



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 29, 2020 – 04:28 PM BST

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

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

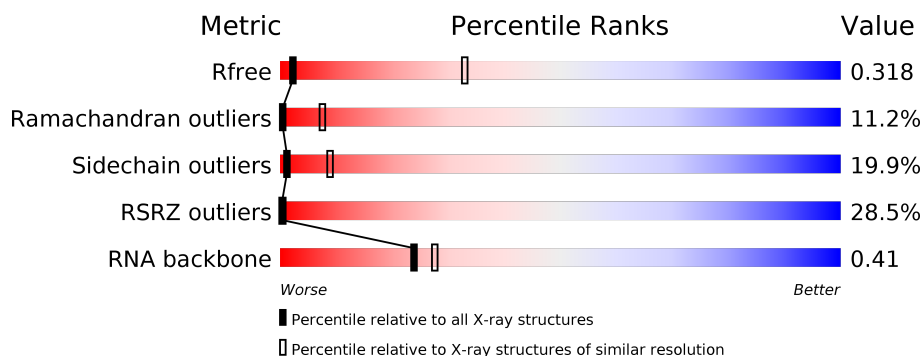
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.86 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1048 (4.10-3.62)
Ramachandran outliers	138981	1069 (4.10-3.62)
Sidechain outliers	138945	1062 (4.10-3.62)
RSRZ outliers	127900	1206 (4.12-3.60)
RNA backbone	3102	1039 (4.70-3.00)

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

Mol	Chain	Length	Quality of chain
1	AB	235	<div> <div>24%</div> <div>74%</div> <div>23%</div> <div>.</div> </div>
1	CB	235	<div> <div>23%</div> <div>75%</div> <div>23%</div> <div>.</div> </div>
2	AC	207	<div> <div>26%</div> <div>73%</div> <div>26%</div> <div>.</div> </div>
2	CC	207	<div> <div>33%</div> <div>71%</div> <div>28%</div> <div>.</div> </div>
3	AD	208	<div> <div>61%</div> <div>74%</div> <div>25%</div> <div>.</div> </div>
3	CD	208	<div> <div>61%</div> <div>80%</div> <div>17%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
4	AE	151	<div> <div>34%</div> <div>79%</div> <div>20%</div> <div>.</div> </div>
4	CE	151	<div> <div>41%</div> <div>80%</div> <div>19%</div> <div>.</div> </div>
5	AF	101	<div> <div>%</div> <div>80%</div> <div>19%</div> <div>.</div> </div>
5	CF	101	<div> <div>%</div> <div>78%</div> <div>20%</div> <div>.</div> </div>
6	AG	155	<div> <div>29%</div> <div>81%</div> <div>19%</div> <div>.</div> </div>
6	CG	155	<div> <div>17%</div> <div>79%</div> <div>20%</div> <div>.</div> </div>
7	AH	138	<div> <div>22%</div> <div>70%</div> <div>28%</div> <div>.</div> </div>
7	CH	138	<div> <div>25%</div> <div>74%</div> <div>25%</div> <div>.</div> </div>
8	AI	127	<div> <div>77%</div> <div>77%</div> <div>21%</div> <div>.</div> </div>
8	CI	127	<div> <div>78%</div> <div>81%</div> <div>17%</div> <div>.</div> </div>
9	AJ	99	<div> <div>39%</div> <div>78%</div> <div>21%</div> <div>.</div> </div>
9	CJ	99	<div> <div>49%</div> <div>79%</div> <div>21%</div> <div>.</div> </div>
10	AK	119	<div> <div>13%</div> <div>79%</div> <div>19%</div> <div>.</div> </div>
10	CK	119	<div> <div>20%</div> <div>82%</div> <div>14%</div> <div>.</div> </div>
11	AL	125	<div> <div>31%</div> <div>60%</div> <div>38%</div> <div>..</div> </div>
11	CL	125	<div> <div>42%</div> <div>59%</div> <div>35%</div> <div>5%</div> <div>.</div> </div>
12	AM	125	<div> <div>30%</div> <div>76%</div> <div>21%</div> <div>.</div> </div>
12	CM	125	<div> <div>38%</div> <div>75%</div> <div>22%</div> <div>.</div> </div>
13	AN	60	<div> <div>73%</div> <div>72%</div> <div>28%</div> <div>.</div> </div>
13	CN	60	<div> <div>70%</div> <div>77%</div> <div>23%</div> <div>.</div> </div>
14	AO	88	<div> <div>22%</div> <div>75%</div> <div>24%</div> <div>.</div> </div>
14	CO	88	<div> <div>30%</div> <div>75%</div> <div>24%</div> <div>.</div> </div>
15	AP	84	<div> <div>75%</div> <div>73%</div> <div>27%</div> <div>.</div> </div>
15	CP	84	<div> <div>79%</div> <div>83%</div> <div>15%</div> <div>.</div> </div>
16	AQ	100	<div> <div>39%</div> <div>73%</div> <div>23%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
16	CQ	100	
17	AR	70	
17	CR	70	
18	AS	79	
18	CS	79	
19	AT	99	
19	CT	99	
20	AA	1511	
20	CA	1511	
21	AV	18	
21	CV	18	
22	AW	77	
22	CW	77	
23	AY	687	
23	CY	687	
24	AU	6	
24	CU	6	
25	BC	228	
25	DC	228	
26	BD	275	
26	DD	275	
27	BE	205	
27	DE	205	
28	BF	208	
28	DF	208	

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Mol	Chain	Length	Quality of chain
29	BG	181	
29	DG	181	
30	BH	167	
30	DH	167	
31	BJ	170	
31	DJ	170	
32	BK	140	
32	DK	140	
33	BO	122	
33	DO	122	
34	BP	146	
34	DP	146	
35	BQ	141	
35	DQ	141	
36	BR	117	
36	DR	117	
37	BS	99	
37	DS	99	
38	BT	138	
38	DT	138	
39	BU	117	
39	DU	117	
40	BV	101	
40	DV	101	
41	BW	113	

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Mol	Chain	Length	Quality of chain
41	DW	113	
42	BX	93	
42	DX	93	
43	BY	107	
43	DY	107	
44	BZ	185	
44	DZ	185	
45	B0	84	
45	D0	84	
46	B1	93	
46	D1	93	
47	B4	35	
47	D4	35	
48	BN	138	
48	DN	138	
49	B2	71	
49	D2	71	
50	B3	60	
50	D3	60	
51	B5	59	
51	D5	59	
52	B6	50	
52	D6	50	
53	B7	49	
53	D7	49	

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Mol	Chain	Length	Quality of chain
54	B8	64	<div> <div>81%</div> <div>66%30%5%</div> </div>
54	D8	64	<div> <div>78%</div> <div>70%25%5%</div> </div>
55	B9	37	<div> <div>100%</div> <div>73%27%</div> </div>
55	D9	37	<div> <div>97%</div> <div>76%24%</div> </div>
56	Be	103	<div> <div>6%</div> <div>87%10%..</div> </div>
56	De	103	<div> <div>9%</div> <div>85%13%..</div> </div>
57	Bf	31	<div> <div>100%</div> </div>
57	Bg	31	<div> <div>100%</div> </div>
57	Df	31	<div> <div>100%</div> </div>
57	Dg	31	<div> <div>100%</div> </div>
58	Bh	30	<div> <div>100%</div> </div>
58	Dh	30	<div> <div>100%</div> </div>
59	BB	119	<div> <div>4%</div> <div>74%25%. .</div> </div>
59	DB	119	<div> <div>8%</div> <div>80%20%</div> </div>
60	BA	2879	<div> <div>10%</div> <div>72%26%. .</div> </div>
60	DA	2879	<div> <div>10%</div> <div>74%25%. .</div> </div>

2 Entry composition

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 21 is a RNA chain called messenger RNA.

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

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

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

- Molecule 23 is a protein called Elongation factor G.

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

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 24 is a protein called Viomycin.

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

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

There are 10 discrepancies between the modelled and reference sequences:

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

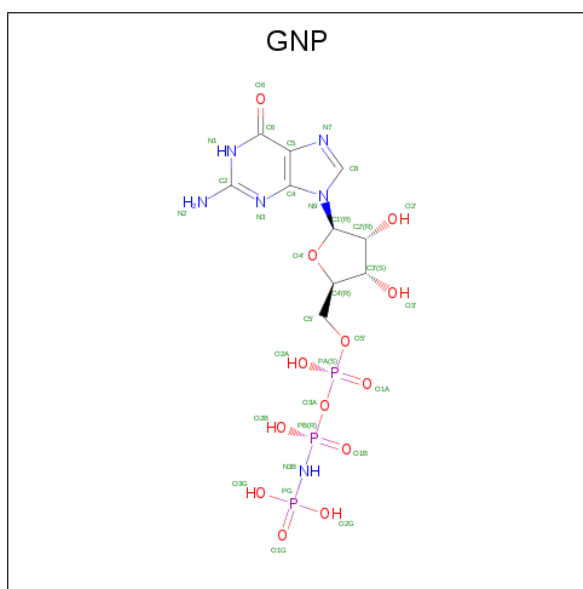
- Molecule 59 is a RNA chain called 5S ribosomal RNA.

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

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

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

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



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

- Molecule 62 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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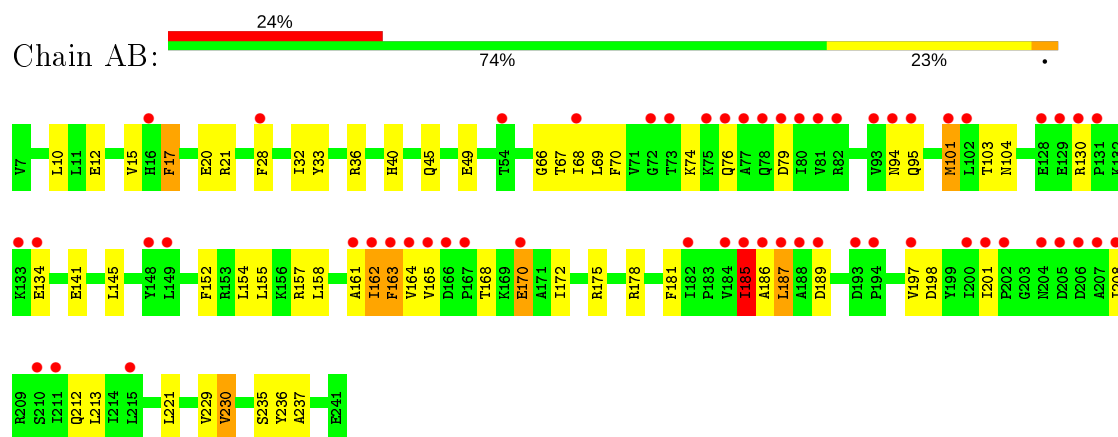
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	CY	1	Total	Mg	0	0
			1	1		

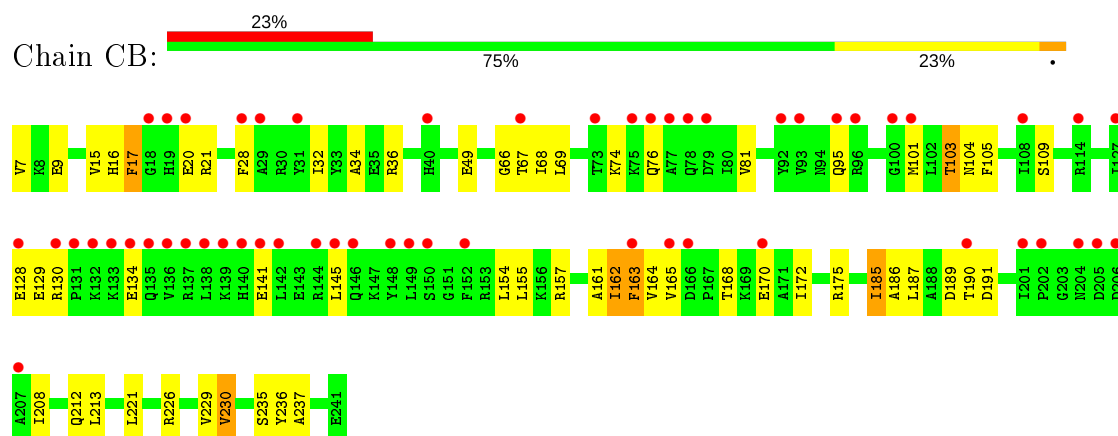
3 Residue-property plots [i](#)

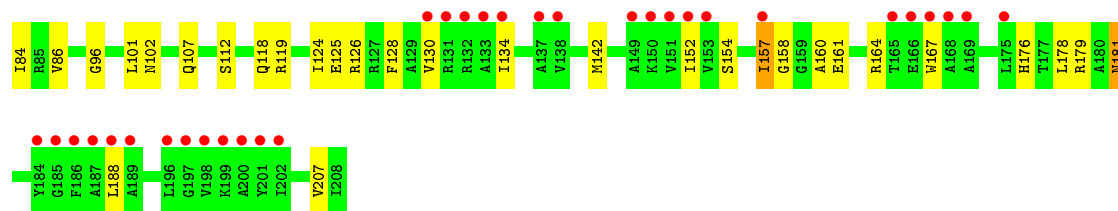
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: 30S ribosomal protein S2

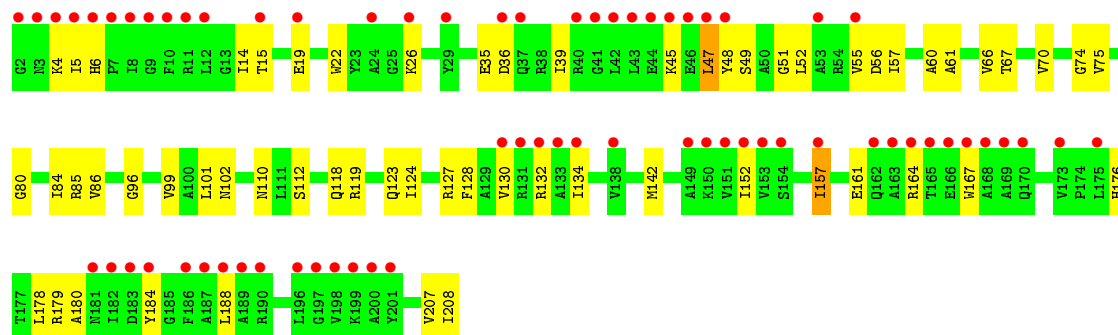
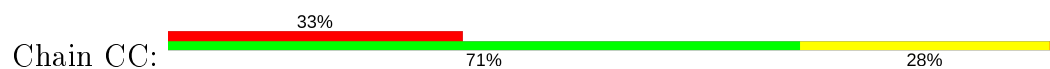


- Molecule 1: 30S ribosomal protein S2

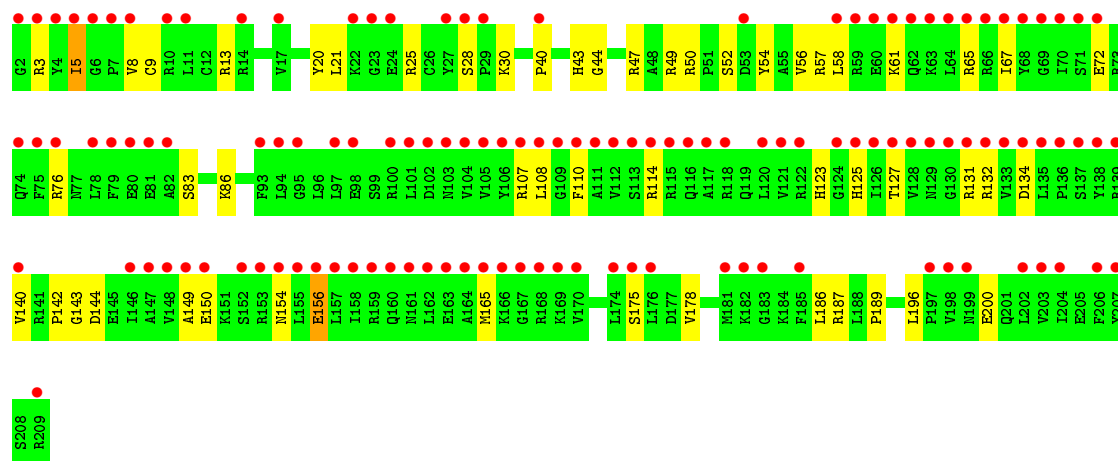
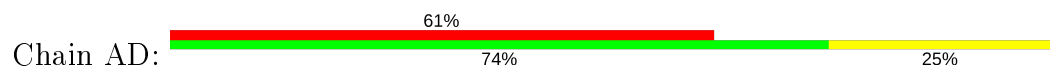




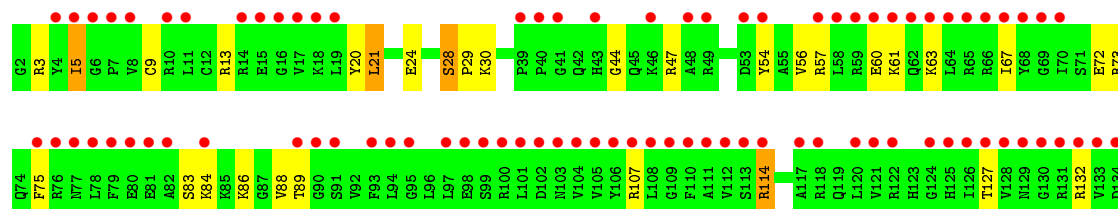
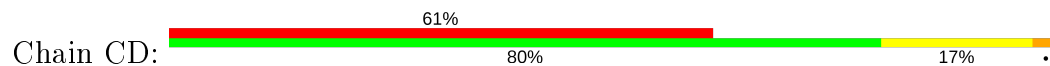
• Molecule 2: 30S ribosomal protein S3

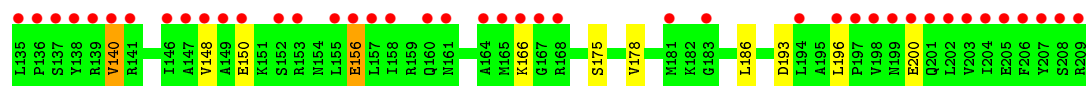


• Molecule 3: 30S ribosomal protein S4

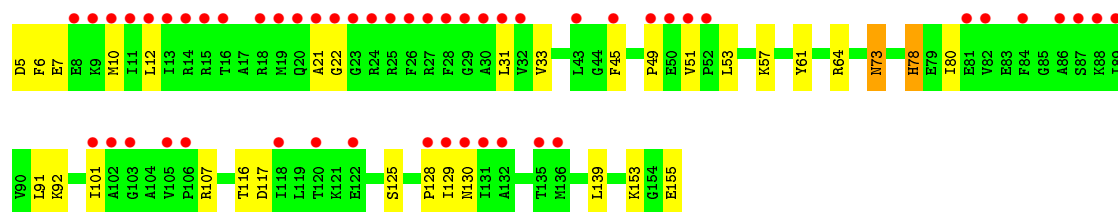
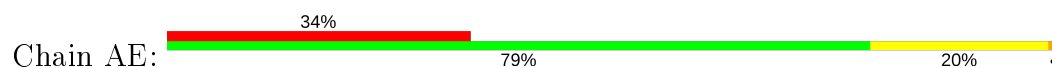


• Molecule 3: 30S ribosomal protein S4

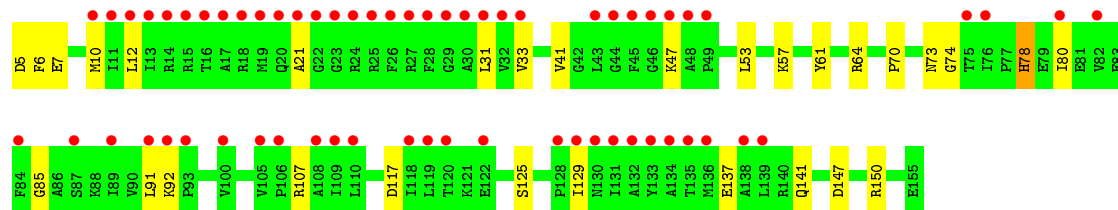
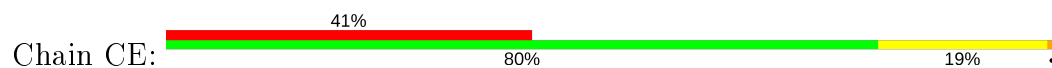




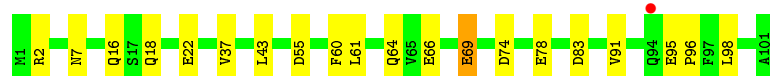
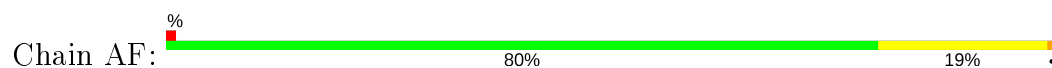
- Molecule 4: 30S ribosomal protein S5



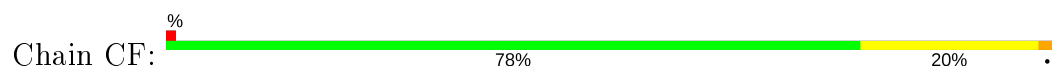
- Molecule 4: 30S ribosomal protein S5



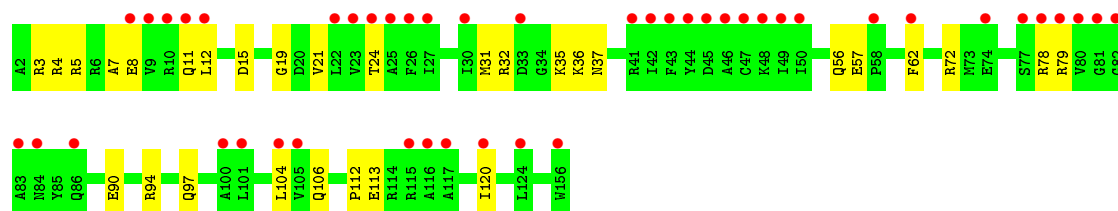
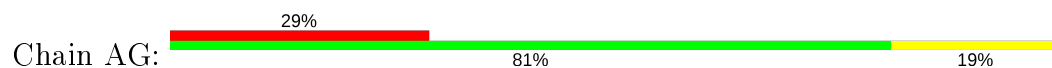
- Molecule 5: 30S ribosomal protein S6



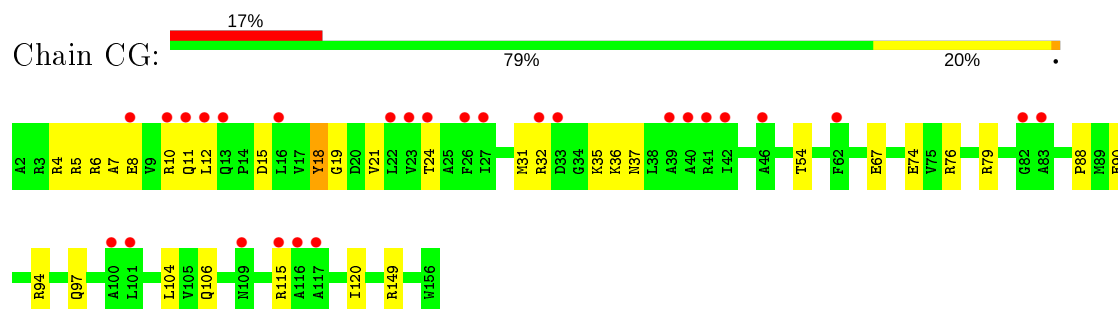
- Molecule 5: 30S ribosomal protein S6



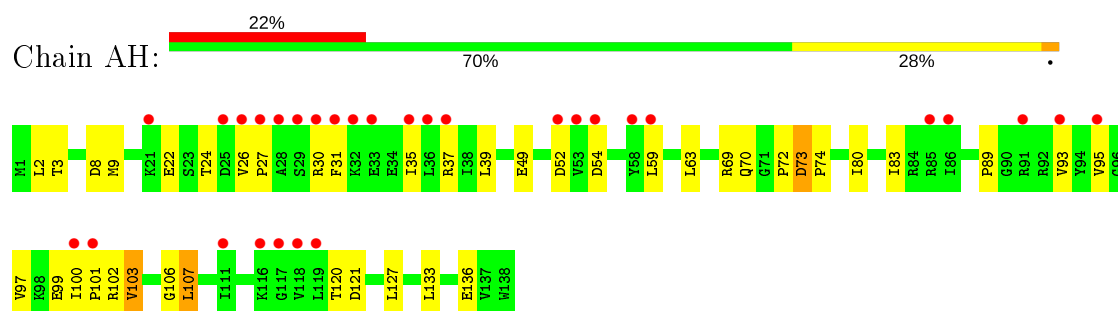
- Molecule 6: 30S ribosomal protein S7



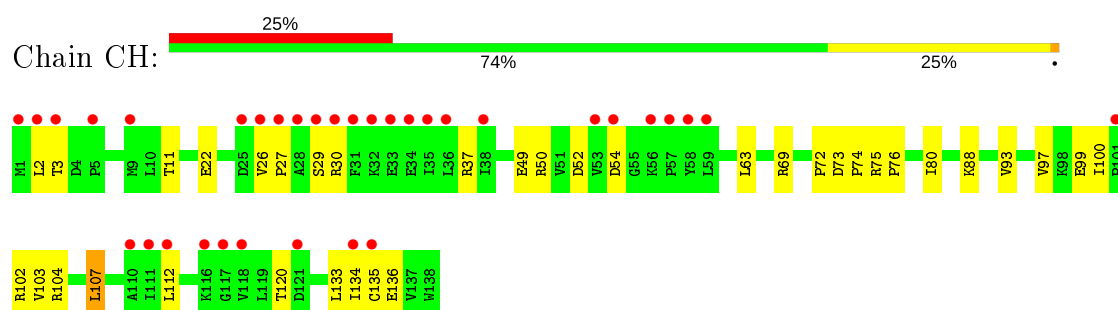
- Molecule 6: 30S ribosomal protein S7



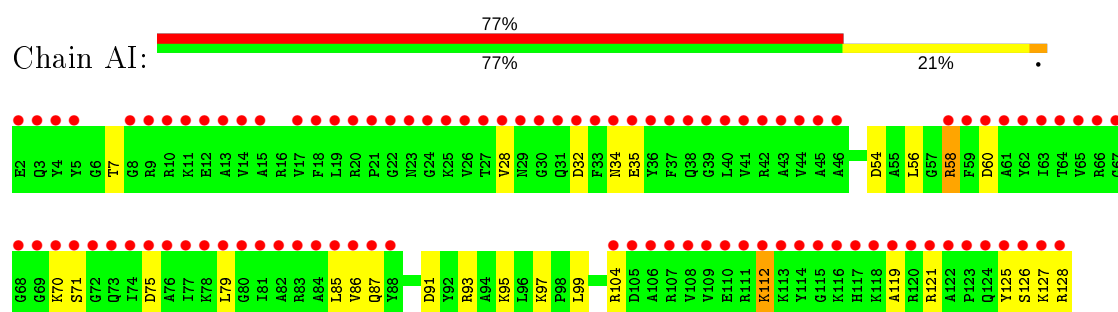
- Molecule 7: 30S ribosomal protein S8



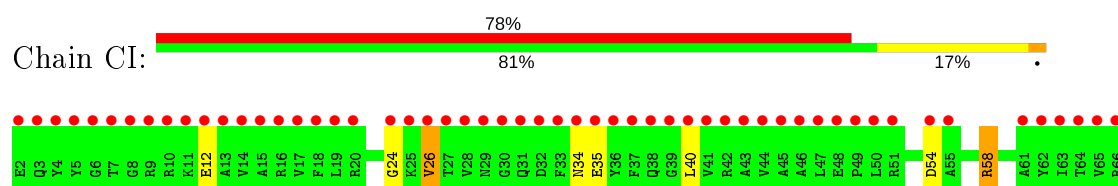
- Molecule 7: 30S ribosomal protein S8



- Molecule 8: 30S ribosomal protein S9

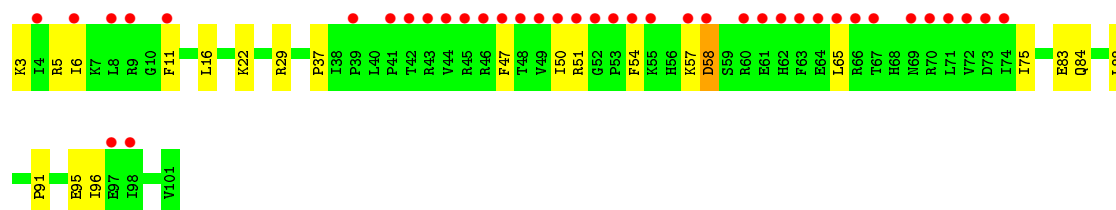
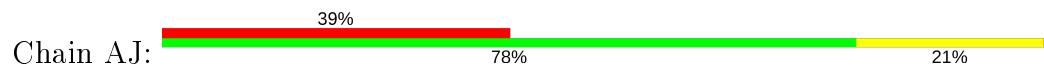


- Molecule 8: 30S ribosomal protein S9

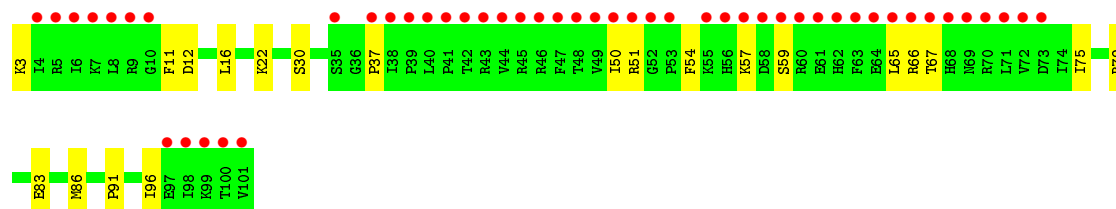
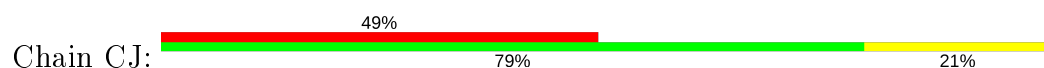




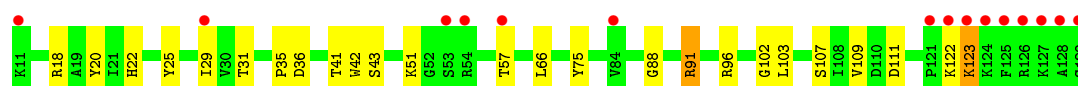
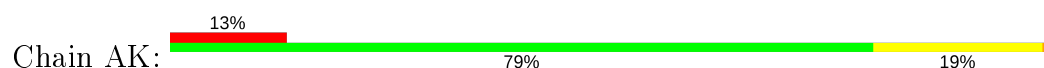
- Molecule 9: 30S ribosomal protein S10



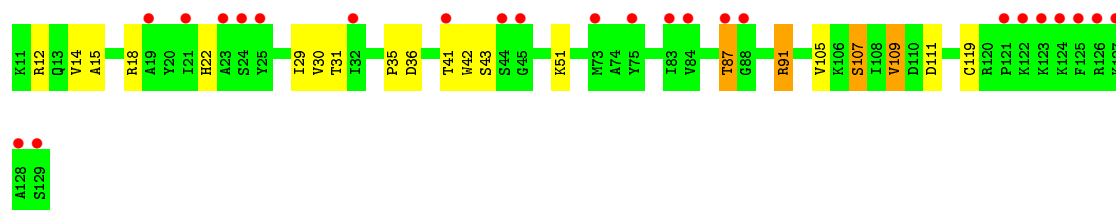
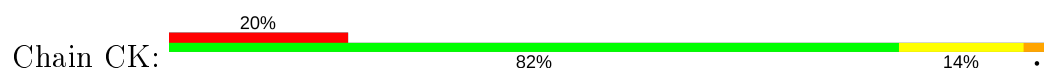
- Molecule 9: 30S ribosomal protein S10



- Molecule 10: 30S ribosomal protein S11

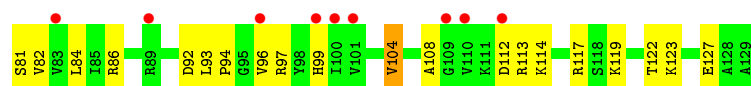


- Molecule 10: 30S ribosomal protein S11

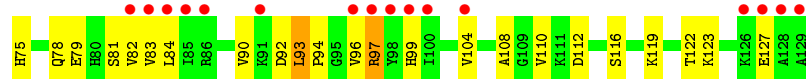
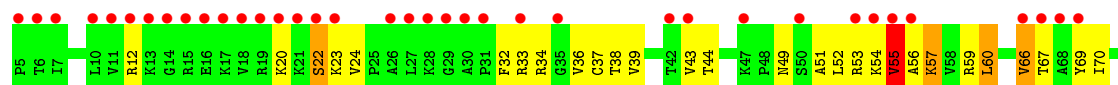
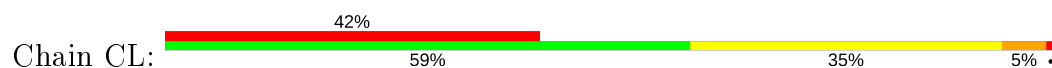


- Molecule 11: 30S ribosomal protein S12

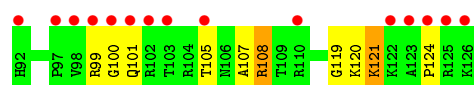
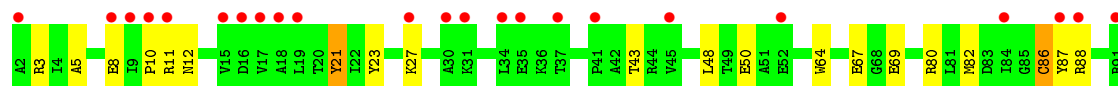
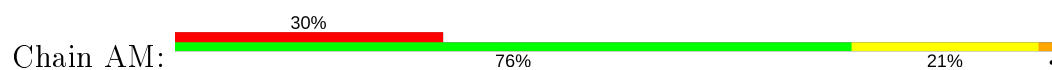




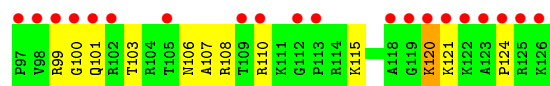
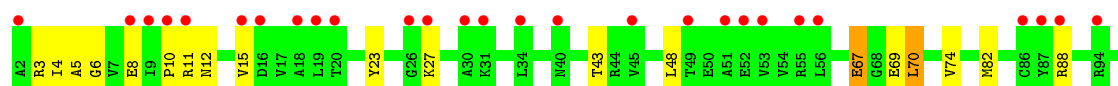
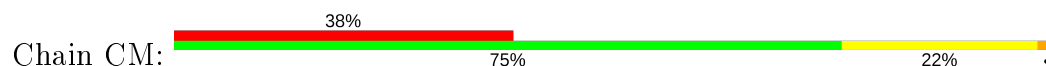
- Molecule 11: 30S ribosomal protein S12



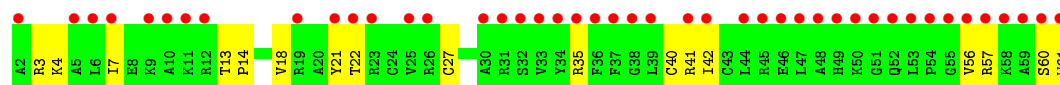
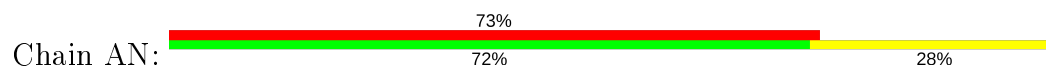
- Molecule 12: 30S ribosomal protein S13



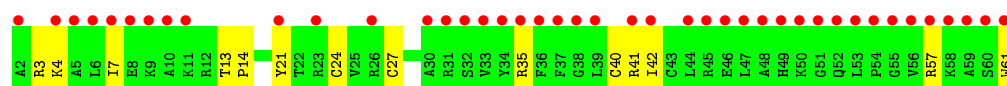
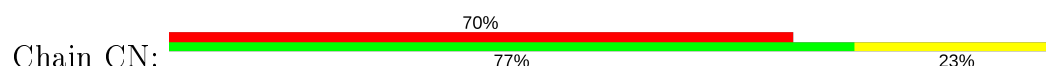
- Molecule 12: 30S ribosomal protein S13



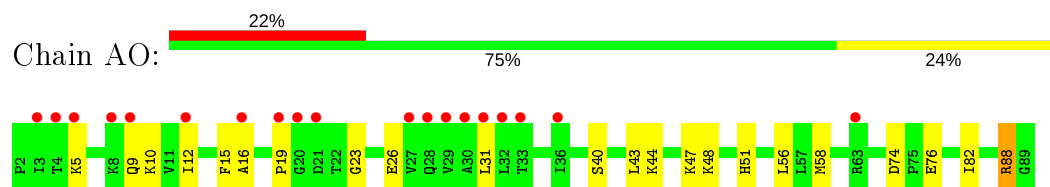
- Molecule 13: 30S ribosomal protein S14 type Z



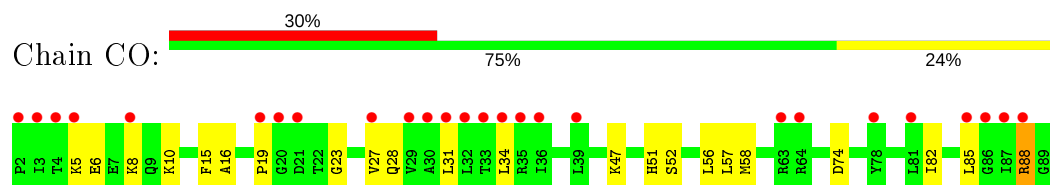
- Molecule 13: 30S ribosomal protein S14 type Z



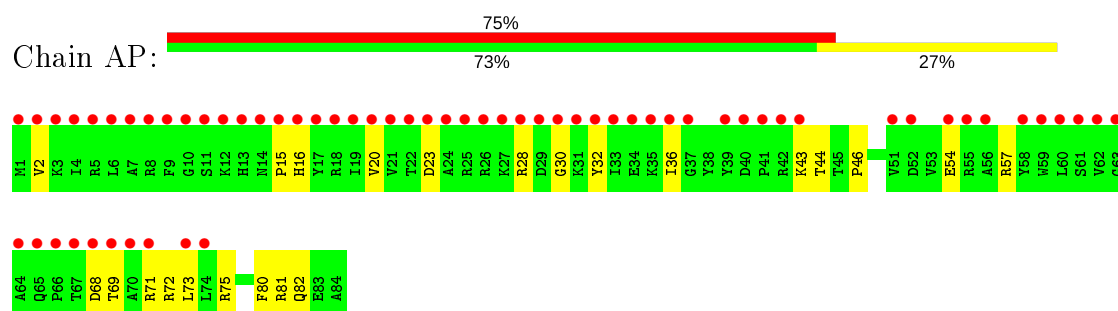
- Molecule 14: 30S ribosomal protein S15



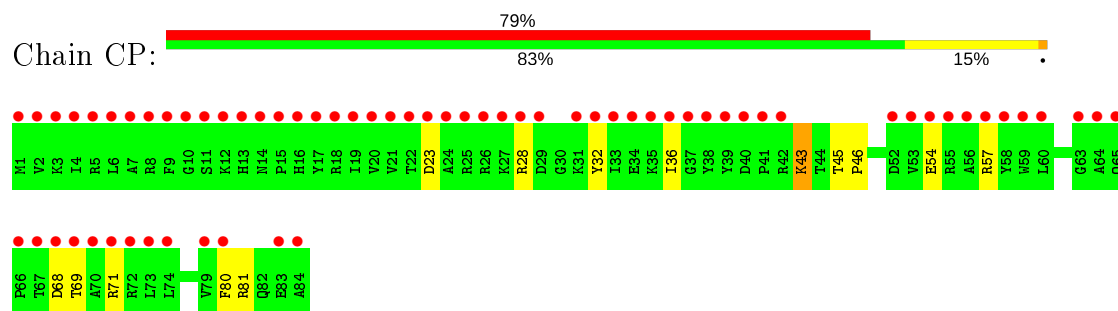
- Molecule 14: 30S ribosomal protein S15



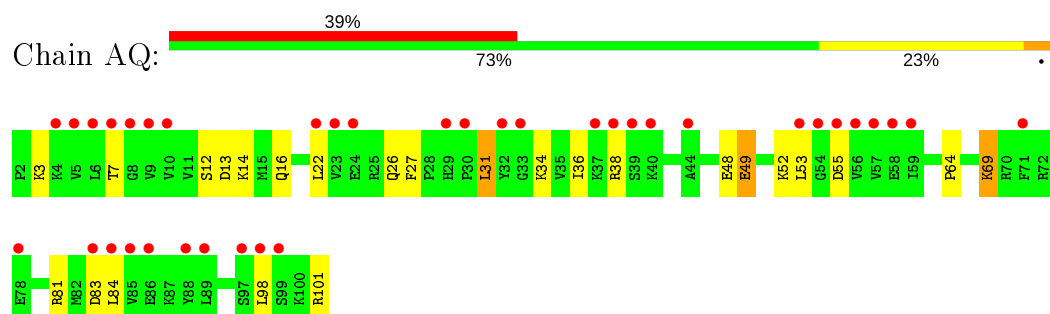
- Molecule 15: 30S ribosomal protein S16



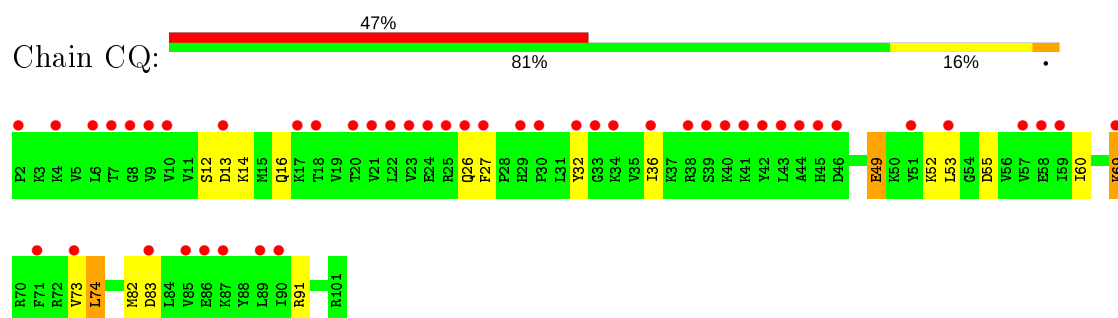
- Molecule 15: 30S ribosomal protein S16



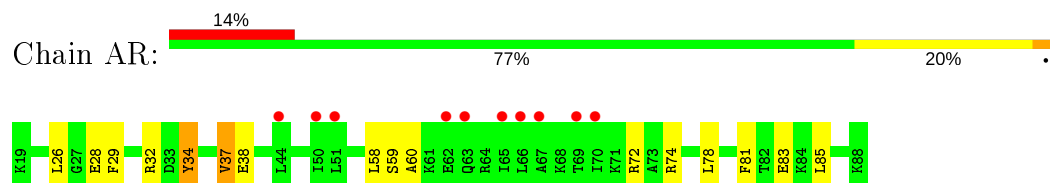
- Molecule 16: 30S ribosomal protein S17



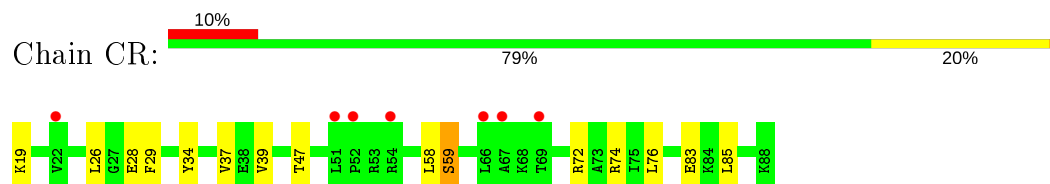
- Molecule 16: 30S ribosomal protein S17



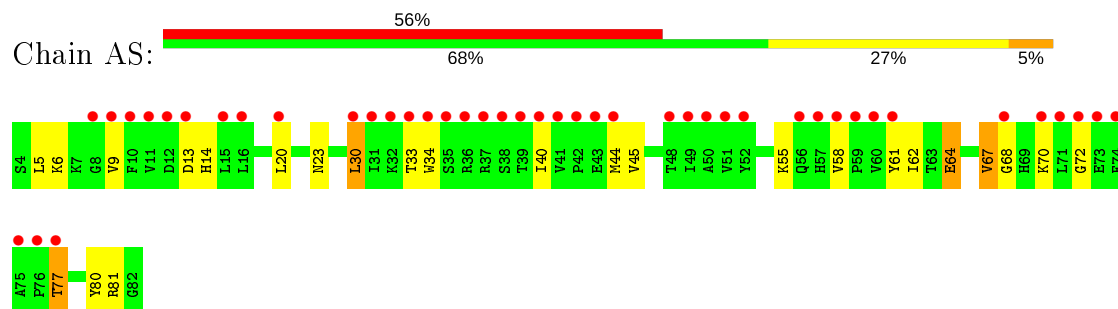
- Molecule 17: 30S ribosomal protein S18



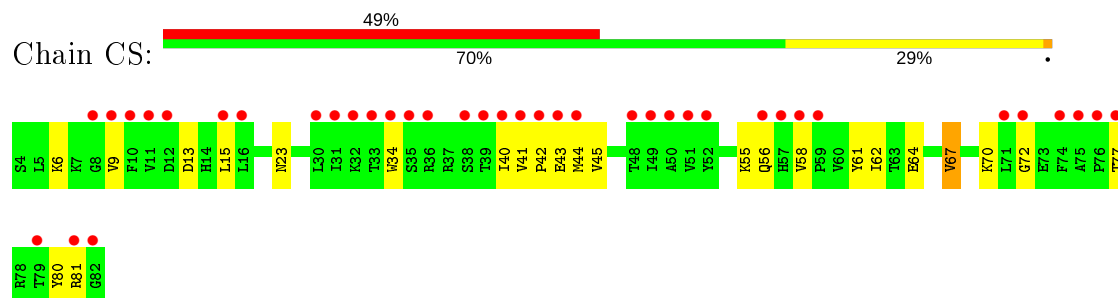
- Molecule 17: 30S ribosomal protein S18



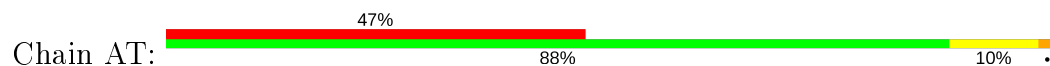
- Molecule 18: 30S ribosomal protein S19

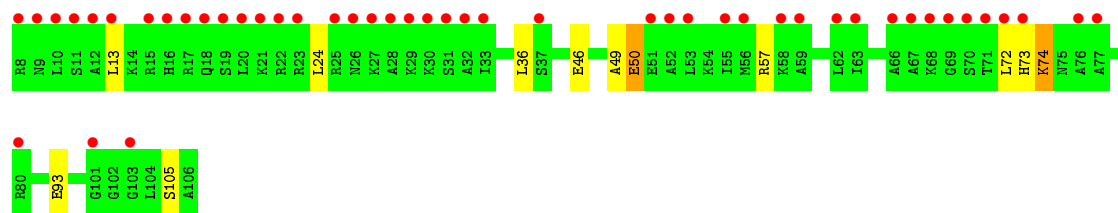


- Molecule 18: 30S ribosomal protein S19

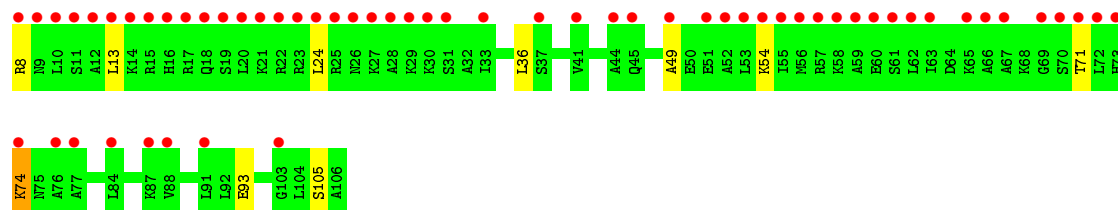
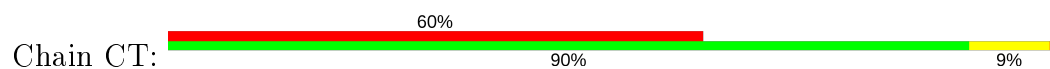


- Molecule 19: 30S ribosomal protein S20

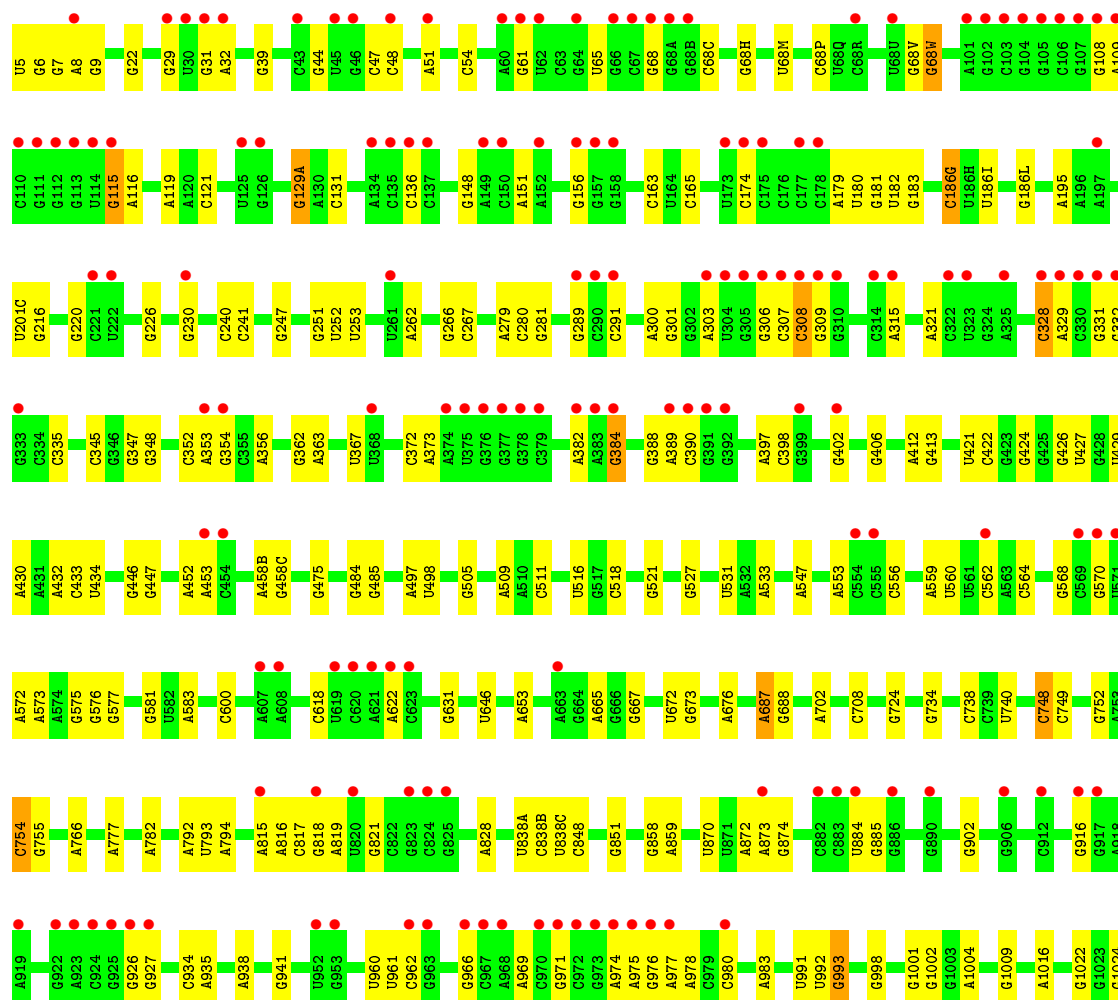
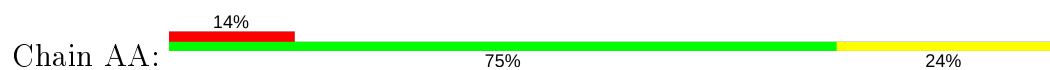


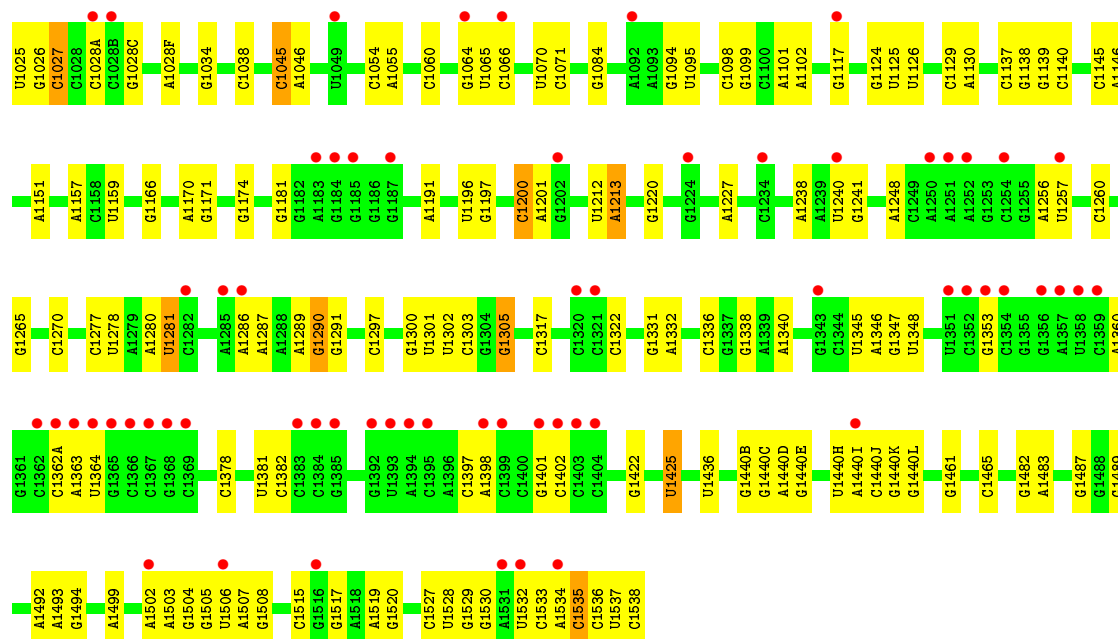


• Molecule 19: 30S ribosomal protein S20

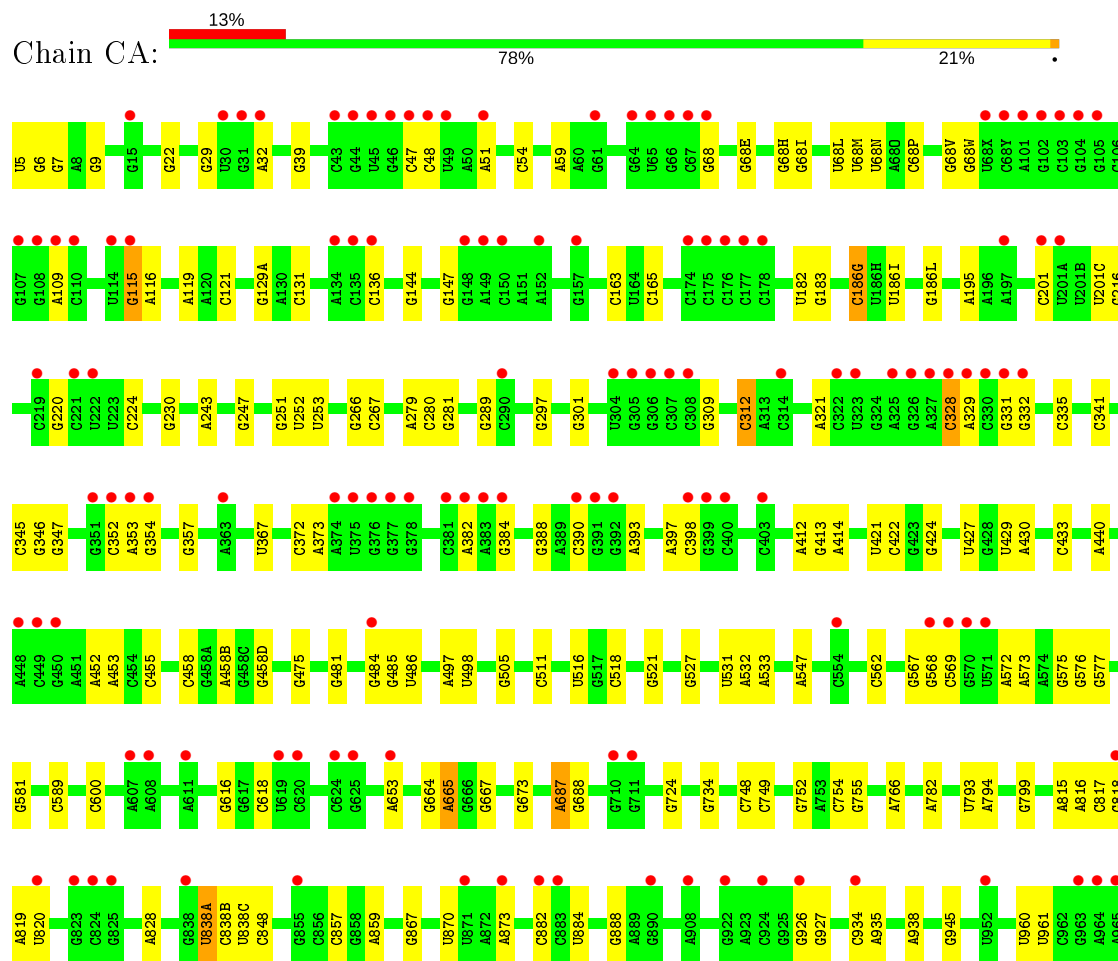


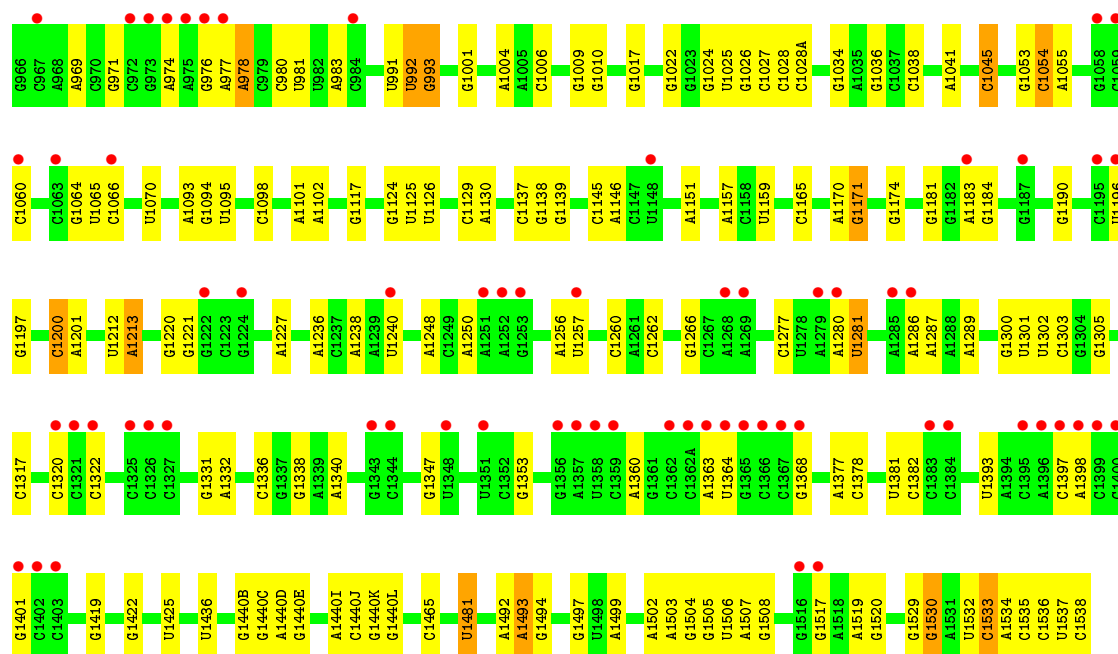
• Molecule 20: 16S ribosomal RNA



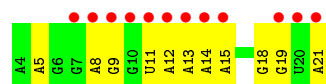


• Molecule 20: 16S ribosomal RNA

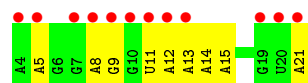




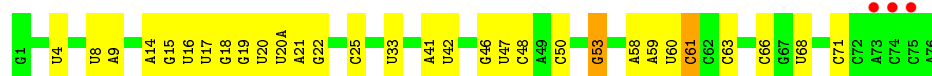
- Molecule 21: messenger RNA



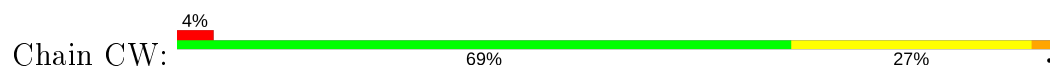
- Molecule 21: messenger RNA



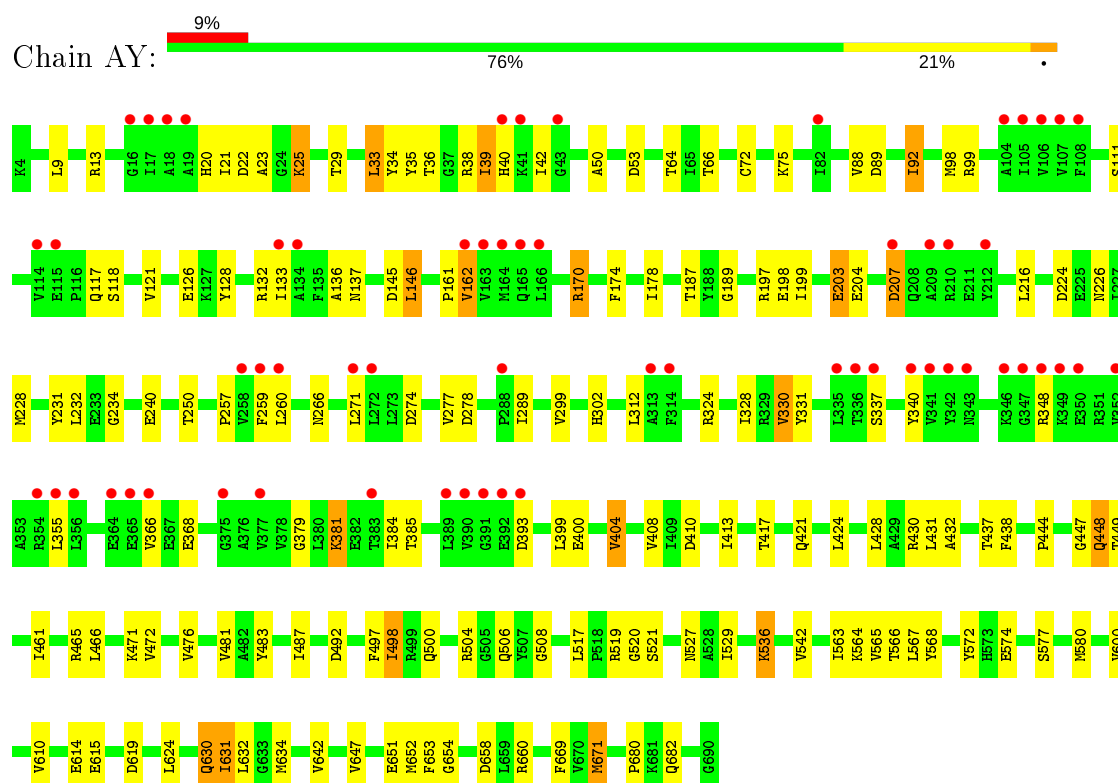
- Molecule 22: tRNA-Met



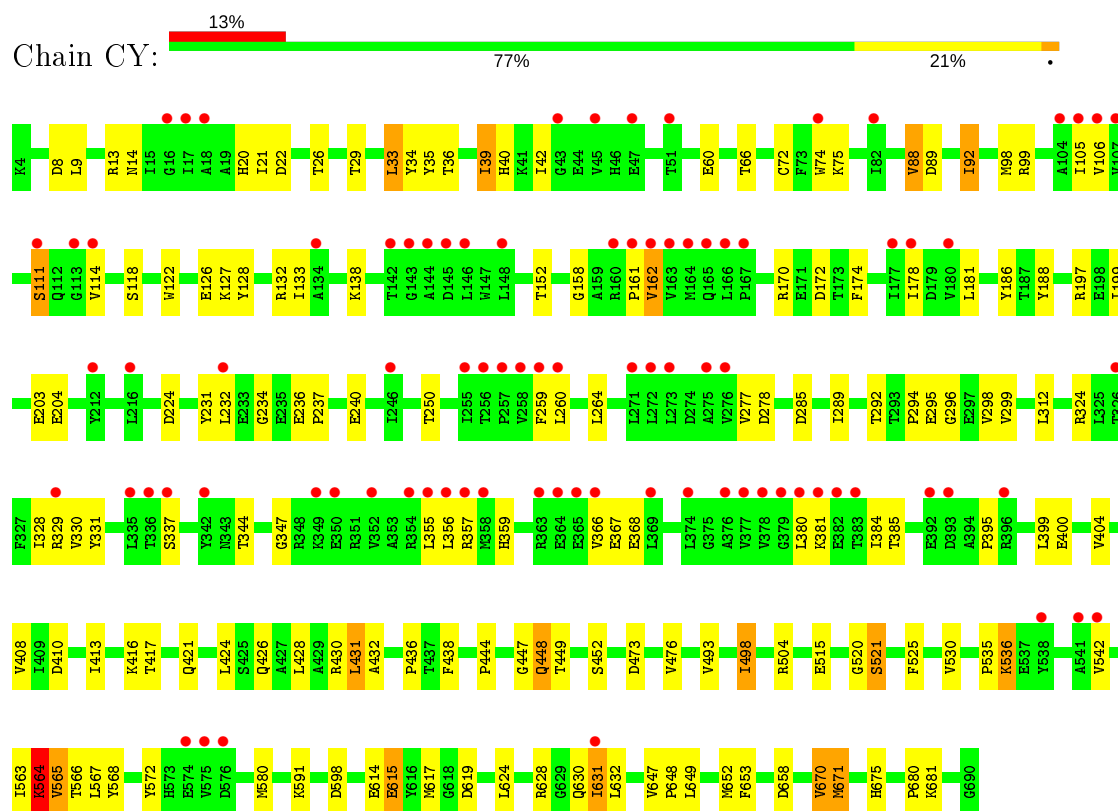
- Molecule 22: tRNA-Met



- Molecule 23: Elongation factor G



• Molecule 23: Elongation factor G



• Molecule 24: Viomycin

Chain AU:  67% 33%



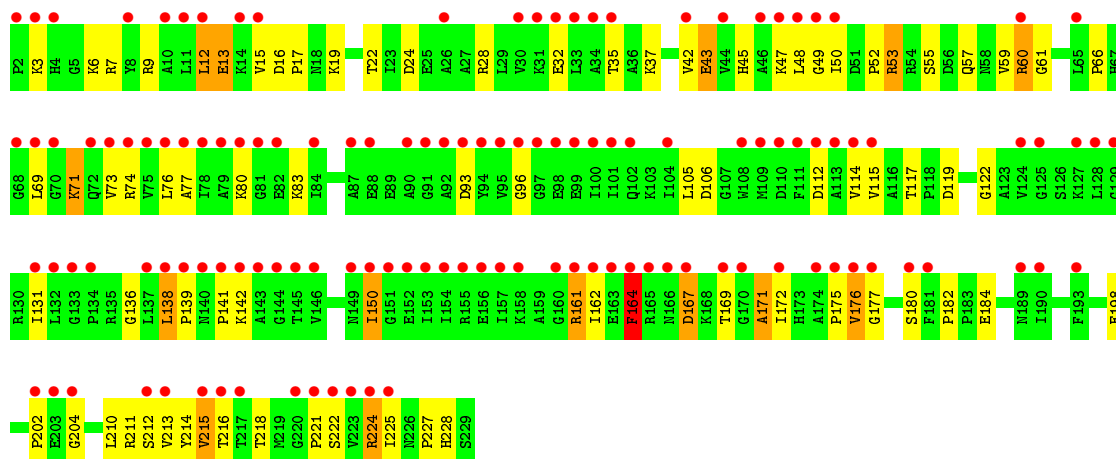
- Molecule 24: Viomycin

Chain CU:  67% 33%



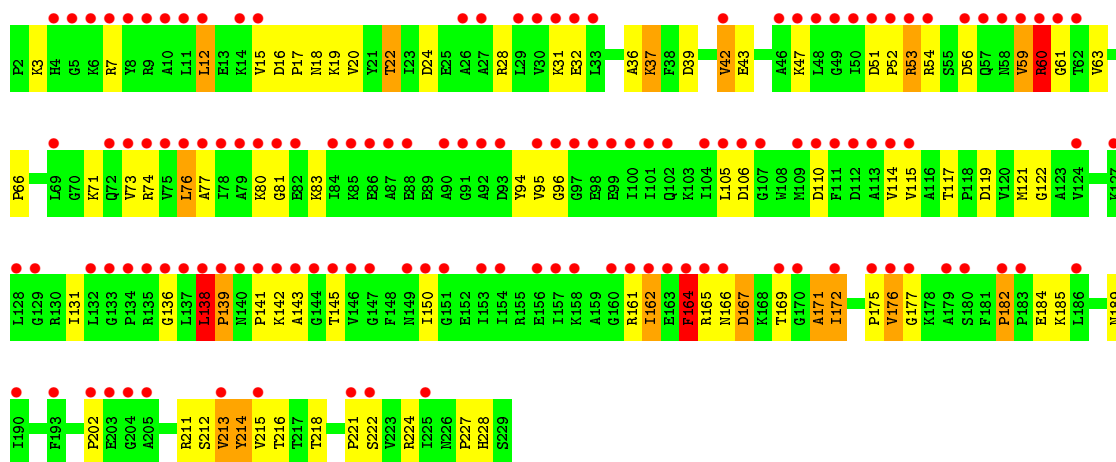
- Molecule 25: 50S ribosomal protein L1

Chain BC:  56% 62% 31% 6%

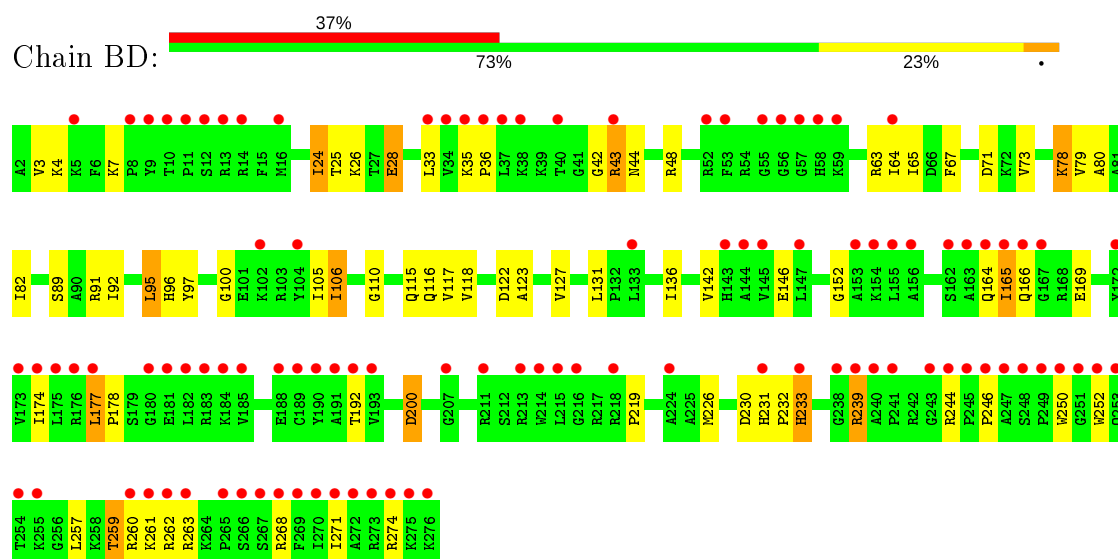


- Molecule 25: 50S ribosomal protein L1

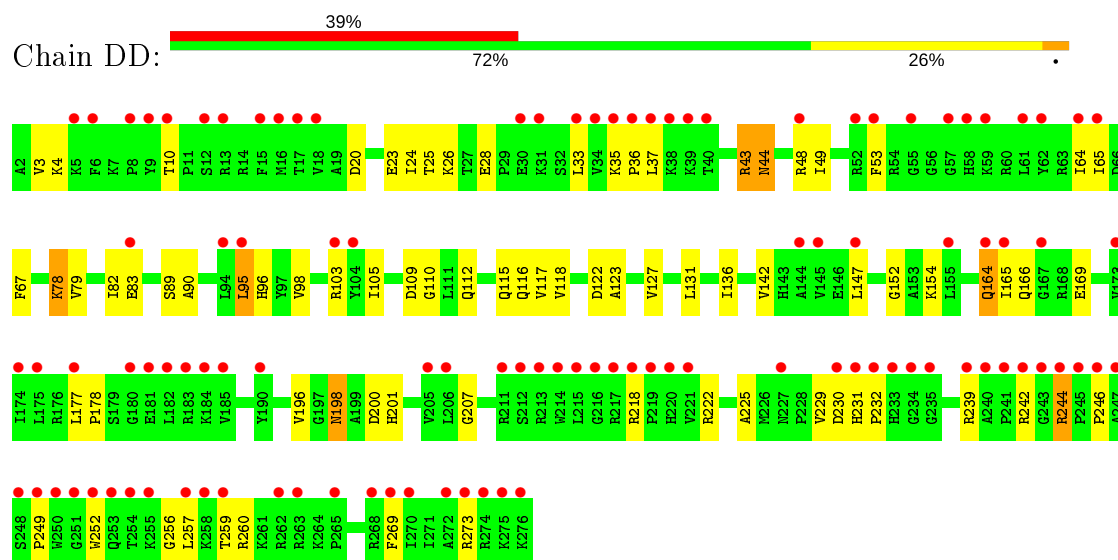
Chain DC:  58% 61% 30% 7%



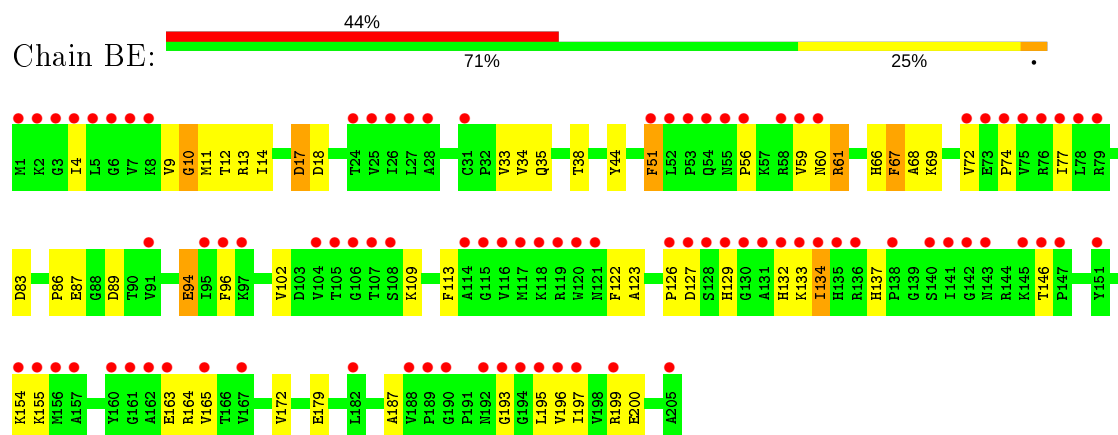
- Molecule 26: 50S ribosomal protein L2



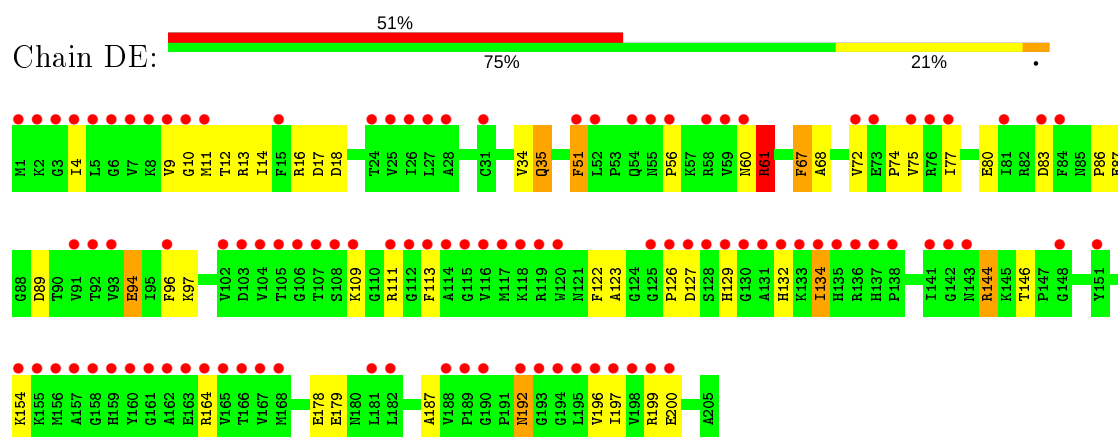
• Molecule 26: 50S ribosomal protein L2



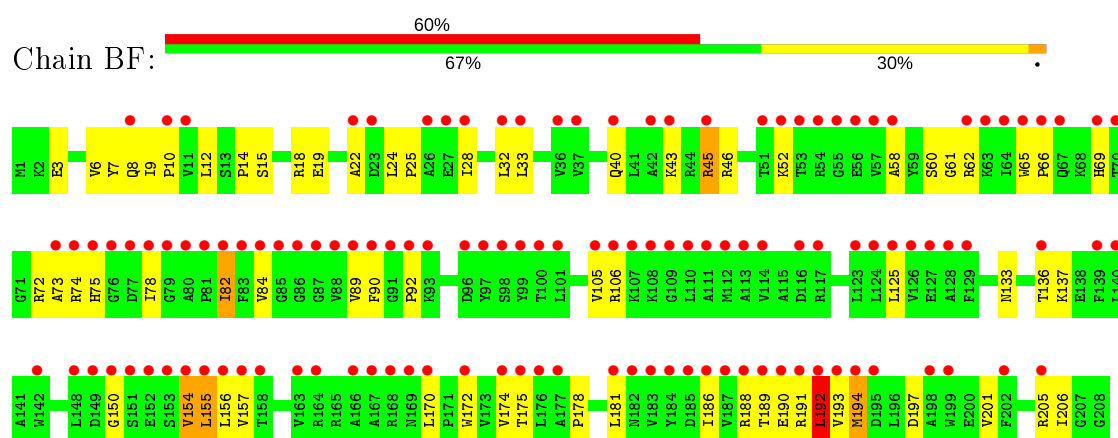
• Molecule 27: 50S ribosomal protein L3



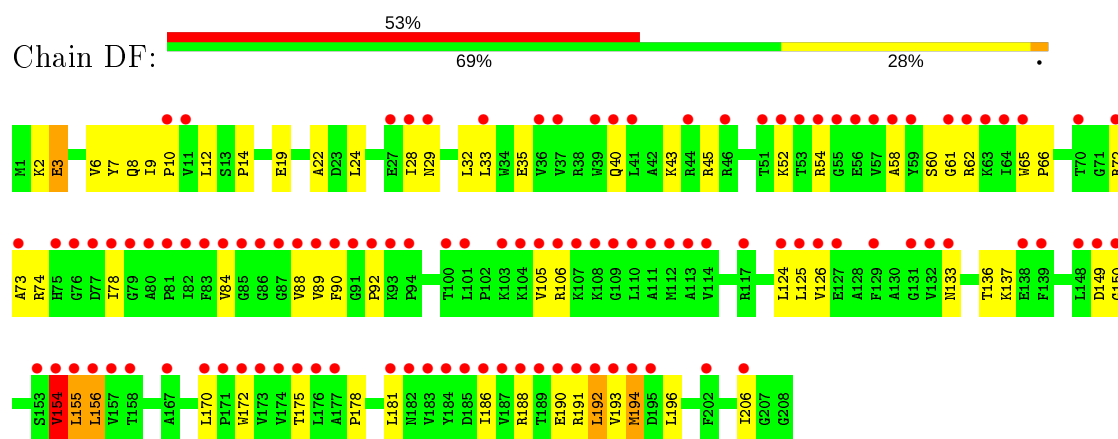
• Molecule 27: 50S ribosomal protein L3



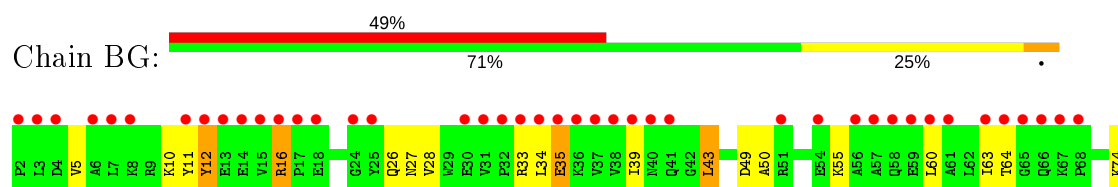
• Molecule 28: 50S ribosomal protein L4

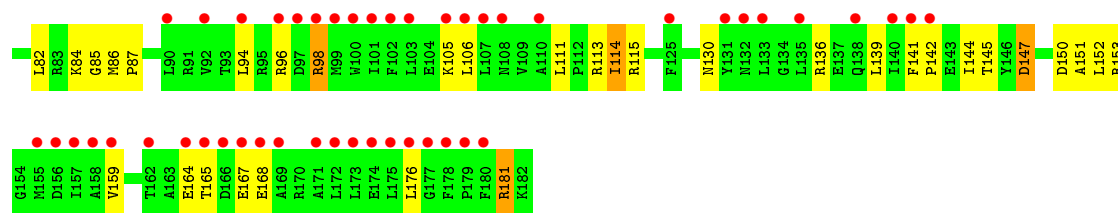


• Molecule 28: 50S ribosomal protein L4

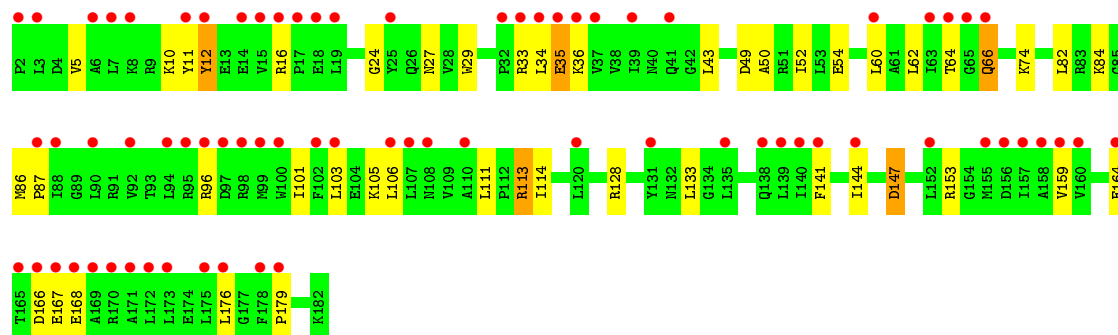
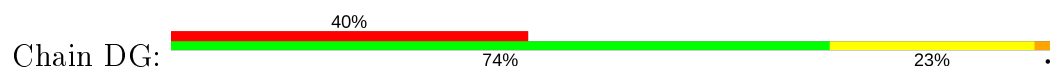


• Molecule 29: 50S ribosomal protein L5

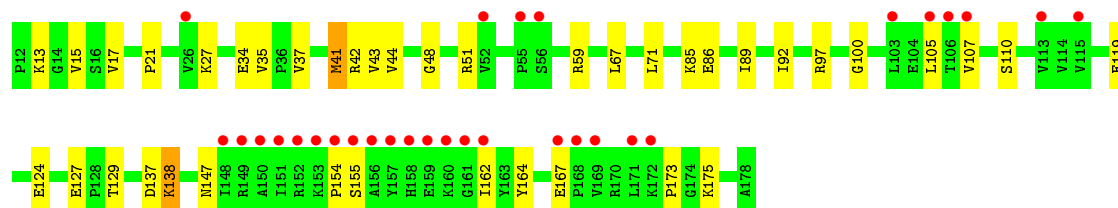
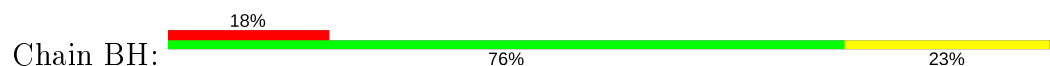




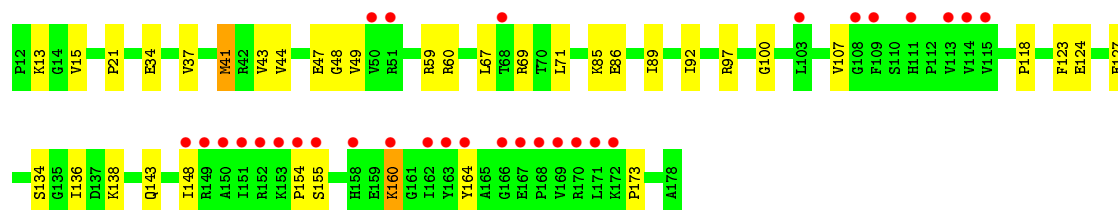
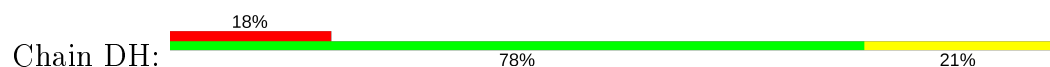
• Molecule 29: 50S ribosomal protein L5



• Molecule 30: 50S ribosomal protein L6



• Molecule 30: 50S ribosomal protein L6

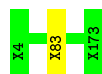


• Molecule 31: 50S ribosomal protein L10




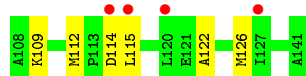
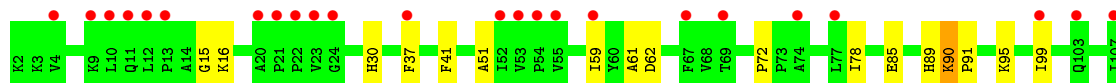
- Molecule 31: 50S ribosomal protein L10

Chain DJ:  99%




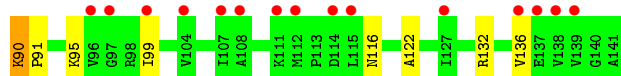
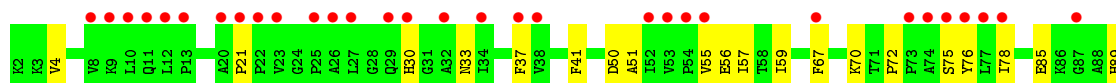
- Molecule 32: 50S ribosomal protein L11

Chain BK:  20% 84% 16%




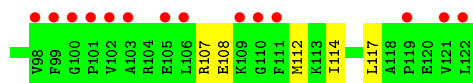
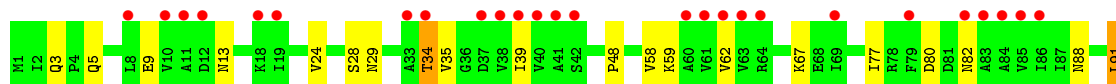
- Molecule 32: 50S ribosomal protein L11

Chain DK:  33% 80% 19%




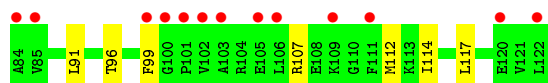
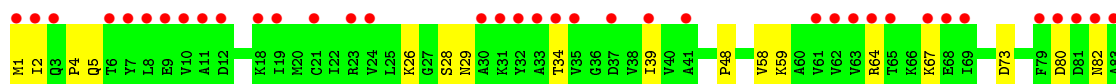
- Molecule 33: 50S ribosomal protein L14

Chain BO:  33% 80% 19%

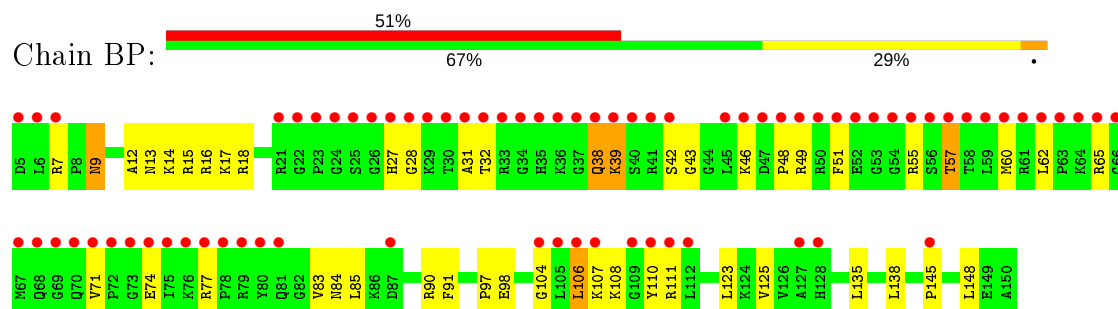


- Molecule 33: 50S ribosomal protein L14

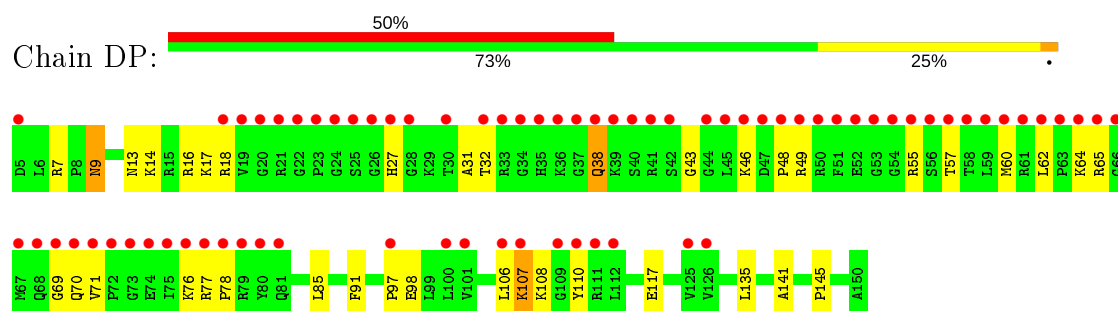
Chain DO:  41% 80% 20%



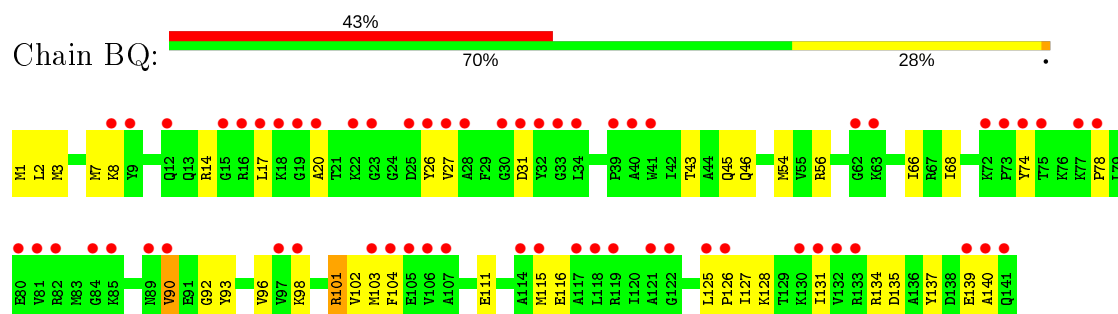
- Molecule 34: 50S ribosomal protein L15



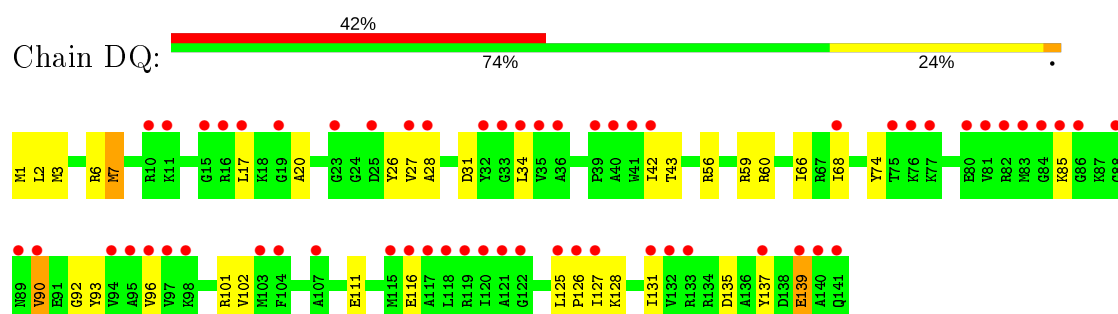
- Molecule 34: 50S ribosomal protein L15



- Molecule 35: 50S ribosomal protein L16

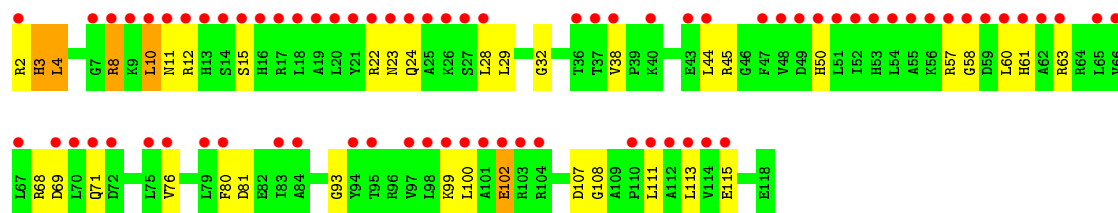


- Molecule 35: 50S ribosomal protein L16

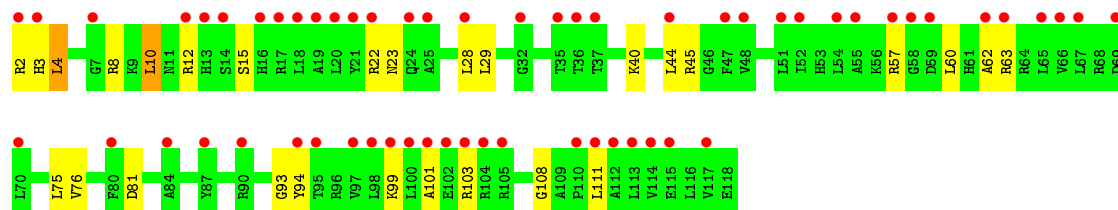
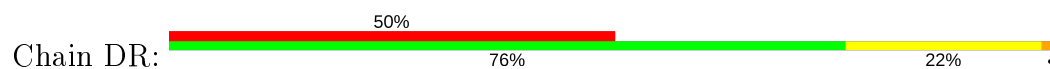


- Molecule 36: 50S ribosomal protein L17

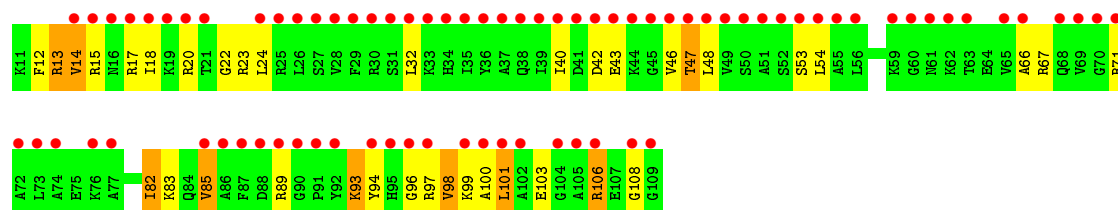
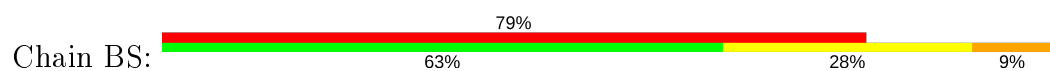




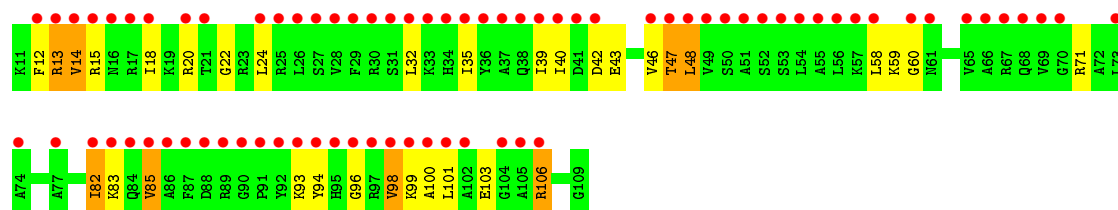
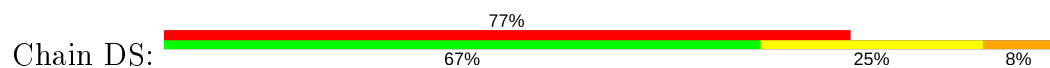
• Molecule 36: 50S ribosomal protein L17



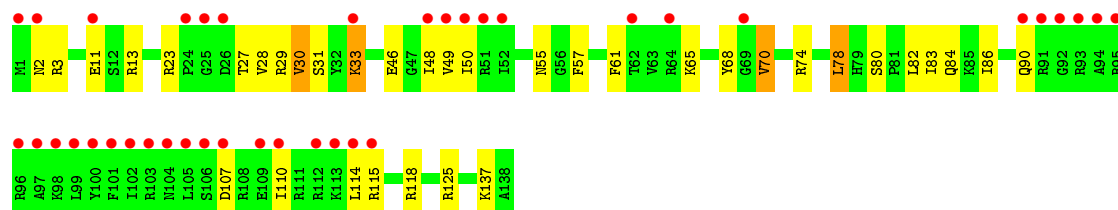
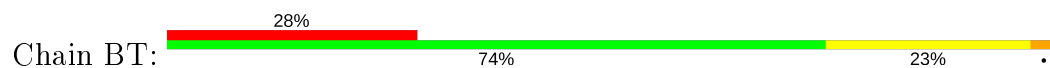
• Molecule 37: 50S ribosomal protein L18



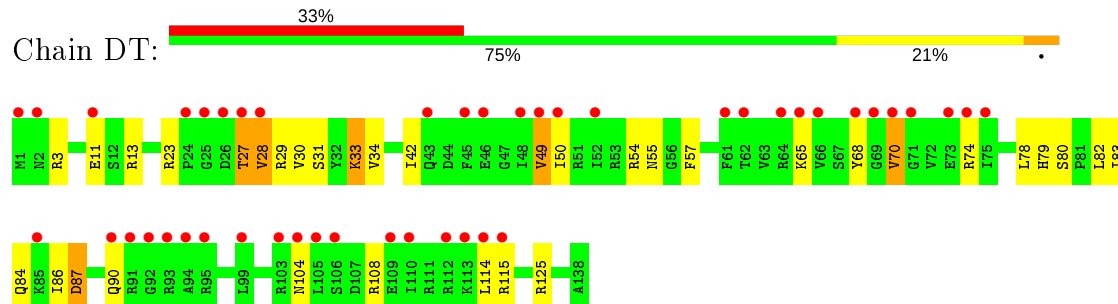
• Molecule 37: 50S ribosomal protein L18



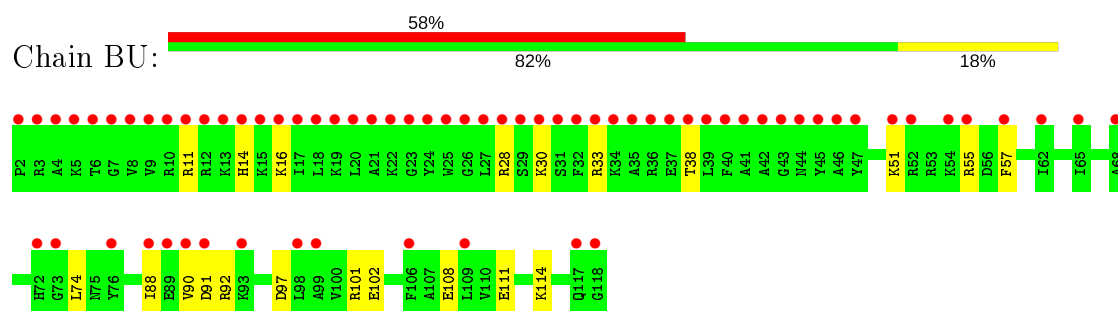
• Molecule 38: 50S ribosomal protein L19



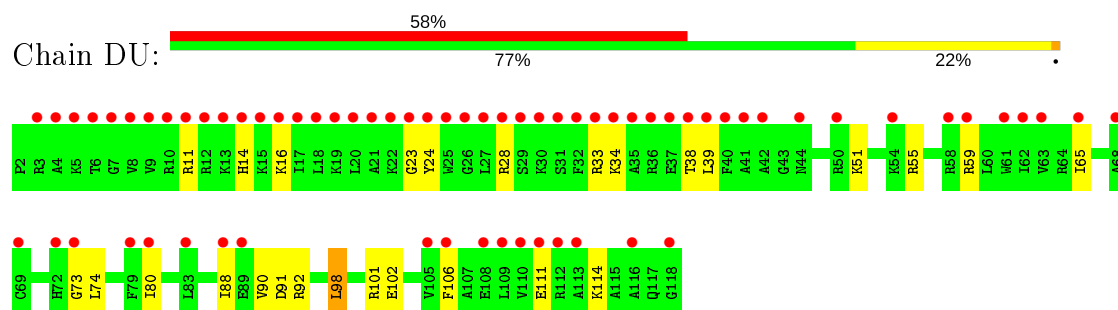
- Molecule 38: 50S ribosomal protein L19



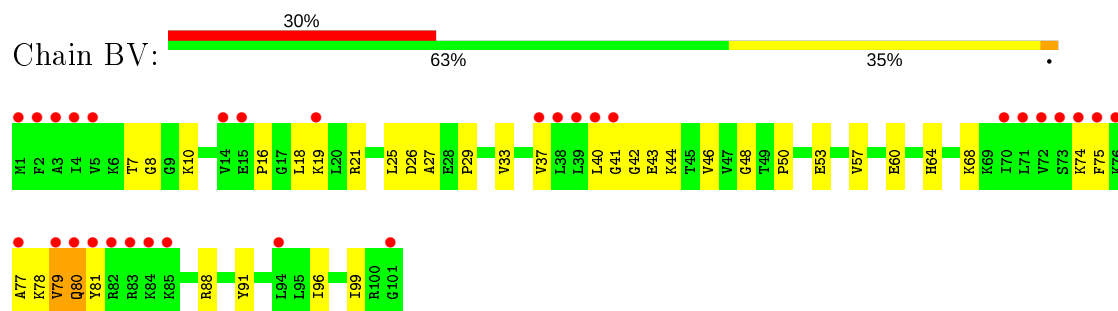
- Molecule 39: 50S ribosomal protein L20



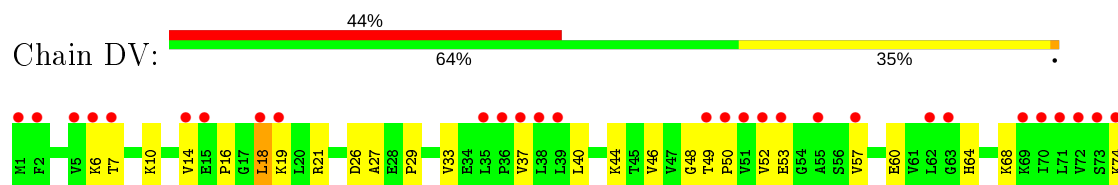
- Molecule 39: 50S ribosomal protein L20

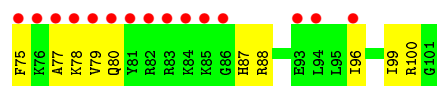


- Molecule 40: 50S ribosomal protein L21

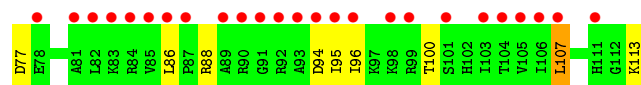
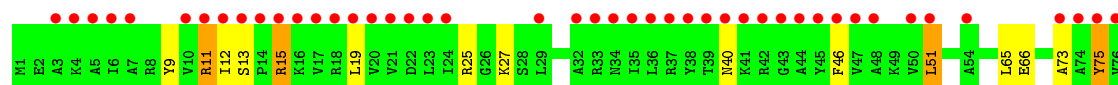
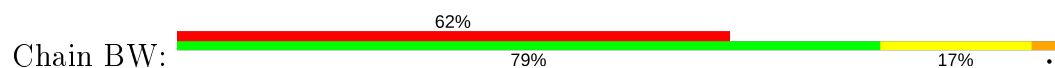


- Molecule 40: 50S ribosomal protein L21

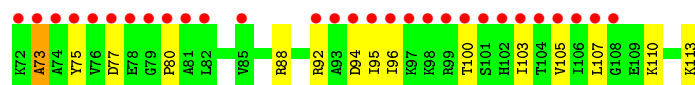
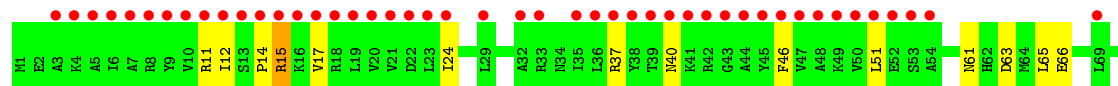
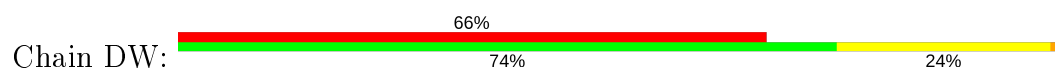




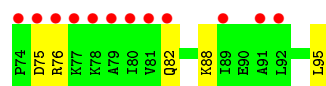
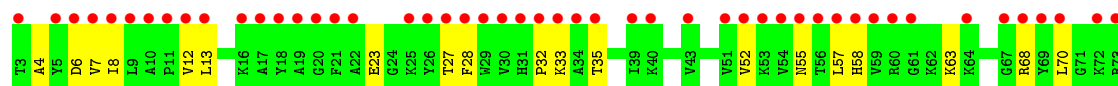
- Molecule 41: 50S ribosomal protein L22



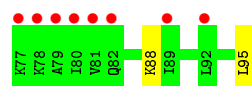
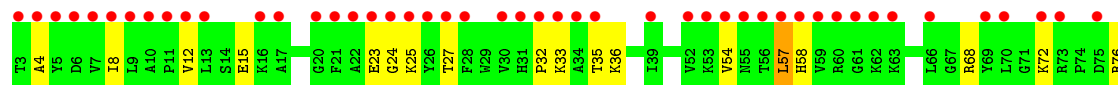
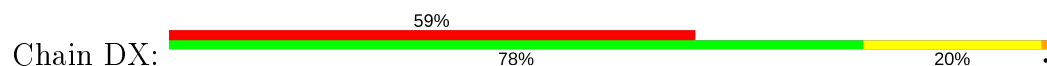
- Molecule 41: 50S ribosomal protein L22



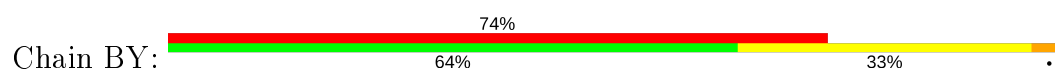
- Molecule 42: 50S ribosomal protein L23

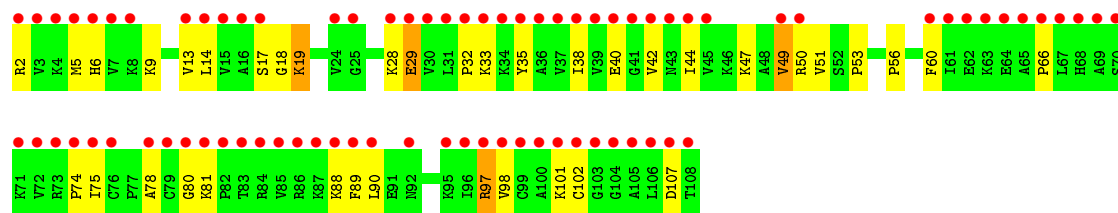


- Molecule 42: 50S ribosomal protein L23

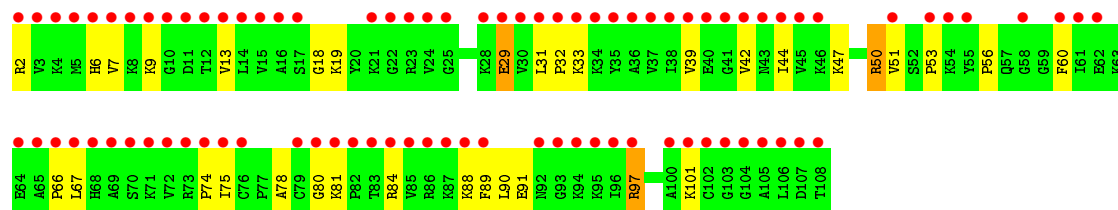
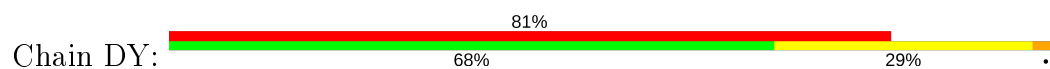


- Molecule 43: 50S ribosomal protein L24

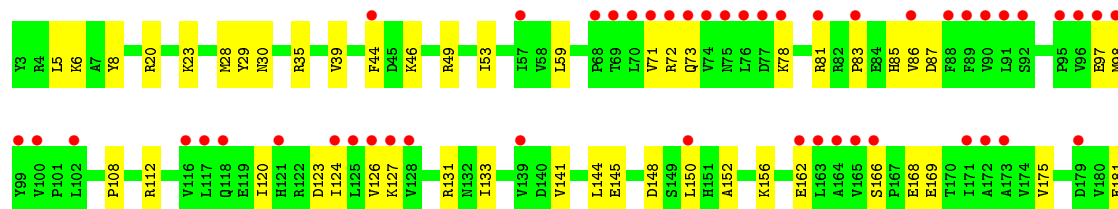
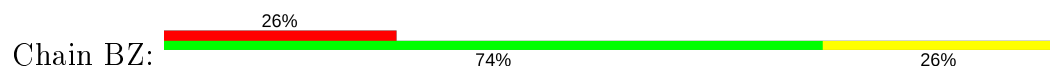




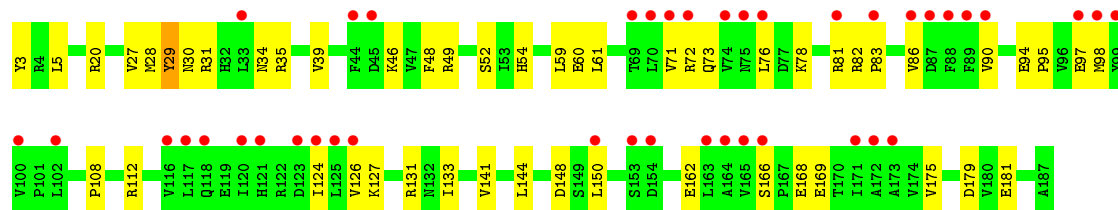
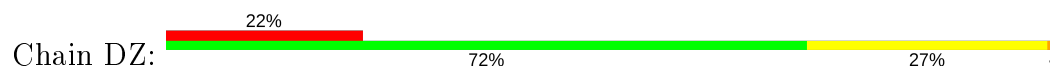
● Molecule 43: 50S ribosomal protein L24



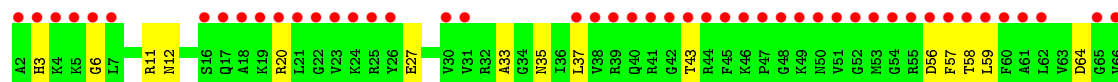
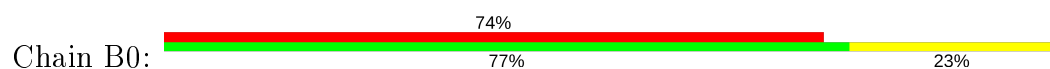
● Molecule 44: 50S ribosomal protein L25

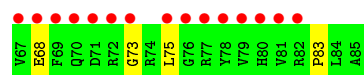


● Molecule 44: 50S ribosomal protein L25

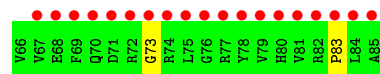
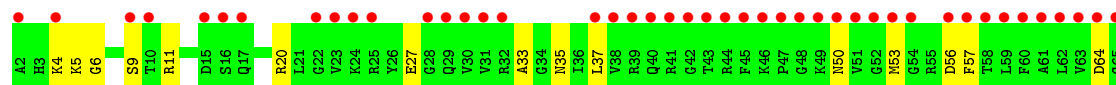
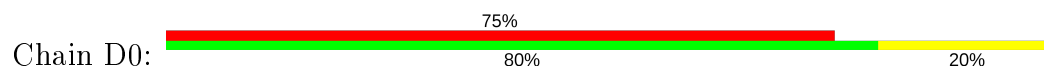


● Molecule 45: 50S ribosomal protein L27

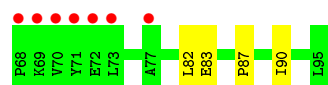




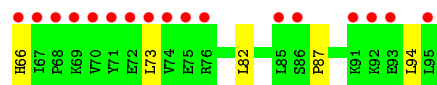
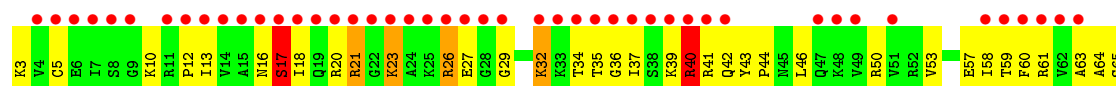
- Molecule 45: 50S ribosomal protein L27



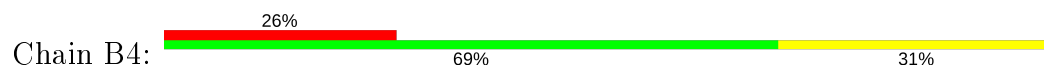
- Molecule 46: 50S ribosomal protein L28



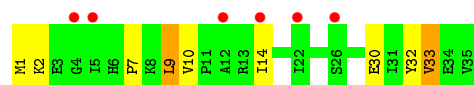
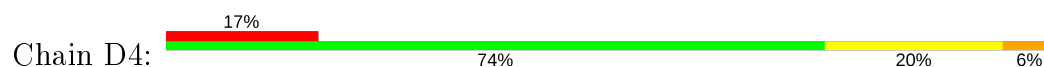
- Molecule 46: 50S ribosomal protein L28



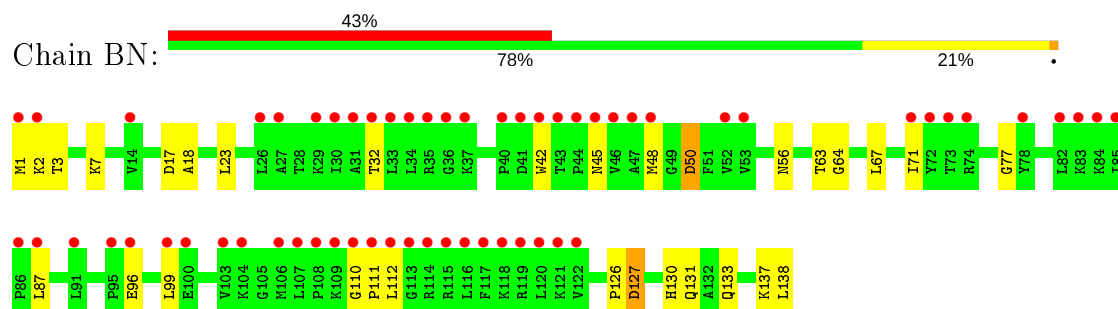
- Molecule 47: 50S ribosomal protein L31



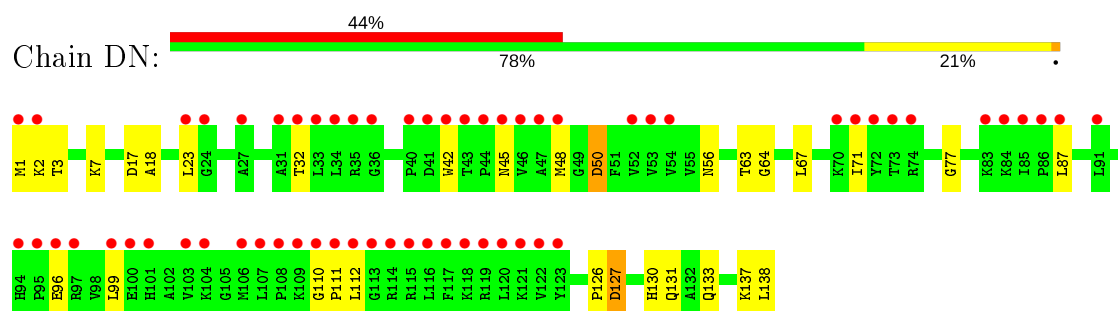
- Molecule 47: 50S ribosomal protein L31



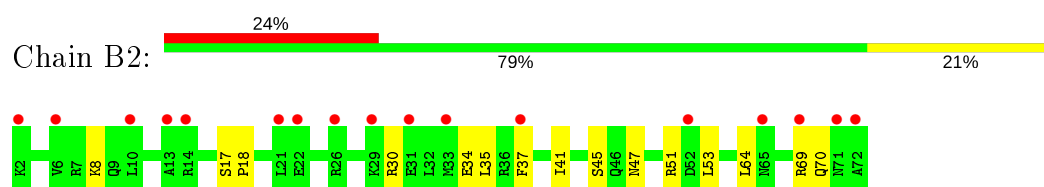
- Molecule 48: 50S ribosomal protein L13



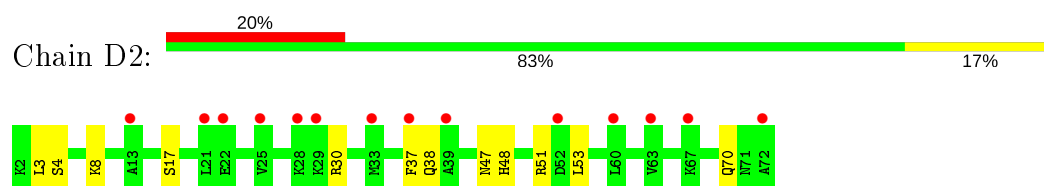
- Molecule 48: 50S ribosomal protein L13



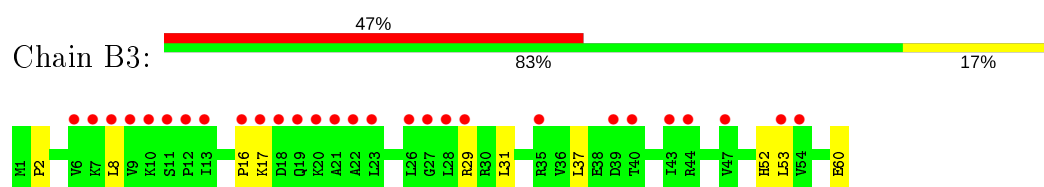
- Molecule 49: 50S ribosomal protein L29



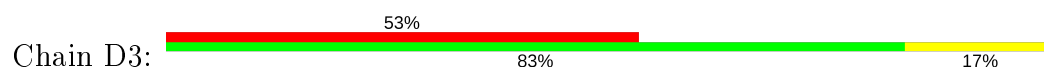
- Molecule 49: 50S ribosomal protein L29



- Molecule 50: 50S ribosomal protein L30

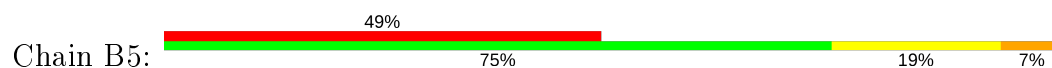


- Molecule 50: 50S ribosomal protein L30

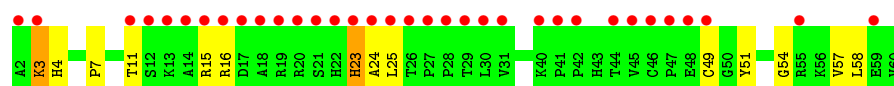
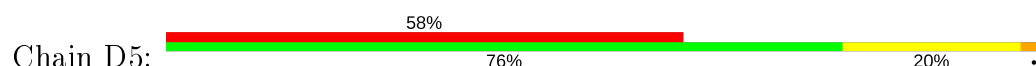




- Molecule 51: 50S ribosomal protein L32



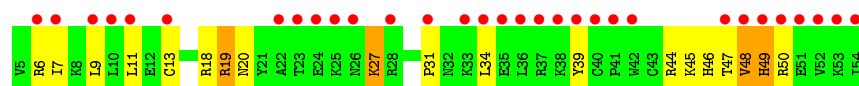
- Molecule 51: 50S ribosomal protein L32



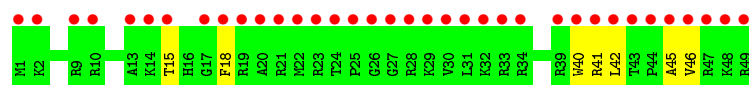
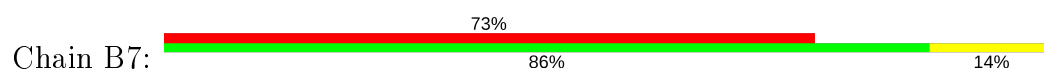
- Molecule 52: 50S ribosomal protein L33



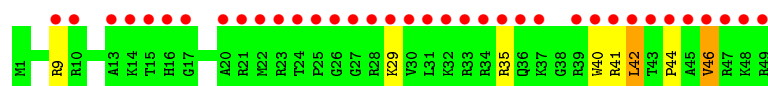
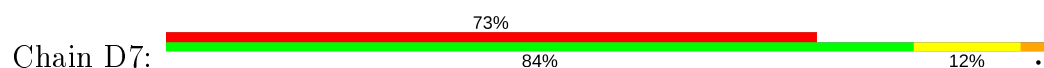
- Molecule 52: 50S ribosomal protein L33




- Molecule 53: 50S ribosomal protein L34

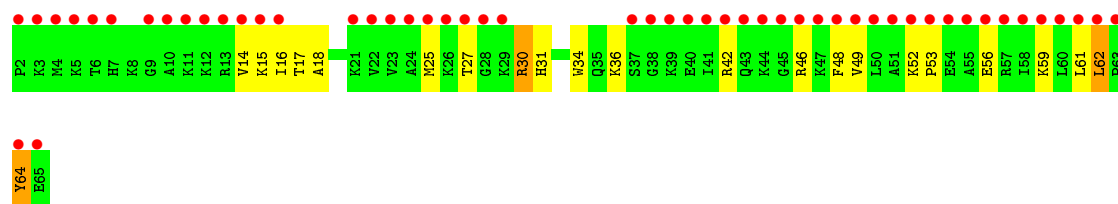


- Molecule 53: 50S ribosomal protein L34




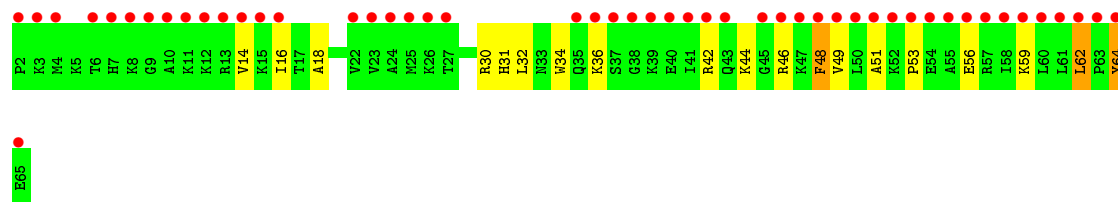
- Molecule 54: 50S ribosomal protein L35

Chain B8: 




- Molecule 54: 50S ribosomal protein L35

Chain D8: 




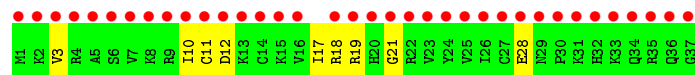
- Molecule 55: 50S ribosomal protein L36

Chain B9: 




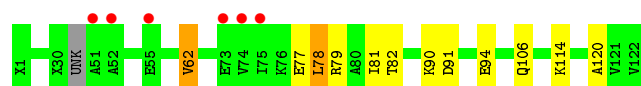
- Molecule 55: 50S ribosomal protein L36

Chain D9: 




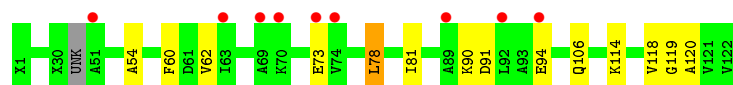
- Molecule 56: 50S ribosomal protein L7/L12

Chain Be: 



- Molecule 56: 50S ribosomal protein L7/L12

Chain De: 



- Molecule 57: 50S ribosomal protein L7/L12

Chain Bf:  100%

There are no outlier residues recorded for this chain.

- Molecule 57: 50S ribosomal protein L7/L12

Chain Bg:  100%

There are no outlier residues recorded for this chain.

- Molecule 57: 50S ribosomal protein L7/L12

Chain Df:  100%

There are no outlier residues recorded for this chain.

- Molecule 57: 50S ribosomal protein L7/L12

Chain Dg:  100%

There are no outlier residues recorded for this chain.

- Molecule 58: 50S ribosomal protein L7/L12

Chain Bh:  100%


There are no outlier residues recorded for this chain.

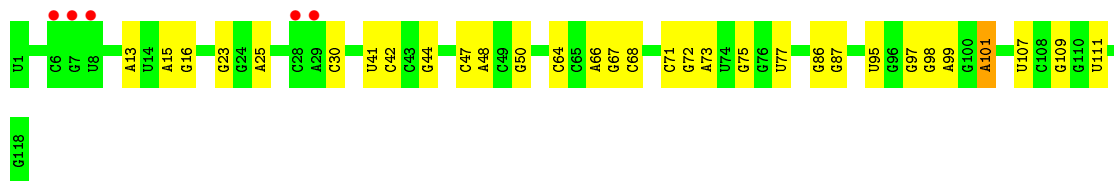
- Molecule 58: 50S ribosomal protein L7/L12

Chain Dh:  100%


There are no outlier residues recorded for this chain.

- Molecule 59: 5S ribosomal RNA

Chain BB:  4% 74% 25%



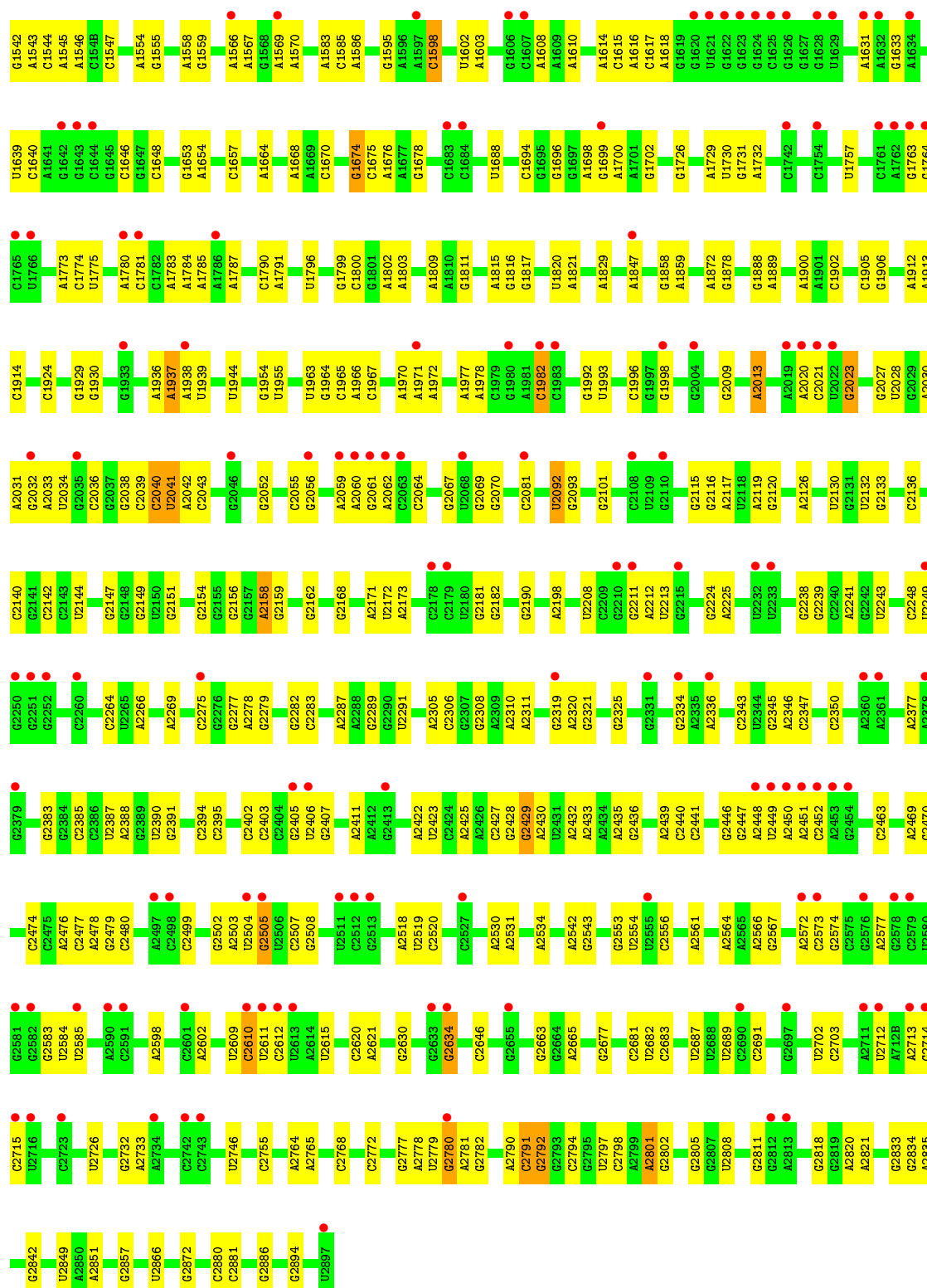
- Molecule 59: 5S ribosomal RNA

Chain DB:  8% 80% 20%

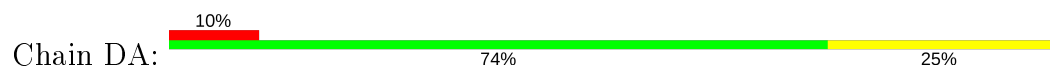


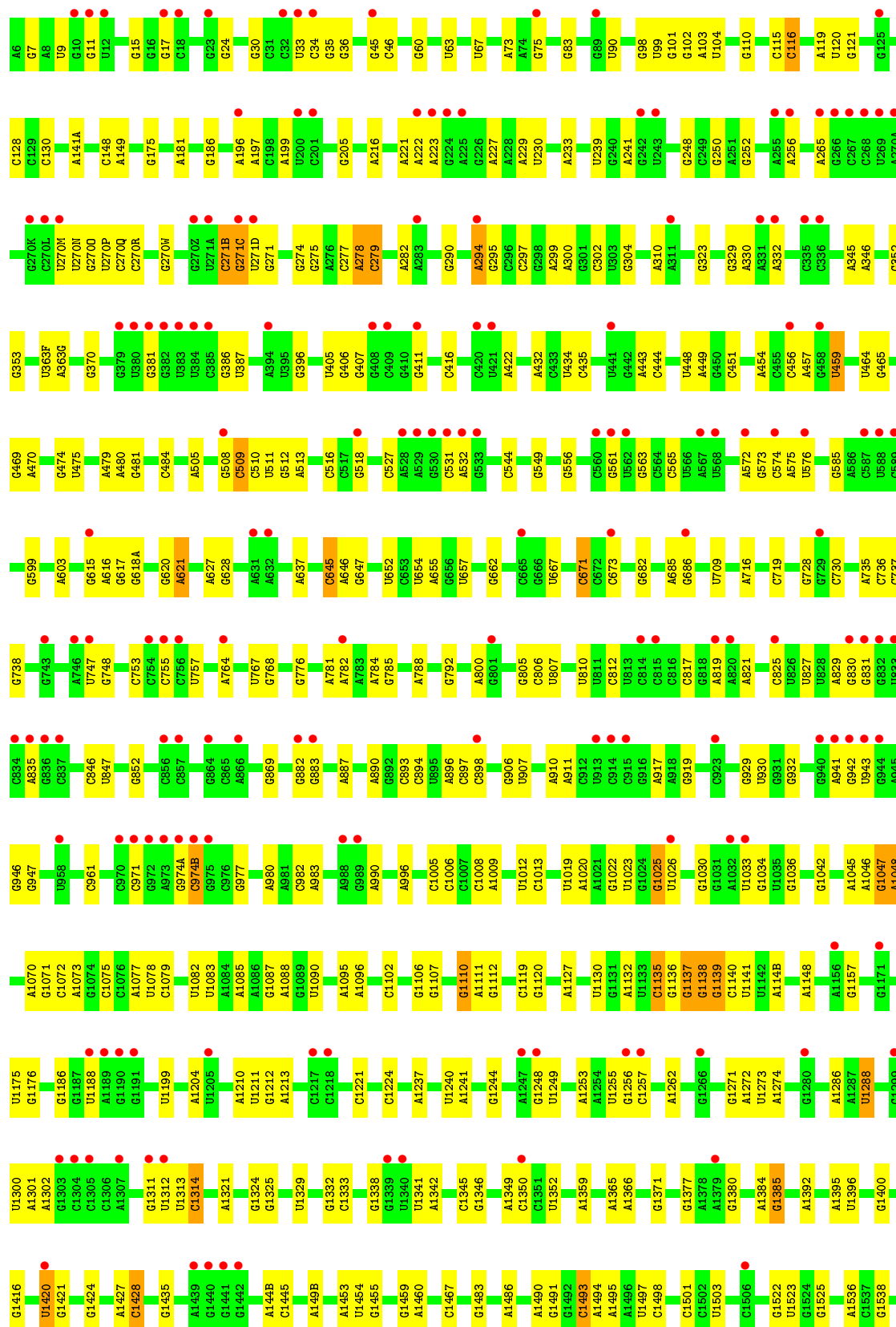
- Molecule 60: 23S ribosomal RNA





• Molecule 60: 23S 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	302.39Å 683.92Å 356.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.86 182.04 – 3.87	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.86) 64.4 (182.04-3.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.34	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 3.89Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.264 , 0.317 0.271 , 0.318	Depositor DCC
R_{free} test set	21652 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	76.3	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 478.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.24$, $\langle L^2 \rangle = 0.09$	Xtriage
Estimated twinning fraction	0.320 for h,-k,-l	Xtriage
F_o, F_c correlation	0.72	EDS
Total number of atoms	308202	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GNP, DPP, MG, KBE, UAL, 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	0.46	0/1945	0.80	9/2621 (0.3%)
1	CB	0.43	0/1945	0.80	6/2621 (0.2%)
2	AC	0.30	0/1645	0.60	0/2216
2	CC	0.30	0/1645	0.58	0/2216
3	AD	0.31	0/1733	0.61	0/2318
3	CD	0.30	0/1733	0.59	0/2318
4	AE	0.30	0/1172	0.57	0/1576
4	CE	0.30	0/1172	0.58	0/1576
5	AF	0.29	0/856	0.54	0/1154
5	CF	0.28	0/856	0.56	0/1154
6	AG	0.29	0/1276	0.54	0/1709
6	CG	0.29	0/1276	0.53	0/1709
7	AH	0.31	0/1136	0.61	0/1527
7	CH	0.31	0/1136	0.61	0/1527
8	AI	0.33	0/1029	0.56	1/1378 (0.1%)
8	CI	0.32	0/1029	0.56	1/1378 (0.1%)
9	AJ	0.29	0/815	0.56	0/1095
9	CJ	0.30	0/815	0.55	0/1095
10	AK	0.37	0/900	0.71	0/1213
10	CK	0.39	0/900	0.67	0/1213
11	AL	0.49	0/992	0.91	2/1327 (0.2%)
11	CL	0.47	0/992	0.88	2/1327 (0.2%)
12	AM	0.30	0/1008	0.61	0/1347
12	CM	0.27	0/1008	0.59	0/1347
13	AN	0.30	0/501	0.46	0/664
13	CN	0.30	0/501	0.49	0/664
14	AO	0.31	0/745	0.56	0/992
14	CO	0.32	0/745	0.62	0/992
15	AP	0.28	0/722	0.54	0/970
15	CP	0.27	0/722	0.52	0/970
16	AQ	0.40	0/848	0.71	0/1131
16	CQ	0.41	0/848	0.73	0/1131

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AR	0.31	0/579	0.64	0/768
17	CR	0.29	0/579	0.61	0/768
18	AS	0.30	0/647	0.60	0/870
18	CS	0.30	0/647	0.61	0/870
19	AT	0.34	0/764	0.62	0/1006
19	CT	0.33	0/764	0.61	0/1006
20	AA	0.39	0/36351	1.06	104/56736 (0.2%)
20	CA	0.38	2/36351 (0.0%)	1.06	96/56736 (0.2%)
21	AV	0.47	0/443	1.09	5/691 (0.7%)
21	CV	0.29	0/443	0.86	0/691
22	AW	0.42	0/1827	1.14	7/2845 (0.2%)
22	CW	0.37	0/1827	1.06	7/2845 (0.2%)
23	AY	0.37	0/5481	0.68	8/7418 (0.1%)
23	CY	0.41	0/5481	0.69	3/7418 (0.0%)
24	AU	1.08	0/11	1.84	0/13
24	CU	1.09	0/11	1.84	0/13
25	BC	0.52	0/1774	0.84	3/2391 (0.1%)
25	DC	0.55	1/1774 (0.1%)	0.93	7/2391 (0.3%)
26	BD	0.34	0/2195	0.65	2/2955 (0.1%)
26	DD	0.34	0/2195	0.64	2/2955 (0.1%)
27	BE	0.37	0/1602	0.68	2/2160 (0.1%)
27	DE	0.34	0/1602	0.65	1/2160 (0.0%)
28	BF	0.47	1/1663 (0.1%)	0.87	6/2249 (0.3%)
28	DF	0.43	0/1663	0.87	6/2249 (0.3%)
29	BG	0.42	1/1499 (0.1%)	1.33	5/2016 (0.2%)
29	DG	0.39	1/1499 (0.1%)	0.63	0/2016
30	BH	0.30	0/1298	0.56	0/1751
30	DH	0.30	0/1298	0.56	0/1751
32	BK	0.28	0/1054	0.55	0/1427
32	DK	0.27	0/1054	0.52	0/1427
33	BO	0.29	0/943	0.58	0/1269
33	DO	0.29	0/943	0.55	0/1269
34	BP	0.32	0/1131	0.68	0/1504
34	DP	0.30	0/1131	0.62	0/1504
35	BQ	0.33	0/1143	0.60	0/1527
35	DQ	0.32	0/1143	0.63	0/1527
36	BR	0.31	0/974	0.63	0/1302
36	DR	0.32	0/974	0.63	0/1302
37	BS	0.36	0/783	0.69	0/1041
37	DS	0.36	0/783	0.68	0/1041
38	BT	0.34	0/1161	0.67	0/1549
38	DT	0.32	0/1161	0.65	0/1549
39	BU	0.38	0/982	0.59	0/1306

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	DU	0.38	0/982	0.61	0/1306
40	BV	0.38	0/790	0.73	0/1057
40	DV	0.34	0/790	0.66	1/1057 (0.1%)
41	BW	0.35	0/911	0.66	2/1220 (0.2%)
41	DW	0.34	0/911	0.63	0/1220
42	BX	0.31	0/748	0.57	0/1004
42	DX	0.29	0/748	0.55	1/1004 (0.1%)
43	BY	0.32	0/831	0.61	0/1108
43	DY	0.31	0/831	0.58	0/1108
44	BZ	0.30	0/1505	0.60	0/2042
44	DZ	0.31	0/1505	0.60	0/2042
45	B0	0.27	0/671	0.54	0/892
45	D0	0.27	0/671	0.53	0/892
46	B1	0.48	0/739	0.77	2/981 (0.2%)
46	D1	0.50	0/739	0.82	3/981 (0.3%)
47	B4	0.40	0/276	0.62	0/372
47	D4	0.36	0/276	0.59	0/372
48	BN	0.34	0/1131	0.66	0/1525
48	DN	0.34	0/1131	0.66	0/1525
49	B2	0.36	0/600	0.62	0/793
49	D2	0.34	0/600	0.58	0/793
50	B3	0.29	0/482	0.53	0/646
50	D3	0.29	0/482	0.53	0/646
51	B5	0.33	0/473	0.65	0/639
51	D5	0.31	0/473	0.58	0/639
52	B6	0.32	0/440	0.67	0/586
52	D6	0.34	0/440	0.66	0/586
53	B7	0.31	0/438	0.56	0/575
53	D7	0.32	0/438	0.55	0/575
54	B8	0.33	0/525	0.66	0/691
54	D8	0.32	0/525	0.63	0/691
55	B9	0.43	0/310	0.69	0/407
55	D9	0.30	0/310	0.63	0/407
56	Be	0.33	0/538	0.56	0/715
56	De	0.31	0/538	0.56	0/715
59	BB	0.39	0/2853	1.12	15/4451 (0.3%)
59	DB	0.38	0/2853	1.07	10/4451 (0.2%)
60	BA	0.39	0/69437	1.09	229/108401 (0.2%)
60	DA	0.38	3/69437 (0.0%)	1.06	187/108401 (0.2%)
All	All	0.38	9/330652 (0.0%)	0.97	735/492274 (0.1%)

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

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

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

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	BG	114	ILE	C-N	10.70	1.58	1.34
20	CA	1393	U	N1-C2	9.25	1.46	1.38
29	DG	114	ILE	N-CA	-7.54	1.31	1.46
25	DC	214	TYR	CD1-CE1	6.83	1.49	1.39
28	BF	157	VAL	CB-CG1	-5.60	1.41	1.52

The worst 5 of 735 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	BG	114	ILE	O-C-N	-51.93	39.62	122.70
60	BA	1006	C	C6-N1-C2	-15.70	114.02	120.30
60	BA	1006	C	N3-C2-O2	-13.26	112.62	121.90

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	AA	1535	C	P-O3'-C3'	12.55	134.76	119.70
60	BA	2505	G	N1-C6-O6	12.54	127.43	119.90

There are no chirality outliers.

5 of 51 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AB	170	GLU	Peptide
1	AB	185	ILE	Peptide
1	AB	68	ILE	Peptide
11	AL	32	PHE	Peptide
23	AY	34	TYR	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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%)	60 (26%)	19 (8%)	1	13
1	CB	233/235 (99%)	164 (70%)	49 (21%)	20 (9%)	1	13
2	AC	205/207 (99%)	140 (68%)	43 (21%)	22 (11%)	0	8
2	CC	205/207 (99%)	136 (66%)	47 (23%)	22 (11%)	0	8
3	AD	206/208 (99%)	146 (71%)	46 (22%)	14 (7%)	1	17
3	CD	206/208 (99%)	140 (68%)	49 (24%)	17 (8%)	1	13
4	AE	149/151 (99%)	118 (79%)	22 (15%)	9 (6%)	1	20
4	CE	149/151 (99%)	125 (84%)	16 (11%)	8 (5%)	2	22
5	AF	99/101 (98%)	82 (83%)	14 (14%)	3 (3%)	4	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	CF	99/101 (98%)	81 (82%)	10 (10%)	8 (8%)	1	14
6	AG	153/155 (99%)	113 (74%)	27 (18%)	13 (8%)	1	13
6	CG	153/155 (99%)	116 (76%)	24 (16%)	13 (8%)	1	13
7	AH	136/138 (99%)	98 (72%)	21 (15%)	17 (12%)	0	5
7	CH	136/138 (99%)	90 (66%)	29 (21%)	17 (12%)	0	5
8	AI	125/127 (98%)	98 (78%)	16 (13%)	11 (9%)	1	12
8	CI	125/127 (98%)	100 (80%)	16 (13%)	9 (7%)	1	16
9	AJ	97/99 (98%)	69 (71%)	22 (23%)	6 (6%)	1	19
9	CJ	97/99 (98%)	71 (73%)	20 (21%)	6 (6%)	1	19
10	AK	117/119 (98%)	81 (69%)	23 (20%)	13 (11%)	0	8
10	CK	117/119 (98%)	82 (70%)	22 (19%)	13 (11%)	0	8
11	AL	123/125 (98%)	55 (45%)	38 (31%)	30 (24%)	0	1
11	CL	123/125 (98%)	54 (44%)	41 (33%)	28 (23%)	0	1
12	AM	123/125 (98%)	85 (69%)	21 (17%)	17 (14%)	0	4
12	CM	123/125 (98%)	85 (69%)	22 (18%)	16 (13%)	0	5
13	AN	58/60 (97%)	46 (79%)	7 (12%)	5 (9%)	1	13
13	CN	58/60 (97%)	45 (78%)	8 (14%)	5 (9%)	1	13
14	AO	86/88 (98%)	59 (69%)	20 (23%)	7 (8%)	1	14
14	CO	86/88 (98%)	60 (70%)	20 (23%)	6 (7%)	1	17
15	AP	82/84 (98%)	61 (74%)	14 (17%)	7 (8%)	1	13
15	CP	82/84 (98%)	59 (72%)	20 (24%)	3 (4%)	3	28
16	AQ	98/100 (98%)	71 (72%)	14 (14%)	13 (13%)	0	4
16	CQ	98/100 (98%)	72 (74%)	17 (17%)	9 (9%)	1	12
17	AR	68/70 (97%)	43 (63%)	17 (25%)	8 (12%)	0	6
17	CR	68/70 (97%)	49 (72%)	16 (24%)	3 (4%)	2	25
18	AS	77/79 (98%)	45 (58%)	21 (27%)	11 (14%)	0	4
18	CS	77/79 (98%)	38 (49%)	29 (38%)	10 (13%)	0	5
19	AT	97/99 (98%)	77 (79%)	16 (16%)	4 (4%)	3	26
19	CT	97/99 (98%)	79 (81%)	14 (14%)	4 (4%)	3	26
23	AY	685/687 (100%)	474 (69%)	144 (21%)	67 (10%)	0	10
23	CY	685/687 (100%)	476 (70%)	143 (21%)	66 (10%)	0	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	AU	2/6 (33%)	2 (100%)	0	0	100	100
24	CU	2/6 (33%)	2 (100%)	0	0	100	100
25	BC	226/228 (99%)	109 (48%)	65 (29%)	52 (23%)	0	1
25	DC	226/228 (99%)	108 (48%)	66 (29%)	52 (23%)	0	1
26	BD	273/275 (99%)	177 (65%)	66 (24%)	30 (11%)	0	8
26	DD	273/275 (99%)	179 (66%)	57 (21%)	37 (14%)	0	4
27	BE	203/205 (99%)	123 (61%)	50 (25%)	30 (15%)	0	4
27	DE	203/205 (99%)	133 (66%)	41 (20%)	29 (14%)	0	4
28	BF	206/208 (99%)	130 (63%)	47 (23%)	29 (14%)	0	4
28	DF	206/208 (99%)	126 (61%)	55 (27%)	25 (12%)	0	6
29	BG	179/181 (99%)	116 (65%)	45 (25%)	18 (10%)	0	10
29	DG	179/181 (99%)	121 (68%)	43 (24%)	15 (8%)	1	13
30	BH	165/167 (99%)	115 (70%)	35 (21%)	15 (9%)	1	12
30	DH	165/167 (99%)	121 (73%)	26 (16%)	18 (11%)	0	8
32	BK	138/140 (99%)	97 (70%)	28 (20%)	13 (9%)	0	11
32	DK	138/140 (99%)	91 (66%)	35 (25%)	12 (9%)	1	12
33	BO	120/122 (98%)	88 (73%)	25 (21%)	7 (6%)	1	20
33	DO	120/122 (98%)	90 (75%)	22 (18%)	8 (7%)	1	18
34	BP	144/146 (99%)	82 (57%)	41 (28%)	21 (15%)	0	4
34	DP	144/146 (99%)	88 (61%)	35 (24%)	21 (15%)	0	4
35	BQ	139/141 (99%)	93 (67%)	32 (23%)	14 (10%)	0	10
35	DQ	139/141 (99%)	99 (71%)	26 (19%)	14 (10%)	0	10
36	BR	115/117 (98%)	72 (63%)	28 (24%)	15 (13%)	0	5
36	DR	115/117 (98%)	78 (68%)	26 (23%)	11 (10%)	0	10
37	BS	97/99 (98%)	54 (56%)	22 (23%)	21 (22%)	0	1
37	DS	97/99 (98%)	52 (54%)	24 (25%)	21 (22%)	0	1
38	BT	136/138 (99%)	84 (62%)	33 (24%)	19 (14%)	0	4
38	DT	136/138 (99%)	89 (65%)	28 (21%)	19 (14%)	0	4
39	BU	115/117 (98%)	89 (77%)	21 (18%)	5 (4%)	2	25
39	DU	115/117 (98%)	84 (73%)	20 (17%)	11 (10%)	0	10
40	BV	99/101 (98%)	59 (60%)	22 (22%)	18 (18%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	DV	99/101 (98%)	63 (64%)	22 (22%)	14 (14%)	0	4
41	BW	111/113 (98%)	88 (79%)	16 (14%)	7 (6%)	1	19
41	DW	111/113 (98%)	90 (81%)	10 (9%)	11 (10%)	0	10
42	BX	91/93 (98%)	71 (78%)	12 (13%)	8 (9%)	1	12
42	DX	91/93 (98%)	69 (76%)	17 (19%)	5 (6%)	2	21
43	BY	105/107 (98%)	48 (46%)	33 (31%)	24 (23%)	0	1
43	DY	105/107 (98%)	50 (48%)	34 (32%)	21 (20%)	0	2
44	BZ	183/185 (99%)	126 (69%)	42 (23%)	15 (8%)	1	13
44	DZ	183/185 (99%)	120 (66%)	45 (25%)	18 (10%)	0	10
45	B0	82/84 (98%)	59 (72%)	15 (18%)	8 (10%)	0	10
45	D0	82/84 (98%)	55 (67%)	20 (24%)	7 (8%)	1	13
46	B1	91/93 (98%)	55 (60%)	19 (21%)	17 (19%)	0	2
46	D1	91/93 (98%)	55 (60%)	17 (19%)	19 (21%)	0	2
47	B4	33/35 (94%)	17 (52%)	13 (39%)	3 (9%)	1	12
47	D4	33/35 (94%)	17 (52%)	11 (33%)	5 (15%)	0	3
48	BN	136/138 (99%)	95 (70%)	25 (18%)	16 (12%)	0	6
48	DN	136/138 (99%)	94 (69%)	26 (19%)	16 (12%)	0	6
49	B2	69/71 (97%)	52 (75%)	13 (19%)	4 (6%)	1	20
49	D2	69/71 (97%)	51 (74%)	14 (20%)	4 (6%)	1	20
50	B3	58/60 (97%)	48 (83%)	7 (12%)	3 (5%)	2	22
50	D3	58/60 (97%)	45 (78%)	10 (17%)	3 (5%)	2	22
51	B5	57/59 (97%)	37 (65%)	10 (18%)	10 (18%)	0	3
51	D5	57/59 (97%)	37 (65%)	13 (23%)	7 (12%)	0	6
52	B6	48/50 (96%)	26 (54%)	11 (23%)	11 (23%)	0	1
52	D6	48/50 (96%)	26 (54%)	11 (23%)	11 (23%)	0	1
53	B7	47/49 (96%)	32 (68%)	11 (23%)	4 (8%)	1	13
53	D7	47/49 (96%)	34 (72%)	9 (19%)	4 (8%)	1	13
54	B8	62/64 (97%)	38 (61%)	18 (29%)	6 (10%)	0	10
54	D8	62/64 (97%)	37 (60%)	17 (27%)	8 (13%)	0	5
55	B9	35/37 (95%)	16 (46%)	14 (40%)	5 (14%)	0	4
55	D9	35/37 (95%)	19 (54%)	12 (34%)	4 (11%)	0	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
56	Be	70/103 (68%)	38 (54%)	25 (36%)	7 (10%)	0	10
56	De	70/103 (68%)	40 (57%)	23 (33%)	7 (10%)	0	10
All	All	13304/13578 (98%)	8936 (67%)	2877 (22%)	1491 (11%)	0	7

5 of 1491 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AB	203/203 (100%)	161 (79%)	42 (21%)	1	8
1	CB	203/203 (100%)	165 (81%)	38 (19%)	1	11
2	AC	161/161 (100%)	124 (77%)	37 (23%)	1	6
2	CC	161/161 (100%)	121 (75%)	40 (25%)	0	5
3	AD	180/180 (100%)	138 (77%)	42 (23%)	1	6
3	CD	180/180 (100%)	149 (83%)	31 (17%)	2	14
4	AE	116/116 (100%)	91 (78%)	25 (22%)	1	7
4	CE	116/116 (100%)	93 (80%)	23 (20%)	1	9
5	AF	90/90 (100%)	72 (80%)	18 (20%)	1	9
5	CF	90/90 (100%)	74 (82%)	16 (18%)	2	13
6	AG	126/126 (100%)	109 (86%)	17 (14%)	4	22
6	CG	126/126 (100%)	106 (84%)	20 (16%)	2	17
7	AH	119/119 (100%)	92 (77%)	27 (23%)	1	6
7	CH	119/119 (100%)	99 (83%)	20 (17%)	2	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	AI	98/98 (100%)	79 (81%)	19 (19%)	1	10
8	CI	98/98 (100%)	82 (84%)	16 (16%)	2	16
9	AJ	89/89 (100%)	72 (81%)	17 (19%)	1	10
9	CJ	89/89 (100%)	74 (83%)	15 (17%)	2	15
10	AK	90/90 (100%)	76 (84%)	14 (16%)	2	17
10	CK	90/90 (100%)	78 (87%)	12 (13%)	4	22
11	AL	104/104 (100%)	83 (80%)	21 (20%)	1	8
11	CL	104/104 (100%)	77 (74%)	27 (26%)	0	4
12	AM	100/100 (100%)	83 (83%)	17 (17%)	2	14
12	CM	100/100 (100%)	82 (82%)	18 (18%)	1	12
13	AN	49/49 (100%)	37 (76%)	12 (24%)	0	5
13	CN	49/49 (100%)	40 (82%)	9 (18%)	1	11
14	AO	79/79 (100%)	63 (80%)	16 (20%)	1	8
14	CO	79/79 (100%)	62 (78%)	17 (22%)	1	7
15	AP	72/72 (100%)	56 (78%)	16 (22%)	1	6
15	CP	72/72 (100%)	60 (83%)	12 (17%)	2	15
16	AQ	95/95 (100%)	77 (81%)	18 (19%)	1	10
16	CQ	95/95 (100%)	82 (86%)	13 (14%)	3	21
17	AR	61/61 (100%)	51 (84%)	10 (16%)	2	15
17	CR	61/61 (100%)	48 (79%)	13 (21%)	1	7
18	AS	69/69 (100%)	51 (74%)	18 (26%)	0	4
18	CS	69/69 (100%)	54 (78%)	15 (22%)	1	7
19	AT	76/76 (100%)	66 (87%)	10 (13%)	4	22
19	CT	76/76 (100%)	69 (91%)	7 (9%)	9	34
23	AY	579/579 (100%)	475 (82%)	104 (18%)	1	12
23	CY	579/579 (100%)	472 (82%)	107 (18%)	1	11
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%)	138 (77%)	42 (23%)	1	6
25	DC	180/180 (100%)	130 (72%)	50 (28%)	0	3
26	BD	217/217 (100%)	164 (76%)	53 (24%)	0	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	DD	217/217 (100%)	173 (80%)	44 (20%)	1	8
27	BE	165/165 (100%)	131 (79%)	34 (21%)	1	8
27	DE	165/165 (100%)	134 (81%)	31 (19%)	1	11
28	BF	165/165 (100%)	127 (77%)	38 (23%)	1	6
28	DF	165/165 (100%)	126 (76%)	39 (24%)	1	5
29	BG	155/155 (100%)	118 (76%)	37 (24%)	0	5
29	DG	155/155 (100%)	121 (78%)	34 (22%)	1	7
30	BH	136/136 (100%)	109 (80%)	27 (20%)	1	9
30	DH	136/136 (100%)	115 (85%)	21 (15%)	2	17
32	BK	105/105 (100%)	94 (90%)	11 (10%)	7	29
32	DK	105/105 (100%)	88 (84%)	17 (16%)	2	16
33	BO	100/100 (100%)	80 (80%)	20 (20%)	1	9
33	DO	100/100 (100%)	84 (84%)	16 (16%)	2	16
34	BP	112/112 (100%)	80 (71%)	32 (29%)	0	2
34	DP	112/112 (100%)	91 (81%)	21 (19%)	1	11
35	BQ	111/111 (100%)	81 (73%)	30 (27%)	0	4
35	DQ	111/111 (100%)	85 (77%)	26 (23%)	1	5
36	BR	100/100 (100%)	72 (72%)	28 (28%)	0	3
36	DR	100/100 (100%)	81 (81%)	19 (19%)	1	10
37	BS	77/77 (100%)	55 (71%)	22 (29%)	0	2
37	DS	77/77 (100%)	60 (78%)	17 (22%)	1	6
38	BT	120/120 (100%)	99 (82%)	21 (18%)	2	13
38	DT	120/120 (100%)	99 (82%)	21 (18%)	2	13
39	BU	93/93 (100%)	77 (83%)	16 (17%)	2	14
39	DU	93/93 (100%)	76 (82%)	17 (18%)	1	11
40	BV	82/82 (100%)	61 (74%)	21 (26%)	0	5
40	DV	82/82 (100%)	60 (73%)	22 (27%)	0	4
41	BW	92/92 (100%)	73 (79%)	19 (21%)	1	8
41	DW	92/92 (100%)	74 (80%)	18 (20%)	1	9
42	BX	75/75 (100%)	59 (79%)	16 (21%)	1	7
42	DX	75/75 (100%)	60 (80%)	15 (20%)	1	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	BY	88/88 (100%)	69 (78%)	19 (22%)	1	7
43	DY	88/88 (100%)	72 (82%)	16 (18%)	1	11
44	BZ	162/162 (100%)	129 (80%)	33 (20%)	1	8
44	DZ	162/162 (100%)	128 (79%)	34 (21%)	1	7
45	B0	66/66 (100%)	55 (83%)	11 (17%)	2	15
45	D0	66/66 (100%)	56 (85%)	10 (15%)	3	18
46	B1	78/78 (100%)	61 (78%)	17 (22%)	1	7
46	D1	78/78 (100%)	53 (68%)	25 (32%)	0	2
47	B4	31/31 (100%)	23 (74%)	8 (26%)	0	4
47	D4	31/31 (100%)	25 (81%)	6 (19%)	1	10
48	BN	117/117 (100%)	100 (86%)	17 (14%)	3	19
48	DN	117/117 (100%)	100 (86%)	17 (14%)	3	19
49	B2	66/66 (100%)	55 (83%)	11 (17%)	2	15
49	D2	66/66 (100%)	58 (88%)	8 (12%)	5	24
50	B3	52/52 (100%)	45 (86%)	7 (14%)	4	22
50	D3	52/52 (100%)	45 (86%)	7 (14%)	4	22
51	B5	51/51 (100%)	42 (82%)	9 (18%)	2	13
51	D5	51/51 (100%)	42 (82%)	9 (18%)	2	13
52	B6	49/49 (100%)	36 (74%)	13 (26%)	0	4
52	D6	49/49 (100%)	37 (76%)	12 (24%)	0	5
53	B7	42/42 (100%)	39 (93%)	3 (7%)	14	44
53	D7	42/42 (100%)	36 (86%)	6 (14%)	3	20
54	B8	54/54 (100%)	35 (65%)	19 (35%)	0	1
54	D8	54/54 (100%)	40 (74%)	14 (26%)	0	4
55	B9	34/34 (100%)	29 (85%)	5 (15%)	3	19
55	D9	34/34 (100%)	29 (85%)	5 (15%)	3	19
56	Be	54/54 (100%)	47 (87%)	7 (13%)	4	23
56	De	54/54 (100%)	46 (85%)	8 (15%)	3	18
All	All	11174/11174 (100%)	8954 (80%)	2220 (20%)	1	9

5 of 2220 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
44	BZ	123	ASP
3	CD	107	ARG
43	DY	44	ILE
46	B1	26	ARG
54	B8	48	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 93 such sidechains are listed below:

Mol	Chain	Res	Type
2	CC	123	GLN
7	CH	78	GLN
46	D1	45	ASN
2	CC	136	GLN
3	CD	125	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
20	AA	1511/1511 (100%)	330 (21%)	21 (1%)
20	CA	1511/1511 (100%)	304 (20%)	18 (1%)
21	AV	17/18 (94%)	8 (47%)	1 (5%)
21	CV	17/18 (94%)	8 (47%)	1 (5%)
22	AW	76/77 (98%)	27 (35%)	2 (2%)
22	CW	76/77 (98%)	22 (28%)	2 (2%)
59	BB	118/119 (99%)	26 (22%)	2 (1%)
59	DB	118/119 (99%)	19 (16%)	1 (0%)
60	BA	2878/2879 (99%)	729 (25%)	26 (0%)
60	DA	2878/2879 (99%)	692 (24%)	22 (0%)
All	All	9200/9208 (99%)	2165 (23%)	96 (1%)

5 of 2165 RNA backbone outliers are listed below:

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

5 of 96 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
60	BA	1913	A
20	CA	115	G
60	DA	1937	A
60	BA	1937	A
60	BA	2158	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	DPP	CU	2	24	3,5,6	0.50	0	1,5,7	0.25	0
24	5OH	AU	6	24	8,12,13	0.75	0	3,16,18	1.07	0
24	KBE	CU	1	24	8,8,9	1.06	0	7,8,10	2.18	1 (14%)
24	UAL	CU	5	24	7,8,9	2.68	3 (42%)	5,9,11	2.09	1 (20%)
24	5OH	CU	6	24	8,12,13	0.75	0	3,16,18	1.07	0
24	DPP	AU	2	24	3,5,6	0.50	0	1,5,7	0.26	0
24	UAL	AU	5	24	7,8,9	2.70	3 (42%)	5,9,11	2.08	1 (20%)
24	KBE	AU	1	24	8,8,9	1.05	0	7,8,10	2.18	1 (14%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	KBE	AU	1	24	-	2/7/7/8	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AU	5	UAL	C-CA	5.54	1.54	1.45
24	CU	5	UAL	C-CA	5.50	1.54	1.45
24	AU	5	UAL	C1-N1	-3.43	1.34	1.40
24	CU	5	UAL	C1-N1	-3.40	1.35	1.40
24	CU	5	UAL	CB-N1	-2.23	1.30	1.35

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	CU	1	KBE	CB-CA-C	5.37	120.16	112.25
24	AU	1	KBE	CB-CA-C	5.36	120.14	112.25
24	CU	5	UAL	O-C-CA	-4.21	120.03	125.39
24	AU	5	UAL	O-C-CA	-4.19	120.06	125.39

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
61	GNP	AY	701	62	28,34,34	2.75	8 (28%)	30,54,54	2.47	10 (33%)
61	GNP	CY	702	62	28,34,34	2.75	8 (28%)	30,54,54	2.47	10 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	GNP	AY	701	62	-	10/17/38/38	0/3/3/3
61	GNP	CY	702	62	-	10/17/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	AY	701	GNP	C5-C6	-8.27	1.38	1.52
61	CY	702	GNP	C5-C6	-8.27	1.38	1.52
61	CY	702	GNP	C4-N9	-8.13	1.36	1.47
61	AY	701	GNP	C4-N9	-8.10	1.37	1.47
61	CY	702	GNP	PG-O1G	4.78	1.53	1.46

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	AY	701	GNP	C4-C5-N7	7.62	112.56	102.46
61	CY	702	GNP	C4-C5-N7	7.59	112.52	102.46
61	CY	702	GNP	C5-C6-N1	-5.27	111.69	118.19
61	AY	701	GNP	C5-C6-N1	-5.25	111.72	118.19
61	AY	701	GNP	PA-O3A-PB	-4.70	116.08	132.62

There are no chirality outliers.

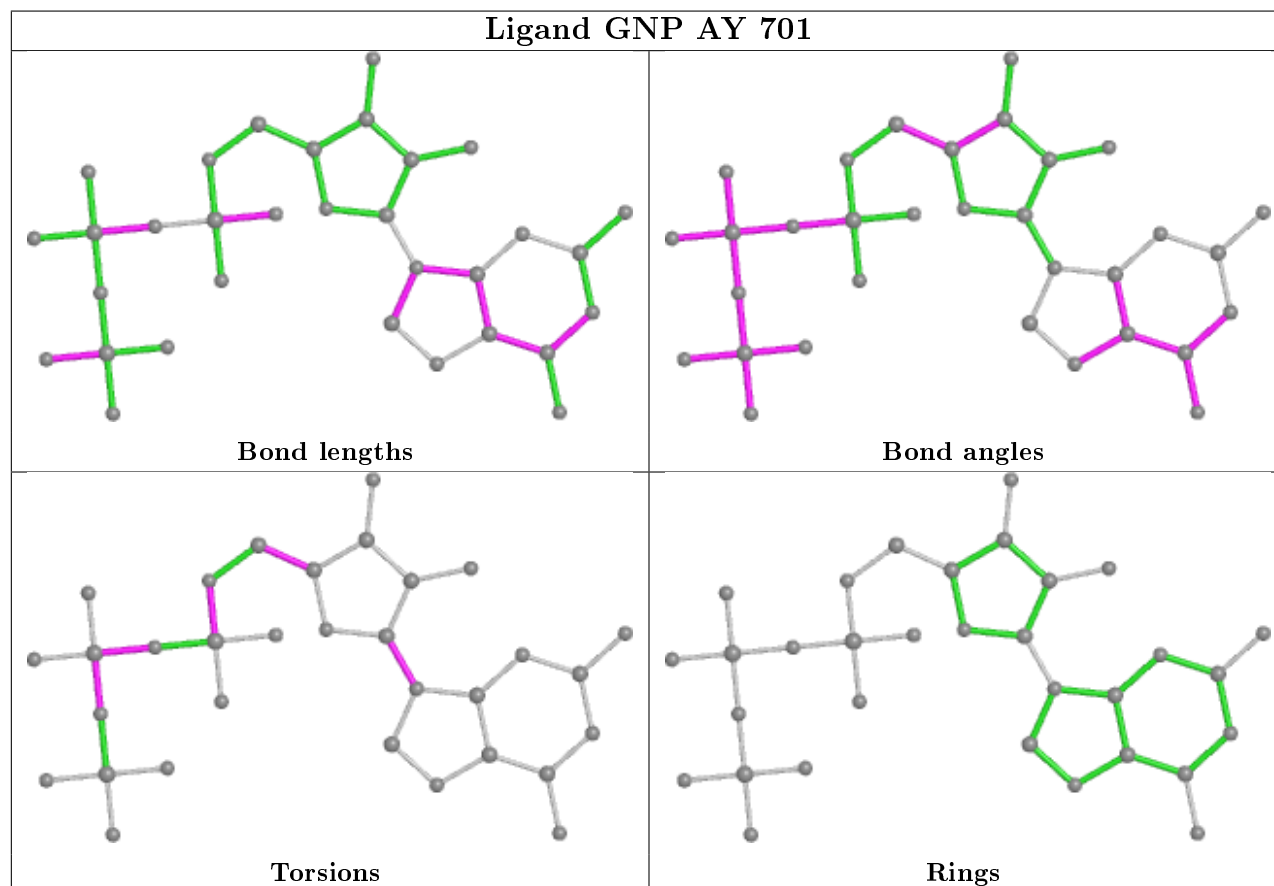
5 of 20 torsion outliers are listed below:

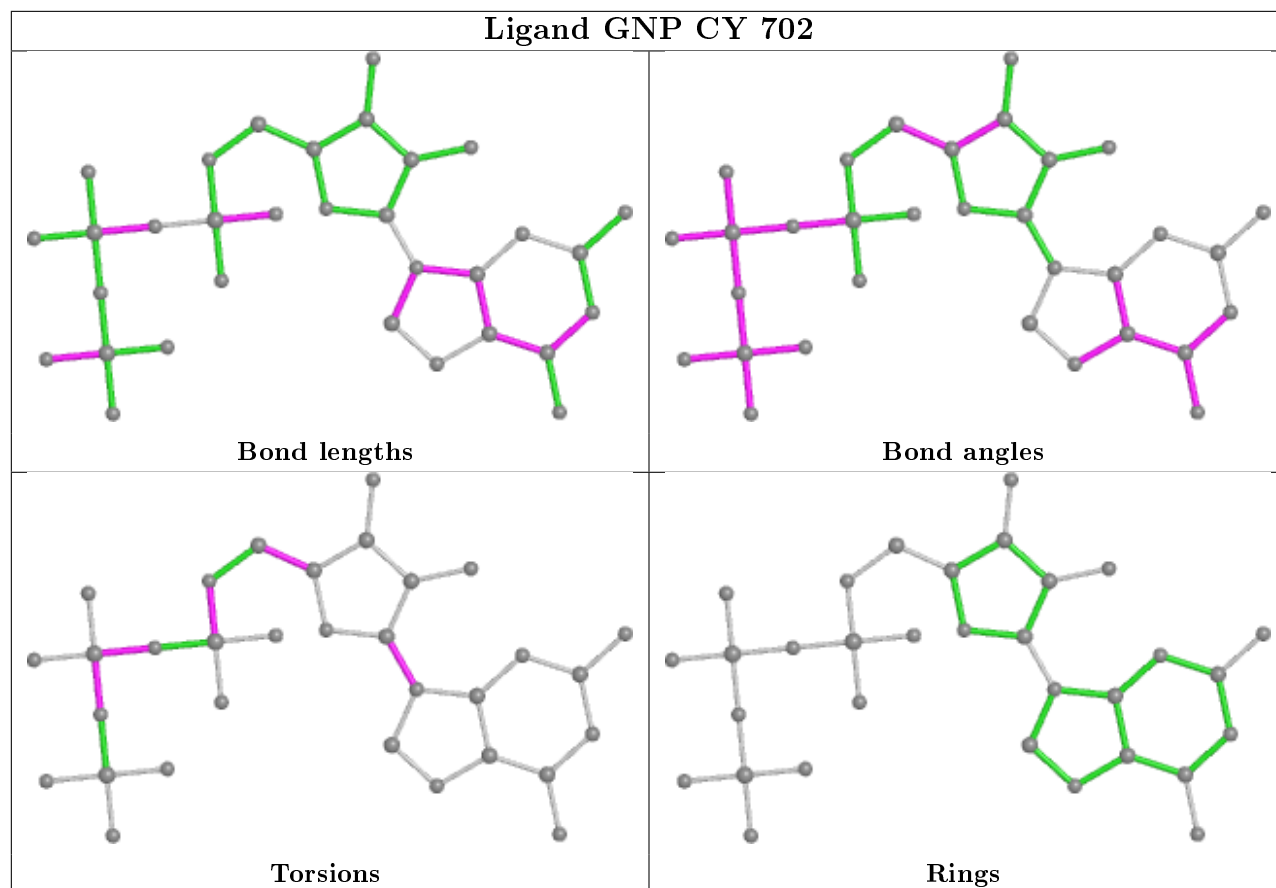
Mol	Chain	Res	Type	Atoms
61	AY	701	GNP	PG-N3B-PB-O1B
61	AY	701	GNP	PG-N3B-PB-O3A
61	AY	701	GNP	PA-O3A-PB-O1B
61	AY	701	GNP	PA-O3A-PB-O2B
61	AY	701	GNP	C5'-O5'-PA-O3A

There are no ring outliers.

No monomer is involved in short contacts.

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AB	235/235 (100%)	0.81	56 (23%) 0 0	13, 75, 147, 218	0
1	CB	235/235 (100%)	0.71	55 (23%) 0 0	26, 78, 150, 182	0
2	AC	207/207 (100%)	1.30	53 (25%) 0 0	21, 64, 129, 194	0
2	CC	207/207 (100%)	1.20	68 (32%) 0 0	33, 66, 122, 164	0
3	AD	208/208 (100%)	2.77	126 (60%) 0 0	24, 71, 131, 187	0
3	CD	208/208 (100%)	3.03	127 (61%) 0 0	16, 79, 141, 186	0
4	AE	151/151 (100%)	1.12	52 (34%) 0 0	10, 57, 124, 176	0
4	CE	151/151 (100%)	2.07	62 (41%) 0 0	23, 71, 126, 185	0
5	AF	101/101 (100%)	-0.63	1 (0%) 82 75	36, 69, 131, 173	0
5	CF	101/101 (100%)	-0.57	1 (0%) 82 75	29, 64, 127, 176	0
6	AG	155/155 (100%)	0.89	45 (29%) 0 0	20, 84, 135, 192	0
6	CG	155/155 (100%)	0.39	27 (17%) 1 1	39, 86, 144, 209	0
7	AH	138/138 (100%)	0.80	30 (21%) 0 1	21, 64, 118, 145	0
7	CH	138/138 (100%)	0.76	34 (24%) 0 0	33, 67, 126, 179	0
8	AI	127/127 (100%)	4.12	98 (77%) 0 0	13, 74, 122, 146	0
8	CI	127/127 (100%)	4.55	99 (77%) 0 0	16, 69, 128, 177	0
9	AJ	99/99 (100%)	1.80	39 (39%) 0 0	34, 74, 129, 147	0
9	CJ	99/99 (100%)	2.34	49 (49%) 0 0	24, 81, 132, 167	0
10	AK	119/119 (100%)	0.19	15 (12%) 3 4	17, 68, 129, 145	0
10	CK	119/119 (100%)	0.85	24 (20%) 1 1	37, 83, 128, 165	0
11	AL	125/125 (100%)	1.33	39 (31%) 0 0	22, 64, 128, 177	0
11	CL	125/125 (100%)	1.93	53 (42%) 0 0	21, 72, 139, 179	0
12	AM	125/125 (100%)	1.38	38 (30%) 0 0	54, 96, 167, 207	0
12	CM	125/125 (100%)	1.60	47 (37%) 0 0	58, 97, 159, 195	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
13	AN	60/60 (100%)	3.82	44 (73%)	0	0	3, 48, 113, 131	0
13	CN	60/60 (100%)	3.60	42 (70%)	0	0	30, 54, 113, 147	0
14	AO	88/88 (100%)	0.85	19 (21%)	0	1	24, 64, 113, 158	0
14	CO	88/88 (100%)	1.15	26 (29%)	0	0	32, 73, 127, 165	0
15	AP	84/84 (100%)	6.13	63 (75%)	0	0	35, 82, 143, 179	0
15	CP	84/84 (100%)	5.62	66 (78%)	0	0	29, 73, 132, 175	0
16	AQ	100/100 (100%)	1.70	39 (39%)	0	0	25, 66, 120, 137	0
16	CQ	100/100 (100%)	2.14	47 (47%)	0	0	42, 74, 130, 159	0
17	AR	70/70 (100%)	0.26	10 (14%)	2	3	29, 54, 107, 143	0
17	CR	70/70 (100%)	0.38	7 (10%)	7	6	26, 69, 132, 198	0
18	AS	79/79 (100%)	3.21	44 (55%)	0	0	25, 95, 172, 193	0
18	CS	79/79 (100%)	2.40	39 (49%)	0	0	26, 89, 165, 199	0
19	AT	99/99 (100%)	2.19	47 (47%)	0	0	16, 66, 130, 188	0
19	CT	99/99 (100%)	2.69	59 (59%)	0	0	27, 80, 144, 169	0
20	AA	1511/1511 (100%)	0.43	216 (14%)	2	3	11, 79, 165, 273	0
20	CA	1511/1511 (100%)	0.44	194 (12%)	3	4	6, 84, 166, 265	0
21	AV	18/18 (100%)	2.58	12 (66%)	0	0	41, 113, 170, 197	0
21	CV	18/18 (100%)	2.94	12 (66%)	0	0	33, 135, 179, 181	0
22	AW	77/77 (100%)	-0.21	3 (3%)	39	31	24, 109, 168, 243	0
22	CW	77/77 (100%)	-0.01	3 (3%)	39	31	43, 116, 183, 208	0
23	AY	687/687 (100%)	-0.02	61 (8%)	9	7	26, 80, 149, 224	0
23	CY	687/687 (100%)	0.10	87 (12%)	3	4	25, 86, 158, 217	0
24	AU	2/6 (33%)	-0.70	0	100	100	66, 66, 66, 66	0
24	CU	2/6 (33%)	-1.14	0	100	100	66, 66, 66, 66	0
25	BC	228/228 (100%)	2.67	127 (55%)	0	0	77, 137, 202, 235	0
25	DC	228/228 (100%)	2.93	132 (57%)	0	0	73, 140, 196, 228	0
26	BD	275/275 (100%)	1.65	103 (37%)	0	0	12, 58, 126, 156	0
26	DD	275/275 (100%)	1.60	106 (38%)	0	0	18, 59, 122, 191	0
27	BE	205/205 (100%)	2.22	90 (43%)	0	0	16, 58, 123, 159	0
27	DE	205/205 (100%)	2.48	104 (50%)	0	0	20, 74, 138, 209	0
28	BF	208/208 (100%)	2.80	124 (59%)	0	0	41, 78, 145, 195	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
28	DF	208/208 (100%)	2.78	110 (52%)	0	0	26, 76, 155, 199	0
29	BG	181/181 (100%)	2.10	89 (49%)	0	0	24, 87, 153, 191	0
29	DG	181/181 (100%)	1.69	73 (40%)	0	0	40, 94, 165, 199	0
30	BH	167/167 (100%)	0.49	30 (17%)	1	1	7, 68, 133, 171	0
30	DH	167/167 (100%)	0.50	30 (17%)	1	1	11, 67, 139, 168	0
31	BJ	0/170	-	-			-	-
31	DJ	0/170	-	-			-	-
32	BK	140/140 (100%)	0.85	28 (20%)	1	1	24, 91, 182, 225	0
32	DK	140/140 (100%)	1.29	46 (32%)	0	0	30, 110, 178, 234	0
33	BO	122/122 (100%)	1.43	40 (32%)	0	0	24, 45, 123, 162	0
33	DO	122/122 (100%)	1.75	50 (40%)	0	0	20, 58, 106, 159	0
34	BP	146/146 (100%)	2.88	74 (50%)	0	0	22, 76, 132, 175	0
34	DP	146/146 (100%)	2.59	73 (50%)	0	0	28, 78, 141, 189	0
35	BQ	141/141 (100%)	1.83	61 (43%)	0	0	17, 63, 130, 200	0
35	DQ	141/141 (100%)	2.09	59 (41%)	0	0	22, 68, 140, 174	0
36	BR	117/117 (100%)	2.73	75 (64%)	0	0	15, 57, 119, 178	0
36	DR	117/117 (100%)	2.13	59 (50%)	0	0	18, 69, 143, 195	0
37	BS	99/99 (100%)	5.89	78 (78%)	0	0	22, 104, 172, 208	0
37	DS	99/99 (100%)	4.96	76 (76%)	0	0	18, 106, 167, 216	0
38	BT	138/138 (100%)	1.13	39 (28%)	0	0	22, 71, 133, 179	0
38	DT	138/138 (100%)	1.27	45 (32%)	0	0	19, 75, 153, 238	0
39	BU	117/117 (100%)	3.44	68 (58%)	0	0	40, 57, 131, 184	0
39	DU	117/117 (100%)	3.07	68 (58%)	0	0	24, 61, 118, 158	0
40	BV	101/101 (100%)	1.70	30 (29%)	0	0	13, 54, 114, 146	0
40	DV	101/101 (100%)	2.41	44 (43%)	0	0	20, 72, 127, 200	0
41	BW	113/113 (100%)	2.88	70 (61%)	0	0	16, 55, 121, 147	0
41	DW	113/113 (100%)	3.79	75 (66%)	0	0	5, 65, 136, 178	0
42	BX	93/93 (100%)	3.08	61 (65%)	0	0	18, 60, 114, 149	0
42	DX	93/93 (100%)	2.97	55 (59%)	0	0	34, 63, 128, 170	0
43	BY	107/107 (100%)	4.27	79 (73%)	0	0	8, 86, 151, 180	0
43	DY	107/107 (100%)	4.05	87 (81%)	0	0	35, 76, 151, 176	0
44	BZ	185/185 (100%)	0.87	48 (25%)	0	0	30, 76, 142, 176	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
44	DZ	185/185 (100%)	0.56	41 (22%)	0	0	36, 82, 147, 226	0
45	B0	84/84 (100%)	5.18	62 (73%)	0	0	18, 92, 159, 181	0
45	D0	84/84 (100%)	5.01	63 (75%)	0	0	19, 85, 145, 160	0
46	B1	93/93 (100%)	3.52	54 (58%)	0	0	26, 91, 161, 204	0
46	D1	93/93 (100%)	4.57	63 (67%)	0	0	38, 92, 166, 194	0
47	B4	35/35 (100%)	0.80	9 (25%)	0	0	49, 106, 171, 203	0
47	D4	35/35 (100%)	0.45	6 (17%)	1	1	82, 115, 164, 187	0
48	BN	138/138 (100%)	2.11	60 (43%)	0	0	59, 83, 108, 111	0
48	DN	138/138 (100%)	2.04	61 (44%)	0	0	58, 84, 107, 116	0
49	B2	71/71 (100%)	1.12	17 (23%)	0	0	38, 79, 143, 185	0
49	D2	71/71 (100%)	0.92	14 (19%)	1	1	42, 70, 130, 187	0
50	B3	60/60 (100%)	1.69	28 (46%)	0	0	34, 62, 117, 150	0
50	D3	60/60 (100%)	2.58	32 (53%)	0	0	53, 68, 130, 149	0
51	B5	59/59 (100%)	2.54	29 (49%)	0	0	26, 56, 131, 149	0
51	D5	59/59 (100%)	2.50	34 (57%)	0	0	16, 83, 166, 185	0
52	B6	50/50 (100%)	1.98	23 (46%)	0	0	63, 99, 159, 175	0
52	D6	50/50 (100%)	3.07	31 (62%)	0	0	61, 118, 161, 188	0
53	B7	49/49 (100%)	3.44	36 (73%)	0	0	18, 47, 122, 156	0
53	D7	49/49 (100%)	3.54	36 (73%)	0	0	33, 61, 140, 186	0
54	B8	64/64 (100%)	4.20	52 (81%)	0	0	29, 63, 152, 160	0
54	D8	64/64 (100%)	5.09	50 (78%)	0	0	28, 75, 142, 191	0
55	B9	37/37 (100%)	10.16	37 (100%)	0	0	71, 109, 177, 183	0
55	D9	37/37 (100%)	12.55	36 (97%)	0	0	102, 132, 185, 210	0
56	Be	72/103 (69%)	-0.04	6 (8%)	11	9	40, 109, 188, 239	0
56	De	72/103 (69%)	0.14	9 (12%)	3	4	46, 118, 183, 199	0
57	Bf	0/31	-	-	-	-	-	-
57	Bg	0/31	-	-	-	-	-	-
57	Df	0/31	-	-	-	-	-	-
57	Dg	0/31	-	-	-	-	-	-
58	Bh	0/30	-	-	-	-	-	-
58	Dh	0/30	-	-	-	-	-	-
59	BB	119/119 (100%)	-0.32	5 (4%)	36	30	27, 111, 173, 187	0
59	DB	119/119 (100%)	-0.18	9 (7%)	13	10	35, 118, 182, 220	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
60	BA	2879/2879 (100%)	0.22	290 (10%) 7 6	7, 78, 171, 308	0
60	DA	2879/2879 (100%)	0.23	286 (9%) 7 6	5, 79, 177, 310	0
All	All	22716/23310 (97%)	1.26	6463 (28%) 0 0	3, 79, 161, 310	0

The worst 5 of 6463 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
55	D9	11	CYS	26.6
55	D9	27	CYS	26.1
60	DA	2250	G	24.1
55	D9	34	GLN	24.1
55	B9	14	CYS	23.5

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	0.89	0.18	65,65,65,65	0
24	KBE	CU	1	9/10	0.92	0.30	65,65,65,65	0
24	DPP	CU	2	6/7	0.92	0.10	65,65,65,65	0
24	KBE	AU	1	9/10	0.93	1.01	65,65,65,65	0
24	UAL	CU	5	9/10	0.94	0.10	65,65,65,65	0
24	5OH	AU	6	12/13	0.96	0.25	99,101,102,102	0
24	DPP	AU	2	6/7	0.96	0.12	65,65,65,65	0
24	5OH	CU	6	12/13	0.97	0.09	99,101,102,102	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

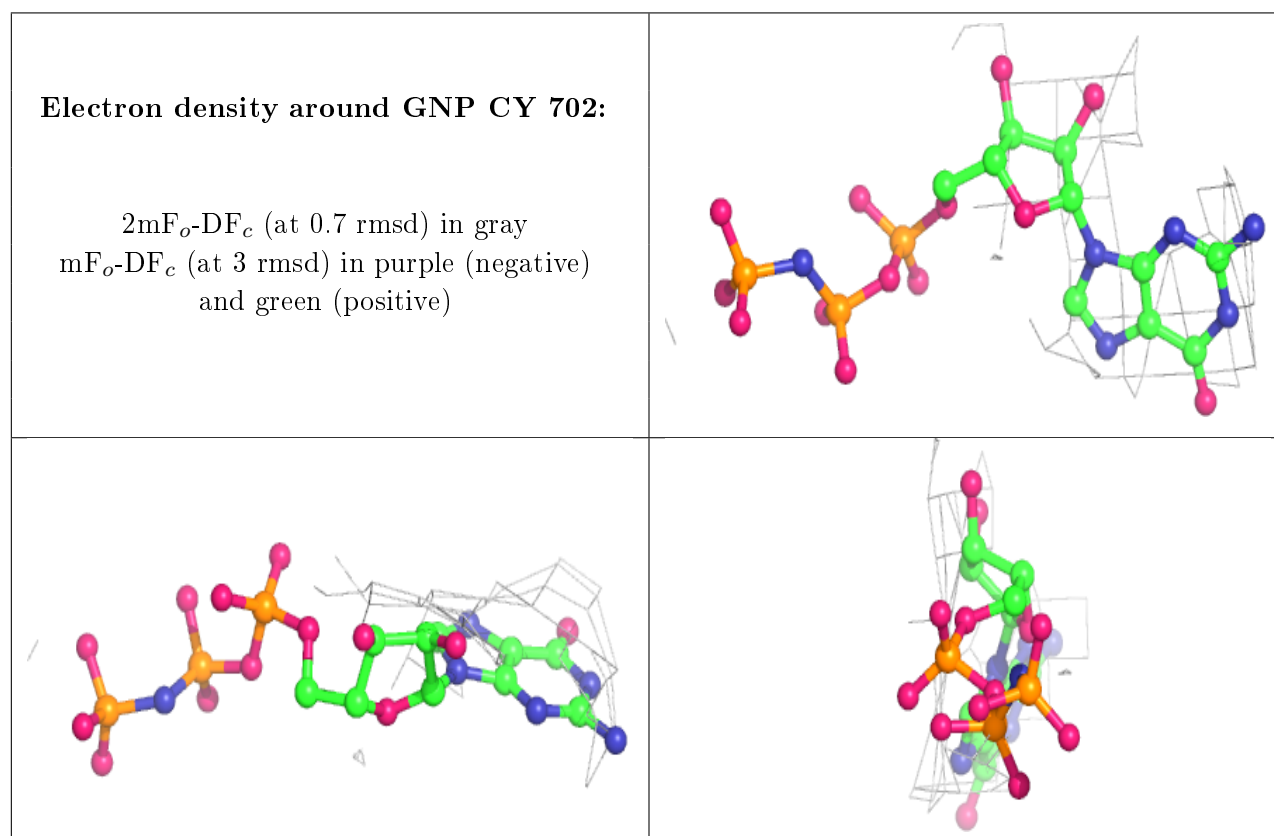
6.4 Ligands [i](#)

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.

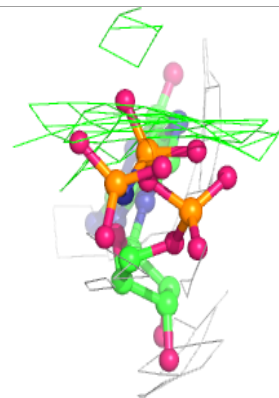
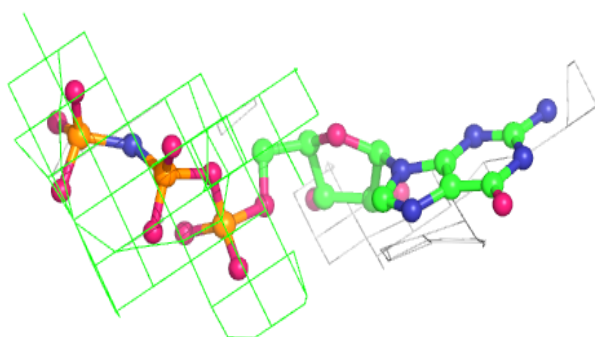
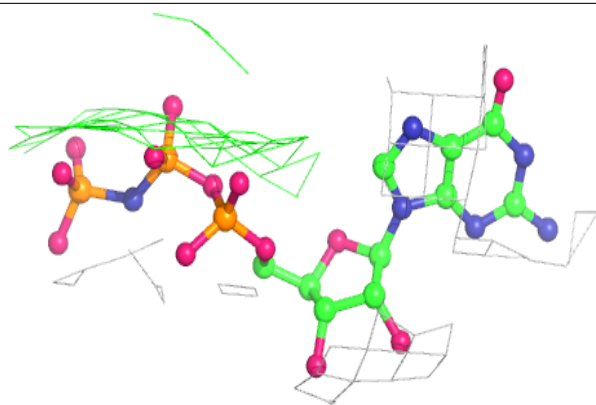
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
61	GNP	CY	702	32/32	0.94	0.13	58,71,81,83	0
61	GNP	AY	701	32/32	0.95	0.20	58,71,81,83	0
62	MG	AY	702	1/1	0.96	0.20	124,124,124,124	0
62	MG	CY	701	1/1	0.97	0.11	104,104,104,104	0

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



Electron density around GNP AY 701:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.