protein L5





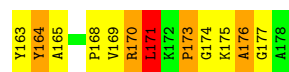
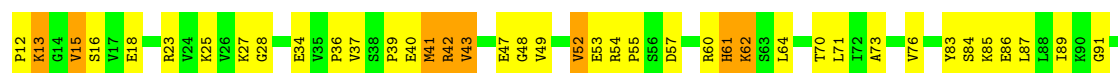
- Molecule 29: 50S ribosomal protein L5



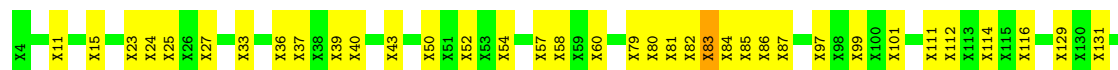
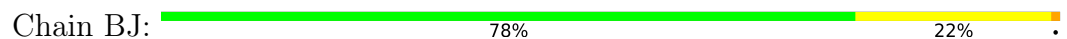
- Molecule 30: 50S ribosomal protein L6

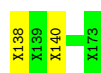


- Molecule 30: 50S ribosomal protein L6



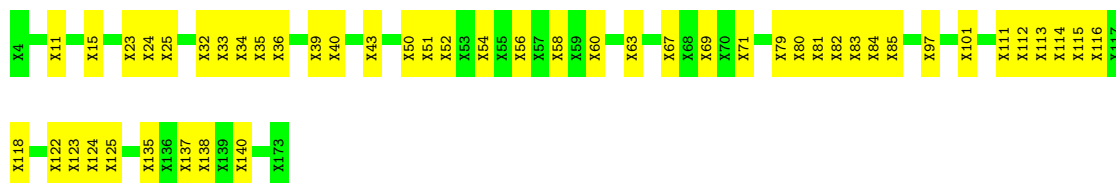
- Molecule 31: 50S RIBOSOMAL PROTEIN L10





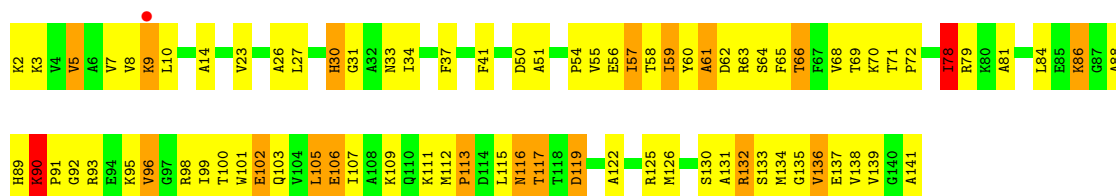
• Molecule 31: 50S RIBOSOMAL PROTEIN L10

Chain DJ: 72% 28%



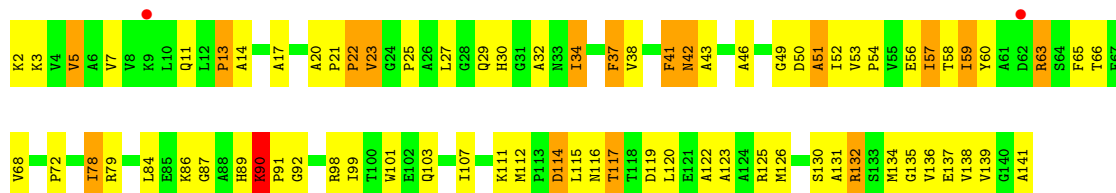
• Molecule 32: 50S ribosomal protein L11

Chain BK: 42% 44% 13%



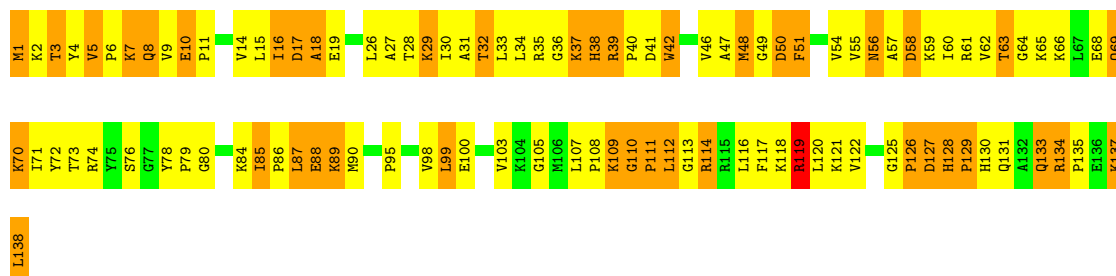
• Molecule 32: 50S ribosomal protein L11

Chain DK: 46% 42% 11%



• Molecule 33: 50S ribosomal protein L13

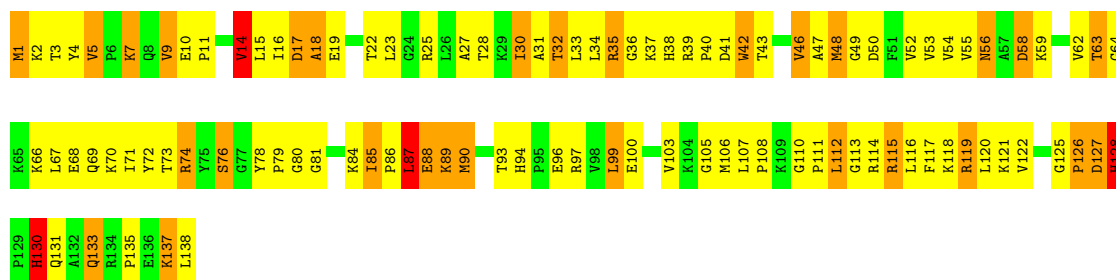
Chain BN: 25% 45% 30%



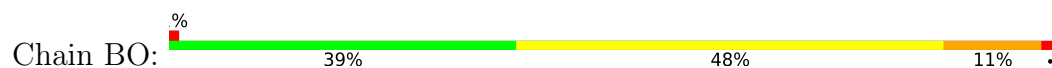
• Molecule 33: 50S ribosomal protein L13

Chain DN: 25% 51% 21%

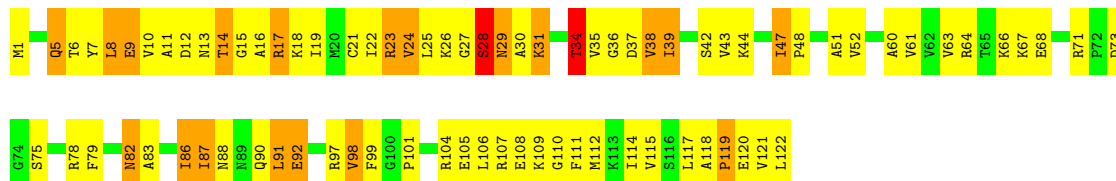




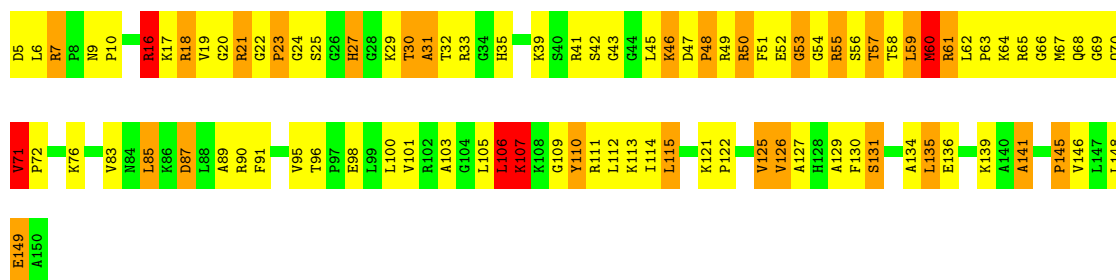
- Molecule 34: 50S ribosomal protein L14



- Molecule 34: 50S ribosomal protein L14

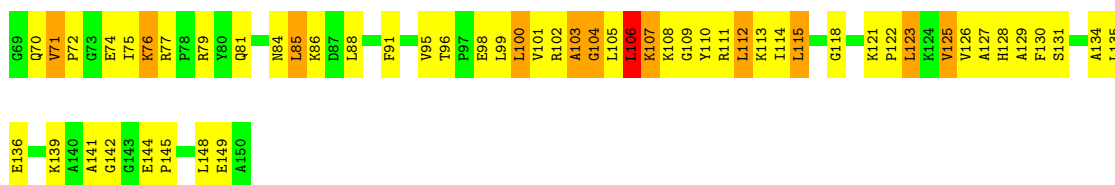


- Molecule 35: 50S ribosomal protein L15

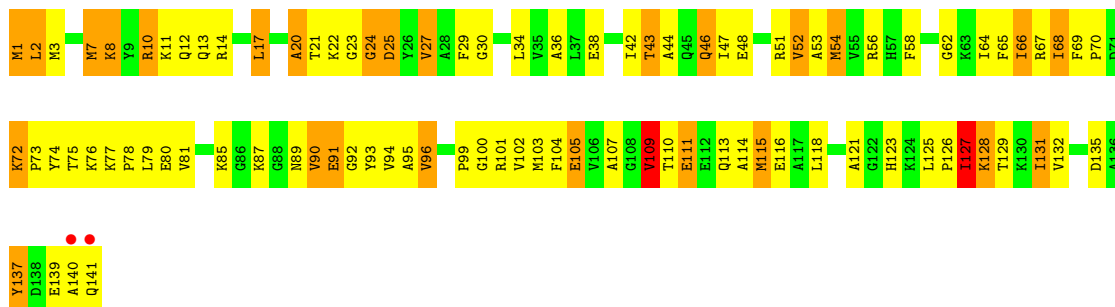
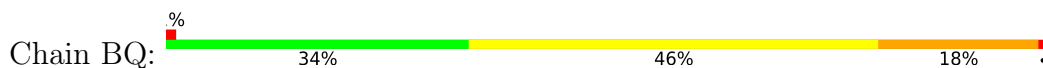


- Molecule 35: 50S ribosomal protein L15

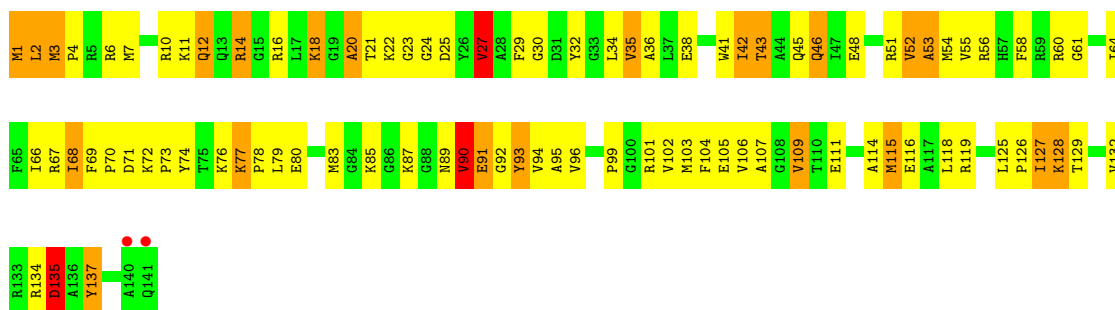




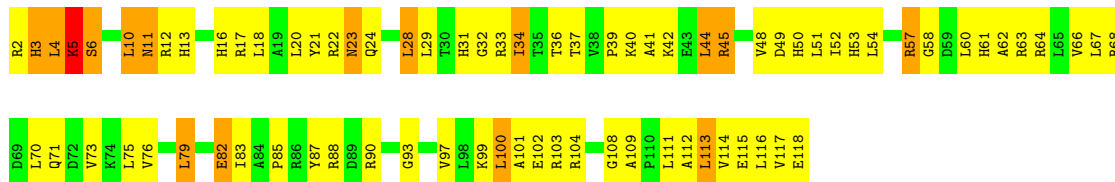
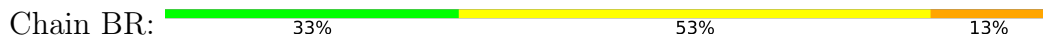
- Molecule 36: 50S ribosomal protein L16



- Molecule 36: 50S ribosomal protein L16

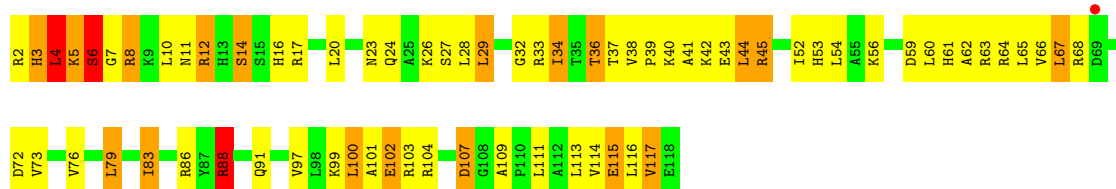


- Molecule 37: 50S ribosomal protein L17



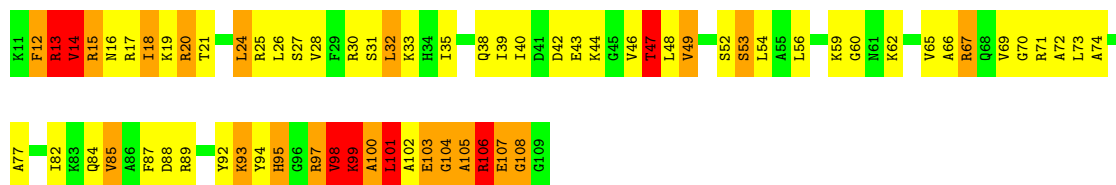
- Molecule 37: 50S ribosomal protein L17





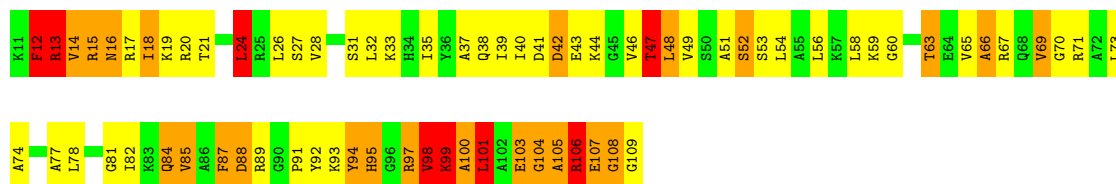
• Molecule 38: 50S ribosomal protein L18

Chain BS: 30% 43% 19% 7%



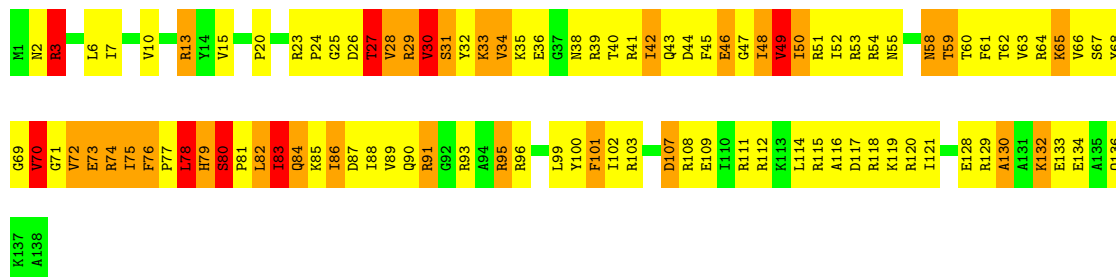
• Molecule 38: 50S ribosomal protein L18

Chain DS: 26% 42% 23% 8%



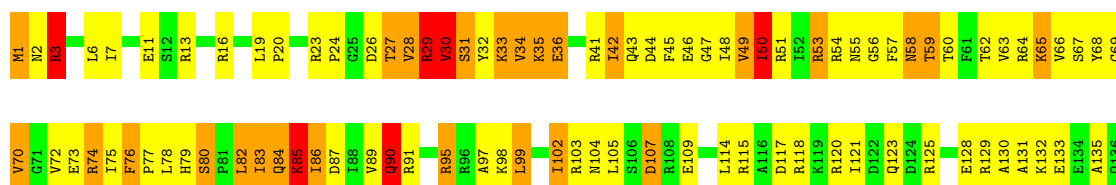
• Molecule 39: 50S ribosomal protein L19

Chain BT: 26% 48% 20% 6%



• Molecule 39: 50S ribosomal protein L19

Chain DT: 30% 46% 19%



K137
A138

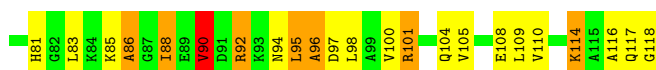
- Molecule 40: 50S ribosomal protein L20

Chain BU:  30% 56% 13%

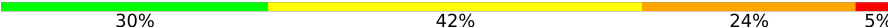
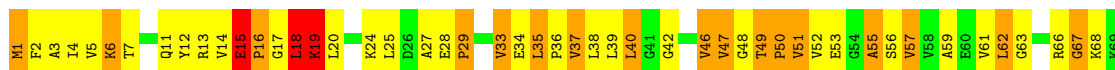
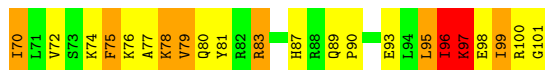


- Molecule 40: 50S ribosomal protein L20

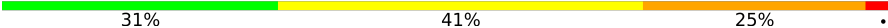
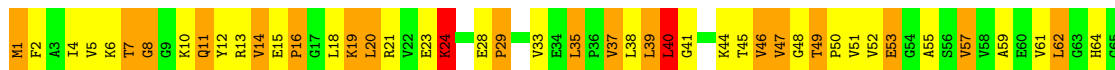
Chain DU:  44% 43% 13%



- Molecule 41: 50S ribosomal protein L21

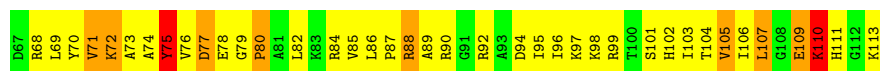
Chain BV:  30% 42% 24% 5%



- Molecule 41: 50S ribosomal protein L21

Chain DV:  31% 41% 25%


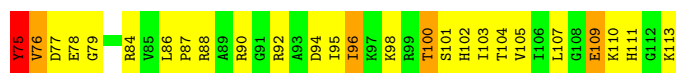

- Molecule 42: 50S ribosomal protein L22

Chain BW:  26% 58% 13%

• Molecule 42: 50S ribosomal protein L22

Chain DW: 41% 48% 9%



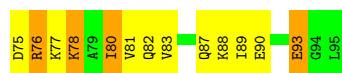
• Molecule 43: 50S ribosomal protein L23

Chain BX: 40% 51% 10%



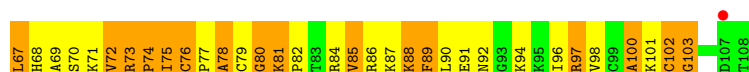
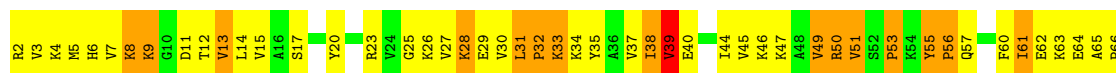
• Molecule 43: 50S ribosomal protein L23

Chain DX: 41% 46% 13%



• Molecule 44: 50S ribosomal protein L24

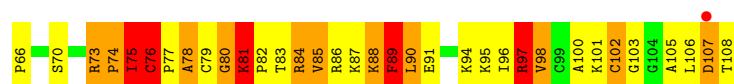
Chain BY: 23% 47% 29%



• Molecule 44: 50S ribosomal protein L24

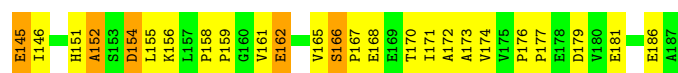
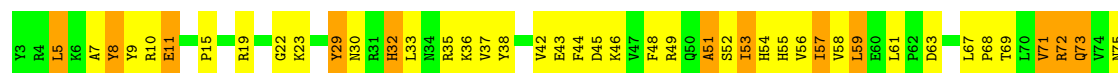
Chain DY: 26% 46% 21% 7%





- Molecule 45: 50S ribosomal protein L25

Chain BZ: 39% 44% 16% .



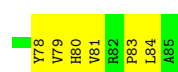
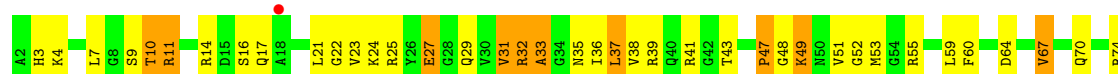
- Molecule 45: 50S ribosomal protein L25

Chain DZ: 41% 48% 11% .



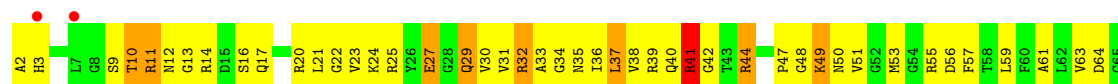
- Molecule 46: 50S ribosomal protein L27

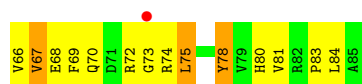
Chain B0: 46% 42% 12%



- Molecule 46: 50S ribosomal protein L27

Chain D0: 30% 56% 13%





- Molecule 47: 50S ribosomal protein L29

Chain B2: 42% 51% 6% .



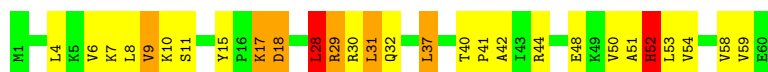
- Molecule 47: 50S ribosomal protein L29

Chain D2: 45% 46% 8% .



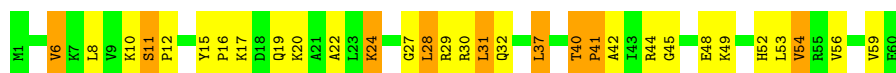
- Molecule 48: 50S ribosomal protein L30

Chain B3: 53% 33% 10% .



- Molecule 48: 50S ribosomal protein L30

Chain D3: 48% 37% 15% .



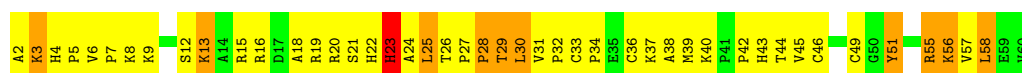
- Molecule 49: 50S ribosomal protein L32

Chain B5: 31% 53% 15% .



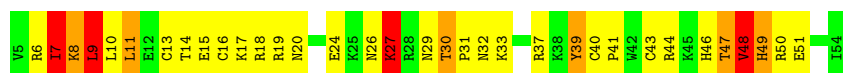
- Molecule 49: 50S ribosomal protein L32

Chain D5: 24% 58% 17% .

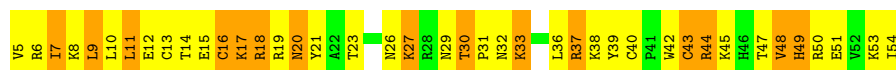
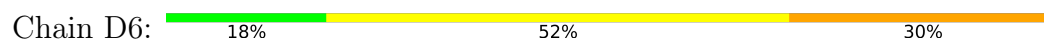


- Molecule 50: 50S ribosomal protein L33

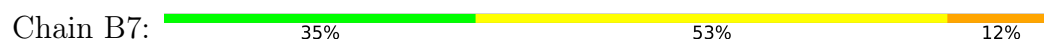
Chain B6: 32% 48% 12% 8% .



- Molecule 50: 50S ribosomal protein L33



- Molecule 51: 50S ribosomal protein L34



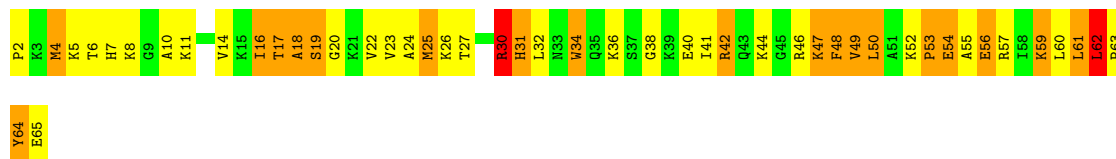
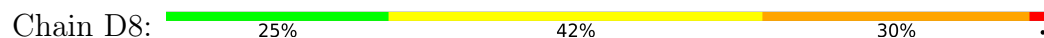
- Molecule 51: 50S ribosomal protein L34



- Molecule 52: 50S ribosomal protein L35



- Molecule 52: 50S ribosomal protein L35



- Molecule 53: 50S ribosomal protein L36



- Molecule 53: 50S ribosomal protein L36

Chain D9:  49% 46% 5%



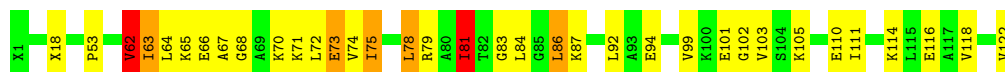
- Molecule 54: 50S ribosomal protein L7/L12

Chain Be:  2% 69% 25% 6%



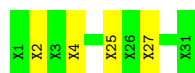
- Molecule 54: 50S ribosomal protein L7/L12

Chain De:  66% 27% 5%

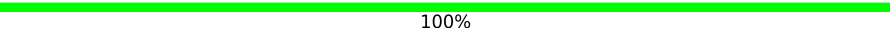


- Molecule 55: 50S RIBOSOMAL PROTEIN L7/L12

Chain Bf:  87% 13%



- Molecule 55: 50S RIBOSOMAL PROTEIN L7/L12

Chain Bg:  100%

There are no outlier residues recorded for this chain.

- Molecule 55: 50S RIBOSOMAL PROTEIN L7/L12

Chain Df:  90% 10%

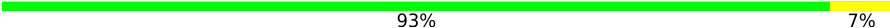


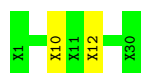
- Molecule 55: 50S RIBOSOMAL PROTEIN L7/L12

Chain Dg:  100%

There are no outlier residues recorded for this chain.

- Molecule 56: 50S RIBOSOMAL PROTEIN L7/L12

Chain Bh:  93% 7%



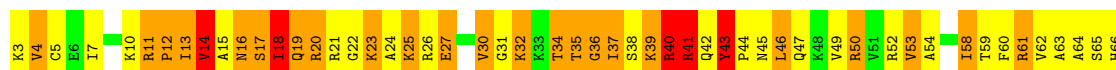
- Molecule 56: 50S RIBOSOMAL PROTEIN L7/L12

Chain Dh: 100%

There are no outlier residues recorded for this chain.

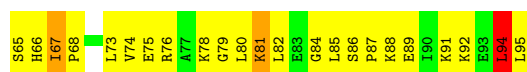
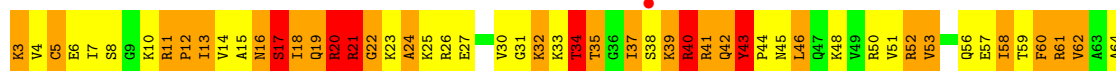
- Molecule 57: 50S ribosomal protein L28

Chain B1: 23% 42% 30% 5%



- Molecule 57: 50S ribosomal protein L28

Chain D1: 18% 47% 27% 8%



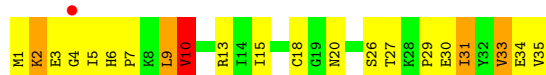
- Molecule 58: 50S ribosomal protein L31

Chain B4: 40% 34% 14% 11%



- Molecule 58: 50S ribosomal protein L31

Chain D4: 3% 40% 46% 11%



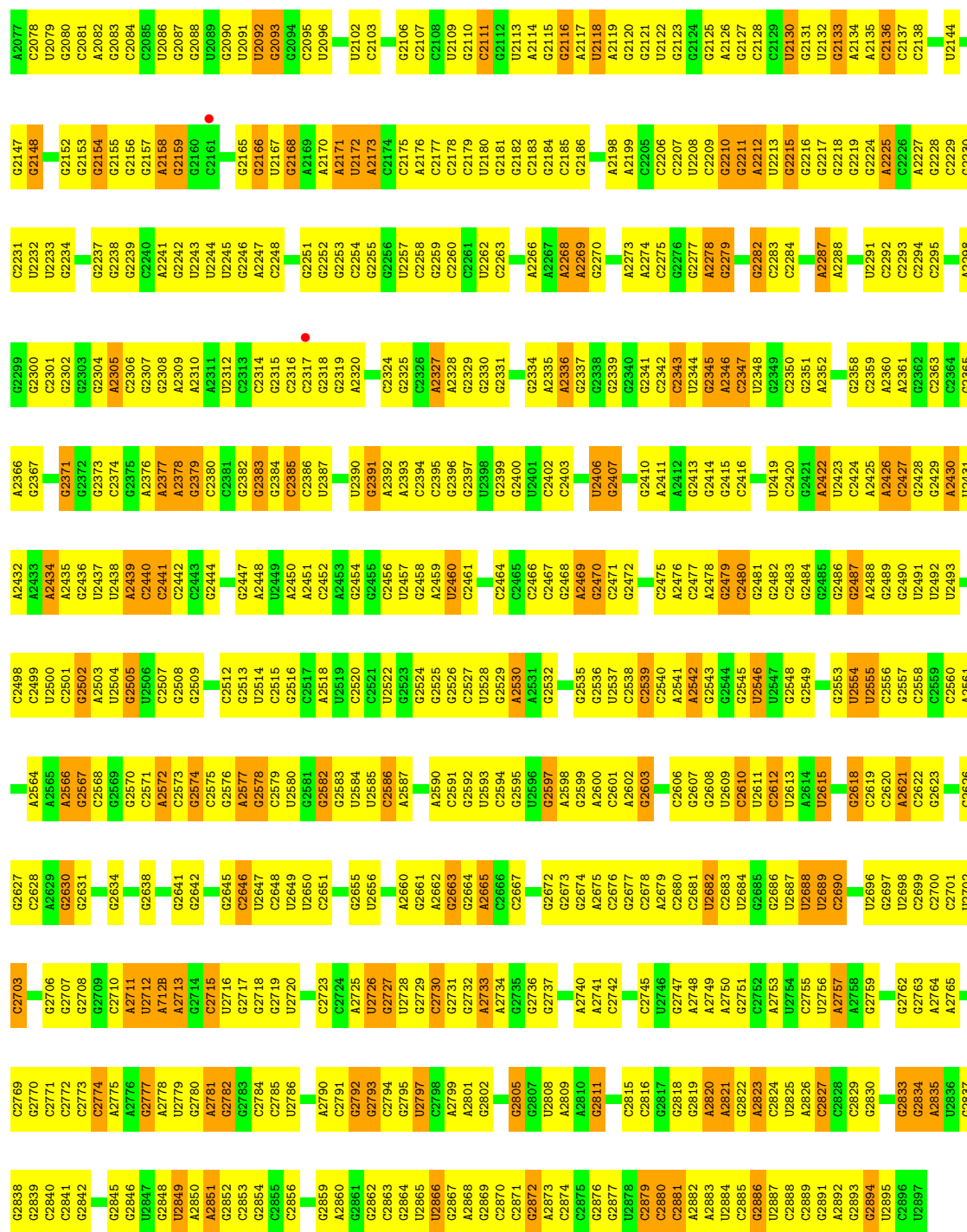
- Molecule 59: 23S ribosomal RNA

Chain BA: 29% 57% 14%



C1006	C1007	C1008	C1009	C1010	C1011	C1012	C1013	C1014	C1015	C1016	C1017	C1018	C1019	A1020	A1021	G1022	G1023	G1024	G1025	U1026	A1027	A1028	A1029	U1033	U1034	U1035	U1036	G1037	C1038	G1039	C1040	G1041	G1042	C1043	G1044	A1045	A1046	G1047	A1048	C1049	A1054	G1055	G1056	A1057	G1058	G1059	U1060	U1061	G1062	G1063	C1064	A1067	A1070	G1071	C1072																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
G946	G947	G948	C949	G950	C951	G954	G955	G956	G957	C958	C959	C960	C961	A962	A963	A964	C965	C966	C967	C968	C969	C970	C971	C972	A973	G974	C975	C976	C977	C978	C979	C980	C981	C982	A983	A984	C985	C986	C987	C988	C989	C990	C991	C992	C993	C994	C995	A996	C997	C998	C999	A1000	A1001	G1002	C1005																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
U747	G748	C749	U750	C751	C752	C753	C754	U755	U756	U757	U758	U759	U760	U761	U762	U763	U764	U765	U766	U767	U768	U769	U770	U771	U772	U773	U774	U775	U776	U777	U778	U779	U780	U781	U782	U783	U784	U785	U786	U787	U788	U789	U790	U791	U792	U793	U794	U795	U796	U797	U798	U799	A800	U801	U802	U803	U804	U805	U806	U807																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
G808	G809	U810	U811	C812	U813	U814	U815	U816	U817	U818	U819	U820	U821	U822	U823	U824	U825	U826	U827	U828	U829	U830	U831	C834	A835	U836	C837	C838	C839	C840	C841	C842	C843	C844	C845	C846	C847	C848	C849	C850	C851	C852	C853	C854	C855	C856	C857	C858	C859	C860	C861	C862	C863	C864	C865	C866	C867	C868	C869	C870																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
A870	U871	A872	G873	G874	G875	G876	G877	G878	G879	G880	G881	G882	G883	G884	G885	G886	G887	G888	G889	G890	G891	G892	G893	G894	G895	G896	G897	G898	G899	G900	G901	G902	G903	G904	G905	G906	G907	G908	G909	G910	G911	G912	G913	G914	G915	G916	G917	G918	G919	G920	G921	G922	G923	G924	G925	G926	G927	G928	G929	G930	G931	G932	G933	G934	G935	G936	G937	G938	G939	G940	G941	G942	G943	G944	G945	G946	G947	G948	G949	G950	G951	G952	G953	G954	G955	G956	G957	G958	G959	G960	G961	G962	G963	G964	G965	G966	G967	G968	G969	G970	G971	G972	G973	G974	G975	G976	G977	G978	G979	G980	G981	G982	G983	G984	G985	G986	G987	G988	G989	G990	G991	G992	G993	G994	G995	G996	G997	G998	G999	A1000	A1001	G1002	C1005																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
U947	U948	U949	U950	U951	U952	U953	U954	U955	U956	U957	U958	U959	U960	U961	U962	U963	U964	U965	U966	U967	U968	U969	U970	U971	U972	U973	U974	U975	U976	U977	U978	U979	U980	U981	U982	U983	U984	U985	U986	U987	U988	U989	U990	U991	U992	U993	U994	U995	U996	U997	U998	U999	A1000	A1001	G1002	C1005																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
U1006	U1007	U1008	U1009	U1010	U1011	U1012	U1013	U1014	U1015	U1016	U1017	U1018	U1019	U1020	U1021	U1022	U1023	U1024	U1025	U1026	U1027	U1028	U1029	U1030	U1031	U1032	U1033	U1034	U1035	U1036	U1037	U1038	U1039	U1040	U1041	U1042	U1043	U1044	U1045	U1046	U1047	U1048	U1049	U1050	U1051	U1052	U1053	U1054	U1055	U1056	U1057	U1058	U1059	U1060	U1061	U1062	U1063	U1064	U1065	U1066	U1067	U1068	U1069	U1070	U1071	U1072																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
C270X	C270Y	C270Z	C271A	C271B	C271C	C271D	C271E	C271F	C271G	C271H	C271I	C271J	C271K	C271L	C271M	C271N	C271O	C271P	C271Q	C271R	C271S	C271T	C271U	C271V	C271W	C271X	C271Y	C271Z	C272A	C272B	C272C	C272D	C272E	C272F	C272G	C272H	C272I	C272J	C272K	C272L	C272M	C272N	C272O	C272P	C272Q	C272R	C272S	C272T	C272U	C272V	C272W	C272X	C272Y	C272Z	C273A	C273B	C273C	C273D	C273E	C273F	C273G	C273H	C273I	C273J	C273K	C273L	C273M	C273N	C273O	C273P	C273Q	C273R	C273S	C273T	C273U	C273V	C273W	C273X	C273Y	C273Z	C274A	C274B	C274C	C274D	C274E	C274F	C274G	C274H	C274I	C274J	C274K	C274L	C274M	C274N	C274O	C274P	C274Q	C274R	C274S	C274T	C274U	C274V	C274W	C274X	C274Y	C274Z	C275A	C275B	C275C	C275D	C275E	C275F	C275G	C275H	C275I	C275J	C275K	C275L	C275M	C275N	C275O	C275P	C275Q	C275R	C275S	C275T	C275U	C275V	C275W	C275X	C275Y	C275Z	C276A	C276B	C276C	C276D	C276E	C276F	C276G	C276H	C276I	C276J	C276K	C276L	C276M	C276N	C276O	C276P	C276Q	C276R	C276S	C276T	C276U	C276V	C276W	C276X	C276Y	C276Z	C277A	C277B	C277C	C277D	C277E	C277F	C277G	C277H	C277I	C277J	C277K	C277L	C277M	C277N	C277O	C277P	C277Q	C277R	C277S	C277T	C277U	C277V	C277W	C277X	C277Y	C277Z	C278A	C278B	C278C	C278D	C278E	C278F	C278G	C278H	C278I	C278J	C278K	C278L	C278M	C278N	C278O	C278P	C278Q	C278R	C278S	C278T	C278U	C278V	C278W	C278X	C278Y	C278Z	C279A	C279B	C279C	C279D	C279E	C279F	C279G	C279H	C279I	C279J	C279K	C279L	C279M	C279N	C279O	C279P	C279Q	C279R	C279S	C279T	C279U	C279V	C279W	C279X	C279Y	C279Z	C280A	C280B	C280C	C280D	C280E	C280F	C280G	C280H	C280I	C280J	C280K	C280L	C280M	C280N	C280O	C280P	C280Q	C280R	C280S	C280T	C280U	C280V	C280W	C280X	C280Y	C280Z	C281A	C281B	C281C	C281D	C281E	C281F	C281G	C281H	C281I	C281J	C281K	C281L	C281M	C281N	C281O	C281P	C281Q	C281R	C281S	C281T	C281U	C281V	C281W	C281X	C281Y	C281Z	C282A	C282B	C282C	C282D	C282E	C282F	C282G	C282H	C282I	C282J	C282K	C282L	C282M	C282N	C282O	C282P	C282Q	C282R	C282S	C282T	C282U	C282V	C282W	C282X	C282Y	C282Z	C283A	C283B	C283C	C283D	C283E	C283F	C283G	C283H	C283I	C283J	C283K	C283L	C283M	C283N	C283O	C283P	C283Q	C283R	C283S	C283T	C283U	C283V	C283W	C283X	C283Y	C283Z	C284A	C284B	C284C	C284D	C284E	C284F	C284G	C284H	C284I	C284J	C284K	C284L	C284M	C284N	C284O	C284P	C284Q	C284R	C284S	C284T	C284U	C284V	C284W	C284X	C284Y	C284Z	C285A	C285B	C285C	C285D	C285E	C285F	C285G	C285H	C285I	C285J	C285K	C285L	C285M	C285N	C285O	C285P	C285Q	C285R	C285S	C285T	C285U	C285V	C285W	C285X	C285Y	C285Z	C286A	C286B	C286C	C286D	C286E	C286F	C286G	C286H	C286I	C286J	C286K	C286L	C286M	C286N	C286O	C286P	C286Q	C286R	C286S	C286T	C286U	C286V	C286W	C286X	C286Y	C286Z	C287A	C287B	C287C	C287D	C287E	C287F	C287G	C287H	C287I	C287J	C287K	C287L	C287M	C287N	C287O	C287P	C287Q	C287R	C287S	C287T	C287U	C287V	C287W	C287X	C287Y	C287Z	C288A	C288B	C288C	C288D	C288E	C288F	C288G	C288H	C288I	C288J	C288K	C288L	C288M	C288N	C288O	C288P	C288Q	C288R	C288S	C288T	C288U	C288V	C288W	C288X	C288Y	C288Z	C289A	C289B	C289C	C289D	C289E	C289F	C289G	C289H	C289I	C289J	C289K	C289L	C289M	C289N	C289O	C289P	C289Q	C289R	C289S	C289T	C289U	C289V	C289W	C289X	C289Y	C289Z	C290A	C290B	C290C	C290D	C290E	C290F	C290G	C290H	C290I	C290J	C290K	C290L	C290M	C290N	C290O	C290P	C290Q	C290R	C290S	C290T	C290U	C290V	C290W	C290X	C290Y	C290Z	C291A	C291B	C291C	C291D	C291E	C291F	C291G	C291H	C291I	C291J	C291K	C291L	C291M	C291N	C291O	C291P	C291Q	C291R	C291S	C291T	C291U	C291V	C291W	C291X	C291Y	C291Z	C292A	C292B	C292C	C292D	C292E	C292F	C292G	C292H	C292I	C292J	C292K	C292L	C292M	C292N	C292O	C292P	C292Q	C292R	C292S	C292T	C292U	C292V	C292W	C292X	C292Y	C292Z	C293A	C293B	C293C	C293D	C293E	C293F	C293G	C293H	C293I	C293J	C293K	C293L	C293M	C293N	C293O	C293P	C293Q	C293R	C293S	C293T	C293U	C293V	C293W	C293X	C293Y	C293Z	C294A	C294B	C294C	C294D	C294E	C294F	C294G	C294H	C294I	C294J	C294K	C294L	C294M	C294N	C294O	C294P	C294Q	C294R	C294S	C294T	C294U	C294V	C294W	C294X	C294Y	C294Z	C295A	C295B	C295C	C295D	C295E	C295F	C295G	C295H	C295I	C295J	C295K	C295L	C295M	C295N	C295O	C295P	C295Q	C295R	C295S	C295T	C295U	C295V	C295W	C295X	C295Y	C295Z	C296A	C296B	C296C	C296D	C296E	C296F	C296G	C296H	C296I	C296J	C296K	C296L	C296M	C296N	C296O	C296P	C296Q	C296R	C296S	C296T	C296U	C296V	C296W	C296X	C296Y	C296Z	C297A	C297B	C297C	C297D	C297E	C297F	C297G	C297H	C297I	C297J	C297K	C297L	C297M	C297N	C297O	C297P	C297Q	C297R	C297S	C297T	C297U	C297V	C297W	C297X	C297Y	C297Z	C298A	C298B	C298C	C298D	C298E	C298F	C298G	C298H	C298I	C298J	C298K	C298L	C298M	C298N	C298O	C298P	C298Q	C298R	C298S	C298T	C298U	C298V	C298W	C298X	C298Y	C298Z	C299A	C299B	C299C	C299D	C299E	C299F	C299G	C299H	C299I	C299J	C299K	C299L	C299M	C299N	C299O	C299P	C299Q	C299R	C299S	C299T	C299U	C299V	C299W	C299X	C299Y	C299Z	C300A	C300B	C300C	C300D	C300E	C300F	C300G	C300H	C300I	C300J	C300K	C300L	C300M	C300N	C300O	C300P	C300Q	C300R	C300S	C300T	C300U	C300V	C300W	C300X	C300Y	C300Z	C301A	C301B	C301C	C301D	C301E	C301F	C301G	C301H	C301I	C301J	C301K	C301L	C301M	C301N	C301O	C301P	C301Q	C301R	C301S	C301T	C301U	C301V	C301W	C301X	C301Y	C301Z	C302A	C302B	C302C	C302D	C302E	C302F	C302G	C302H	C302I	C302J	C302K	C302L	C302M	C302N	C302O	C302P	C302Q	C302R	C302S	C302T	C302U	C302V	C302W	C302X	C302Y	C302Z	C303A	C303B	C303C	C303D	C303E	C303F	C303G	C303H	C303I	C303J	C303K	C303L	C303M	C303N	C303O	C303P	C303Q	C303R	C303S	C303T	C303U	C303V	C303W	C303X	C303Y	C303Z	C304A	C304B	C304C	C304D	C304E	C304F	C304G	C304H	C304I	C304J	C304K	C304L	C304M	C304N	C304O	C304P	C304Q	C304R	C304S	C304T

A2014	G1950	G1859	A1802	C1711	A1641	A1570	G1500	G1429	G1356	U1288	C1221	C1144	C1075
A2015	U1951	C1870	A1803	G1717	G1642	A1571	C1501	C1430	G1357	C1289	C122A	C1145	C1076
U2016	A1952	A1871	C1904	G1718	C1643	A1572	C1502	A1434	G1358	C1290	G1222	A1148	A1077
U2017	A1953	A1872	U1805	G1725	G1644	U1576	A1508	G1435	A1359	C1291	G1223	G1149	U1079
G2018	G1954	C1806	G1807	G1726	G1645	C1577	A1509	G1436	A1360	U1292	A1226	C1150	C1078
A2019	U1955	G1807	G1808	G1727	G1646	U1578	A1510	C1437	G1361	C1293	A1226	G1151	C1080
A2020	C1881	C1808	U1808	G1728	G1647	U1579	A1511	U1438	C1362	U1294	A1226	G1152	U1081
C2021	C1957	A1809	A1809	G1729	G1648	A1579	A1512	U1439	C1363	C1295	G1230	C1153	U1082
U2022	A1884	A1810	G1811	A1729	G1649	C1580	A1513	G1440	A1364	G1296	G1231	G1154	U1083
G2023	A1885	G1811	G1811	A1730	G1650	C1581	A1514	G1441	A1365	G1297	G1232	A1155	U1084
G2024	C1886	A1812	A1812	A1732	G1651	C1582	C1515	G1442	A1366	U1300	G1233	A1156	A1085
G2025	C1887	G1813	G1813	G1733	A1652	C1583	C1516	G1443	A1367	A1301	G1234	A1157	A1086
A2030	G1888	G1814	G1814	C1742	A1653	C1584	A1517	A1444	G1371	A1302	G1235	G1157	A1087
A2031	A1889	A1815	A1815	C1742	A1654	A1586	C1518	A1445	C1375	G1162	G1236	G1157	A1088
A2032	A1890	G1816	G1816	C1742	A1655	A1587	C1519	A1446	C1376	G1163	A1237	G1157	A1089
A2033	G1891	G1817	G1817	G1748	A1656	C1588	A1520	C1447	C1377	G1164	U1240	U1165	U1090
A2034	C1892	U1818	U1818	A1749	C1657	C1589	U1523	G1448	A1378	U1165	A1241	U1166	G1091
G2035	G1893	A1819	A1819	G1753	C1658	U1590	G1524	A1498	A1379	U1167	A1242	U1167	U1092
G2036	U1894	U1820	U1820	G1754	U1659	G1591	G1525	A1499	A1384	U1167	G1243	U1167	U1093
A2037	G1895	A1821	A1821	C1755	C1663	C1592	G1526	C1451	A1385	U1167	G1244	U1167	A1098
G2038	U1896	G1822	G1822	A1756	A1664	G1595	A1529	U1453	G1386	G1171	A1247	G1171	G1099
G2039	G1897	A1823	A1823	G1756	A1665	A1596	G1530	U1454	C1387	G1172	A1247	G1172	C1100
C2040	A1900	A1824	A1824	U1757	A1666	A1597	G1531	G1455	G1388	U1173	G1248	U1174	U1101
U2041	G1901	G1825	G1825	G1758	G1666	A1598	C1532	C1456	C1389	U1175	U1249	U1175	C1102
G2042	C1902	C1826	C1826	A1759	G1667	C1599	C1533	C1457	G1390	G1176	G1250	U1176	A1103
A2043	G1903	G1827	G1827	U1760	A1668	C1600	G1534	C1458	U1390	A1177	G1251	U1177	U1104
C2044	U1904	A1828	A1828	G1761	A1669	C1601	G1535	C1459	U1391	G1182	G1252	U1182	G1106
G2045	G1905	G1829	G1829	A1762	A1670	U1602	U1536	G1460	U1392	G1183	A1253	G1107	C1107
G2046	A1912	C1830	C1830	C1763	U1671	U1603	A1537	C1461	U1393	G1184	U1254	U1108	U1108
U2047	A1913	G1831	G1831	C1765	G1672	C1604	G1538	C1462	U1394	G1185	U1255	C1109	C1109
G2048	C1914	U1833	U1833	U1766	C1673	C1605	G1539	C1463	U1395	G1186	U1256	G1110	G1110
G2049	U1915	U1834	U1834	C1771	C1674	C1606	G1540	C1464	U1396	G1187	G1257	G1111	G1111
A2051	A1916	C1838	C1838	G1772	A1675	C1607	U1541	C1465	U1397	G1192	G1260	G1112	U1113
G2052	U1917	G1839	G1839	A1773	A1676	C1608	G1542	C1466	C1398	G1195	U1261	G1120	G1120
A2053	U1917	G1840	G1840	G1773	G1677	A1609	A1543	C1467	C1399	G1196	C1261	G1121	C1121
G2054	U1917	U1841	U1841	U1778	G1681	A1610	G1544	C1468	G1401	G1197	A1262	G1122	G1122
C2055	U1918	G1842	G1842	U1779	G1682	C1611	C1545	C1474	C1402	G1198	U1263	G1123	C1123
G2056	U1919	C1843	C1843	A1780	C1683	C1612	A1546	G1475	C1403	G1200	G1264	G1124	G1124
A2057	G1920	G1844	G1844	C1781	A1690	G1613	C1547	G1478	U1405	G1201	G1265	G1125	G1125
A2058	U1921	G1845	G1845	A1782	A1691	C1614	C1548	G1479	C1406	G1202	U1267	G1126	A1126
A2059	G1922	G1846	G1846	A1783	U1692	C1615	C1549	U1480	C1407	G1203	A1268	A1127	A1127
G2060	U1923	A1847	A1847	A1784	C1693	A1616	C1550	U1481	C1408	G1204	G1269	A1128	A1128
G2061	G1924	G1848	G1848	A1785	C1694	C1617	G1551	G1482	C1409	G1205	A1270	A1129	A1129
A2062	U1925	G1849	G1849	A1786	G1695	G1623	G1552	G1483	C1410	G1206	G1271	G1206	G1206
G2063	G1926	U1850	U1850	A1787	G1696	G1624	A1553	A1486	C1411	G1207	A1272	A1205	A1205
A2064	U1927	C1851	C1851	C1788	G1697	G1625	A1554	G1487	C1412	G1208	U1273	G1206	G1206
G2065	G1928	U1852	U1852	A1789	G1698	G1626	C1557	G1488	C1413	G1209	A1274	G1209	G1209
G2066	A1929	A1853	A1853	A1790	A1698	C1627	C1558	U1489	U1415	A1210	A1275	G1135	G1135
G2067	U1930	G1854	G1854	A1791	G1699	C1628	A1559	A1490	G1416	A1211	A1276	G1136	G1136
A2068	A1931	U1855	U1855	G1792	A1700	A1631	G1560	G1491	C1417	G1212	G1277	G1137	G1137
A2069	G1932	G1856	G1856	C1793	A1701	A1632	G1561	G1492	C1418	G1213	A1278	G1138	G1138
G2070	U1933	G1857	G1857	U1794	G1702	G1633	G1562	C1493	G1419	G1214	G1279	G1139	G1139
C2071	C1941	G1858	G1858	C1795	A1634	A1634	G1563	C1494	A1419	G1215	G1280	G1215	G1215
A2071	G1935	U1859	U1859	U1796	G1635	C1635	C1564	A1495	G1420	G1216	G1281	G1216	G1216
G2072	C1942	A1859	A1859	C1797	G1636	C1636	A1565	A1496	G1421	G1217	U1282	G1217	G1217
U2073	U1943	G1860	G1860	U1798	G1707	A1637	A1566	A1497	G1422	G1218	A1286	G1218	G1218
G2074	G1861	C1861	C1861	U1799	G1708	A1638	A1567	U1498	C1423	G1219	A1287	G1219	G1219
U2075	C1947	G1862	G1862	U1800	U1709	U1639	A1568	C1499	C1428	G1220	A1288	G1220	G1220
A2076	G1948	G1863	G1863	G1801	C1710	C1640	A1569	C1499	C1428	G1221	A1289	G1221	G1221



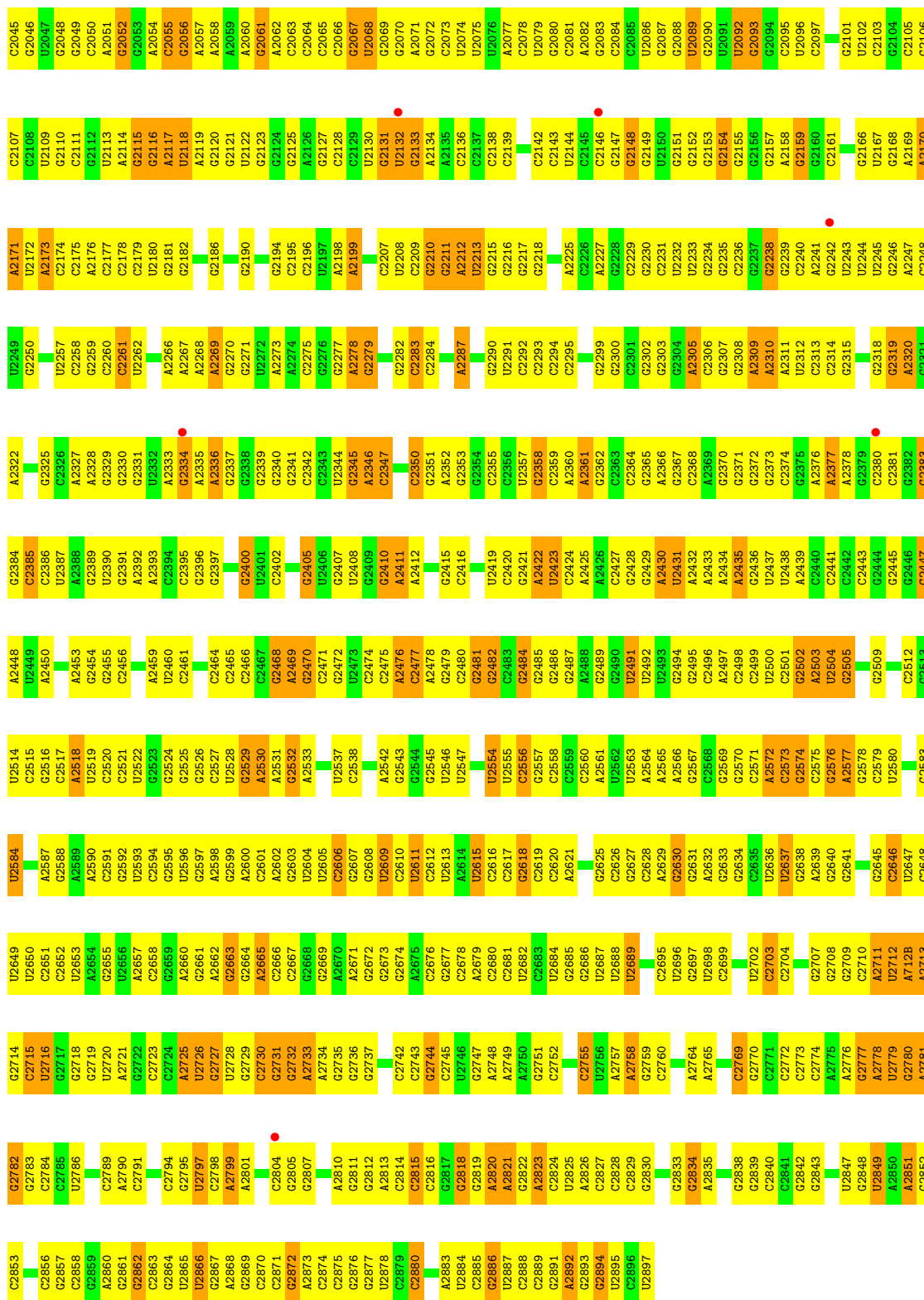
Molecule 59: 23S ribosomal RNA

Chain DA:



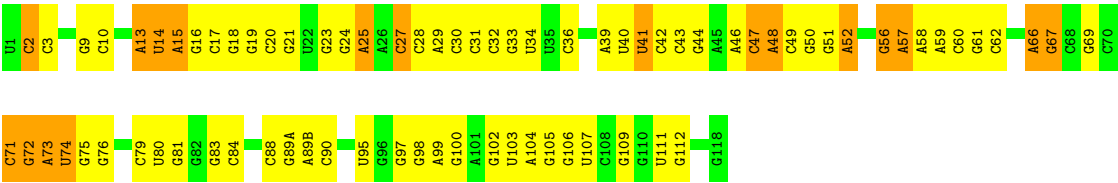


A1981	G1903	G1823	G1758	A1664	G1595	A1529	G1459	G1389	G1324	C1258	G1186	G1102	C1052
C1982	G1904	G1824	G1759	A1665	C1598	G1530	A1460	U1590	G1325	G1259	G1187	C1101	C1053
G1983	A1825	A1826	C1666	G1667	C1599	G1531	G1461	U1394	U1326	G1260	A1188	G1102	G1054
G1984	G1826	G1827	A1668	A1669	U1602	C1532	C1463	U1395	G1327	C1261	A1189	G1102	G1055
A1986	A1912	G1828	G1763	A1670	A1603	U1535	G1465	U1397	G1329	U1263	U1190	C1124	A1057
G1989	A1913	G1829	G1764	C1670	C1604	A1536	G1466	U1398	C1330	G1264	G1193	G1125	G1058
G1990	C1924	G1830	U1766	U1671	C1605	A1537	G1467	C1399	A1331	G1265	A1194	G1126	G1059
G1991	C1923	C1832	U1766	G1674	G1606	G1538	G1468	G1400	G1332	G1266	G1195	A1127	G1060
G1992	G1833	U1833	G1770	C1675	G1607	G1539	A1469	G1401	G1333	U1267	G1196	A1128	G1061
U1993	C1924	C1836	G1771	A1676	A1609	U1541	G1470	C1402	G1334	A1268	G1197	A1129	G1062
U1994	A1927	G1837	G1772	A1677	A1610	G1542	A1471	C1403	U1335	A1269	U1198	U1130	G1063
U1995	A1928	G1838	G1773	G1678	G1611	G1543	A1472	C1404	A1336	C1270	U1199	G1131	C1064
G1996	G1929	C1838	C1774	G1681	C1612	A1544	G1473	C1405	G1337	G1271	C1200	U1065	U1066
G1997	G1930	U1841	G1775	G1682	G1613	C1544	C1474	U1406	G1338	A1272	C1201	G1135	U1067
G1998	U1931	U1842	G1776	C1683	A1614	A1545	G1475	C1407	G1339	U1273	C1202	G1136	A1069
G1999	A1932	G1843	U1777	U1778	G1615	A1546	G1476	C1408	U1340	A1274	G1203	G1137	A1070
G2000	G1933	C1843	U1778	G1687	C1616	G1547	A1477	C1409	A1342	U1205	U1206	G1138	G1071
A2001	C1934	U1854	U1779	U1688	A1616	C1548	G1478	G1410	G1343	A1278	G1207	C1140	C1072
G2002	G1935	A1847	A1780	U1688	C1617	G1548	G1479	C1411	U1352	G1279	C1207	U1141	A1073
G2003	A1936	G1856	C1781	A1689	G1618	C1549	G1480	G1416	A1353	G1283	G1208	U1142	G1074
G2004	A1937	G1858	C1782	A1690	A1619	C1550	U1481	C1417	A1354	A1284	G1209	A114B	C1075
A2005	A1938	A1859	A1783	C1691	G1620	C1551	G1483	G1418	A1349	G1285	U1211	A1143	C1076
C2006	U1939	G1860	A1784	U1692	U1621	C1552	U1486	G1419	U1352	A1286	G1212	G1144	A1077
C2007	U1940	G1855	A1785	U1693	G1622	A1553	G1487	U1419	A1353	U1287	A1213	C1145	U1078
C2008	U1941	G1856	A1786	C1694	G1623	A1554	U1487	U1420	A1354	A1288	A1214	G1149	C1079
G2009	U1943	G1857	A1787	U1695	G1624	C1555	U1488	U1421	A1355	U1289	G1215	C1150	C1080
G2010	U1944	G1858	C1788	G1696	G1625	C1556	A1490	G1423	G1355	C1289	G1216	G1151	U1081
U2011	U1945	A1859	A1789	G1697	G1626	C1557	G1491	G1424	G1356	C1290	G1217	G1152	U1082
G2012	G1948	G1860	A1790	A1698	C1627	A1558	G1492	G1425	U1357	C1291	C1217	G1153	U1083
A2013	G1949	U1860	C1791	U1699	A1631	G1559	C1493	G1425	A1358	C1292	C1221	G1154	A1084
A2014	U1952	U1864	G1792	A1700	A1634	G1560	A1494	G1426	A1359	U1293	C1222	G1154	A1085
A2015	A1953	A1872	U1796	A1701	G1635	C1564	A1495	C1428	A1360	U1294	C1223	G1157	A1086
U2016	G1954	G1878	C1797	G1703	A1636	C1565	A1496	G1429	U1367	G1295	G1224	G1158	G1087
U2017	G1955	C1879	U1798	G1704	A1637	A1566	U1497	C1430	A1366	G1296	G1225	U1159	A1088
U2018	U1955	G1880	G1799	G1705	C1638	A1567	C1498	U1431	A1367	U1299	A1226	G1162	G1089
A2019	U1956	C1881	C1800	G1707	U1639	G1568	G1500	A1434	A1367	U1300	G1227	G1163	U1090
A2020	C1957	C1882	C1801	C1708	C1640	A1569	C1501	G1435	G1368	A1301	U1230	G1164	C1091
C2021	C1958	G1883	A1802	U1709	A1641	A1570	C1502	G1436	G1369	A1302	G1231	U1165	C1092
U2022	U1962	A1884	C1803	C1710	G1642	A1571	U1503	C1437	C1370	G1305	G1232	G1166	U1094
G2023	U1963	A1885	C1804	C1711	G1643	A1572	A1508	U1438	U1372	C1306	G1371	U1167	A1095
G2024	G1964	C1886	U1805	G1718	C1646	C1575	A1509	U1438	A1373	A1307	G1239	G1168	A1096
C2025	C1965	G1887	C1806	G1719	G1647	U1576	A1510	G1441	G1374	A1307	U1240	G1169	U1097
A2030	A1966	G1888	G1807	U1727	C1648	C1577	A1511	U1448	A1375	A1308	A1241	U1177	U1101
A2031	C1967	A1889	A1810	G1728	G1649	U1578	G1512	C1445	C1376	A1309	U1242	G1173	C1102
G2032	G1968	A1890	G1811	A1729	G1650	A1579	C1513	C1446	G1377	G1310	G1243	A1174	A1103
A2033	A1969	G1891	A1812	U1730	G1651	A1580	U1514	C1446	A1378	G1311	G1244	U1175	C1104
U2034	C1892	C1893	G1813	G1731	A1652	G1581	C1515	G1447	A1379	U1312	G1244	U1176	U1105
G2035	A1971	C1894	G1814	A1732	G1653	C1582	U1516	G1448	G1380	C1314	A1247	A1177	G1106
C2036	A1972	C1895	A1815	G1733	A1654	A1583	G1517	G1449	G1381	G1315	G1248	C1178	G1107
G2037	G1973	G1896	G1816	C1741	A1655	C1585	C1518	G1449	G1382	U1316	U1249	C1179	C1108
G2038	C1974	G1897	G1817	G1741	A1656	A1586	G1519	C1451	C1383	A1317	A1253	C1180	G1112
C2039	G1975	G1898	U1818	C1657	C1656	U1520	U1520	A1451	A1384	C1318	A1254	C1181	U1113
C2040	U1976	G1899	U1819	C1658	C1657	C1589	G1524	A1453	G1385	U1321	A1254	A1182	G1114
U2041	A1977	G1900	A1820	U1659	C1658	U1590	G1525	U1454	C1386	A1322	U1255	G1183	G1115
A2042	A1978	A1901	A1821	C1659	U1659	G1591	G1526	U1455	C1387	U1323	G1257	G1184	C1116
C2043	C1979	C1902	G1822	G1753	C1663	U1591	G1526	U1456	G1388			C1257	G1117



● Molecule 60: 5S ribosomal RNA

Chain BB:



• 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	308.96Å 670.66Å 347.77Å 90.00° 92.52° 90.00°	Depositor
Resolution (Å)	40.00 – 3.50 40.00 – 3.56	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.50) 74.7 (40.00-3.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 3.58Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.284 , 0.328 0.290 , 0.329	Depositor DCC
R_{free} test set	33495 reflections (4.00%)	wwPDB-VP
Wilson B-factor (Å ²)	57.8	Xtriage
Anisotropy	0.660	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.18 , 294.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.25$, $\langle L^2 \rangle = 0.10$	Xtriage
Estimated twinning fraction	0.258 for h,-k,-l	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	308166	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% 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: KBE, DPP, MG, FUA, UAL, GDP, 5OH

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AB	0.54	0/1945	1.15	18/2621 (0.7%)
1	CB	0.53	1/1945 (0.1%)	1.07	11/2621 (0.4%)
2	AC	0.37	0/1645	0.86	2/2216 (0.1%)
2	CC	0.39	0/1645	0.94	3/2216 (0.1%)
3	AD	0.39	0/1733	0.92	3/2318 (0.1%)
3	CD	0.39	0/1733	0.98	6/2318 (0.3%)
4	AE	0.43	0/1172	0.93	3/1576 (0.2%)
4	CE	0.41	0/1172	0.94	4/1576 (0.3%)
5	AF	0.39	0/856	0.92	2/1154 (0.2%)
5	CF	0.37	0/856	0.87	0/1154
6	AG	0.38	0/1276	0.90	2/1709 (0.1%)
6	CG	0.36	0/1276	0.89	1/1709 (0.1%)
7	AH	0.42	0/1136	0.91	4/1527 (0.3%)
7	CH	0.41	0/1136	0.95	4/1527 (0.3%)
8	AI	0.40	0/1029	0.86	1/1379 (0.1%)
8	CI	0.37	0/1029	0.84	2/1379 (0.1%)
9	AJ	0.37	0/815	0.89	0/1095
9	CJ	0.40	0/815	0.90	0/1095
10	AK	0.47	0/900	1.06	5/1213 (0.4%)
10	CK	0.52	0/900	1.14	8/1213 (0.7%)
11	AL	0.59	0/992	1.25	13/1327 (1.0%)
11	CL	0.58	0/992	1.25	10/1327 (0.8%)
12	AM	0.40	0/1008	0.96	4/1347 (0.3%)
12	CM	0.39	0/1008	0.87	0/1347
13	AN	0.38	0/501	0.88	0/664
13	CN	0.34	0/501	0.84	2/664 (0.3%)
14	AO	0.40	0/745	0.87	3/992 (0.3%)
14	CO	0.39	0/745	0.83	0/992
15	AP	0.38	0/722	0.81	0/970
15	CP	0.35	0/722	0.84	0/970
16	AQ	0.46	0/848	1.07	5/1131 (0.4%)
16	CQ	0.46	0/848	1.14	10/1131 (0.9%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AR	0.39	0/579	0.90	0/768
17	CR	0.37	0/579	0.85	1/768 (0.1%)
18	AS	0.45	0/647	0.99	5/870 (0.6%)
18	CS	0.42	0/647	1.03	7/870 (0.8%)
19	AT	0.43	0/765	0.91	1/1007 (0.1%)
19	CT	0.41	0/765	0.87	0/1007
20	AA	0.20	0/36351	0.41	1/56736 (0.0%)
20	CA	0.19	0/36351	0.40	2/56736 (0.0%)
21	AW	0.18	0/1827	0.43	0/2845
21	CW	0.18	0/1827	0.41	0/2845
22	AV	0.15	0/568	0.36	0/886
22	CV	0.16	0/568	0.40	0/886
23	AY	0.48	1/5317 (0.0%)	1.07	35/7198 (0.5%)
23	CY	0.54	5/5317 (0.1%)	1.02	22/7198 (0.3%)
24	AU	0.92	0/11	1.48	0/13
24	CU	0.86	0/11	1.35	0/13
25	BC	0.61	0/1774	1.24	25/2391 (1.0%)
25	DC	0.65	2/1774 (0.1%)	1.19	28/2391 (1.2%)
26	BD	0.47	0/2195	1.06	13/2955 (0.4%)
26	DD	0.49	0/2195	1.04	17/2955 (0.6%)
27	BE	0.47	0/1602	1.13	16/2160 (0.7%)
27	DE	0.44	0/1602	1.11	11/2160 (0.5%)
28	BF	0.49	0/1663	1.12	21/2249 (0.9%)
28	DF	0.50	1/1663 (0.1%)	1.15	20/2249 (0.9%)
29	BG	0.61	5/1499 (0.3%)	1.05	6/2016 (0.3%)
29	DG	0.55	3/1499 (0.2%)	1.06	7/2016 (0.3%)
30	BH	0.43	0/1298	0.94	1/1751 (0.1%)
30	DH	0.40	0/1298	0.93	2/1751 (0.1%)
32	BK	0.42	0/1054	0.92	6/1427 (0.4%)
32	DK	0.42	0/1054	0.93	5/1427 (0.4%)
33	BN	0.66	0/1131	1.19	11/1525 (0.7%)
33	DN	0.66	0/1131	1.09	6/1525 (0.4%)
34	BO	0.39	0/943	1.02	6/1269 (0.5%)
34	DO	0.39	0/943	0.91	3/1269 (0.2%)
35	BP	0.41	0/1131	0.98	5/1504 (0.3%)
35	DP	0.42	0/1131	0.99	5/1504 (0.3%)
36	BQ	0.46	0/1143	1.01	3/1527 (0.2%)
36	DQ	0.41	0/1143	0.96	1/1527 (0.1%)
37	BR	0.43	0/974	0.94	1/1302 (0.1%)
37	DR	0.43	0/974	0.94	2/1302 (0.2%)
38	BS	0.50	0/783	1.12	8/1041 (0.8%)
38	DS	0.46	0/783	1.11	7/1041 (0.7%)
39	BT	0.48	0/1161	1.05	6/1549 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	DT	0.50	0/1161	1.05	5/1549 (0.3%)
40	BU	0.47	0/982	0.88	0/1306
40	DU	0.53	0/982	0.91	1/1306 (0.1%)
41	BV	0.51	0/790	1.11	6/1057 (0.6%)
41	DV	0.49	0/790	1.06	6/1057 (0.6%)
42	BW	0.44	0/911	0.95	1/1220 (0.1%)
42	DW	0.44	0/911	1.03	2/1220 (0.2%)
43	BX	0.36	0/748	0.92	3/1004 (0.3%)
43	DX	0.37	0/748	0.88	0/1004
44	BY	0.46	0/831	1.12	8/1108 (0.7%)
44	DY	0.48	0/831	1.11	11/1108 (1.0%)
45	BZ	0.39	0/1505	0.99	5/2042 (0.2%)
45	DZ	0.40	0/1505	1.01	6/2042 (0.3%)
46	B0	0.33	0/671	0.75	0/892
46	D0	0.37	0/671	0.83	2/892 (0.2%)
47	B2	0.37	0/600	0.91	1/793 (0.1%)
47	D2	0.38	0/600	0.93	2/793 (0.3%)
48	B3	0.42	0/482	0.95	1/646 (0.2%)
48	D3	0.37	0/482	1.03	5/646 (0.8%)
49	B5	0.49	0/473	1.00	3/639 (0.5%)
49	D5	0.45	0/473	0.96	0/639
50	B6	0.42	0/440	1.02	2/586 (0.3%)
50	D6	0.40	0/440	0.91	1/586 (0.2%)
51	B7	0.41	0/438	0.97	0/575
51	D7	0.39	0/438	0.94	0/575
52	B8	0.46	0/525	1.10	2/691 (0.3%)
52	D8	0.43	0/525	1.04	5/691 (0.7%)
53	B9	0.40	0/310	0.89	0/407
53	D9	0.41	0/310	0.88	0/407
54	Be	0.41	0/538	0.90	4/715 (0.6%)
54	De	0.36	0/538	0.88	1/715 (0.1%)
57	B1	0.71	0/739	1.36	17/981 (1.7%)
57	D1	0.73	1/739 (0.1%)	1.38	13/981 (1.3%)
58	B4	0.55	0/276	1.07	3/372 (0.8%)
58	D4	0.56	0/276	1.07	1/372 (0.3%)
59	BA	0.21	0/69437	0.44	3/108401 (0.0%)
59	DA	0.21	0/69437	0.43	3/108401 (0.0%)
60	BB	0.19	0/2853	0.41	0/4451
60	DB	0.18	0/2853	0.38	0/4451
All	All	0.32	19/330576 (0.0%)	0.66	565/492228 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AB	0	3
1	CB	0	1
11	CL	0	2
23	AY	0	3
23	CY	0	2
25	BC	0	1
25	DC	0	3
26	BD	0	1
26	DD	0	2
28	BF	0	2
28	DF	0	2
29	BG	0	2
29	DG	0	2
31	BJ	0	1
31	DJ	0	1
35	DP	0	1
38	BS	0	3
38	DS	0	3
42	BW	0	1
42	DW	0	1
57	B1	0	2
57	D1	0	2
All	All	0	41

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	CY	506	GLN	C-N	14.48	1.53	1.33
29	BG	114	ILE	N-CA	-12.45	1.31	1.46
23	CY	25	LYS	C-N	11.49	1.48	1.33
29	DG	114	ILE	N-CA	-10.93	1.31	1.46
23	AY	506	GLN	C-N	-8.34	1.21	1.33

The worst 5 of 565 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	AY	506	GLN	O-C-N	-16.55	102.72	122.58
29	DG	111	LEU	CA-C-N	-15.72	103.76	119.64
29	DG	111	LEU	C-N-CA	-15.72	103.76	119.64
29	BG	111	LEU	CA-C-N	-15.72	103.77	119.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	BG	111	LEU	C-N-CA	-15.72	103.77	119.64

There are no chirality outliers.

5 of 41 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AB	162	ILE	Peptide
1	AB	170	GLU	Peptide
1	AB	185	ILE	Peptide
23	AY	133	ILE	Peptide
23	AY	503	GLY	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AB	1910	0	1957	138	0
1	CB	1910	0	1957	109	0
2	AC	1621	0	1688	90	0
2	CC	1621	0	1688	67	0
3	AD	1703	0	1763	108	0
3	CD	1703	0	1763	109	0
4	AE	1156	0	1213	70	0
4	CE	1156	0	1213	58	0
5	AF	843	0	857	47	0
5	CF	843	0	857	33	0
6	AG	1257	0	1296	55	0
6	CG	1257	0	1296	56	0
7	AH	1116	0	1177	68	0
7	CH	1116	0	1177	73	0
8	AI	1010	0	1037	79	0
8	CI	1010	0	1037	56	0
9	AJ	802	0	849	44	0
9	CJ	802	0	849	48	0
10	AK	885	0	904	56	0
10	CK	885	0	904	61	0
11	AL	976	0	1062	118	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	CL	976	0	1062	107	0
12	AM	997	0	1072	69	0
12	CM	997	0	1072	49	0
13	AN	492	0	529	39	0
13	CN	492	0	529	26	0
14	AO	734	0	771	49	0
14	CO	734	0	771	44	0
15	AP	706	0	725	45	0
15	CP	706	0	725	29	0
16	AQ	835	0	904	65	0
16	CQ	835	0	904	60	0
17	AR	574	0	644	39	0
17	CR	574	0	644	39	0
18	AS	634	0	655	37	0
18	CS	634	0	655	45	0
19	AT	763	0	861	39	0
19	CT	763	0	861	38	0
20	AA	32474	0	16393	1005	0
20	CA	32474	0	16393	1037	0
21	AW	1635	0	831	63	0
21	CW	1635	0	831	53	0
22	AV	503	0	252	12	0
22	CV	503	0	252	15	0
23	AY	5219	0	5290	333	0
23	CY	5219	0	5291	334	0
24	AU	48	0	39	1	0
24	CU	48	0	39	3	0
25	BC	1742	0	1798	178	0
25	DC	1742	0	1798	184	0
26	BD	2145	0	2234	209	0
26	DD	2145	0	2234	204	0
27	BE	1569	0	1634	129	0
27	DE	1569	0	1634	122	0
28	BF	1628	0	1680	137	0
28	DF	1628	0	1680	156	0
29	BG	1474	0	1535	74	0
29	DG	1474	0	1535	76	0
30	BH	1274	0	1342	60	0
30	DH	1274	0	1342	52	0
31	BJ	851	0	197	31	0
31	DJ	851	0	193	39	0
32	BK	1035	0	1082	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	DK	1035	0	1082	59	0
33	BN	1104	0	1180	88	0
33	DN	1104	0	1180	104	0
34	BO	933	0	996	65	0
34	DO	933	0	996	77	0
35	BP	1114	0	1187	89	0
35	DP	1114	0	1187	90	0
36	BQ	1122	0	1179	80	0
36	DQ	1122	0	1179	75	0
37	BR	960	0	1021	71	0
37	DR	960	0	1021	63	0
38	BS	775	0	835	71	0
38	DS	775	0	835	64	0
39	BT	1147	0	1207	104	0
39	DT	1147	0	1207	103	0
40	BU	964	0	1022	89	0
40	DU	964	0	1022	62	1
41	BV	779	0	852	68	0
41	DV	779	0	852	72	0
42	BW	900	0	964	70	0
42	DW	900	0	964	50	0
43	BX	734	0	789	44	0
43	DX	734	0	789	42	0
44	BY	818	0	908	58	0
44	DY	818	0	908	60	0
45	BZ	1473	0	1497	81	0
45	DZ	1473	0	1497	70	0
46	B0	662	0	688	34	0
46	D0	662	0	688	47	0
47	B2	598	0	653	29	0
47	D2	598	0	653	31	0
48	B3	477	0	529	24	0
48	D3	477	0	529	20	0
49	B5	459	0	477	46	0
49	D5	459	0	477	48	0
50	B6	433	0	461	28	0
50	D6	433	0	461	38	0
51	B7	430	0	480	41	0
51	D7	430	0	480	36	0
52	B8	517	0	582	52	0
52	D8	517	0	582	47	0
53	B9	307	0	338	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	D9	307	0	335	18	0
54	Be	686	0	615	19	0
54	De	686	0	616	27	0
55	Bf	156	0	40	2	0
55	Bg	156	0	41	0	0
55	Df	156	0	40	2	0
55	Dg	156	0	37	0	0
56	Bh	151	0	39	1	0
56	Dh	151	0	40	0	0
57	B1	732	0	808	76	0
57	D1	732	0	808	81	0
58	B4	271	0	284	20	0
58	D4	271	0	284	18	0
59	BA	61997	0	31250	2052	1
59	DA	61997	0	31250	2211	0
60	BB	2551	0	1295	84	0
60	DB	2551	0	1295	85	0
61	AY	37	0	47	6	0
61	CY	37	0	47	7	0
62	AY	28	0	12	12	0
62	CY	28	0	12	13	0
63	BA	1	0	0	0	0
63	CY	1	0	0	0	0
All	All	308166	0	213086	12592	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

The worst 5 of 12592 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)
23:CY:19:ALA:H	23:CY:25:LYS:CE	1.38	1.34
59:DA:2405:G:H21	59:DA:2412:A:N6	1.28	1.26
23:CY:19:ALA:N	23:CY:25:LYS:HE3	1.49	1.26
59:DA:2405:G:N2	59:DA:2412:A:H62	1.29	1.25
21:AW:15:G:N2	21:AW:48:C:H42	1.36	1.24

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:BA:1015:G:O2'	40:DU:118:GLY:O[3_545]	2.09	0.11

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%)	154 (66%)	51 (22%)	28 (12%)	0	4
1	CB	233/235 (99%)	159 (68%)	50 (22%)	24 (10%)	0	5
2	AC	205/207 (99%)	154 (75%)	32 (16%)	19 (9%)	0	6
2	CC	205/207 (99%)	156 (76%)	36 (18%)	13 (6%)	1	12
3	AD	206/208 (99%)	149 (72%)	31 (15%)	26 (13%)	0	4
3	CD	206/208 (99%)	153 (74%)	32 (16%)	21 (10%)	0	6
4	AE	149/151 (99%)	117 (78%)	22 (15%)	10 (7%)	1	11
4	CE	149/151 (99%)	117 (78%)	25 (17%)	7 (5%)	2	17
5	AF	99/101 (98%)	75 (76%)	15 (15%)	9 (9%)	0	7
5	CF	99/101 (98%)	74 (75%)	16 (16%)	9 (9%)	0	7
6	AG	153/155 (99%)	121 (79%)	25 (16%)	7 (5%)	2	17
6	CG	153/155 (99%)	124 (81%)	22 (14%)	7 (5%)	2	17
7	AH	136/138 (99%)	97 (71%)	27 (20%)	12 (9%)	0	7
7	CH	136/138 (99%)	97 (71%)	28 (21%)	11 (8%)	1	8
8	AI	125/127 (98%)	93 (74%)	27 (22%)	5 (4%)	2	19
8	CI	125/127 (98%)	99 (79%)	22 (18%)	4 (3%)	3	24
9	AJ	97/99 (98%)	75 (77%)	13 (13%)	9 (9%)	0	6
9	CJ	97/99 (98%)	75 (77%)	17 (18%)	5 (5%)	1	14
10	AK	117/119 (98%)	82 (70%)	21 (18%)	14 (12%)	0	4
10	CK	117/119 (98%)	82 (70%)	22 (19%)	13 (11%)	0	5
11	AL	123/125 (98%)	38 (31%)	52 (42%)	33 (27%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	CL	123/125 (98%)	47 (38%)	43 (35%)	33 (27%)	0	0
12	AM	123/125 (98%)	93 (76%)	20 (16%)	10 (8%)	1	8
12	CM	123/125 (98%)	91 (74%)	25 (20%)	7 (6%)	1	13
13	AN	58/60 (97%)	44 (76%)	7 (12%)	7 (12%)	0	4
13	CN	58/60 (97%)	44 (76%)	10 (17%)	4 (7%)	1	10
14	AO	86/88 (98%)	65 (76%)	14 (16%)	7 (8%)	1	8
14	CO	86/88 (98%)	60 (70%)	21 (24%)	5 (6%)	1	13
15	AP	82/84 (98%)	66 (80%)	15 (18%)	1 (1%)	10	41
15	CP	82/84 (98%)	64 (78%)	14 (17%)	4 (5%)	1	16
16	AQ	98/100 (98%)	70 (71%)	18 (18%)	10 (10%)	0	6
16	CQ	98/100 (98%)	70 (71%)	18 (18%)	10 (10%)	0	6
17	AR	68/70 (97%)	51 (75%)	10 (15%)	7 (10%)	0	5
17	CR	68/70 (97%)	48 (71%)	13 (19%)	7 (10%)	0	5
18	AS	77/79 (98%)	41 (53%)	23 (30%)	13 (17%)	0	2
18	CS	77/79 (98%)	46 (60%)	17 (22%)	14 (18%)	0	1
19	AT	97/99 (98%)	82 (84%)	11 (11%)	4 (4%)	2	19
19	CT	97/99 (98%)	79 (81%)	12 (12%)	6 (6%)	1	12
23	AY	663/687 (96%)	451 (68%)	138 (21%)	74 (11%)	0	5
23	CY	663/687 (96%)	461 (70%)	134 (20%)	68 (10%)	0	5
24	AU	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
24	CU	2/6 (33%)	1 (50%)	0	1 (50%)	0	0
25	BC	226/228 (99%)	110 (49%)	66 (29%)	50 (22%)	0	1
25	DC	226/228 (99%)	123 (54%)	59 (26%)	44 (20%)	0	1
26	BD	273/275 (99%)	174 (64%)	47 (17%)	52 (19%)	0	1
26	DD	273/275 (99%)	165 (60%)	61 (22%)	47 (17%)	0	2
27	BE	203/205 (99%)	128 (63%)	40 (20%)	35 (17%)	0	2
27	DE	203/205 (99%)	122 (60%)	45 (22%)	36 (18%)	0	1
28	BF	206/208 (99%)	130 (63%)	46 (22%)	30 (15%)	0	3
28	DF	206/208 (99%)	128 (62%)	44 (21%)	34 (16%)	0	2
29	BG	179/181 (99%)	122 (68%)	48 (27%)	9 (5%)	1	15
29	DG	179/181 (99%)	134 (75%)	36 (20%)	9 (5%)	1	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	BH	165/167 (99%)	118 (72%)	27 (16%)	20 (12%)	0	4
30	DH	165/167 (99%)	111 (67%)	33 (20%)	21 (13%)	0	3
32	BK	138/140 (99%)	96 (70%)	30 (22%)	12 (9%)	0	7
32	DK	138/140 (99%)	97 (70%)	34 (25%)	7 (5%)	1	15
33	BN	136/138 (99%)	86 (63%)	28 (21%)	22 (16%)	0	2
33	DN	136/138 (99%)	88 (65%)	35 (26%)	13 (10%)	0	6
34	BO	120/122 (98%)	86 (72%)	24 (20%)	10 (8%)	0	7
34	DO	120/122 (98%)	87 (72%)	25 (21%)	8 (7%)	1	11
35	BP	144/146 (99%)	85 (59%)	39 (27%)	20 (14%)	0	3
35	DP	144/146 (99%)	81 (56%)	38 (26%)	25 (17%)	0	2
36	BQ	139/141 (99%)	96 (69%)	27 (19%)	16 (12%)	0	5
36	DQ	139/141 (99%)	97 (70%)	29 (21%)	13 (9%)	0	6
37	BR	115/117 (98%)	80 (70%)	27 (24%)	8 (7%)	1	10
37	DR	115/117 (98%)	83 (72%)	20 (17%)	12 (10%)	0	5
38	BS	97/99 (98%)	56 (58%)	21 (22%)	20 (21%)	0	1
38	DS	97/99 (98%)	56 (58%)	21 (22%)	20 (21%)	0	1
39	BT	136/138 (99%)	80 (59%)	31 (23%)	25 (18%)	0	1
39	DT	136/138 (99%)	85 (62%)	29 (21%)	22 (16%)	0	2
40	BU	115/117 (98%)	84 (73%)	25 (22%)	6 (5%)	1	14
40	DU	115/117 (98%)	90 (78%)	16 (14%)	9 (8%)	1	8
41	BV	99/101 (98%)	66 (67%)	16 (16%)	17 (17%)	0	2
41	DV	99/101 (98%)	63 (64%)	22 (22%)	14 (14%)	0	3
42	BW	111/113 (98%)	85 (77%)	11 (10%)	15 (14%)	0	3
42	DW	111/113 (98%)	85 (77%)	15 (14%)	11 (10%)	0	6
43	BX	91/93 (98%)	72 (79%)	15 (16%)	4 (4%)	2	17
43	DX	91/93 (98%)	72 (79%)	14 (15%)	5 (6%)	1	13
44	BY	105/107 (98%)	51 (49%)	30 (29%)	24 (23%)	0	1
44	DY	105/107 (98%)	46 (44%)	26 (25%)	33 (31%)	0	0
45	BZ	183/185 (99%)	132 (72%)	33 (18%)	18 (10%)	0	6
45	DZ	183/185 (99%)	132 (72%)	32 (18%)	19 (10%)	0	5
46	B0	82/84 (98%)	59 (72%)	16 (20%)	7 (8%)	0	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	D0	82/84 (98%)	57 (70%)	15 (18%)	10 (12%)	0	4
47	B2	69/71 (97%)	51 (74%)	14 (20%)	4 (6%)	1	13
47	D2	69/71 (97%)	56 (81%)	10 (14%)	3 (4%)	2	18
48	B3	58/60 (97%)	48 (83%)	6 (10%)	4 (7%)	1	10
48	D3	58/60 (97%)	42 (72%)	10 (17%)	6 (10%)	0	5
49	B5	57/59 (97%)	43 (75%)	11 (19%)	3 (5%)	1	14
49	D5	57/59 (97%)	41 (72%)	12 (21%)	4 (7%)	1	10
50	B6	48/50 (96%)	28 (58%)	13 (27%)	7 (15%)	0	3
50	D6	48/50 (96%)	29 (60%)	8 (17%)	11 (23%)	0	1
51	B7	47/49 (96%)	35 (74%)	8 (17%)	4 (8%)	0	7
51	D7	47/49 (96%)	32 (68%)	9 (19%)	6 (13%)	0	3
52	B8	62/64 (97%)	35 (56%)	17 (27%)	10 (16%)	0	2
52	D8	62/64 (97%)	36 (58%)	18 (29%)	8 (13%)	0	3
53	B9	35/37 (95%)	18 (51%)	12 (34%)	5 (14%)	0	3
53	D9	35/37 (95%)	24 (69%)	8 (23%)	3 (9%)	0	7
54	Be	70/102 (69%)	38 (54%)	24 (34%)	8 (11%)	0	5
54	De	70/102 (69%)	41 (59%)	23 (33%)	6 (9%)	0	7
57	B1	91/93 (98%)	60 (66%)	19 (21%)	12 (13%)	0	3
57	D1	91/93 (98%)	56 (62%)	18 (20%)	17 (19%)	0	1
58	B4	33/35 (94%)	15 (46%)	13 (39%)	5 (15%)	0	2
58	D4	33/35 (94%)	17 (52%)	9 (27%)	7 (21%)	0	1
All	All	13260/13576 (98%)	9009 (68%)	2708 (20%)	1543 (12%)	0	4

5 of 1543 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AB	9	GLU
1	AB	76	GLN
1	AB	165	VAL
1	AB	194	PRO
2	AC	4	LYS

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%)	164 (81%)	39 (19%)	1	8
1	CB	203/203 (100%)	161 (79%)	42 (21%)	1	6
2	AC	161/161 (100%)	132 (82%)	29 (18%)	2	10
2	CC	161/161 (100%)	134 (83%)	27 (17%)	2	13
3	AD	180/180 (100%)	150 (83%)	30 (17%)	2	13
3	CD	180/180 (100%)	151 (84%)	29 (16%)	2	14
4	AE	116/116 (100%)	91 (78%)	25 (22%)	1	6
4	CE	116/116 (100%)	96 (83%)	20 (17%)	2	12
5	AF	90/90 (100%)	83 (92%)	7 (8%)	11	36
5	CF	90/90 (100%)	77 (86%)	13 (14%)	3	18
6	AG	126/126 (100%)	111 (88%)	15 (12%)	5	23
6	CG	126/126 (100%)	117 (93%)	9 (7%)	13	38
7	AH	119/119 (100%)	100 (84%)	19 (16%)	2	14
7	CH	119/119 (100%)	108 (91%)	11 (9%)	8	32
8	AI	98/98 (100%)	82 (84%)	16 (16%)	2	14
8	CI	98/98 (100%)	84 (86%)	14 (14%)	3	18
9	AJ	89/89 (100%)	76 (85%)	13 (15%)	3	17
9	CJ	89/89 (100%)	72 (81%)	17 (19%)	1	8
10	AK	90/90 (100%)	72 (80%)	18 (20%)	1	7
10	CK	90/90 (100%)	72 (80%)	18 (20%)	1	7
11	AL	104/104 (100%)	70 (67%)	34 (33%)	0	2
11	CL	104/104 (100%)	76 (73%)	28 (27%)	0	3
12	AM	100/100 (100%)	80 (80%)	20 (20%)	1	7
12	CM	100/100 (100%)	84 (84%)	16 (16%)	2	14
13	AN	49/49 (100%)	43 (88%)	6 (12%)	5	22
13	CN	49/49 (100%)	44 (90%)	5 (10%)	7	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	AO	79/79 (100%)	71 (90%)	8 (10%)	7	28
14	CO	79/79 (100%)	67 (85%)	12 (15%)	3	16
15	AP	72/72 (100%)	65 (90%)	7 (10%)	8	30
15	CP	72/72 (100%)	63 (88%)	9 (12%)	4	22
16	AQ	95/95 (100%)	80 (84%)	15 (16%)	2	15
16	CQ	95/95 (100%)	76 (80%)	19 (20%)	1	7
17	AR	61/61 (100%)	51 (84%)	10 (16%)	2	14
17	CR	61/61 (100%)	54 (88%)	7 (12%)	5	24
18	AS	69/69 (100%)	56 (81%)	13 (19%)	1	9
18	CS	69/69 (100%)	54 (78%)	15 (22%)	1	6
19	AT	76/76 (100%)	64 (84%)	12 (16%)	2	15
19	CT	76/76 (100%)	68 (90%)	8 (10%)	6	27
23	AY	563/579 (97%)	462 (82%)	101 (18%)	2	10
23	CY	563/579 (97%)	449 (80%)	114 (20%)	1	7
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%)	136 (76%)	44 (24%)	1	4
25	DC	180/180 (100%)	136 (76%)	44 (24%)	1	4
26	BD	217/217 (100%)	164 (76%)	53 (24%)	1	4
26	DD	217/217 (100%)	167 (77%)	50 (23%)	1	5
27	BE	165/165 (100%)	133 (81%)	32 (19%)	1	8
27	DE	165/165 (100%)	132 (80%)	33 (20%)	1	7
28	BF	165/165 (100%)	129 (78%)	36 (22%)	1	6
28	DF	165/165 (100%)	135 (82%)	30 (18%)	2	10
29	BG	155/155 (100%)	130 (84%)	25 (16%)	2	14
29	DG	155/155 (100%)	123 (79%)	32 (21%)	1	7
30	BH	136/136 (100%)	117 (86%)	19 (14%)	3	19
30	DH	136/136 (100%)	120 (88%)	16 (12%)	5	23
32	BK	105/105 (100%)	88 (84%)	17 (16%)	2	14
32	DK	105/105 (100%)	89 (85%)	16 (15%)	3	16
33	BN	117/117 (100%)	91 (78%)	26 (22%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	DN	117/117 (100%)	88 (75%)	29 (25%)	1	4
34	BO	100/100 (100%)	79 (79%)	21 (21%)	1	6
34	DO	100/100 (100%)	82 (82%)	18 (18%)	2	10
35	BP	112/112 (100%)	87 (78%)	25 (22%)	1	5
35	DP	112/112 (100%)	92 (82%)	20 (18%)	2	10
36	BQ	111/111 (100%)	83 (75%)	28 (25%)	0	4
36	DQ	111/111 (100%)	86 (78%)	25 (22%)	1	5
37	BR	100/100 (100%)	85 (85%)	15 (15%)	3	17
37	DR	100/100 (100%)	81 (81%)	19 (19%)	1	8
38	BS	77/77 (100%)	63 (82%)	14 (18%)	2	10
38	DS	77/77 (100%)	58 (75%)	19 (25%)	1	4
39	BT	120/120 (100%)	92 (77%)	28 (23%)	1	5
39	DT	120/120 (100%)	92 (77%)	28 (23%)	1	5
40	BU	93/93 (100%)	72 (77%)	21 (23%)	1	5
40	DU	93/93 (100%)	70 (75%)	23 (25%)	1	4
41	BV	82/82 (100%)	58 (71%)	24 (29%)	0	2
41	DV	82/82 (100%)	57 (70%)	25 (30%)	0	2
42	BW	92/92 (100%)	71 (77%)	21 (23%)	1	5
42	DW	92/92 (100%)	73 (79%)	19 (21%)	1	6
43	BX	75/75 (100%)	67 (89%)	8 (11%)	6	27
43	DX	75/75 (100%)	60 (80%)	15 (20%)	1	7
44	BY	88/88 (100%)	71 (81%)	17 (19%)	1	8
44	DY	88/88 (100%)	71 (81%)	17 (19%)	1	8
45	BZ	162/162 (100%)	132 (82%)	30 (18%)	1	9
45	DZ	162/162 (100%)	138 (85%)	24 (15%)	3	17
46	B0	66/66 (100%)	55 (83%)	11 (17%)	2	13
46	D0	66/66 (100%)	54 (82%)	12 (18%)	2	10
47	B2	66/66 (100%)	59 (89%)	7 (11%)	6	27
47	D2	66/66 (100%)	59 (89%)	7 (11%)	6	27
48	B3	52/52 (100%)	43 (83%)	9 (17%)	2	11
48	D3	52/52 (100%)	45 (86%)	7 (14%)	4	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	B5	51/51 (100%)	43 (84%)	8 (16%)	2	15
49	D5	51/51 (100%)	39 (76%)	12 (24%)	1	4
50	B6	49/49 (100%)	38 (78%)	11 (22%)	1	5
50	D6	49/49 (100%)	39 (80%)	10 (20%)	1	7
51	B7	42/42 (100%)	36 (86%)	6 (14%)	3	18
51	D7	42/42 (100%)	38 (90%)	4 (10%)	8	31
52	B8	54/54 (100%)	38 (70%)	16 (30%)	0	2
52	D8	54/54 (100%)	38 (70%)	16 (30%)	0	2
53	B9	34/34 (100%)	29 (85%)	5 (15%)	3	17
53	D9	34/34 (100%)	32 (94%)	2 (6%)	18	44
54	Be	54/54 (100%)	47 (87%)	7 (13%)	4	21
54	De	54/54 (100%)	44 (82%)	10 (18%)	1	9
57	B1	78/78 (100%)	56 (72%)	22 (28%)	0	3
57	D1	78/78 (100%)	58 (74%)	20 (26%)	0	3
58	B4	31/31 (100%)	22 (71%)	9 (29%)	0	2
58	D4	31/31 (100%)	26 (84%)	5 (16%)	2	14
All	All	11142/11174 (100%)	9050 (81%)	2092 (19%)	1	9

5 of 2092 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
39	DT	72	VAL
41	DV	80	GLN
39	DT	65	LYS
57	D1	60	PHE
37	BR	117	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 150 such sidechains are listed below:

Mol	Chain	Res	Type
29	DG	41	GLN
47	D2	48	HIS
30	DH	147	ASN
39	DT	104	ASN
34	BO	82	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
20	AA	1510/1511 (99%)	305 (20%)	17 (1%)
20	CA	1510/1511 (99%)	285 (18%)	16 (1%)
21	AW	76/77 (98%)	23 (30%)	1 (1%)
21	CW	76/77 (98%)	22 (28%)	1 (1%)
22	AV	22/23 (95%)	8 (36%)	1 (4%)
22	CV	22/23 (95%)	8 (36%)	2 (9%)
59	BA	2878/2879 (99%)	666 (23%)	27 (0%)
59	DA	2878/2879 (99%)	666 (23%)	21 (0%)
60	BB	118/119 (99%)	21 (17%)	1 (0%)
60	DB	118/119 (99%)	17 (14%)	1 (0%)
All	All	9208/9218 (99%)	2021 (21%)	88 (0%)

5 of 2021 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
20	AA	6	G
20	AA	9	G
20	AA	13	U
20	AA	15	G
20	AA	29	G

5 of 88 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
20	CA	1145	C
59	DA	479	A
20	CA	1504	G
22	CV	18	G
59	DA	1558	A

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	UAL	CU	5	24	6,8,9	2.63	2 (33%)	4,9,11	1.88	1 (25%)
24	KBE	AU	1	24	8,8,9	0.60	0	6,8,10	1.53	1 (16%)
24	5OH	CU	6	24	7,12,13	0.69	0	4,16,18	1.89	2 (50%)
24	KBE	CU	1	24	8,8,9	0.63	0	6,8,10	1.85	1 (16%)
24	UAL	AU	5	24	6,8,9	2.53	2 (33%)	4,9,11	1.53	1 (25%)
24	DPP	AU	2	24	4,5,6	0.44	0	1,5,7	1.18	0
24	5OH	AU	6	24	7,12,13	0.66	0	4,16,18	2.65	1 (25%)
24	DPP	CU	2	24	4,5,6	0.34	0	1,5,7	0.52	0

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	CU	5	UAL	C-CA	5.08	1.53	1.45
24	AU	5	UAL	C-CA	5.07	1.53	1.45
24	CU	5	UAL	C1-N1	-3.32	1.35	1.40
24	AU	5	UAL	C1-N1	-2.92	1.35	1.40

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AU	6	5OH	CR-CB-CA	4.75	117.65	112.61
24	CU	1	KBE	CB-CA-C	4.25	119.03	112.17
24	CU	5	UAL	O-C-CA	-3.68	120.78	125.39
24	AU	1	KBE	CB-CA-C	3.14	117.24	112.17
24	AU	5	UAL	O-C-CA	-2.78	121.90	125.39

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	AU	1	KBE	C-CA-CB-N
24	CU	1	KBE	C-CA-CB-N
24	CU	6	5OH	C-CA-CB-CR
24	CU	1	KBE	C-CA-CB-CG
24	CU	1	KBE	N-CB-CG-CD

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	CU	1	KBE	2	0
24	CU	2	DPP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
62	GDP	AY	702	-	29,30,30	1.06	1 (3%)	45,47,47	1.71	9 (20%)
62	GDP	CY	702	-	29,30,30	1.06	1 (3%)	45,47,47	1.71	9 (20%)
61	FUA	CY	701	-	39,40,40	1.71	7 (17%)	50,64,64	2.22	15 (30%)
61	FUA	AY	701	-	39,40,40	1.73	7 (17%)	50,64,64	2.00	14 (28%)

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
62	GDP	AY	702	-	-	2/16/32/32	0/3/3/3
62	GDP	CY	702	-	-	2/16/32/32	0/3/3/3
61	FUA	CY	701	-	-	6/16/92/92	0/4/4/4
61	FUA	AY	701	-	-	7/16/92/92	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	CY	701	FUA	C29-C22	4.74	1.54	1.47
61	AY	701	FUA	C23-C24	-4.39	1.39	1.53
61	AY	701	FUA	C23-C22	-4.35	1.40	1.51
61	AY	701	FUA	C29-C22	4.22	1.53	1.47
61	CY	701	FUA	C23-C24	-4.19	1.39	1.53

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	CY	701	FUA	C24-C23-C22	6.89	127.40	112.72
61	CY	701	FUA	C13-C12-C11	-6.17	102.94	111.90
61	AY	701	FUA	C24-C23-C22	6.06	125.63	112.72
61	AY	701	FUA	C13-C12-C11	-5.63	103.73	111.90
62	AY	702	GDP	C2-N3-C4	5.33	121.47	112.30

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
61	AY	701	FUA	C13-C17-C22-C23
61	AY	701	FUA	C13-C17-C22-C29
61	AY	701	FUA	C29-C22-C23-C24
61	CY	701	FUA	C13-C17-C22-C23
61	CY	701	FUA	C13-C17-C22-C29

There are no ring outliers.

4 monomers are involved in 38 short contacts:

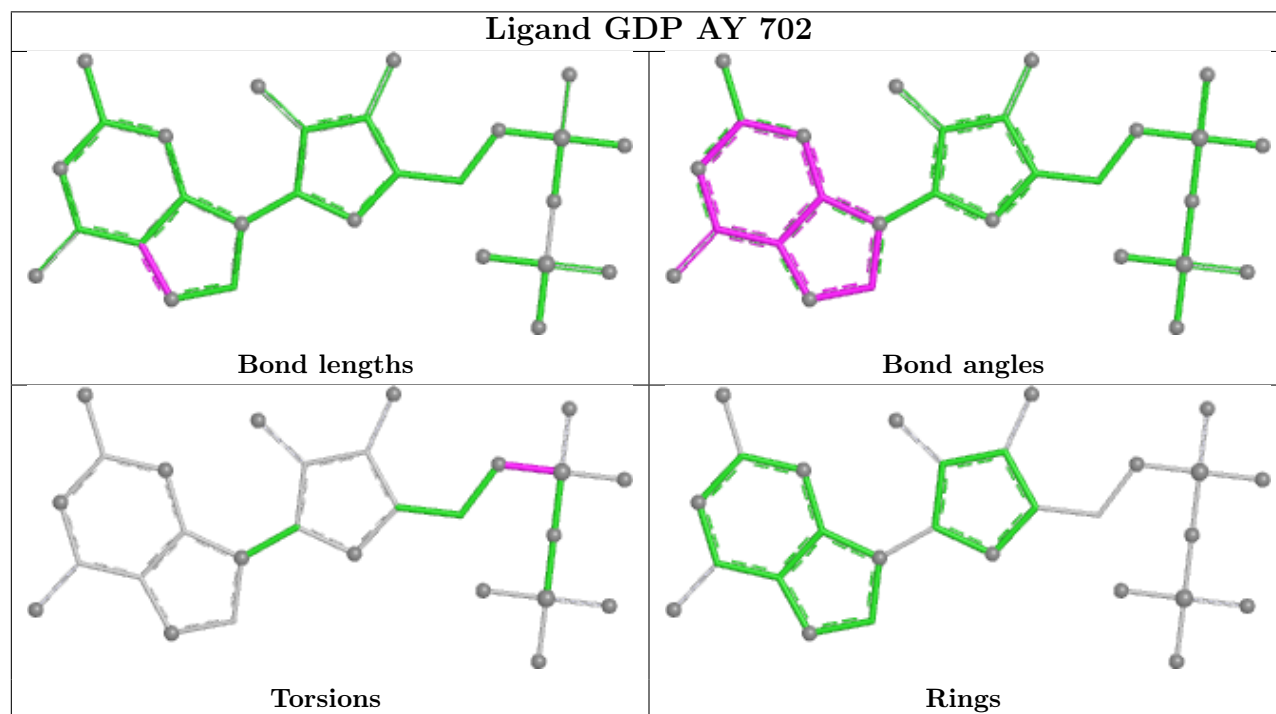
Mol	Chain	Res	Type	Clashes	Symm-Clashes
62	AY	702	GDP	12	0

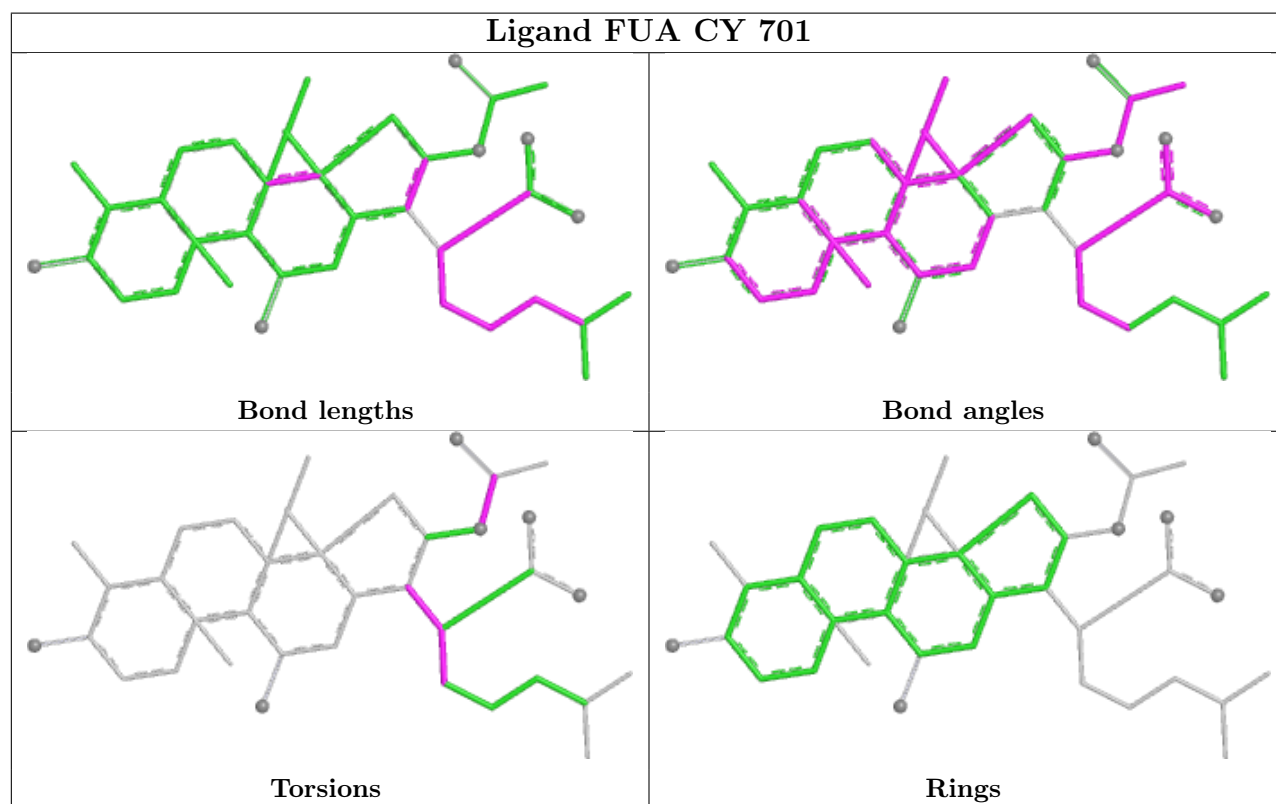
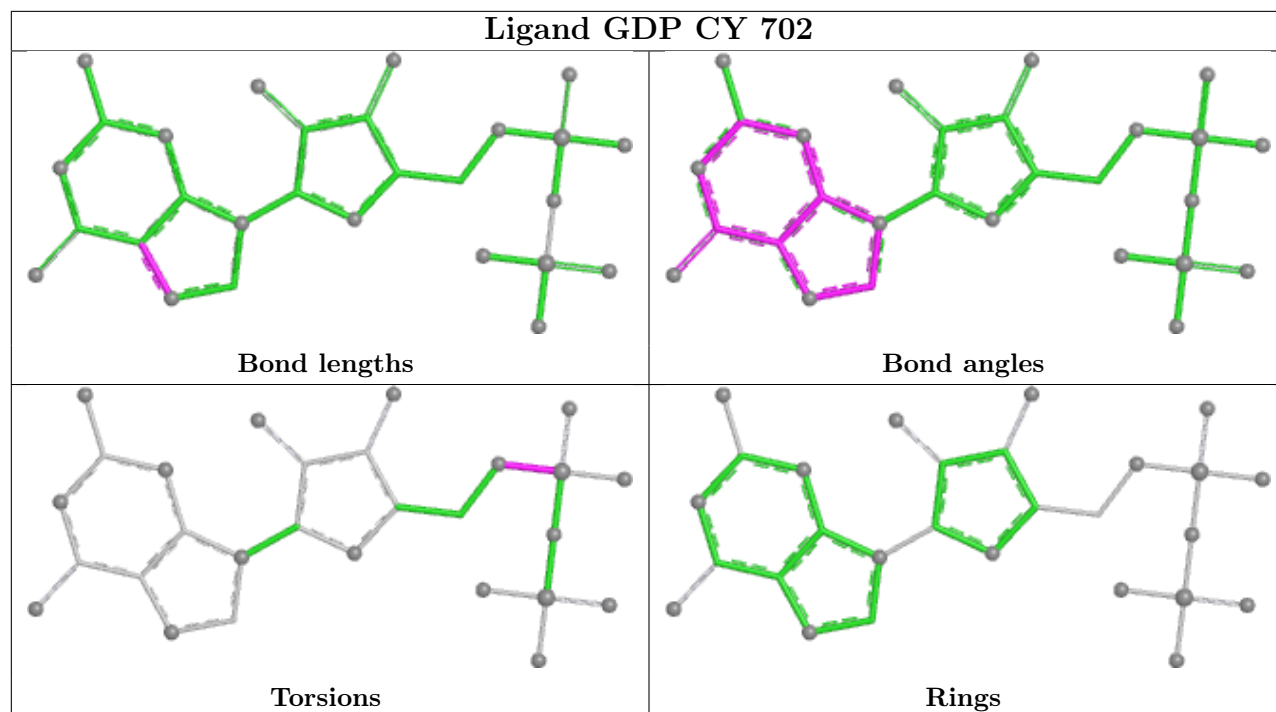
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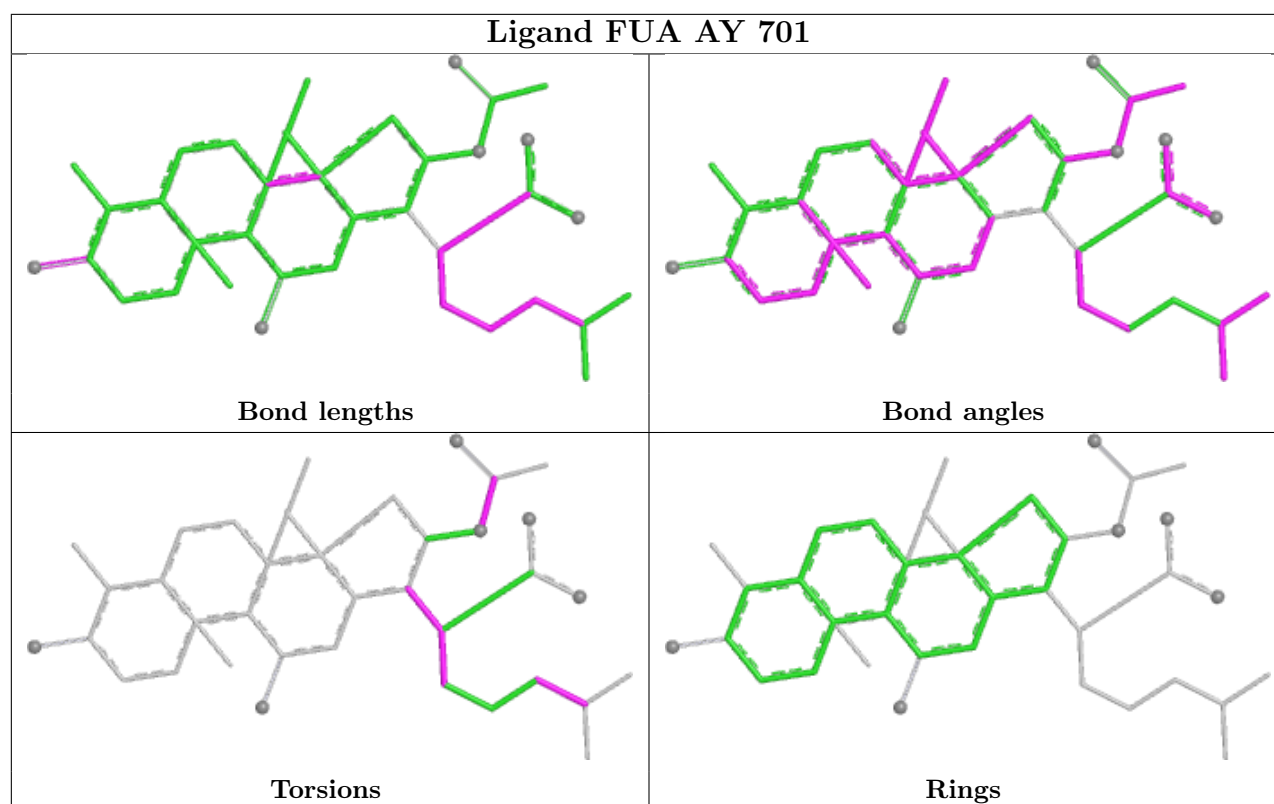
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
62	CY	702	GDP	13	0
61	CY	701	FUA	7	0
61	AY	701	FUA	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
54	De	1
54	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	37.69
1	Be	30:UNK	C	51:ALA	N	36.65

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%)	-1.06	0 100 100	4, 59, 144, 223	0
1	CB	235/235 (100%)	-0.99	1 (0%) 88 72	5, 60, 155, 214	0
2	AC	207/207 (100%)	-0.88	1 (0%) 87 68	4, 63, 136, 190	0
2	CC	207/207 (100%)	-0.97	1 (0%) 87 68	3, 57, 130, 186	0
3	AD	208/208 (100%)	-0.86	1 (0%) 87 68	4, 57, 142, 206	0
3	CD	208/208 (100%)	-0.78	1 (0%) 87 68	14, 72, 144, 196	0
4	AE	151/151 (100%)	-0.73	1 (0%) 84 63	5, 34, 122, 151	0
4	CE	151/151 (100%)	-0.76	0 100 100	4, 35, 133, 165	0
5	AF	101/101 (100%)	-1.11	0 100 100	4, 27, 93, 145	0
5	CF	101/101 (100%)	-1.10	1 (0%) 79 56	5, 37, 115, 163	0
6	AG	155/155 (100%)	-1.18	0 100 100	10, 78, 153, 229	0
6	CG	155/155 (100%)	-1.02	0 100 100	3, 84, 172, 210	0
7	AH	138/138 (100%)	-1.24	0 100 100	3, 31, 89, 166	0
7	CH	138/138 (100%)	-1.19	0 100 100	1, 37, 130, 199	0
8	AI	127/127 (100%)	-0.98	0 100 100	6, 72, 140, 199	0
8	CI	127/127 (100%)	-0.70	3 (2%) 59 35	14, 84, 152, 237	0
9	AJ	99/99 (100%)	-0.55	3 (3%) 52 30	9, 68, 136, 163	0
9	CJ	99/99 (100%)	-0.59	2 (2%) 65 39	13, 65, 154, 217	0
10	AK	119/119 (100%)	-0.92	1 (0%) 82 60	7, 56, 137, 180	0
10	CK	119/119 (100%)	-0.79	1 (0%) 82 60	8, 55, 145, 175	0
11	AL	125/125 (100%)	-0.90	1 (0%) 82 60	5, 39, 105, 171	0
11	CL	125/125 (100%)	-0.92	0 100 100	8, 52, 134, 176	0
12	AM	125/125 (100%)	-0.86	1 (0%) 82 60	23, 90, 167, 199	0
12	CM	125/125 (100%)	-0.90	0 100 100	14, 90, 166, 190	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AN	60/60 (100%)	-1.22	0 100 100	8, 38, 114, 139	0
13	CN	60/60 (100%)	-1.14	0 100 100	8, 42, 131, 166	0
14	AO	88/88 (100%)	-1.24	0 100 100	5, 37, 108, 158	0
14	CO	88/88 (100%)	-1.10	0 100 100	8, 49, 130, 197	0
15	AP	84/84 (100%)	-1.02	0 100 100	18, 68, 131, 171	0
15	CP	84/84 (100%)	-1.08	0 100 100	8, 79, 159, 224	0
16	AQ	100/100 (100%)	-0.88	0 100 100	9, 43, 120, 169	0
16	CQ	100/100 (100%)	-0.84	1 (1%) 79 56	5, 43, 118, 142	0
17	AR	70/70 (100%)	-1.08	0 100 100	7, 30, 134, 185	0
17	CR	70/70 (100%)	-1.07	0 100 100	7, 28, 130, 193	0
18	AS	79/79 (100%)	-0.96	0 100 100	15, 78, 159, 206	0
18	CS	79/79 (100%)	-1.00	1 (1%) 75 50	10, 80, 154, 204	0
19	AT	99/99 (100%)	-0.92	0 100 100	4, 64, 120, 186	0
19	CT	99/99 (100%)	-0.84	0 100 100	16, 71, 155, 187	0
20	AA	1511/1511 (100%)	-1.08	22 (1%) 72 47	3, 62, 163, 289	0
20	CA	1511/1511 (100%)	-1.10	22 (1%) 72 47	5, 63, 173, 323	0
21	AW	77/77 (100%)	-1.19	0 100 100	21, 91, 179, 234	0
21	CW	77/77 (100%)	-1.22	0 100 100	44, 97, 221, 273	0
22	AV	23/23 (100%)	-0.50	1 (4%) 40 21	56, 136, 187, 205	0
22	CV	23/23 (100%)	-0.59	1 (4%) 40 21	66, 119, 215, 230	0
23	AY	667/687 (97%)	-0.95	1 (0%) 92 86	5, 64, 147, 208	0
23	CY	667/687 (97%)	-0.91	5 (0%) 84 63	4, 68, 150, 203	0
24	AU	2/6 (33%)	-0.64	0 100 100	155, 155, 155, 155	0
24	CU	2/6 (33%)	-0.75	0 100 100	81, 81, 81, 88	0
25	BC	228/228 (100%)	-1.03	0 100 100	45, 128, 217, 259	0
25	DC	228/228 (100%)	-1.03	1 (0%) 88 72	33, 153, 230, 287	0
26	BD	275/275 (100%)	-0.89	2 (0%) 84 63	4, 26, 103, 166	0
26	DD	275/275 (100%)	-0.90	0 100 100	4, 25, 107, 210	0
27	BE	205/205 (100%)	-1.12	0 100 100	1, 31, 135, 229	0
27	DE	205/205 (100%)	-1.07	0 100 100	6, 41, 144, 221	0
28	BF	208/208 (100%)	-0.83	1 (0%) 87 68	6, 49, 162, 216	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DF	208/208 (100%)	-0.87	0 100 100	10, 62, 162, 266	0
29	BG	181/181 (100%)	-0.93	0 100 100	11, 91, 152, 197	0
29	DG	181/181 (100%)	-1.01	1 (0%) 85 65	33, 105, 176, 209	0
30	BH	167/167 (100%)	-1.22	0 100 100	3, 47, 130, 224	0
30	DH	167/167 (100%)	-1.03	0 100 100	6, 56, 141, 187	0
31	BJ	0/170	-	-	-	-
31	DJ	0/170	-	-	-	-
32	BK	140/140 (100%)	-0.83	1 (0%) 84 63	17, 104, 194, 230	0
32	DK	140/140 (100%)	-0.94	2 (1%) 73 48	37, 124, 205, 244	0
33	BN	138/138 (100%)	-0.81	0 100 100	59, 83, 108, 111	0
33	DN	138/138 (100%)	-0.83	0 100 100	59, 81, 104, 111	0
34	BO	122/122 (100%)	-1.01	1 (0%) 82 60	5, 33, 94, 148	0
34	DO	122/122 (100%)	-0.96	0 100 100	4, 30, 131, 183	0
35	BP	146/146 (100%)	-0.88	0 100 100	7, 55, 131, 173	0
35	DP	146/146 (100%)	-0.87	1 (0%) 84 63	1, 60, 152, 204	0
36	BQ	141/141 (100%)	-0.95	2 (1%) 73 48	20, 43, 113, 170	0
36	DQ	141/141 (100%)	-0.94	2 (1%) 73 48	8, 32, 107, 219	0
37	BR	117/117 (100%)	-1.07	0 100 100	7, 38, 125, 156	0
37	DR	117/117 (100%)	-1.01	1 (0%) 81 58	2, 38, 126, 213	0
38	BS	99/99 (100%)	-0.90	0 100 100	27, 104, 191, 225	0
38	DS	99/99 (100%)	-0.85	0 100 100	11, 106, 194, 248	0
39	BT	138/138 (100%)	-0.96	0 100 100	6, 53, 139, 225	0
39	DT	138/138 (100%)	-0.85	0 100 100	3, 68, 141, 201	0
40	BU	117/117 (100%)	-1.08	0 100 100	11, 22, 80, 175	0
40	DU	117/117 (100%)	-1.06	1 (0%) 81 58	6, 20, 94, 136	0
41	BV	101/101 (100%)	-1.12	0 100 100	0, 32, 104, 143	0
41	DV	101/101 (100%)	-1.08	0 100 100	2, 32, 117, 147	0
42	BW	113/113 (100%)	-1.00	0 100 100	8, 32, 103, 140	0
42	DW	113/113 (100%)	-0.89	0 100 100	2, 31, 116, 157	0
43	BX	93/93 (100%)	-1.04	0 100 100	5, 51, 118, 172	0
43	DX	93/93 (100%)	-0.96	0 100 100	7, 50, 136, 198	0
44	BY	107/107 (100%)	-0.91	1 (0%) 81 58	12, 69, 151, 213	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	DY	107/107 (100%)	-0.95	1 (0%) 81 58	6, 70, 150, 196	0
45	BZ	185/185 (100%)	-1.15	0 100 100	13, 52, 123, 175	0
45	DZ	185/185 (100%)	-1.10	0 100 100	10, 61, 135, 194	0
46	B0	84/84 (100%)	-0.67	1 (1%) 76 52	6, 53, 127, 163	0
46	D0	84/84 (100%)	-0.76	3 (3%) 46 25	7, 58, 132, 217	0
47	B2	71/71 (100%)	-1.24	0 100 100	12, 61, 137, 175	0
47	D2	71/71 (100%)	-1.17	0 100 100	9, 60, 127, 145	0
48	B3	60/60 (100%)	-1.14	0 100 100	8, 31, 96, 111	0
48	D3	60/60 (100%)	-1.04	0 100 100	13, 29, 101, 126	0
49	B5	59/59 (100%)	-1.07	0 100 100	8, 37, 148, 208	0
49	D5	59/59 (100%)	-1.00	0 100 100	6, 44, 156, 223	0
50	B6	50/50 (100%)	-1.09	0 100 100	12, 92, 147, 163	0
50	D6	50/50 (100%)	-0.95	0 100 100	31, 89, 175, 242	0
51	B7	49/49 (100%)	-1.14	0 100 100	9, 16, 135, 218	0
51	D7	49/49 (100%)	-1.00	0 100 100	11, 32, 107, 180	0
52	B8	64/64 (100%)	-0.96	0 100 100	5, 46, 98, 130	0
52	D8	64/64 (100%)	-0.85	0 100 100	7, 56, 123, 178	0
53	B9	37/37 (100%)	-1.03	0 100 100	10, 26, 148, 246	0
53	D9	37/37 (100%)	-0.93	0 100 100	8, 19, 104, 158	0
54	Be	72/102 (70%)	-0.86	2 (2%) 55 32	24, 113, 183, 201	0
54	De	72/102 (70%)	-1.07	0 100 100	18, 114, 206, 259	0
55	Bf	0/31	-	-	-	-
55	Bg	0/31	-	-	-	-
55	Df	0/31	-	-	-	-
55	Dg	0/31	-	-	-	-
56	Bh	0/30	-	-	-	-
56	Dh	0/30	-	-	-	-
57	B1	93/93 (100%)	-0.47	0 100 100	1, 79, 187, 243	0
57	D1	93/93 (100%)	-0.31	1 (1%) 78 54	8, 72, 174, 241	0
58	B4	35/35 (100%)	-1.16	0 100 100	74, 144, 233, 266	0
58	D4	35/35 (100%)	-0.83	1 (2%) 53 31	64, 158, 226, 275	0
59	BA	2879/2879 (100%)	-1.29	12 (0%) 88 72	3, 43, 145, 276	0
59	DA	2879/2879 (100%)	-1.25	14 (0%) 87 68	0, 47, 163, 315	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
60	BB	119/119 (100%)	-1.42	0	100	100	21, 108, 175, 210	0
60	DB	119/119 (100%)	-1.29	0	100	100	23, 97, 186, 258	0
All	All	22686/23318 (97%)	-1.06	125 (0%)	85	65	0, 57, 160, 323	0

The worst 5 of 125 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	CJ	58	ASP	5.5
44	DY	107	ASP	5.1
59	BA	382	G	5.0
20	CA	1099	G	4.8
44	BY	107	ASP	4.8

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
24	UAL	AU	5	9/10	0.93	0.12	149,151,153,154	0
24	UAL	CU	5	9/10	0.96	0.09	89,90,91,91	0
24	DPP	CU	2	6/7	0.97	0.10	77,79,80,82	0
24	5OH	CU	6	12/13	0.97	0.08	84,88,89,89	0
24	KBE	CU	1	9/10	0.98	0.10	69,74,77,77	0
24	5OH	AU	6	12/13	0.98	0.11	151,153,154,154	0
24	DPP	AU	2	6/7	0.98	0.06	153,153,154,154	0
24	KBE	AU	1	9/10	0.99	0.09	154,155,156,156	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

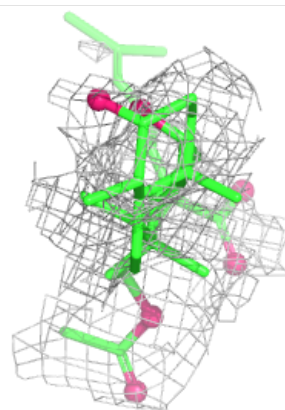
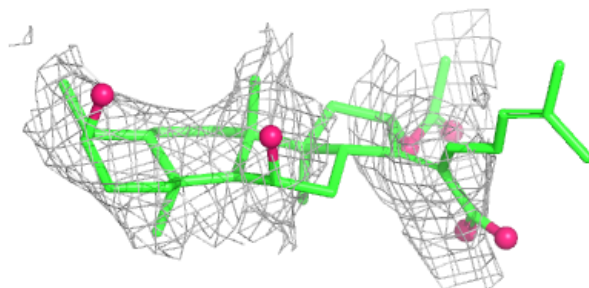
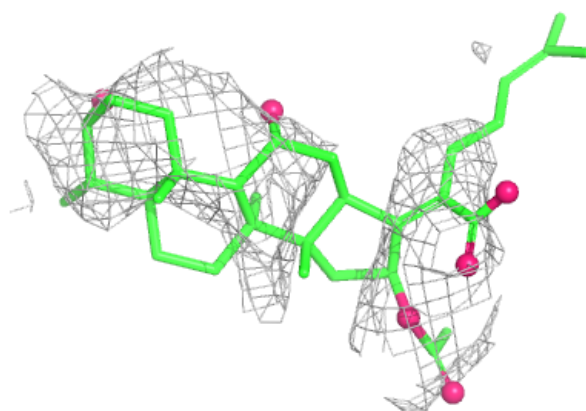
labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
61	FUA	AY	701	37/37	0.97	0.09	154,155,156,156	0
61	FUA	CY	701	37/37	0.97	0.09	199,200,202,202	0
62	GDP	CY	702	28/28	0.97	0.07	78,82,83,84	0
62	GDP	AY	702	28/28	0.98	0.04	78,82,83,84	0
63	MG	BA	2901	1/1	1.00	0.11	5,5,5,5	0
63	MG	CY	703	1/1	1.00	0.07	1,1,1,1	0

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

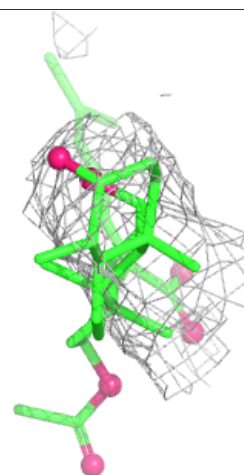
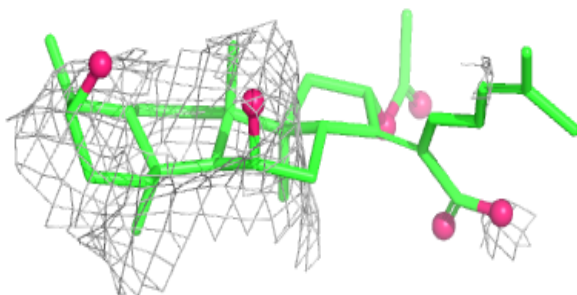
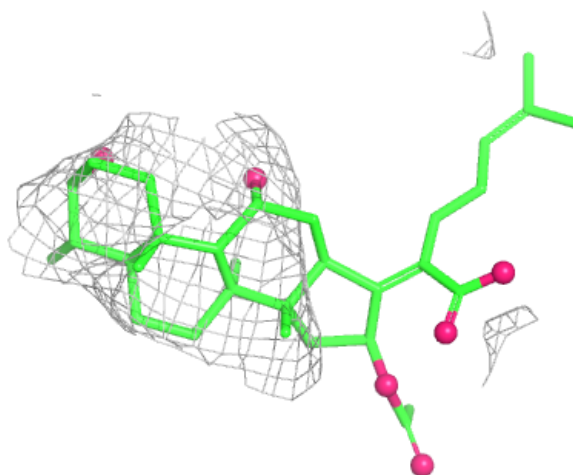
Electron density around FUA AY 701:

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



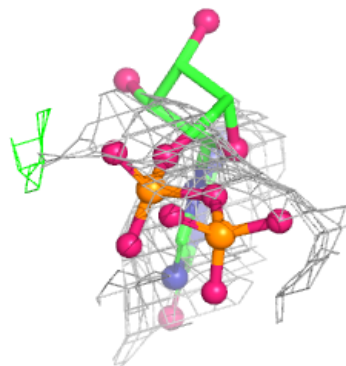
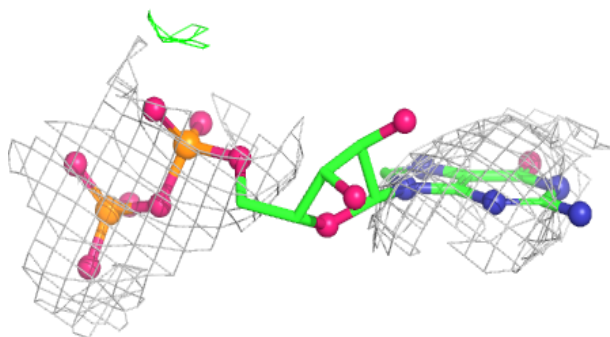
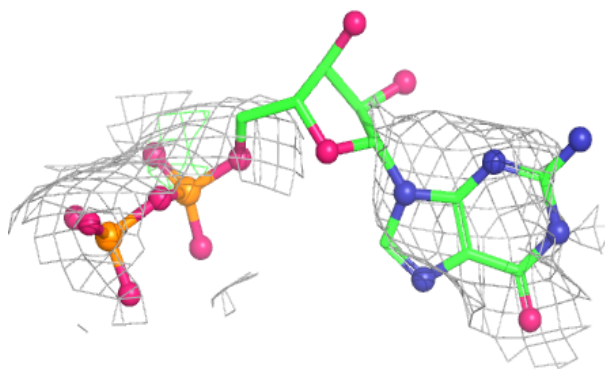
Electron density around FUA CY 701:

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

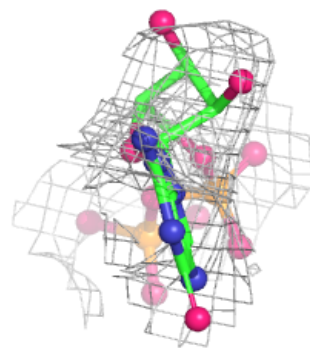
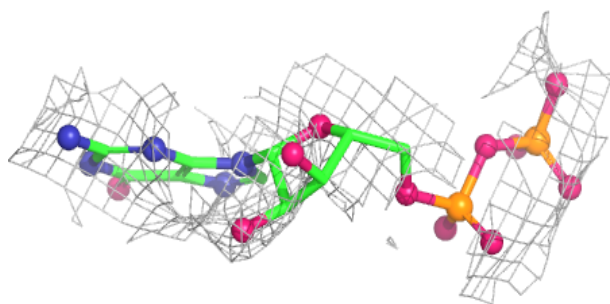
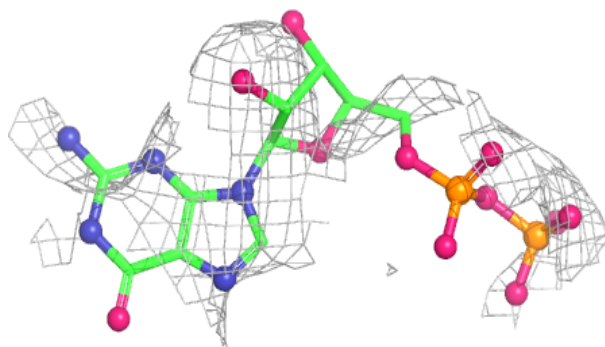


Electron density around GDP CY 702:

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

**Electron density around GDP AY 702:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.