



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 26, 2020 – 06:04 AM BST

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

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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

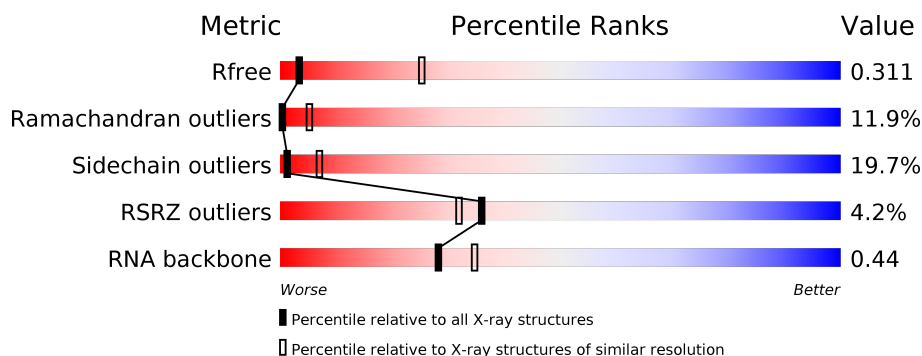
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

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






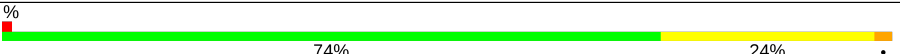
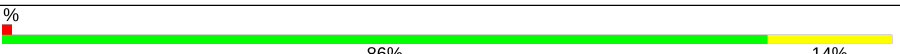
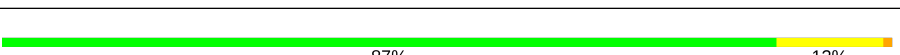
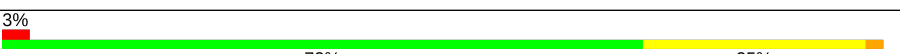
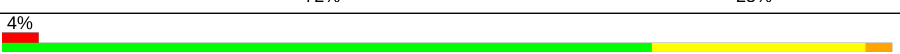

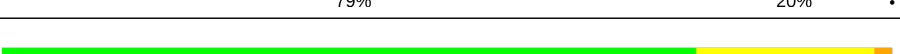

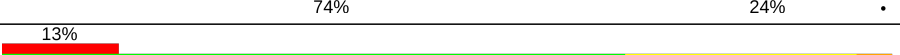
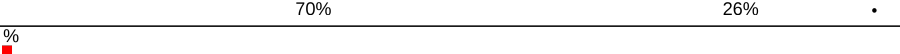
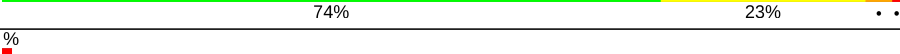











Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)
RNA backbone	3102	1002 (4.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	AB	235	<div> <div>3%</div> <div>76%</div> <div>21%</div> <div>.</div> </div>
1	CB	235	<div> <div>7%</div> <div>80%</div> <div>17%</div> <div>.</div> </div>
2	AC	207	<div> <div>7%</div> <div>73%</div> <div>25%</div> <div>.</div> </div>
2	CC	207	<div> <div>20%</div> <div>74%</div> <div>23%</div> <div>.</div> </div>
3	AD	208	<div> <div>76%</div> <div>22%</div> <div>.</div> </div>
3	CD	208	<div> <div>%</div> <div>78%</div> <div>21%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
4	AE	151	
4	CE	151	
5	AF	101	
5	CF	101	
6	AG	155	
6	CG	155	
7	AH	138	
7	CH	138	
8	AI	127	
8	CI	127	
9	AJ	99	
9	CJ	99	
10	AK	119	
10	CK	119	
11	AL	125	
11	CL	125	
12	AM	125	
12	CM	125	
13	AN	60	
13	CN	60	
14	AO	88	
14	CO	88	
15	AP	84	
15	CP	84	
16	AQ	100	

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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	AY	687	
20	CY	687	
21	AA	1511	
21	CA	1511	
22	AW	77	
22	CW	77	
23	AV	23	
23	CV	23	
24	AU	6	
24	CU	6	
25	BC	228	
25	DC	228	
26	BD	275	
26	DD	275	
27	BE	205	
27	DE	205	
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	BN	138	
33	DN	138	
34	BO	122	
34	DO	122	
35	BP	146	
35	DP	146	
36	BQ	141	
36	DQ	141	
37	BR	117	
37	DR	117	
38	BS	99	
38	DS	99	
39	BT	138	
39	DT	138	
40	BU	117	
40	DU	117	
41	BV	101	

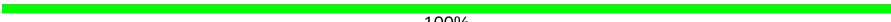
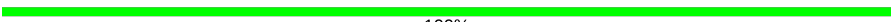







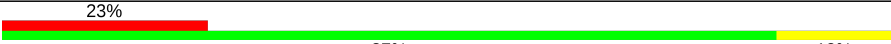
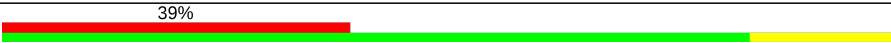

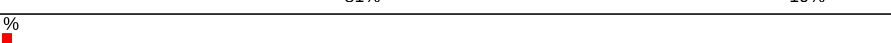
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Mol	Chain	Length	Quality of chain
41	DV	101	
42	BW	113	
42	DW	113	
43	BX	93	
43	DX	93	
44	BY	107	
44	DY	107	
45	BZ	185	
45	DZ	185	
46	B0	84	
46	D0	84	
47	B2	71	
47	D2	71	
48	B3	60	
48	D3	60	
49	B5	59	
49	D5	59	
50	B6	50	
50	D6	50	
51	B7	49	
51	D7	49	
52	B8	64	
52	D8	64	
53	B9	37	
53	D9	37	

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Mol	Chain	Length	Quality of chain
54	Bf	31	 100%
54	Bg	31	 100%
54	Df	31	 100%
54	Dg	31	 100%
55	Bh	30	 100%
55	Dh	30	 100%
56	B1	93	 5% 62% 32% . .
56	D1	93	 11% 63% 32% . .
57	B4	35	 23% 60% 34% 6%
57	D4	35	 29% 54% 37% 9%
58	Be	102	 23% 87% 13%
58	De	102	 39% 84% 16%
59	BA	2879	 76% 23% .
59	DA	2879	 77% 22% .
60	BB	119	 % 81% 19%
60	DB	119	 % 82% 18%

2 Entry composition

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 20 is a protein called Elongation factor G.

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

- Molecule 22 is a RNA chain called transfer RNA.

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

- Molecule 23 is a RNA chain called messenger RNA.

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

- Molecule 24 is a protein called VIOMYCIN.

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

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

There are 10 discrepancies between the modelled and reference sequences:

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 35 is a protein called 50S ribosomal protein L15.

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 37 is a protein called 50S ribosomal protein L17.

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

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

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 40 is a protein called 50S ribosomal protein L20.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 47 is a protein called 50S ribosomal protein L29.

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 57 is a protein called 50S ribosomal protein L31.

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

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

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

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

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

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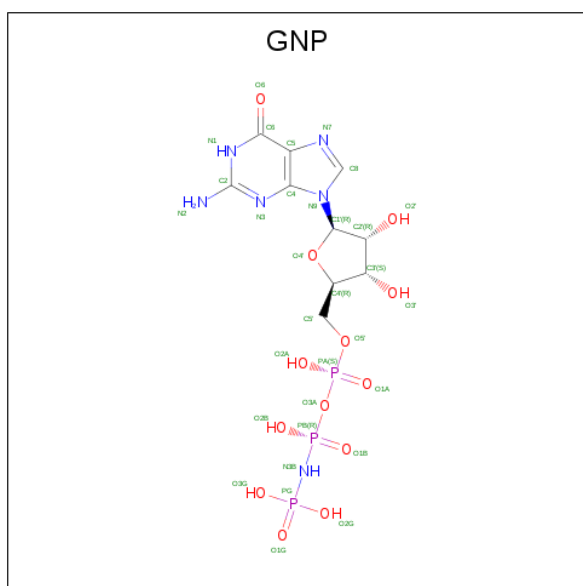
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	DA	2879	Total	C	N	O	P	0	0	0
			61997	27594	11582	19943	2878			

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

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

- Molecule 61 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (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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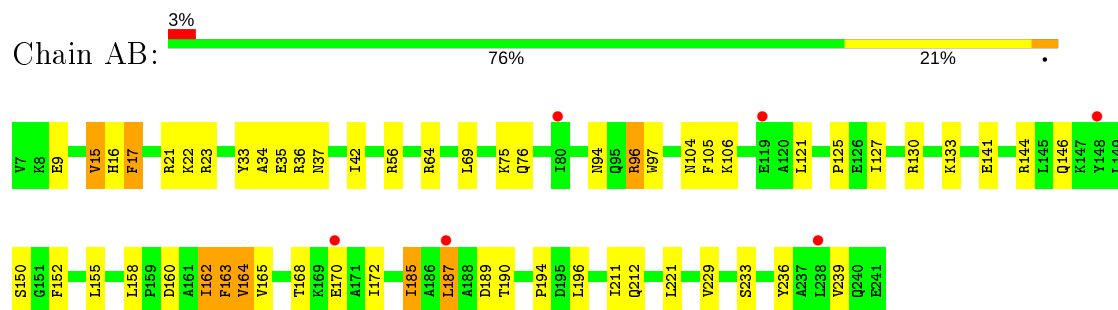
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	CY	1	Total	Mg	0	0
			1	1		

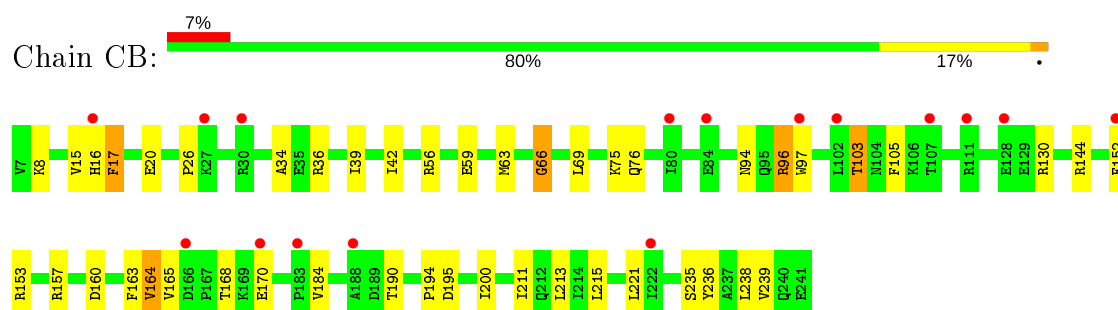
3 Residue-property plots [i](#)

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.

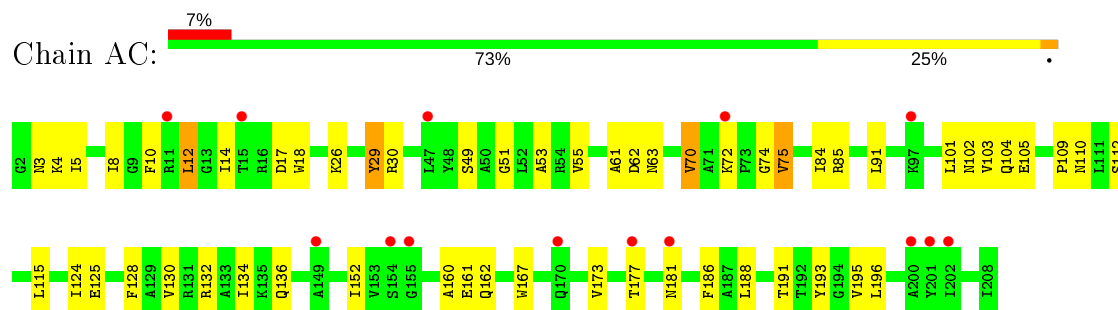
- Molecule 1: 30S ribosomal protein S2



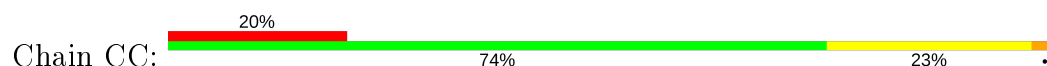
- Molecule 1: 30S ribosomal protein S2

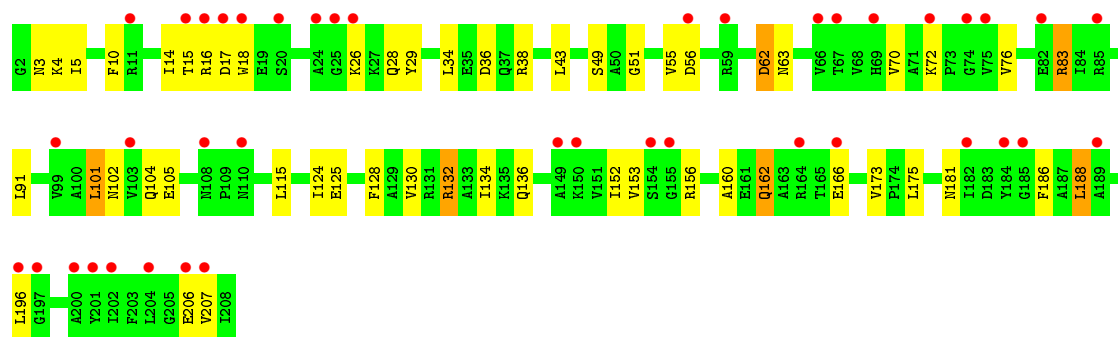


- Molecule 2: 30S ribosomal protein S3



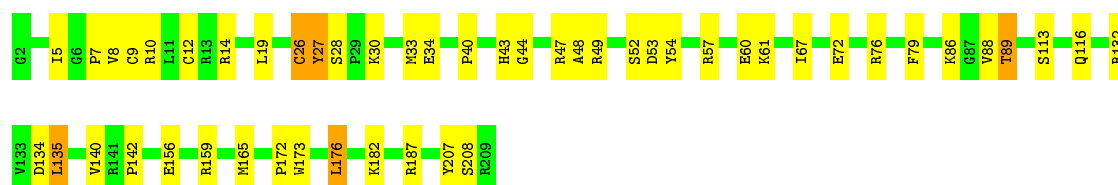
- Molecule 2: 30S ribosomal protein S3





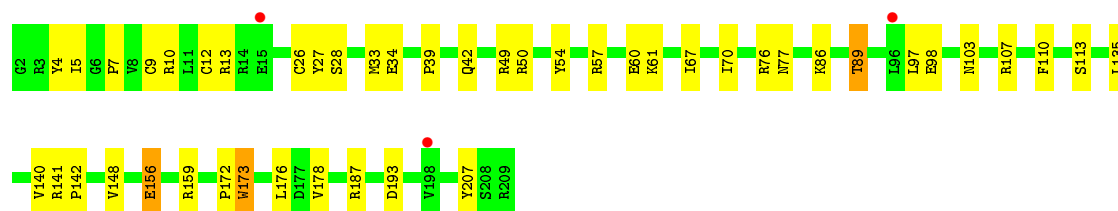
- Molecule 3: 30S ribosomal protein S4

Chain AD: 76% 22% .



- Molecule 3: 30S ribosomal protein S4

Chain CD: 78% 21% .



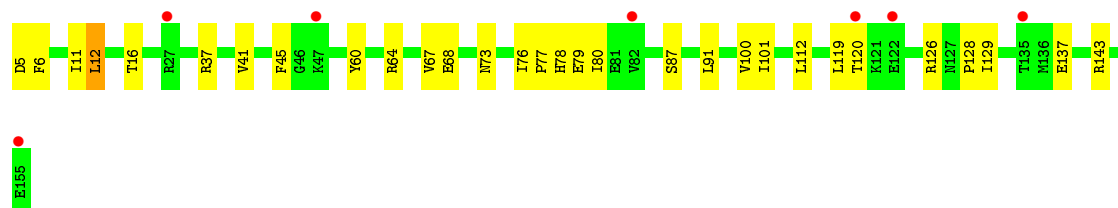
- Molecule 4: 30S ribosomal protein S5

Chain AE: 81% 18% ..

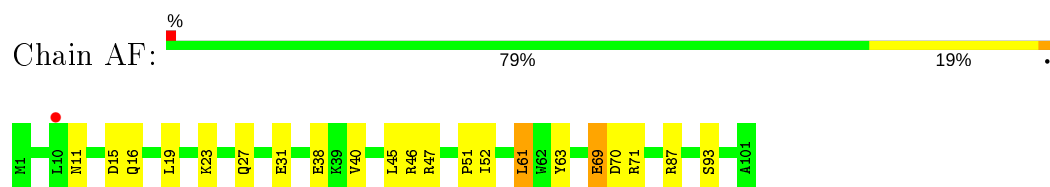


- Molecule 4: 30S ribosomal protein S5

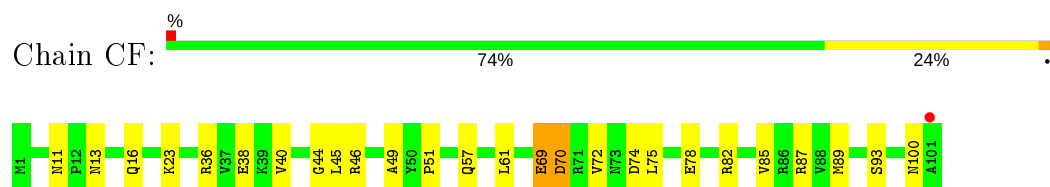
Chain CE: 80% 19% .



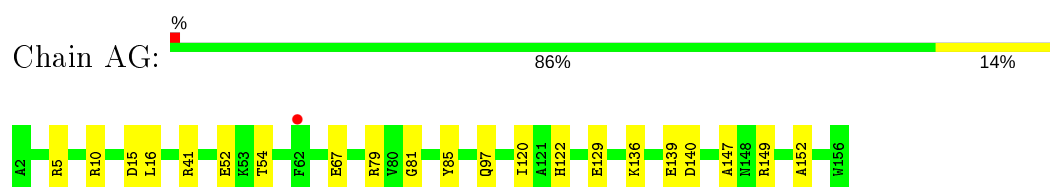
- Molecule 5: 30S ribosomal protein S6



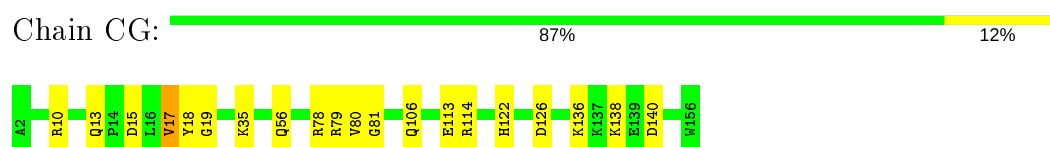
- Molecule 5: 30S ribosomal protein S6



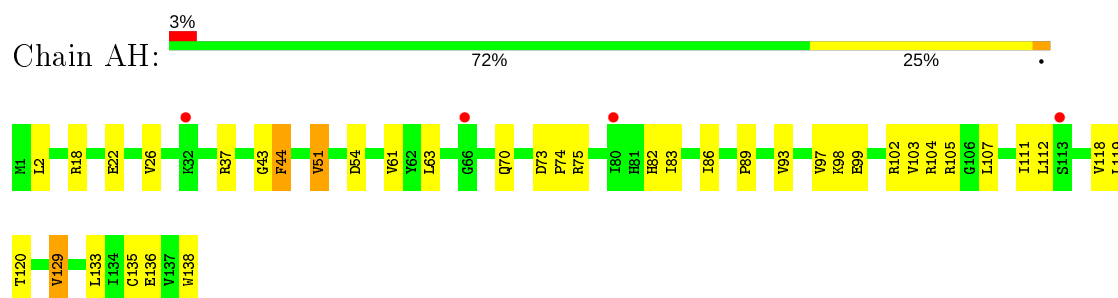
- Molecule 6: 30S ribosomal protein S7



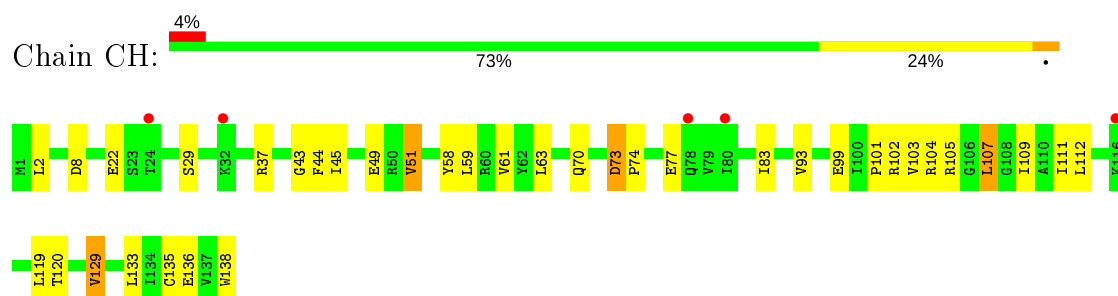
- Molecule 6: 30S ribosomal protein S7




- Molecule 7: 30S ribosomal protein S8



- Molecule 7: 30S ribosomal protein S8



- Molecule 8: 30S ribosomal protein S9

Chain AI:  79% 20%



- Molecule 8: 30S ribosomal protein S9

Chain CI:  78% 20%



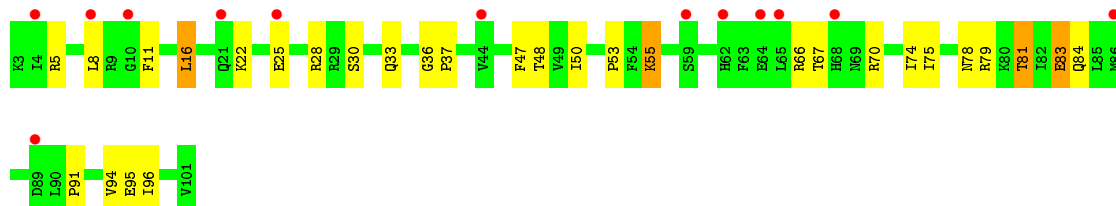
- Molecule 9: 30S ribosomal protein S10

Chain AJ:  6% 74% 24%



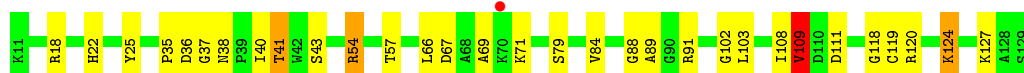
- Molecule 9: 30S ribosomal protein S10

Chain CJ:  13% 70% 26%




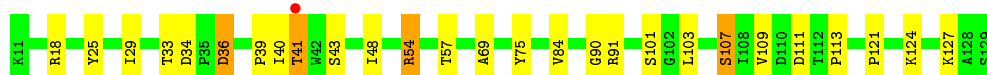
- Molecule 10: 30S ribosomal protein S11

Chain AK:  % 74% 23%



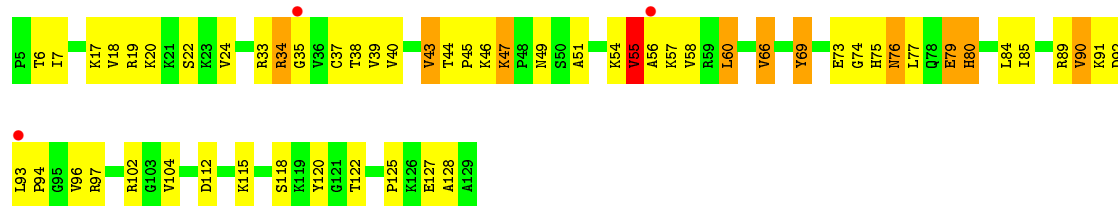
- Molecule 10: 30S ribosomal protein S11

Chain CK:  % 77% 19%

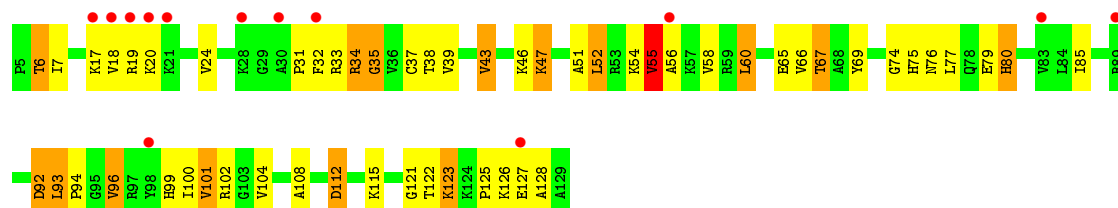


- Molecule 11: 30S ribosomal protein S12

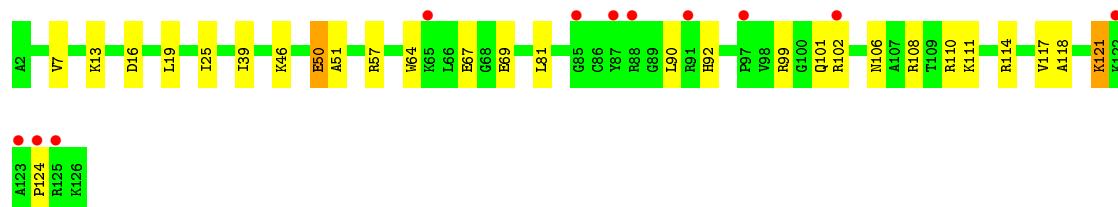
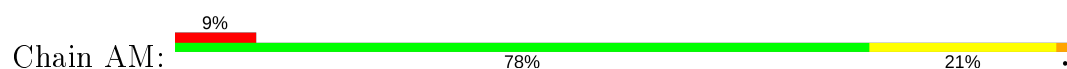
Chain AL:  2% 54% 37% 8%



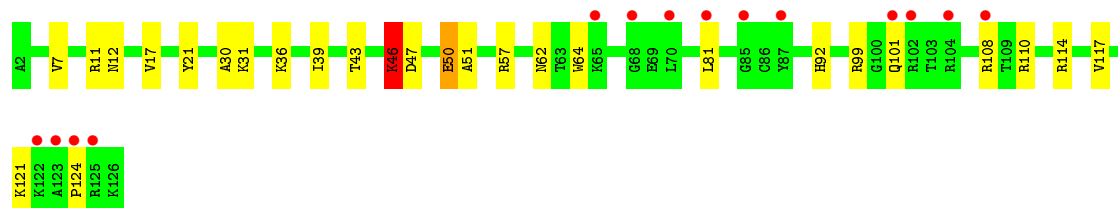
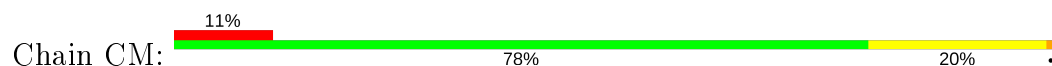
• Molecule 11: 30S ribosomal protein S12



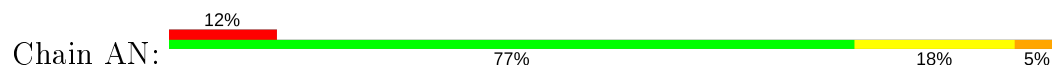
• Molecule 12: 30S ribosomal protein S13



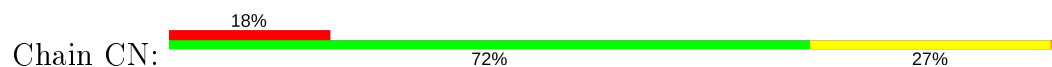
• Molecule 12: 30S ribosomal protein S13

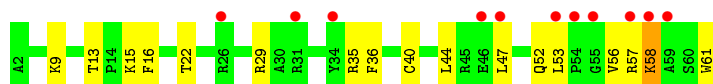


• Molecule 13: 30S ribosomal protein S14 type Z



• Molecule 13: 30S ribosomal protein S14 type Z

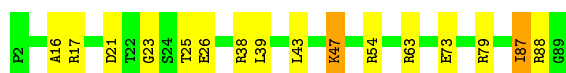
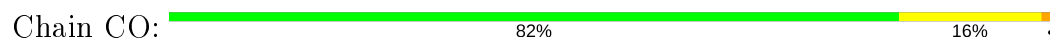




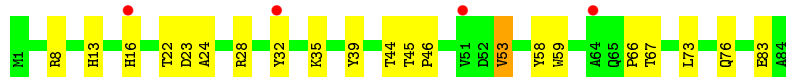
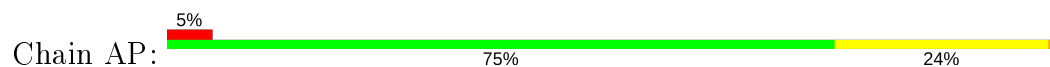
- Molecule 14: 30S ribosomal protein S15



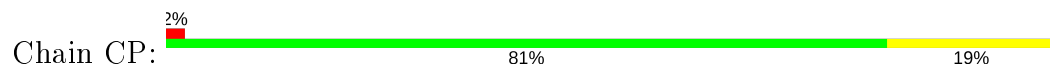
- Molecule 14: 30S ribosomal protein S15



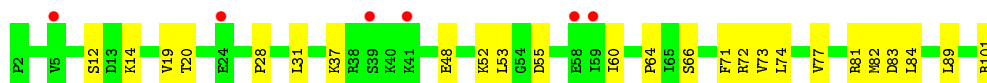
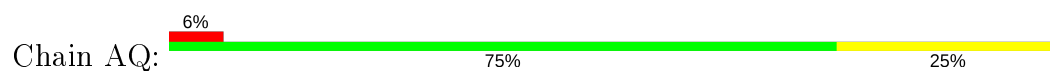
- Molecule 15: 30S ribosomal protein S16



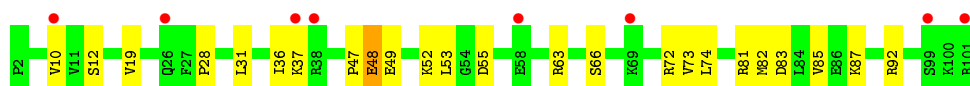
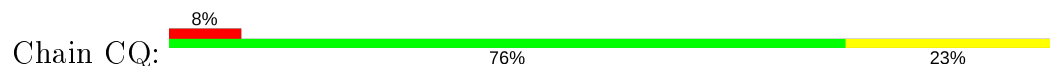
- Molecule 15: 30S ribosomal protein S16



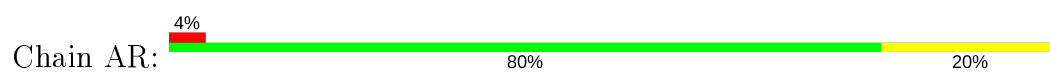
- Molecule 16: 30S ribosomal protein S17



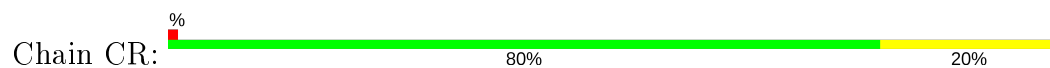
- Molecule 16: 30S ribosomal protein S17



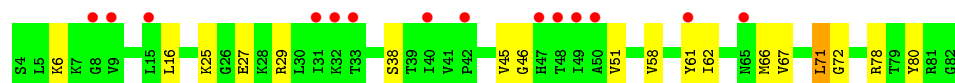
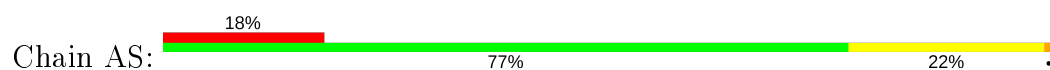
- Molecule 17: 30S ribosomal protein S18



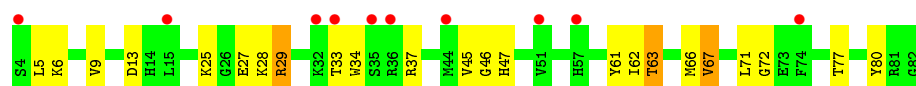
- Molecule 17: 30S ribosomal protein S18



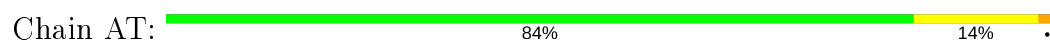
- Molecule 18: 30S ribosomal protein S19



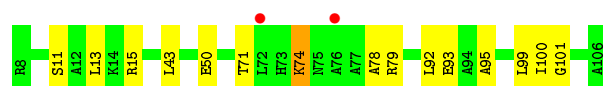
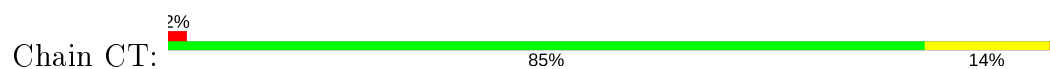
- Molecule 18: 30S ribosomal protein S19



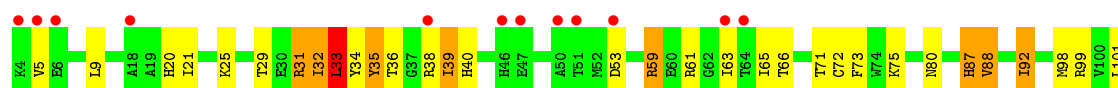
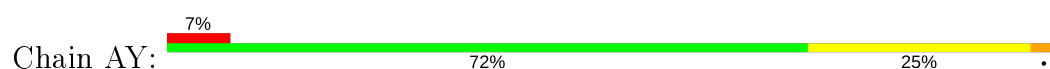
- Molecule 19: 30S ribosomal protein S20

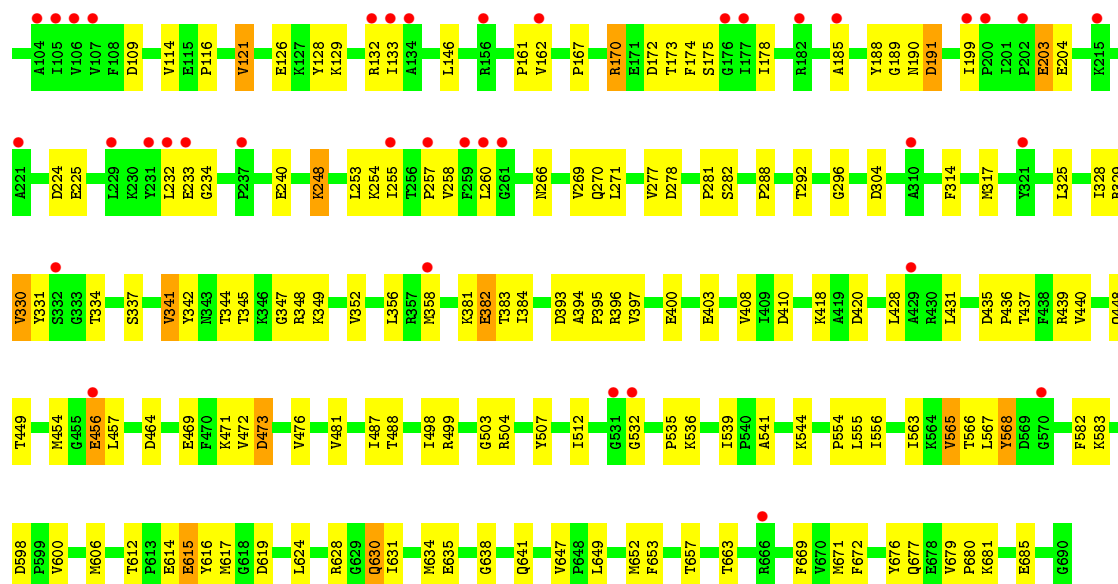


- Molecule 19: 30S ribosomal protein S20

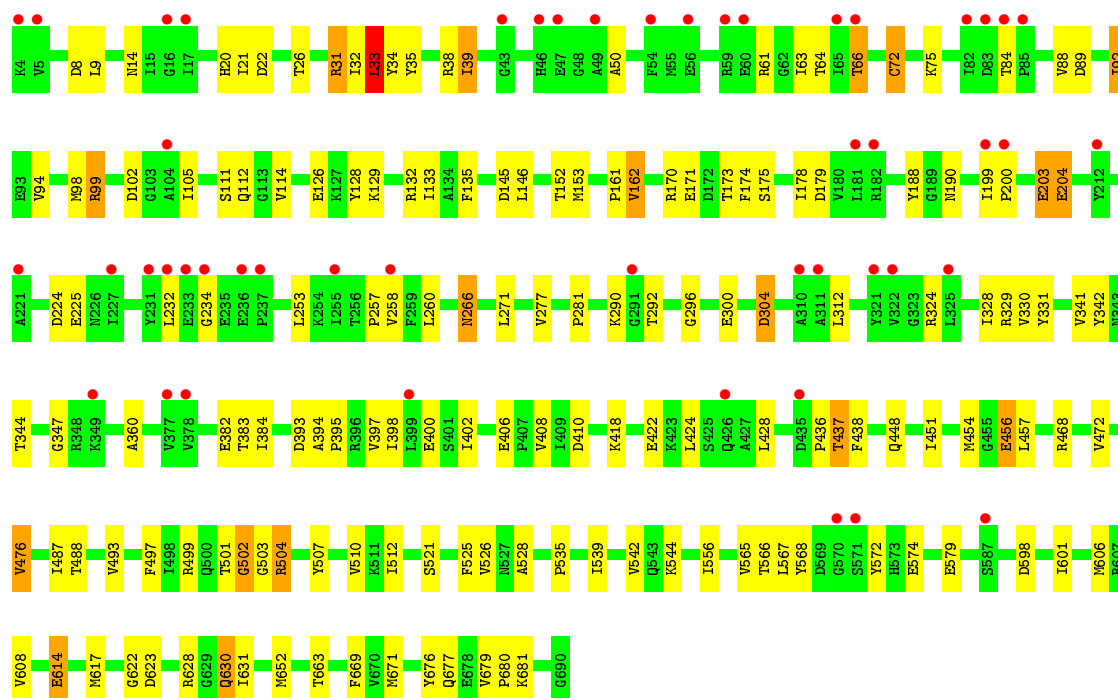
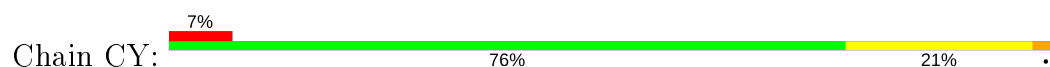


- Molecule 20: Elongation factor G

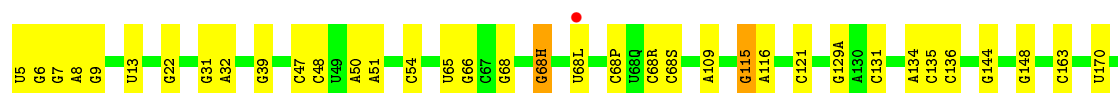
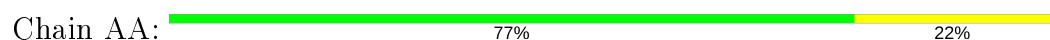


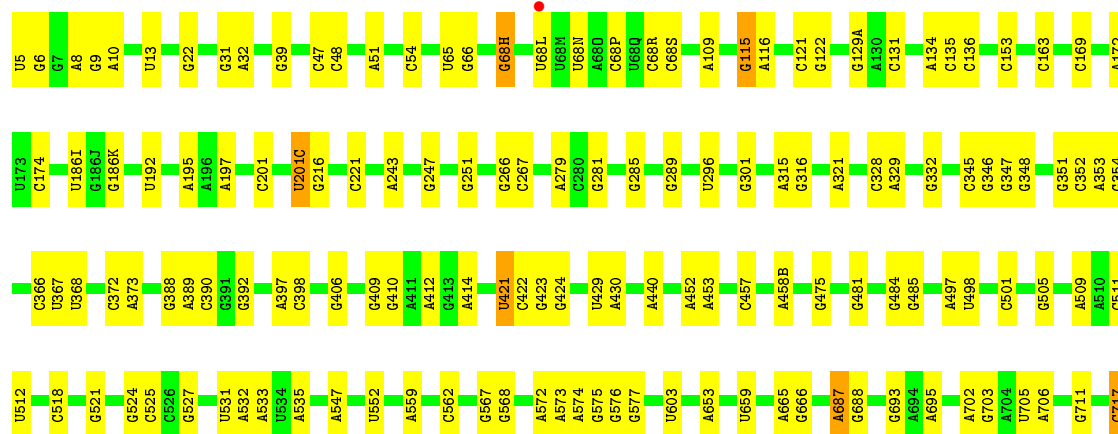


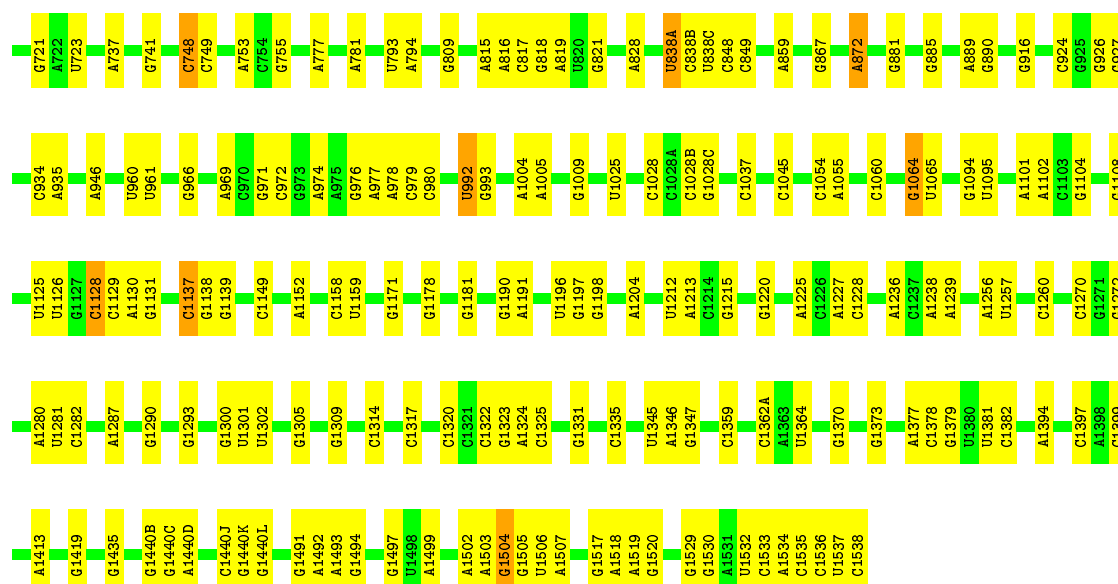
• Molecule 20: Elongation factor G



• Molecule 21: ribosomal RNA 16S







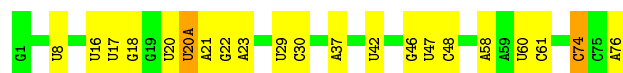
- Molecule 22: transfer RNA

Chain AW: 69% 27%



- Molecule 22: transfer RNA

Chain CW: 73% 25%



- Molecule 23: messenger RNA

Chain AV: 43% 39% 17%



- Molecule 23: messenger RNA

Chain CV: 4% 52% 30% 17%



- Molecule 24: VIOMYCIN

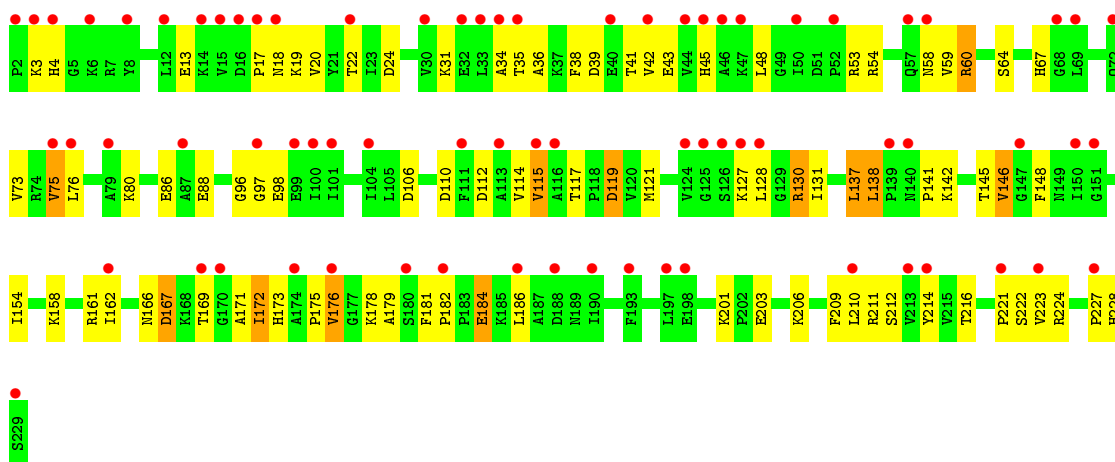
Chain AU: 67% 33%



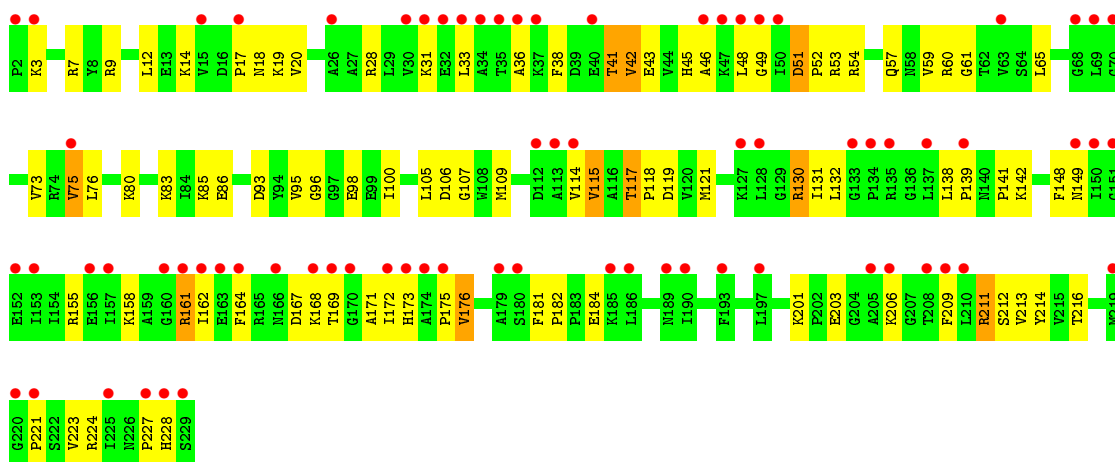
- Molecule 24: VIOMYCIN



- Molecule 25: 50S ribosomal protein L1

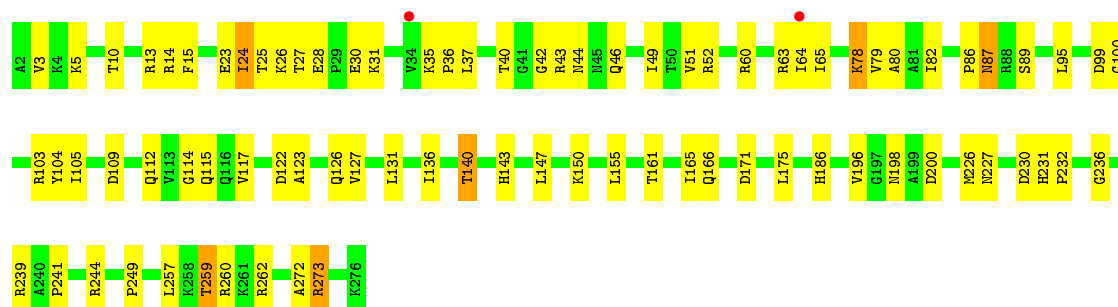


- Molecule 25: 50S ribosomal protein L1

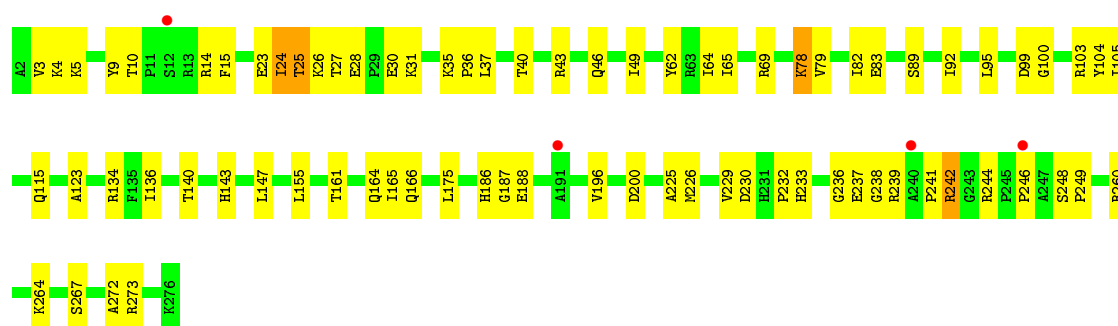
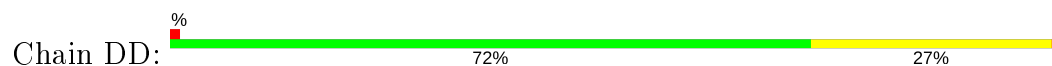


- Molecule 26: 50S ribosomal protein L2

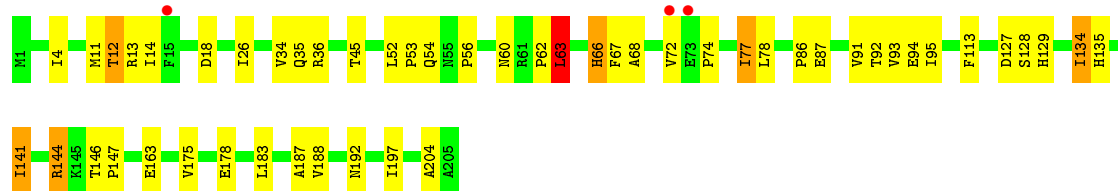
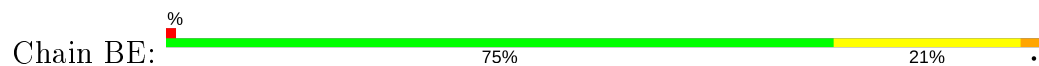




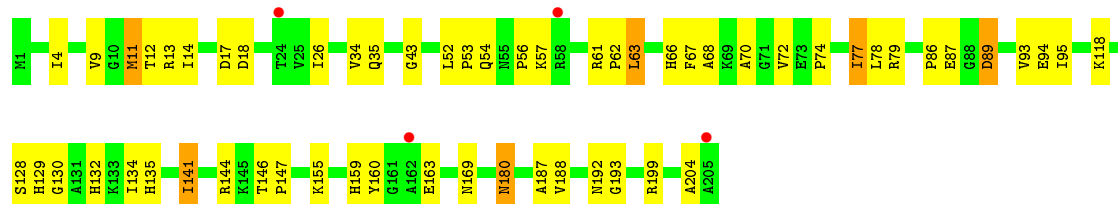
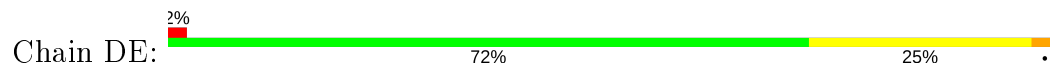
- Molecule 26: 50S ribosomal protein L2



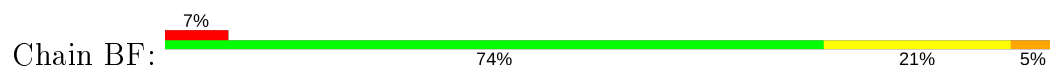
- Molecule 27: 50S ribosomal protein L3

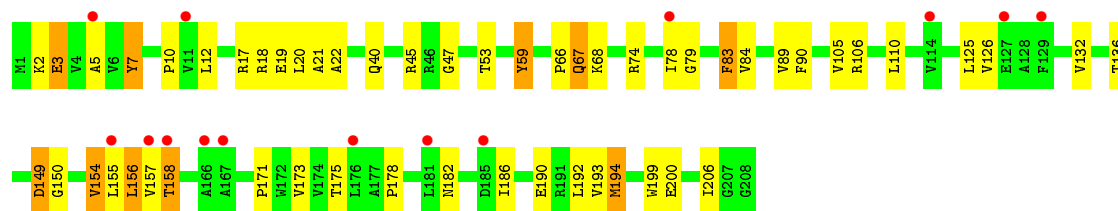


- Molecule 27: 50S ribosomal protein L3

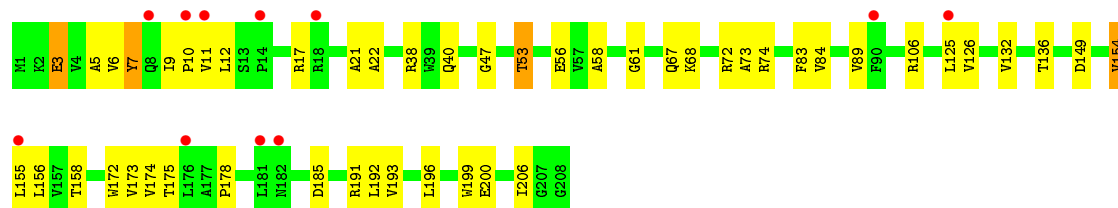
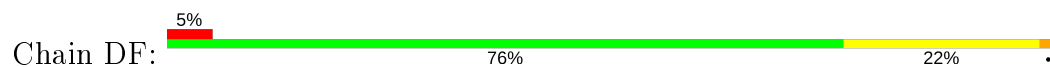


- Molecule 28: 50S ribosomal protein L4

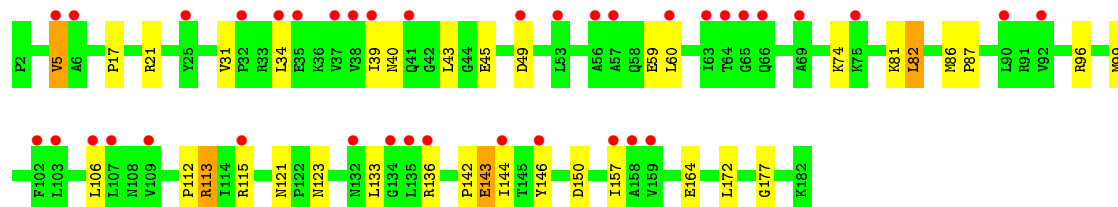
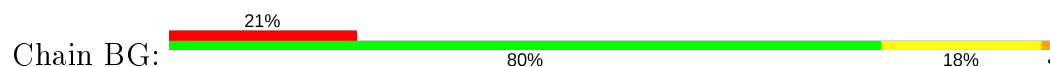




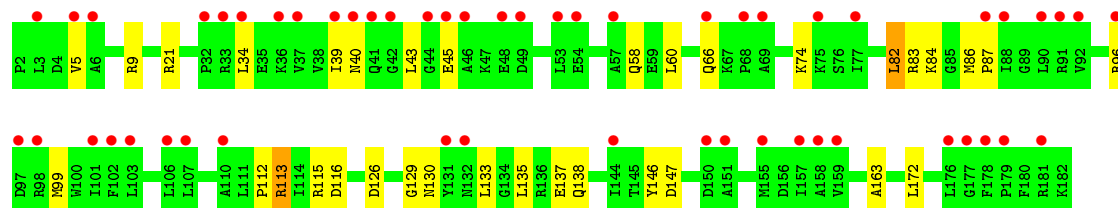
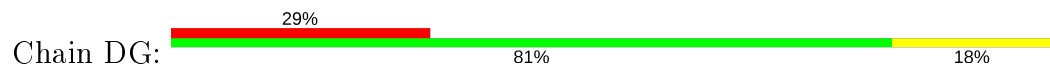
• Molecule 28: 50S ribosomal protein L4



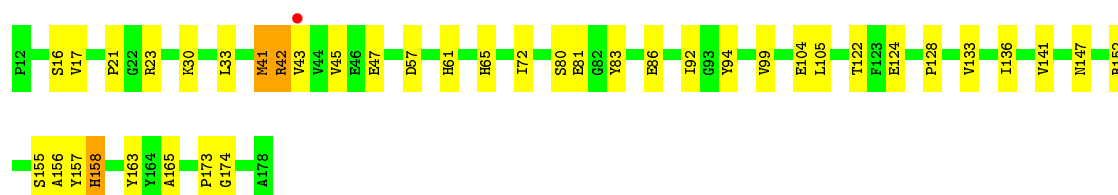
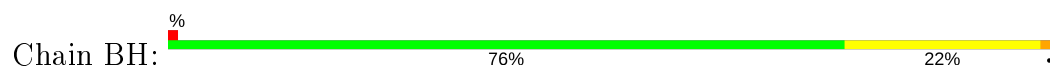
• Molecule 29: 50S ribosomal protein L5



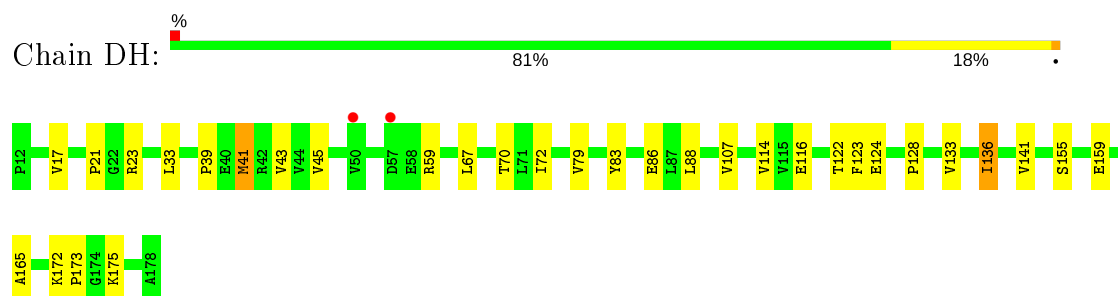
• Molecule 29: 50S ribosomal protein L5



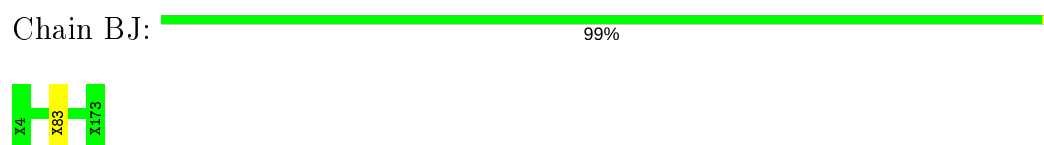
• Molecule 30: 50S ribosomal protein L6



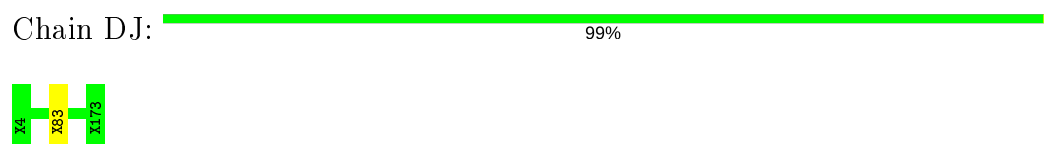
- Molecule 30: 50S ribosomal protein L6



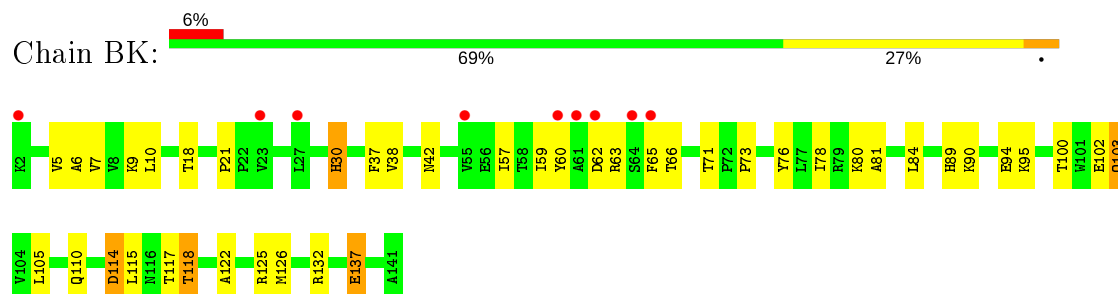
- Molecule 31: 50S RIBOSOMAL PROTEIN L10



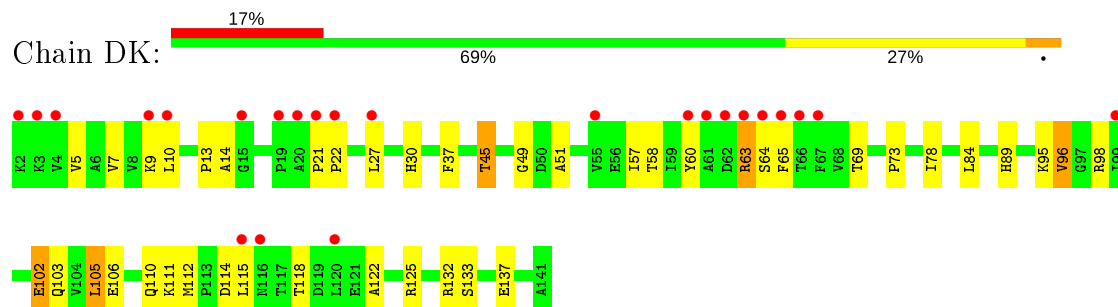
- Molecule 31: 50S RIBOSOMAL PROTEIN L10



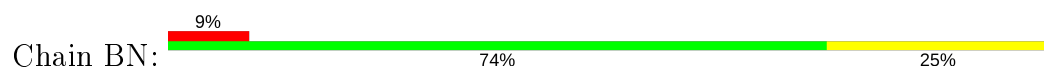
- Molecule 32: 50S ribosomal protein L11

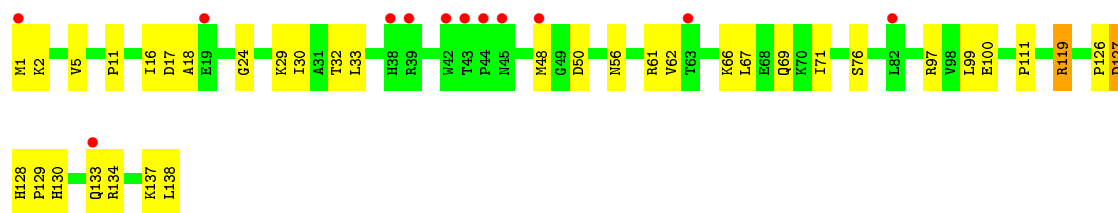


- Molecule 32: 50S ribosomal protein L11

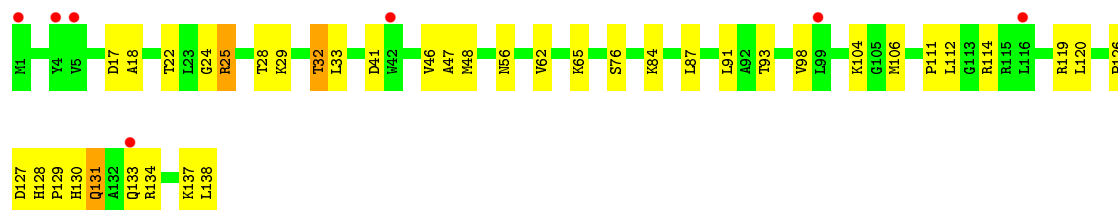
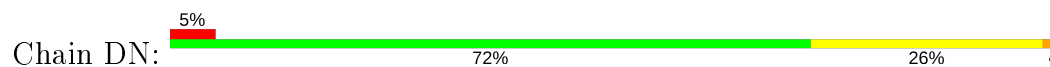


- Molecule 33: 50S ribosomal protein L13

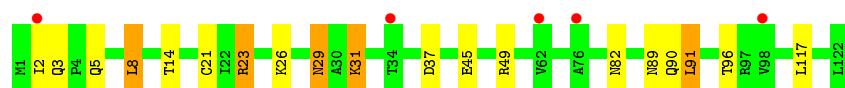
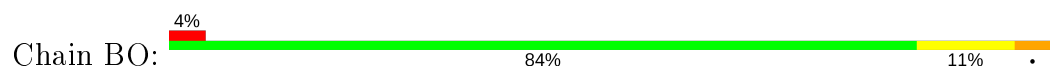




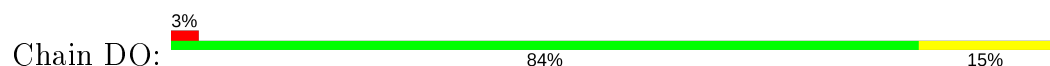
• Molecule 33: 50S ribosomal protein L13



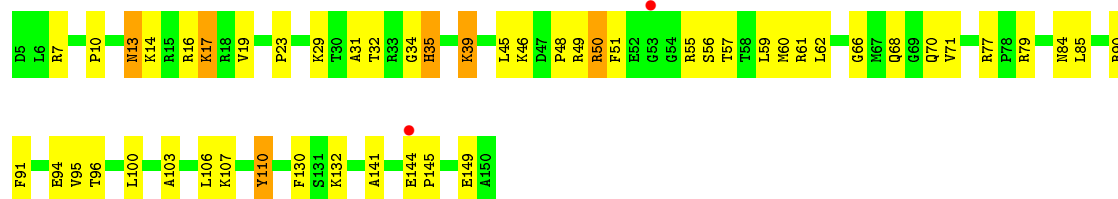
• Molecule 34: 50S ribosomal protein L14



• Molecule 34: 50S ribosomal protein L14



• Molecule 35: 50S ribosomal protein L15

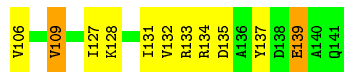
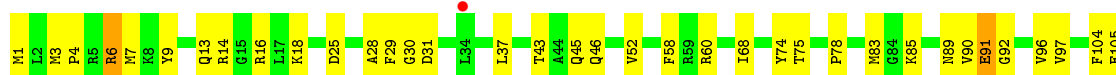


• Molecule 35: 50S ribosomal protein L15

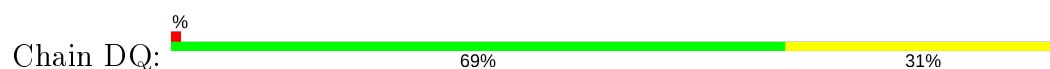




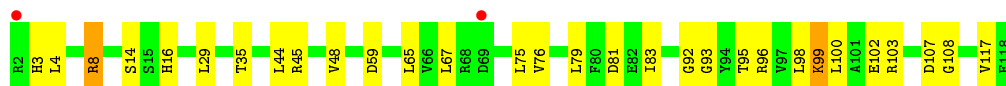
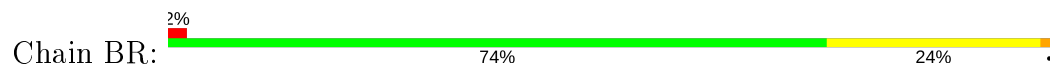
- Molecule 36: 50S ribosomal protein L16



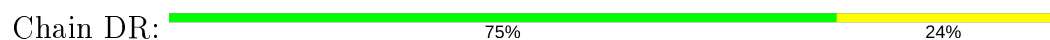
- Molecule 36: 50S ribosomal protein L16



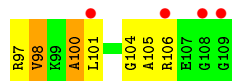
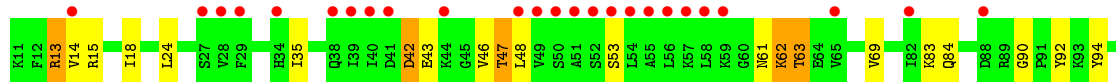
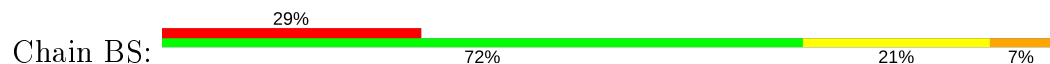
- Molecule 37: 50S ribosomal protein L17



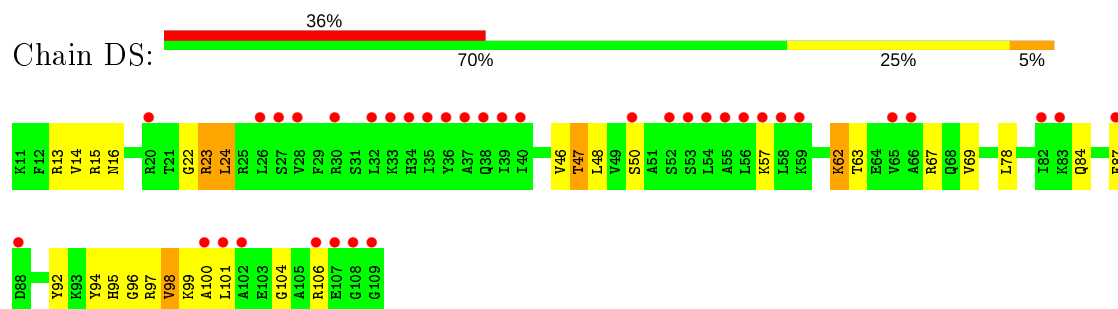
- Molecule 37: 50S ribosomal protein L17



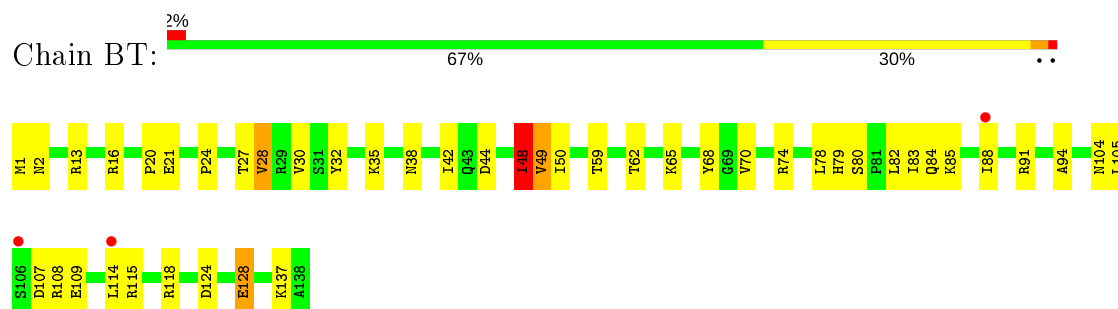
- Molecule 38: 50S ribosomal protein L18



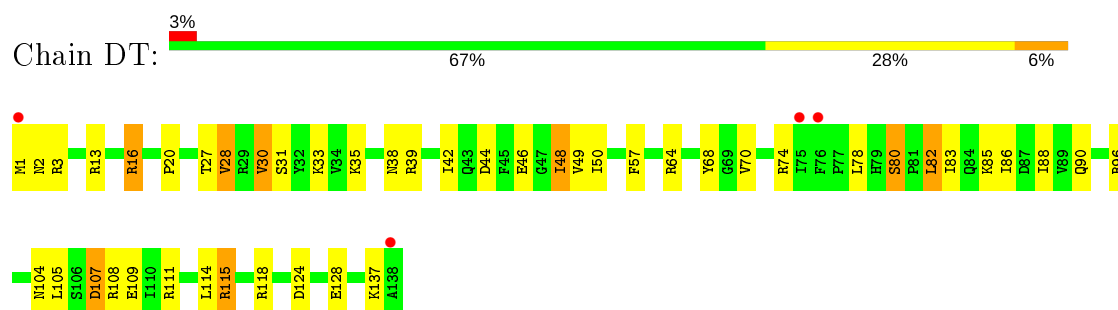
- Molecule 38: 50S ribosomal protein L18



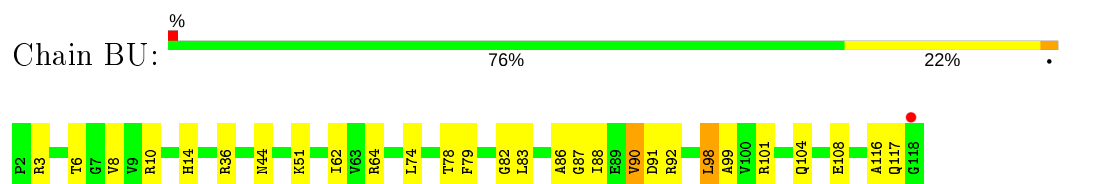
- Molecule 39: 50S ribosomal protein L19



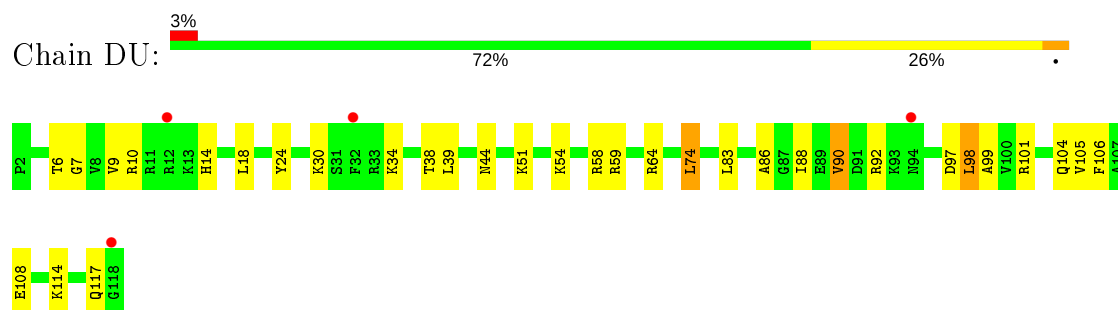
- Molecule 39: 50S ribosomal protein L19



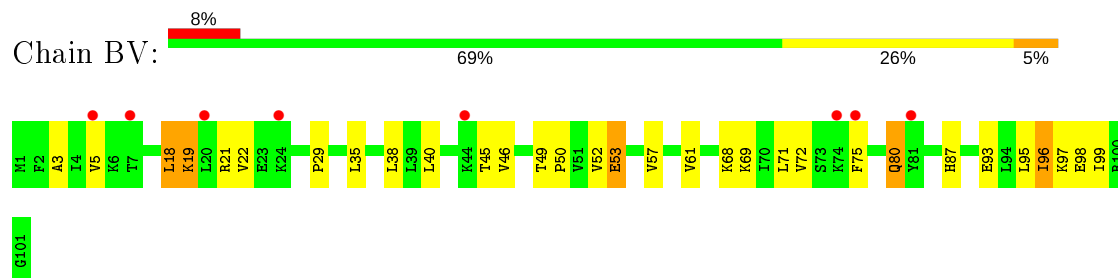
- Molecule 40: 50S ribosomal protein L20



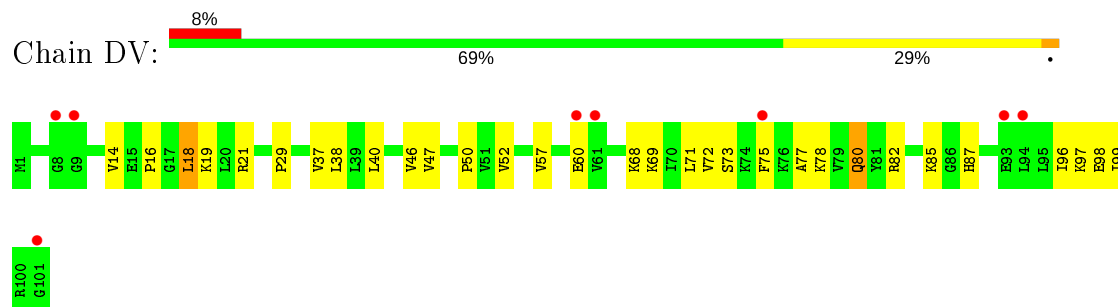
- Molecule 40: 50S ribosomal protein L20



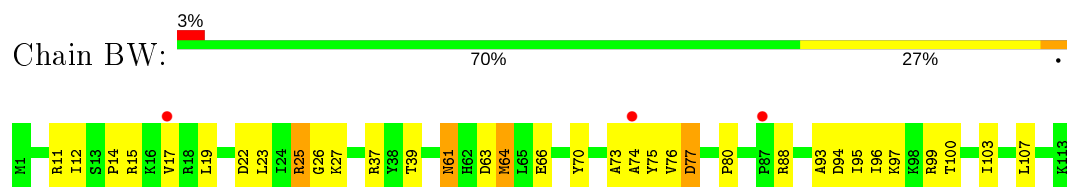
- Molecule 41: 50S ribosomal protein L21



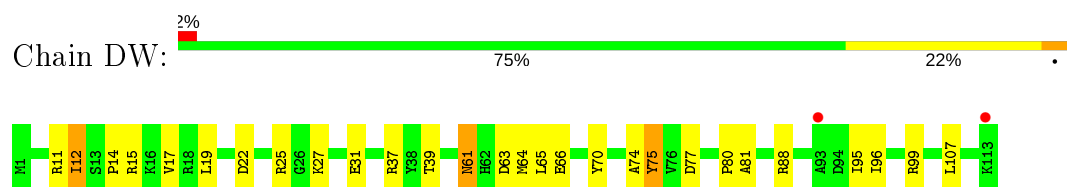
- Molecule 41: 50S ribosomal protein L21



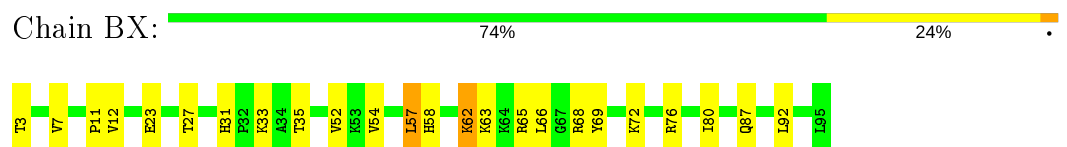
- Molecule 42: 50S ribosomal protein L22



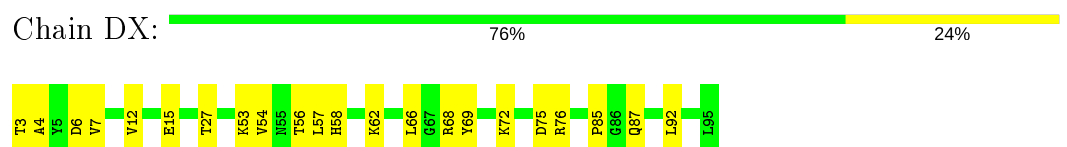
- Molecule 42: 50S ribosomal protein L22



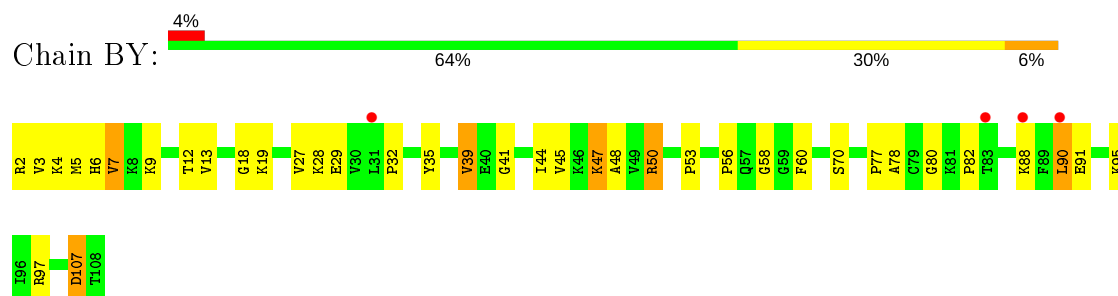
- Molecule 43: 50S ribosomal protein L23



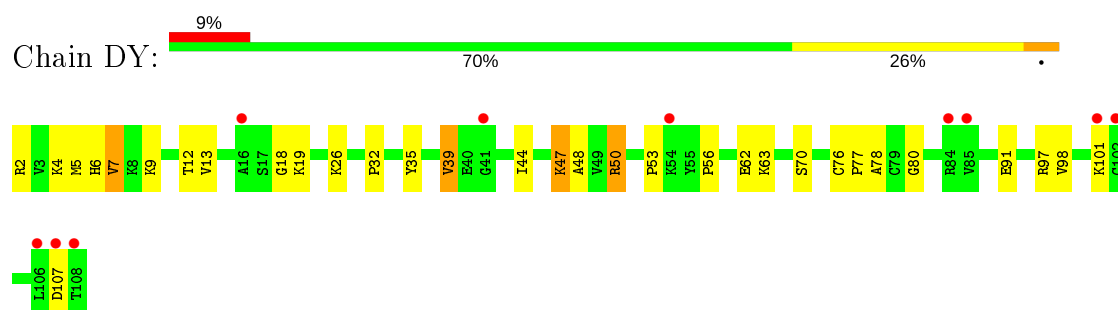
- Molecule 43: 50S ribosomal protein L23



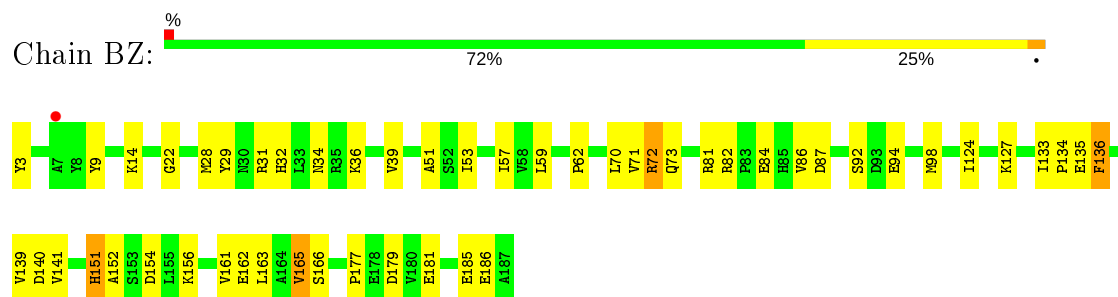
- Molecule 44: 50S ribosomal protein L24



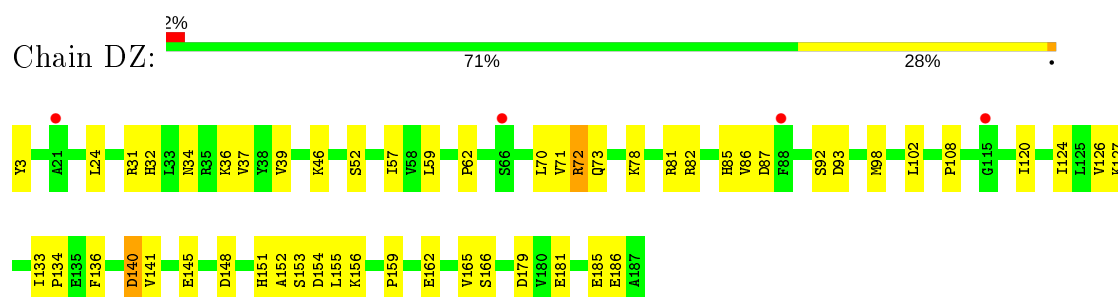
- Molecule 44: 50S ribosomal protein L24



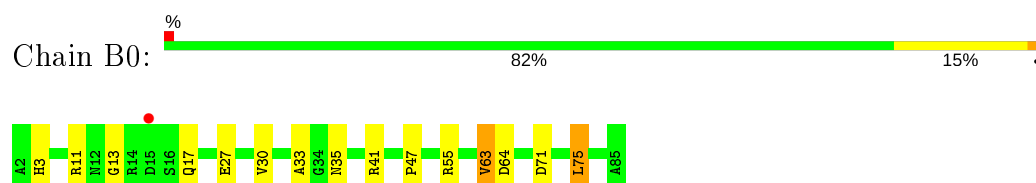
- Molecule 45: 50S ribosomal protein L25



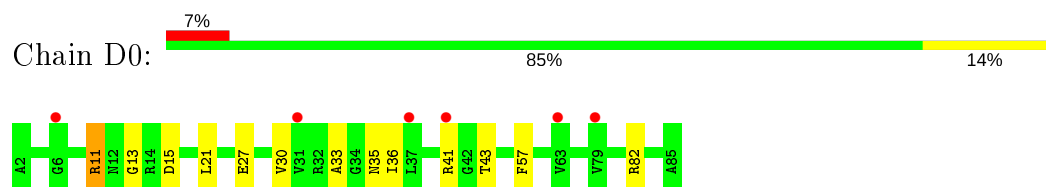
- Molecule 45: 50S ribosomal protein L25



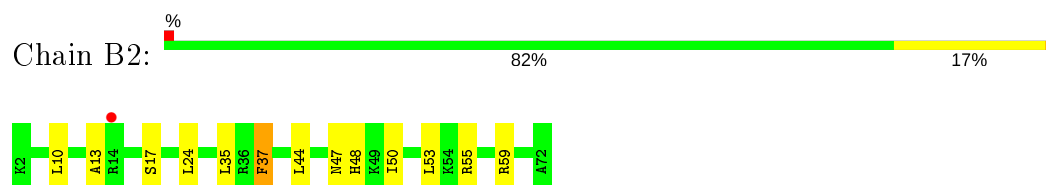
- Molecule 46: 50S ribosomal protein L27



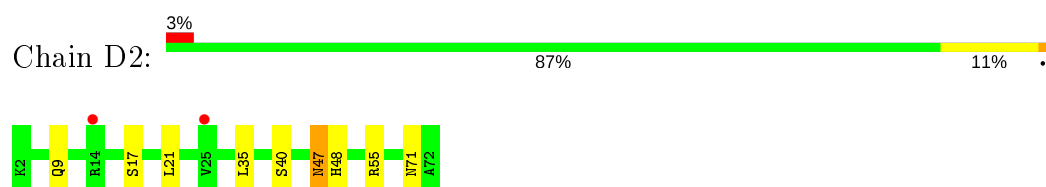
• Molecule 46: 50S ribosomal protein L27



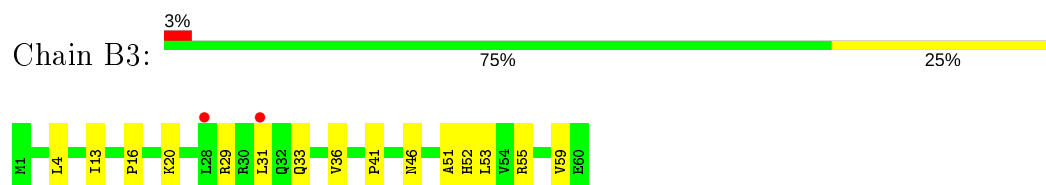
• Molecule 47: 50S ribosomal protein L29



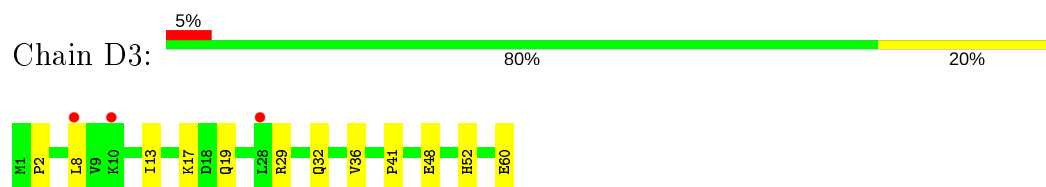
• Molecule 47: 50S ribosomal protein L29



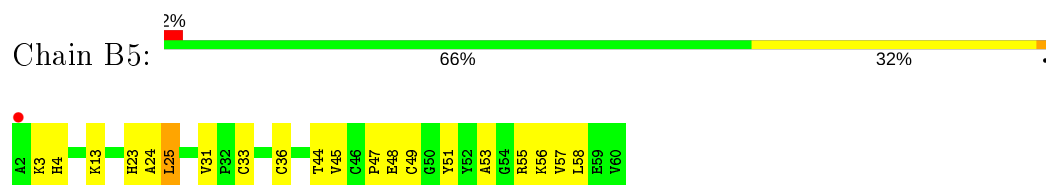
• Molecule 48: 50S ribosomal protein L30



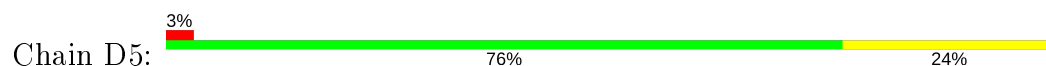
• Molecule 48: 50S ribosomal protein L30

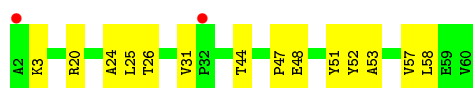


• Molecule 49: 50S ribosomal protein L32



• Molecule 49: 50S ribosomal protein L32

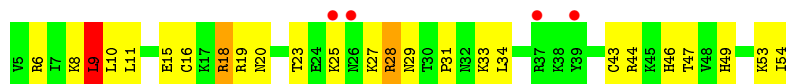




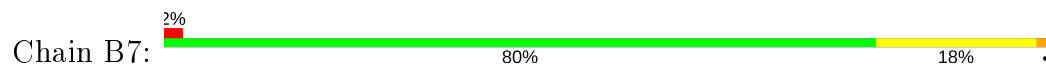
- Molecule 50: 50S ribosomal protein L33



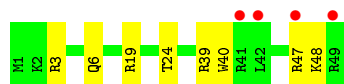
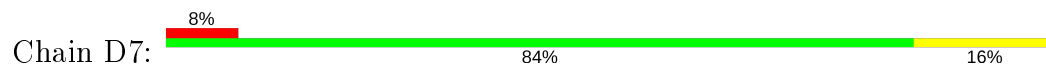
- Molecule 50: 50S ribosomal protein L33



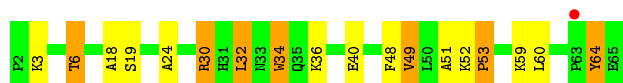
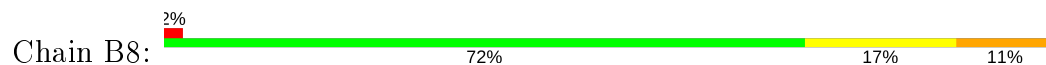
- Molecule 51: 50S ribosomal protein L34



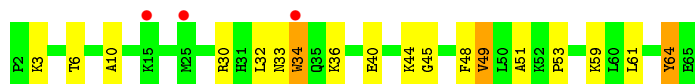
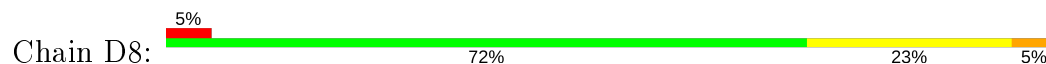
- Molecule 51: 50S ribosomal protein L34



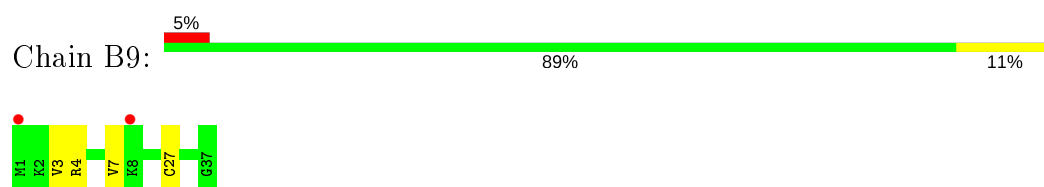
- Molecule 52: 50S ribosomal protein L35



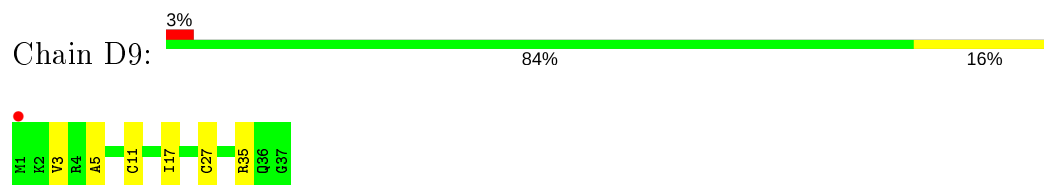
- Molecule 52: 50S ribosomal protein L35



- Molecule 53: 50S ribosomal protein L36



- Molecule 53: 50S ribosomal protein L36



- Molecule 54: 50S RIBOSOMAL PROTEIN L7/L12



There are no outlier residues recorded for this chain.

- Molecule 54: 50S RIBOSOMAL PROTEIN L7/L12



There are no outlier residues recorded for this chain.

- Molecule 54: 50S RIBOSOMAL PROTEIN L7/L12



There are no outlier residues recorded for this chain.

- Molecule 54: 50S RIBOSOMAL PROTEIN L7/L12



There are no outlier residues recorded for this chain.

- Molecule 55: 50S RIBOSOMAL PROTEIN L7/L12



There are no outlier residues recorded for this chain.

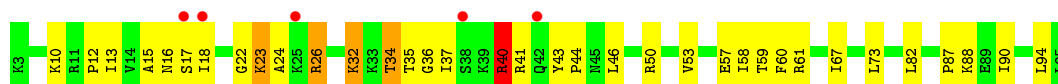
- Molecule 55: 50S RIBOSOMAL PROTEIN L7/L12



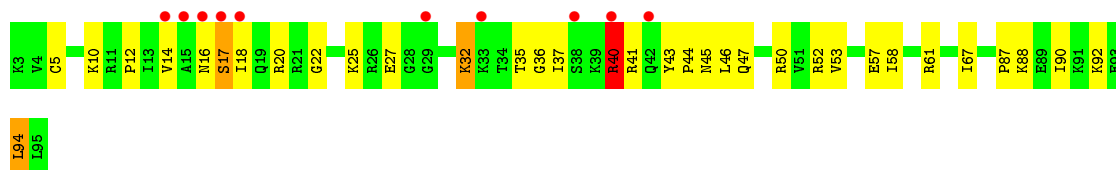
There are no outlier residues recorded for this chain.

- Molecule 56: 50S ribosomal protein L28

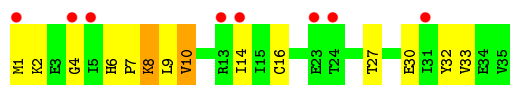




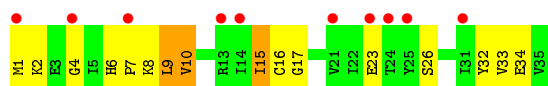
- Molecule 56: 50S ribosomal protein L28



- Molecule 57: 50S ribosomal protein L31



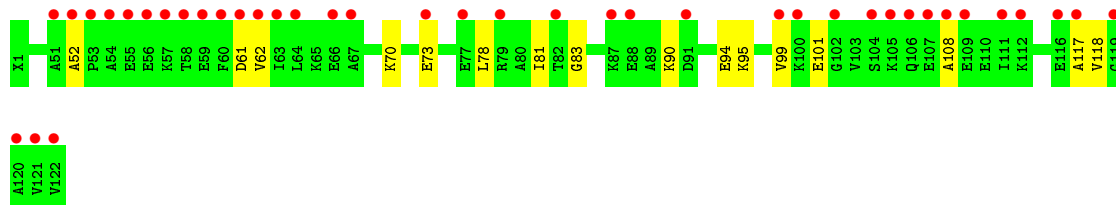
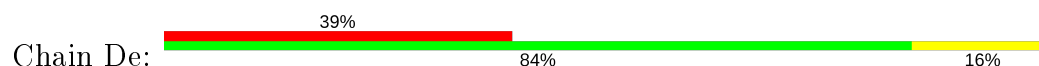
- Molecule 57: 50S ribosomal protein L31



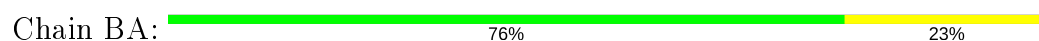
- Molecule 58: 50S ribosomal protein L7/L12



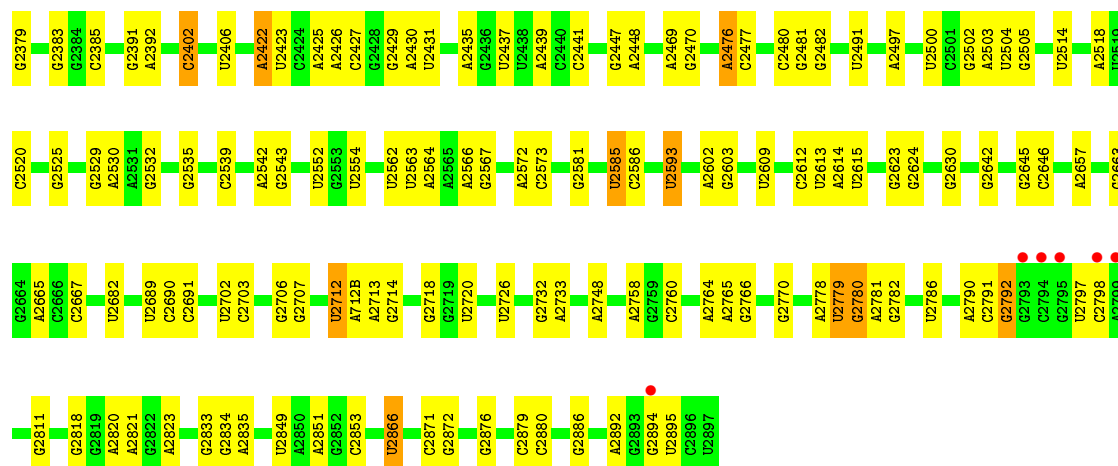
- Molecule 58: 50S ribosomal protein L7/L12



- Molecule 59: 23S ribosomal RNA

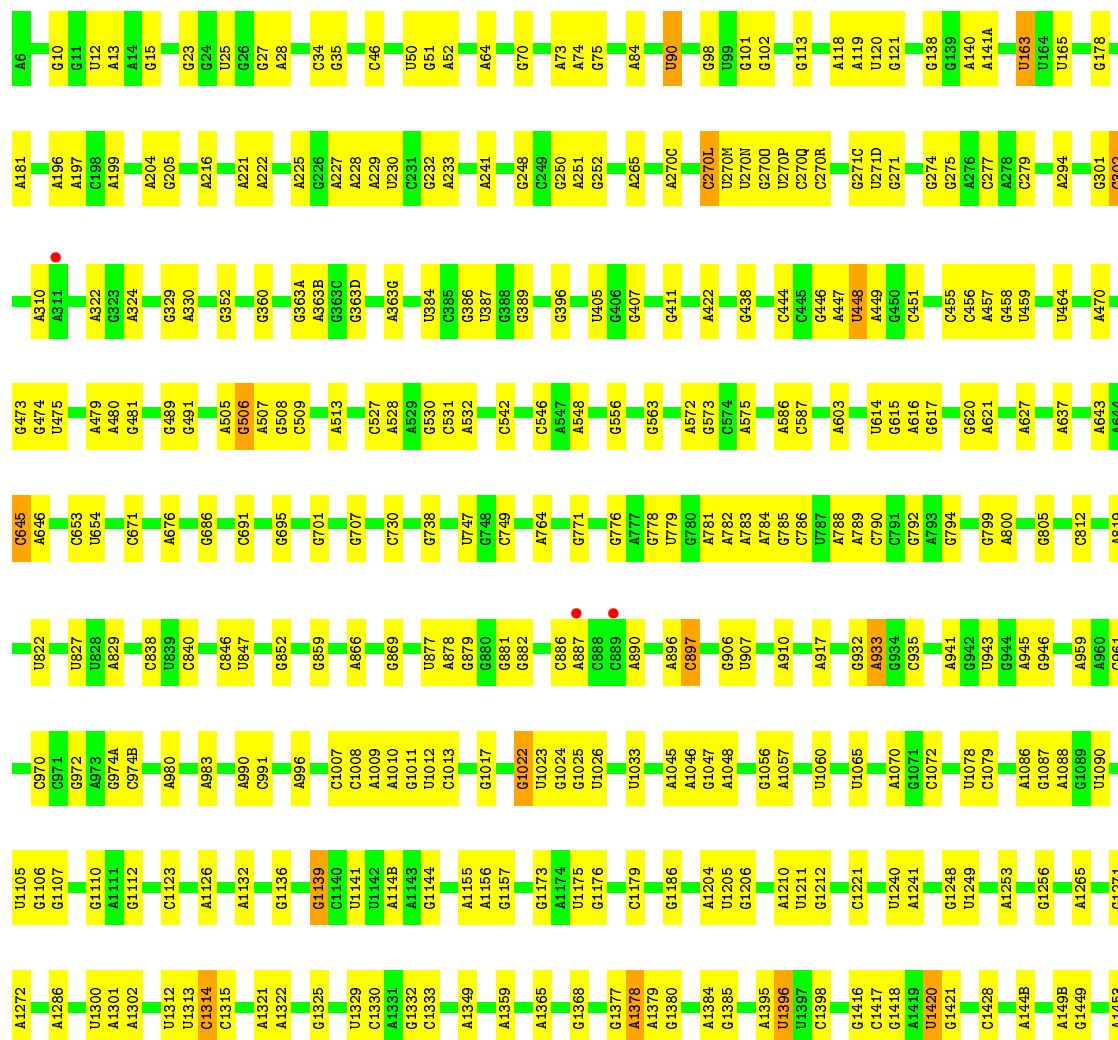


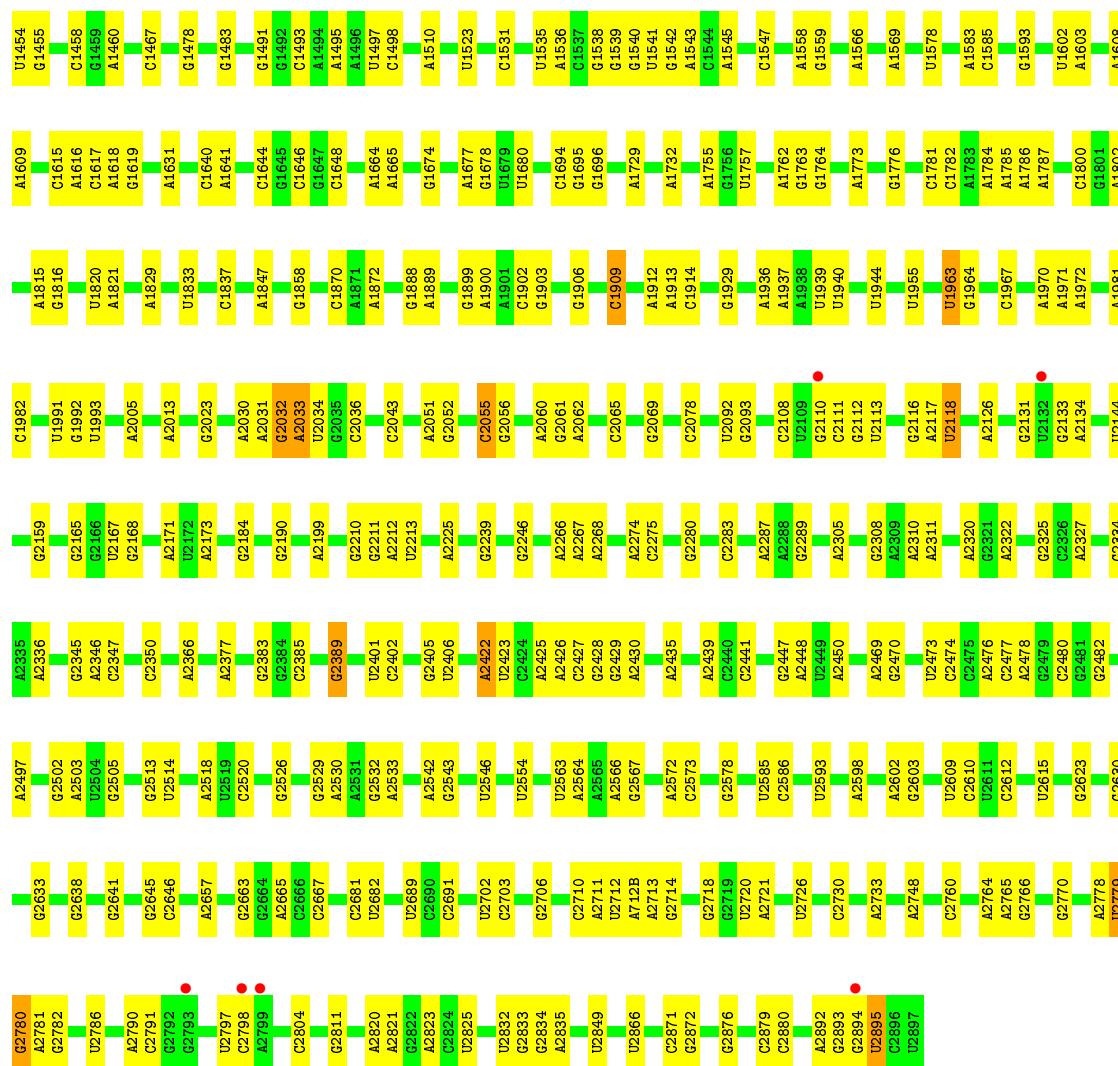
G2211	C2043	U1911	G1540	A1384	U1240	C1072	U943	G805	A627	U475	A322	A181	A6
A2212	C2044	A1912	U1541	G1385	A1241	A1077	G946	C812	C634	G476	G323	A196	U9
U2213	A2051	A1913	A1542	A1395	A1247	U1078	C951	G819	C637	A479	G325	A197	U13
A2225	G2052	C1914	C1543	U1396	G1248	C1079	G952	A819	A637	G480	G329	C198	A12
G2238	C2055	G1929	A1546	C1398	A1283	A1086	A953	A820	C645	G481	A330	A199	U13
G2239	G2056	U1931	C154B	U1397	A1286	G1087	A821	A821	A646	G489	A331	A204	G27
G2246	A2060	G1935	G1547	G1416	G1286	U1088	A959	U822	A655	G491	G352	G205	C34
U2249	A2062	A1937	A1558	C1417	G1286	U1090	C961	A824	C653	A492	G353	G214	C34
G2252	G2069	U1939	G1559	U1418	A1265	U1096	C970	U827	U654	A505	G354	G215	C47
A2269	U2092	U1940	A1566	G1421	G1271	U1097	C974	U831	C671	G508	G363A	A216	G46
A2274	G2093	U1944	A1569	C1428	A1272	U1105	C974B	G832	A675	C509	A363B	A221	A49
C2275	C2111	U1955	A1580	C1429	U1294	G1110	A980	C846	C675	A513	A363G	A222	G51
G2279	U2112	G1963	C1582	A144B	U1300	A1111	A983	U847	G682	C527	G372	A227	G61
G2280	G2113	G1964	A1583	A149B	A1301	A1112	C991	G852	C684	A528	G372	A228	G68
C2281	G2116	C1967	C1585	G1449	A1302	C1123	A996	G859	G686	G530	G386	U230	C69
G2282	U2117	U1970	U1602	G1498	A1302	C1123	A996	U860	C687	C531	U387	C231	C69
U2218	A2118	A1972	A1603	A1453	G1309	A1128	G997	U861	G717	A532	G388	G232	A71
A2219	G2120	A1971	A1608	U1454	G1310	A1129	C998	A866	C730	C544	G389	A233	U72
G2287	U2121	A1972	A1609	G1455	U1311	U1130	U999	A866	G723	G545	G396	G248	A73
G2289	A2126	C1979	A1616	C1458	U1312	G1136	C1008	G869	C730	C546	U405	G252	A74
A2305	G2131	G1980	A1617	G1459	U1313	G1139	A1010	A870	G738	A547	G408	C264	A84
C2306	U2132	A1981	C1617	A1460	A1321	U1140	G1011	U877	U747	A548	A411	A265	U90
G2307	G2133	G1982	A1618	C1467	A1322	U1141	U1012	A878	U748	C560	A412	A266	C93
G2308	A2134	G1992	G1635	G1478	G1325	U1142	C1013	G880	G748	G563	G425	C270L	G94
A2311	U2144	U1993	U1639	G1483	U1329	A1143	G1017	G881	A752	U568	C444	U270M	G98
G2320	G2152	C1996	C1640	G1483	C1330	G1144	A1021	G882	C753	U569	C444	G2700	U99
G2321	G2153	C2007	C1644	A1490	A1331	G1154	G1022	A887	C758	A572	A447	U270P	G101
A2322	G2154	G2007	G1645	G1491	G1332	A1155	U1023	C888	U779	G573	U448	C270Q	G102
G2325	G2159	A2013	C1646	G1492	C1333	U1175	G1024	C890	A764	G574	A449	C270R	A103
C2326	G2160	G2020	C1647	C1493	U1341	G1176	U1025	A890	C776	C574	G450	G271C	U104
A2327	C2161	A2020	C1648	A1494	U1342	G1179	A1027	U895	A777	A575	C451	U271D	G113
G2334	U2166	C2021	A1654	A1495	G1343	C1179	G1030	A896	C778	A586	A454	G271	C116
A2335	G2167	G2022	A1655	U1497	A1343	G1186	U1033	C897	U779	C587	C455	G274	G117
A2336	G2168	G2024	C1656	C1498	A1349	U1199	G1034	A910	A782	G599	C456	A278	A118
G2345	A2171	G2027	C1672	A1509	U1352	U1204	G1047	C914	A784	A603	U464	C279	A119
A2346	U2172	U2028	U1673	A1510	A1359	U1205	A1048	A917	C795	G604	U464	G295	U120
C2347	A2173	A2030	C1691	A1528	A1360	A1210	U1060	G929	A788	U614	G465	A300	G138
U2348	C2174	G2032	C1694	A1535	A1365	U1211	U1061	G932	A789	G616	A466	G301	G138
G2362	G2184	A2033	C1694	U1536	A1377	G1212	G1062	A933	G792	A617	A470	C302	A149
G2365	A2188	U2034	A1729	A1536	A1377	G1221	G1063	A941	A793	G620	G473	A310	U163
A2377	G2199	G2035	G1537	C1537	A1378	A1220	A1070	G942	A800	G474	G474		U164
A2378	G2210	C2036	G1538	G1539	A1379	C1221	A1071						



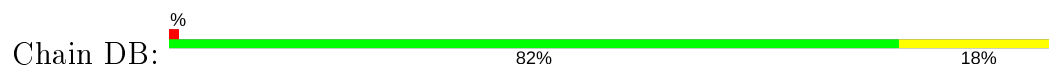
• Molecule 59: 23S ribosomal RNA

Chain DA: 77% 22%





• Molecule 60: 5S ribosomal RNA



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	306.01Å 673.49Å 351.98Å 90.00° 92.69° 90.00°	Depositor
Resolution (Å)	40.00 – 3.50 131.34 – 3.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.50) 74.9 (131.34-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 3.49Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.262 , 0.309 0.270 , 0.311	Depositor DCC
R_{free} test set	38188 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	80.5	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 85.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.26$, $\langle L^2 \rangle = 0.11$	Xtriage
Estimated twinning fraction	0.247 for h,-k,-l	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	308422	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.42	0/1945	0.73	4/2621 (0.2%)
1	CB	0.40	0/1945	0.69	1/2621 (0.0%)
2	AC	0.35	0/1645	0.60	0/2216
2	CC	0.33	0/1645	0.58	1/2216 (0.0%)
3	AD	0.37	0/1733	0.60	0/2318
3	CD	0.34	0/1733	0.61	0/2318
4	AE	0.35	0/1172	0.63	1/1576 (0.1%)
4	CE	0.34	0/1172	0.63	1/1576 (0.1%)
5	AF	0.38	0/856	0.67	2/1154 (0.2%)
5	CF	0.35	0/856	0.64	1/1154 (0.1%)
6	AG	0.34	0/1276	0.58	0/1709
6	CG	0.35	0/1276	0.58	0/1709
7	AH	0.34	0/1136	0.58	0/1527
7	CH	0.33	0/1136	0.57	0/1527
8	AI	0.36	0/1029	0.63	1/1378 (0.1%)
8	CI	0.36	0/1029	0.61	1/1378 (0.1%)
9	AJ	0.37	0/815	0.64	1/1095 (0.1%)
9	CJ	0.33	0/815	0.65	1/1095 (0.1%)
10	AK	0.40	0/900	0.65	0/1213
10	CK	0.37	0/900	0.63	0/1213
11	AL	0.47	0/992	0.89	3/1327 (0.2%)
11	CL	0.47	0/992	0.88	4/1327 (0.3%)
12	AM	0.33	0/1008	0.61	0/1347
12	CM	0.32	0/1008	0.58	0/1347
13	AN	0.37	0/501	0.57	0/664
13	CN	0.35	0/501	0.57	0/664
14	AO	0.39	0/745	0.62	0/992
14	CO	0.35	0/745	0.59	0/992
15	AP	0.34	0/722	0.58	0/970
15	CP	0.33	0/722	0.56	0/970
16	AQ	0.45	0/848	0.75	0/1131
16	CQ	0.42	0/848	0.71	0/1131

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AR	0.33	0/579	0.59	0/768
17	CR	0.31	0/579	0.57	0/768
18	AS	0.32	0/647	0.59	0/870
18	CS	0.31	0/647	0.56	0/870
19	AT	0.36	0/764	0.57	0/1006
19	CT	0.37	0/764	0.62	0/1006
20	AY	0.47	6/5481 (0.1%)	0.72	5/7418 (0.1%)
20	CY	0.52	7/5481 (0.1%)	0.76	12/7418 (0.2%)
21	AA	0.39	0/36351	0.97	36/56736 (0.1%)
21	CA	0.38	0/36351	0.95	35/56736 (0.1%)
22	AW	0.40	0/1827	1.06	9/2845 (0.3%)
22	CW	0.41	1/1827 (0.1%)	1.06	9/2845 (0.3%)
23	AV	0.78	1/568 (0.2%)	1.49	16/886 (1.8%)
23	CV	0.95	3/568 (0.5%)	1.74	19/886 (2.1%)
24	AU	1.05	0/11	1.28	0/13
24	CU	1.06	0/11	1.28	0/13
25	BC	0.44	0/1774	0.74	1/2391 (0.0%)
25	DC	0.50	1/1774 (0.1%)	0.76	0/2391
26	BD	0.38	0/2195	0.65	0/2955
26	DD	0.38	0/2195	0.67	0/2955
27	BE	0.39	0/1602	0.69	1/2160 (0.0%)
27	DE	0.35	0/1602	0.67	1/2160 (0.0%)
28	BF	0.41	0/1663	0.80	5/2249 (0.2%)
28	DF	0.41	0/1663	0.79	4/2249 (0.2%)
29	BG	0.57	1/1499 (0.1%)	0.60	0/2016
29	DG	0.59	1/1499 (0.1%)	0.67	3/2016 (0.1%)
30	BH	0.34	0/1298	0.59	0/1751
30	DH	0.34	0/1298	0.62	0/1751
32	BK	0.34	0/1054	0.60	0/1427
32	DK	0.34	0/1054	0.56	1/1427 (0.1%)
33	BN	0.58	0/1131	0.85	0/1525
33	DN	0.54	0/1131	0.80	0/1525
34	BO	0.36	0/943	0.65	1/1269 (0.1%)
34	DO	0.36	0/943	0.64	1/1269 (0.1%)
35	BP	0.34	0/1131	0.71	0/1504
35	DP	0.34	0/1131	0.71	0/1504
36	BQ	0.37	0/1143	0.64	0/1527
36	DQ	0.36	0/1143	0.60	0/1527
37	BR	0.38	0/974	0.65	0/1302
37	DR	0.34	0/974	0.62	1/1302 (0.1%)
38	BS	0.40	0/783	0.76	0/1041
38	DS	0.40	0/783	0.75	0/1041
39	BT	0.39	0/1161	0.76	3/1549 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	DT	0.37	0/1161	0.67	0/1549
40	BU	0.39	0/982	0.67	1/1306 (0.1%)
40	DU	0.42	0/982	0.68	1/1306 (0.1%)
41	BV	0.37	0/790	0.66	0/1057
41	DV	0.38	0/790	0.71	0/1057
42	BW	0.38	0/911	0.65	0/1220
42	DW	0.37	0/911	0.65	0/1220
43	BX	0.35	0/748	0.59	1/1004 (0.1%)
43	DX	0.35	0/748	0.60	0/1004
44	BY	0.35	0/831	0.65	0/1108
44	DY	0.34	0/831	0.60	0/1108
45	BZ	0.33	0/1505	0.60	0/2042
45	DZ	0.32	0/1505	0.59	0/2042
46	B0	0.33	0/671	0.55	0/892
46	D0	0.31	0/671	0.56	0/892
47	B2	0.37	0/600	0.65	1/793 (0.1%)
47	D2	0.34	0/600	0.60	0/793
48	B3	0.34	0/482	0.63	0/646
48	D3	0.31	0/482	0.58	0/646
49	B5	0.33	0/473	0.58	0/639
49	D5	0.34	0/473	0.60	0/639
50	B6	0.38	0/440	0.81	0/586
50	D6	0.35	0/440	0.79	1/586 (0.2%)
51	B7	0.38	0/438	0.62	0/575
51	D7	0.48	0/438	0.69	0/575
52	B8	0.37	0/525	0.67	0/691
52	D8	0.36	0/525	0.64	0/691
53	B9	0.32	0/310	0.55	0/407
53	D9	0.29	0/310	0.55	0/407
56	B1	0.53	0/739	0.83	1/981 (0.1%)
56	D1	0.54	0/739	0.84	2/981 (0.2%)
57	B4	0.40	0/276	0.65	0/372
57	D4	0.45	0/276	0.66	0/372
58	Be	0.36	0/538	0.55	0/715
58	De	0.35	0/538	0.61	0/715
59	BA	0.41	2/69437 (0.0%)	0.99	82/108401 (0.1%)
59	DA	0.40	1/69437 (0.0%)	0.97	72/108401 (0.1%)
60	BB	0.34	0/2853	0.93	0/4451
60	DB	0.34	0/2853	0.90	1/4451 (0.0%)
All	All	0.40	24/330902 (0.0%)	0.90	348/492664 (0.1%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AB	0	2
1	CB	0	1
10	AK	0	1
11	AL	0	1
11	CL	0	1
20	AY	0	3
20	CY	0	8
25	BC	0	3
25	DC	0	2
26	DD	0	1
28	BF	0	2
28	DF	0	2
29	BG	0	1
29	DG	0	1
31	BJ	0	1
31	DJ	0	1
38	BS	0	2
38	DS	0	2
39	BT	0	2
39	DT	0	1
42	DW	0	1
56	B1	0	2
56	D1	0	3
All	All	0	44

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	CY	502	GLY	C-O	18.54	1.53	1.23
29	DG	112	PRO	CA-C	17.59	1.88	1.52
29	BG	112	PRO	CA-C	17.54	1.88	1.52
23	CV	16	A	O3'-P	-10.50	1.48	1.61
20	AY	499	ARG	C-N	9.84	1.56	1.34

The worst 5 of 348 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	CW	37	A	P-O3'-C3'	19.49	143.09	119.70
23	CV	16	A	P-O3'-C3'	18.93	142.41	119.70
20	CY	502	GLY	O-C-N	-12.85	101.35	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	CY	502	GLY	CA-C-N	12.59	141.38	116.20
20	CY	502	GLY	C-N-CA	11.35	146.14	122.30

There are no chirality outliers.

5 of 44 planarity outliers are listed below:

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

5.2 Too-close contacts [i](#)

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%)	173 (74%)	40 (17%)	20 (9%)	1	9
1	CB	233/235 (99%)	174 (75%)	36 (16%)	23 (10%)	0	7
2	AC	205/207 (99%)	137 (67%)	44 (22%)	24 (12%)	0	5
2	CC	205/207 (99%)	152 (74%)	34 (17%)	19 (9%)	0	8
3	AD	206/208 (99%)	146 (71%)	42 (20%)	18 (9%)	1	9
3	CD	206/208 (99%)	149 (72%)	46 (22%)	11 (5%)	2	17
4	AE	149/151 (99%)	107 (72%)	31 (21%)	11 (7%)	1	11
4	CE	149/151 (99%)	116 (78%)	24 (16%)	9 (6%)	1	15
5	AF	99/101 (98%)	75 (76%)	17 (17%)	7 (7%)	1	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	CF	99/101 (98%)	81 (82%)	7 (7%)	11 (11%)	0	6
6	AG	153/155 (99%)	120 (78%)	27 (18%)	6 (4%)	3	25
6	CG	153/155 (99%)	119 (78%)	27 (18%)	7 (5%)	2	21
7	AH	136/138 (99%)	98 (72%)	22 (16%)	16 (12%)	0	5
7	CH	136/138 (99%)	102 (75%)	21 (15%)	13 (10%)	0	8
8	AI	125/127 (98%)	88 (70%)	26 (21%)	11 (9%)	1	8
8	CI	125/127 (98%)	92 (74%)	25 (20%)	8 (6%)	1	14
9	AJ	97/99 (98%)	71 (73%)	17 (18%)	9 (9%)	0	8
9	CJ	97/99 (98%)	71 (73%)	16 (16%)	10 (10%)	0	7
10	AK	117/119 (98%)	74 (63%)	25 (21%)	18 (15%)	0	3
10	CK	117/119 (98%)	78 (67%)	26 (22%)	13 (11%)	0	6
11	AL	123/125 (98%)	42 (34%)	46 (37%)	35 (28%)	0	0
11	CL	123/125 (98%)	39 (32%)	44 (36%)	40 (32%)	0	0
12	AM	123/125 (98%)	86 (70%)	24 (20%)	13 (11%)	0	7
12	CM	123/125 (98%)	91 (74%)	18 (15%)	14 (11%)	0	6
13	AN	58/60 (97%)	40 (69%)	11 (19%)	7 (12%)	0	5
13	CN	58/60 (97%)	40 (69%)	14 (24%)	4 (7%)	1	12
14	AO	86/88 (98%)	65 (76%)	14 (16%)	7 (8%)	1	9
14	CO	86/88 (98%)	66 (77%)	15 (17%)	5 (6%)	1	16
15	AP	82/84 (98%)	55 (67%)	18 (22%)	9 (11%)	0	6
15	CP	82/84 (98%)	59 (72%)	18 (22%)	5 (6%)	1	15
16	AQ	98/100 (98%)	68 (69%)	18 (18%)	12 (12%)	0	5
16	CQ	98/100 (98%)	68 (69%)	20 (20%)	10 (10%)	0	7
17	AR	68/70 (97%)	50 (74%)	12 (18%)	6 (9%)	1	8
17	CR	68/70 (97%)	52 (76%)	10 (15%)	6 (9%)	1	8
18	AS	77/79 (98%)	51 (66%)	18 (23%)	8 (10%)	0	7
18	CS	77/79 (98%)	56 (73%)	12 (16%)	9 (12%)	0	5
19	AT	97/99 (98%)	72 (74%)	17 (18%)	8 (8%)	1	9
19	CT	97/99 (98%)	75 (77%)	14 (14%)	8 (8%)	1	9
20	AY	685/687 (100%)	431 (63%)	168 (24%)	86 (13%)	0	5
20	CY	685/687 (100%)	457 (67%)	156 (23%)	72 (10%)	0	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	AU	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
24	CU	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
25	BC	226/228 (99%)	108 (48%)	70 (31%)	48 (21%)	0	1
25	DC	226/228 (99%)	105 (46%)	75 (33%)	46 (20%)	0	1
26	BD	273/275 (99%)	180 (66%)	54 (20%)	39 (14%)	0	3
26	DD	273/275 (99%)	188 (69%)	47 (17%)	38 (14%)	0	3
27	BE	203/205 (99%)	130 (64%)	43 (21%)	30 (15%)	0	3
27	DE	203/205 (99%)	133 (66%)	36 (18%)	34 (17%)	0	2
28	BF	206/208 (99%)	126 (61%)	54 (26%)	26 (13%)	0	5
28	DF	206/208 (99%)	137 (66%)	47 (23%)	22 (11%)	0	6
29	BG	179/181 (99%)	120 (67%)	46 (26%)	13 (7%)	1	11
29	DG	179/181 (99%)	127 (71%)	44 (25%)	8 (4%)	2	21
30	BH	165/167 (99%)	118 (72%)	29 (18%)	18 (11%)	0	6
30	DH	165/167 (99%)	118 (72%)	32 (19%)	15 (9%)	1	8
32	BK	138/140 (99%)	88 (64%)	33 (24%)	17 (12%)	0	5
32	DK	138/140 (99%)	86 (62%)	33 (24%)	19 (14%)	0	3
33	BN	136/138 (99%)	93 (68%)	24 (18%)	19 (14%)	0	3
33	DN	136/138 (99%)	91 (67%)	27 (20%)	18 (13%)	0	4
34	BO	120/122 (98%)	92 (77%)	20 (17%)	8 (7%)	1	13
34	DO	120/122 (98%)	95 (79%)	20 (17%)	5 (4%)	3	23
35	BP	144/146 (99%)	81 (56%)	36 (25%)	27 (19%)	0	2
35	DP	144/146 (99%)	76 (53%)	35 (24%)	33 (23%)	0	1
36	BQ	139/141 (99%)	87 (63%)	32 (23%)	20 (14%)	0	3
36	DQ	139/141 (99%)	91 (66%)	31 (22%)	17 (12%)	0	5
37	BR	115/117 (98%)	83 (72%)	21 (18%)	11 (10%)	0	8
37	DR	115/117 (98%)	91 (79%)	17 (15%)	7 (6%)	1	15
38	BS	97/99 (98%)	56 (58%)	25 (26%)	16 (16%)	0	2
38	DS	97/99 (98%)	57 (59%)	25 (26%)	15 (16%)	0	3
39	BT	136/138 (99%)	76 (56%)	41 (30%)	19 (14%)	0	3
39	DT	136/138 (99%)	82 (60%)	28 (21%)	26 (19%)	0	2
40	BU	115/117 (98%)	79 (69%)	25 (22%)	11 (10%)	0	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	DU	115/117 (98%)	80 (70%)	23 (20%)	12 (10%)	0	7
41	BV	99/101 (98%)	57 (58%)	28 (28%)	14 (14%)	0	3
41	DV	99/101 (98%)	64 (65%)	22 (22%)	13 (13%)	0	4
42	BW	111/113 (98%)	82 (74%)	14 (13%)	15 (14%)	0	4
42	DW	111/113 (98%)	81 (73%)	16 (14%)	14 (13%)	0	5
43	BX	91/93 (98%)	73 (80%)	12 (13%)	6 (7%)	1	13
43	DX	91/93 (98%)	70 (77%)	16 (18%)	5 (6%)	2	17
44	BY	105/107 (98%)	50 (48%)	30 (29%)	25 (24%)	0	0
44	DY	105/107 (98%)	50 (48%)	34 (32%)	21 (20%)	0	1
45	BZ	183/185 (99%)	116 (63%)	46 (25%)	21 (12%)	0	6
45	DZ	183/185 (99%)	121 (66%)	44 (24%)	18 (10%)	0	7
46	B0	82/84 (98%)	59 (72%)	16 (20%)	7 (8%)	1	9
46	D0	82/84 (98%)	65 (79%)	13 (16%)	4 (5%)	2	19
47	B2	69/71 (97%)	49 (71%)	14 (20%)	6 (9%)	1	9
47	D2	69/71 (97%)	50 (72%)	17 (25%)	2 (3%)	4	31
48	B3	58/60 (97%)	46 (79%)	7 (12%)	5 (9%)	1	9
48	D3	58/60 (97%)	44 (76%)	9 (16%)	5 (9%)	1	9
49	B5	57/59 (97%)	44 (77%)	4 (7%)	9 (16%)	0	2
49	D5	57/59 (97%)	42 (74%)	11 (19%)	4 (7%)	1	12
50	B6	48/50 (96%)	28 (58%)	9 (19%)	11 (23%)	0	1
50	D6	48/50 (96%)	27 (56%)	8 (17%)	13 (27%)	0	0
51	B7	47/49 (96%)	30 (64%)	13 (28%)	4 (8%)	1	9
51	D7	47/49 (96%)	34 (72%)	11 (23%)	2 (4%)	2	22
52	B8	62/64 (97%)	42 (68%)	7 (11%)	13 (21%)	0	1
52	D8	62/64 (97%)	40 (64%)	11 (18%)	11 (18%)	0	2
53	B9	35/37 (95%)	28 (80%)	5 (14%)	2 (6%)	1	16
53	D9	35/37 (95%)	29 (83%)	4 (11%)	2 (6%)	1	16
56	B1	91/93 (98%)	56 (62%)	17 (19%)	18 (20%)	0	1
56	D1	91/93 (98%)	59 (65%)	18 (20%)	14 (15%)	0	3
57	B4	33/35 (94%)	15 (46%)	11 (33%)	7 (21%)	0	1
57	D4	33/35 (94%)	15 (46%)	9 (27%)	9 (27%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
58	Be	70/102 (69%)	36 (51%)	29 (41%)	5 (7%)	1	12
58	De	70/102 (69%)	40 (57%)	22 (31%)	8 (11%)	0	6
All	All	13304/13576 (98%)	8904 (67%)	2822 (21%)	1578 (12%)	0	5

5 of 1578 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AB	203/203 (100%)	164 (81%)	39 (19%)	1	7
1	CB	203/203 (100%)	177 (87%)	26 (13%)	4	22
2	AC	161/161 (100%)	125 (78%)	36 (22%)	1	4
2	CC	161/161 (100%)	122 (76%)	39 (24%)	0	4
3	AD	180/180 (100%)	143 (79%)	37 (21%)	1	6
3	CD	180/180 (100%)	142 (79%)	38 (21%)	1	5
4	AE	116/116 (100%)	96 (83%)	20 (17%)	2	11
4	CE	116/116 (100%)	95 (82%)	21 (18%)	1	9
5	AF	90/90 (100%)	76 (84%)	14 (16%)	2	16
5	CF	90/90 (100%)	74 (82%)	16 (18%)	2	10
6	AG	126/126 (100%)	111 (88%)	15 (12%)	5	25
6	CG	126/126 (100%)	112 (89%)	14 (11%)	6	28
7	AH	119/119 (100%)	94 (79%)	25 (21%)	1	5
7	CH	119/119 (100%)	91 (76%)	28 (24%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	AI	98/98 (100%)	82 (84%)	16 (16%)	2	13
8	CI	98/98 (100%)	77 (79%)	21 (21%)	1	5
9	AJ	89/89 (100%)	71 (80%)	18 (20%)	1	6
9	CJ	89/89 (100%)	66 (74%)	23 (26%)	0	3
10	AK	90/90 (100%)	73 (81%)	17 (19%)	1	8
10	CK	90/90 (100%)	72 (80%)	18 (20%)	1	7
11	AL	104/104 (100%)	74 (71%)	30 (29%)	0	2
11	CL	104/104 (100%)	77 (74%)	27 (26%)	0	3
12	AM	100/100 (100%)	83 (83%)	17 (17%)	2	12
12	CM	100/100 (100%)	86 (86%)	14 (14%)	3	19
13	AN	49/49 (100%)	39 (80%)	10 (20%)	1	6
13	CN	49/49 (100%)	35 (71%)	14 (29%)	0	3
14	AO	79/79 (100%)	70 (89%)	9 (11%)	5	26
14	CO	79/79 (100%)	66 (84%)	13 (16%)	2	13
15	AP	72/72 (100%)	59 (82%)	13 (18%)	1	9
15	CP	72/72 (100%)	61 (85%)	11 (15%)	2	17
16	AQ	95/95 (100%)	82 (86%)	13 (14%)	3	20
16	CQ	95/95 (100%)	80 (84%)	15 (16%)	2	15
17	AR	61/61 (100%)	53 (87%)	8 (13%)	4	21
17	CR	61/61 (100%)	53 (87%)	8 (13%)	4	21
18	AS	69/69 (100%)	58 (84%)	11 (16%)	2	14
18	CS	69/69 (100%)	52 (75%)	17 (25%)	0	4
19	AT	76/76 (100%)	66 (87%)	10 (13%)	4	21
19	CT	76/76 (100%)	68 (90%)	8 (10%)	7	31
20	AY	579/579 (100%)	459 (79%)	120 (21%)	1	6
20	CY	579/579 (100%)	483 (83%)	96 (17%)	2	13
24	AU	2/2 (100%)	2 (100%)	0	100	100
24	CU	2/2 (100%)	2 (100%)	0	100	100
25	BC	180/180 (100%)	132 (73%)	48 (27%)	0	3
25	DC	180/180 (100%)	128 (71%)	52 (29%)	0	2
26	BD	217/217 (100%)	167 (77%)	50 (23%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	DD	217/217 (100%)	175 (81%)	42 (19%)	1	7
27	BE	165/165 (100%)	137 (83%)	28 (17%)	2	12
27	DE	165/165 (100%)	136 (82%)	29 (18%)	2	10
28	BF	165/165 (100%)	133 (81%)	32 (19%)	1	7
28	DF	165/165 (100%)	140 (85%)	25 (15%)	3	17
29	BG	155/155 (100%)	130 (84%)	25 (16%)	2	14
29	DG	155/155 (100%)	130 (84%)	25 (16%)	2	14
30	BH	136/136 (100%)	111 (82%)	25 (18%)	1	8
30	DH	136/136 (100%)	117 (86%)	19 (14%)	3	19
32	BK	105/105 (100%)	74 (70%)	31 (30%)	0	2
32	DK	105/105 (100%)	77 (73%)	28 (27%)	0	3
33	BN	117/117 (100%)	98 (84%)	19 (16%)	2	14
33	DN	117/117 (100%)	93 (80%)	24 (20%)	1	6
34	BO	100/100 (100%)	85 (85%)	15 (15%)	3	17
34	DO	100/100 (100%)	86 (86%)	14 (14%)	3	19
35	BP	112/112 (100%)	82 (73%)	30 (27%)	0	3
35	DP	112/112 (100%)	85 (76%)	27 (24%)	0	4
36	BQ	111/111 (100%)	80 (72%)	31 (28%)	0	3
36	DQ	111/111 (100%)	84 (76%)	27 (24%)	0	4
37	BR	100/100 (100%)	79 (79%)	21 (21%)	1	5
37	DR	100/100 (100%)	78 (78%)	22 (22%)	1	5
38	BS	77/77 (100%)	60 (78%)	17 (22%)	1	5
38	DS	77/77 (100%)	59 (77%)	18 (23%)	1	4
39	BT	120/120 (100%)	94 (78%)	26 (22%)	1	5
39	DT	120/120 (100%)	93 (78%)	27 (22%)	1	4
40	BU	93/93 (100%)	75 (81%)	18 (19%)	1	7
40	DU	93/93 (100%)	70 (75%)	23 (25%)	0	4
41	BV	82/82 (100%)	60 (73%)	22 (27%)	0	3
41	DV	82/82 (100%)	62 (76%)	20 (24%)	0	4
42	BW	92/92 (100%)	69 (75%)	23 (25%)	0	4
42	DW	92/92 (100%)	76 (83%)	16 (17%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	BX	75/75 (100%)	56 (75%)	19 (25%)	0	3
43	DX	75/75 (100%)	58 (77%)	17 (23%)	1	4
44	BY	88/88 (100%)	69 (78%)	19 (22%)	1	5
44	DY	88/88 (100%)	73 (83%)	15 (17%)	2	12
45	BZ	162/162 (100%)	128 (79%)	34 (21%)	1	5
45	DZ	162/162 (100%)	125 (77%)	37 (23%)	1	4
46	B0	66/66 (100%)	56 (85%)	10 (15%)	3	17
46	D0	66/66 (100%)	56 (85%)	10 (15%)	3	17
47	B2	66/66 (100%)	59 (89%)	7 (11%)	6	30
47	D2	66/66 (100%)	58 (88%)	8 (12%)	5	24
48	B3	52/52 (100%)	42 (81%)	10 (19%)	1	7
48	D3	52/52 (100%)	45 (86%)	7 (14%)	4	21
49	B5	51/51 (100%)	39 (76%)	12 (24%)	1	4
49	D5	51/51 (100%)	41 (80%)	10 (20%)	1	7
50	B6	49/49 (100%)	37 (76%)	12 (24%)	0	4
50	D6	49/49 (100%)	34 (69%)	15 (31%)	0	2
51	B7	42/42 (100%)	35 (83%)	7 (17%)	2	12
51	D7	42/42 (100%)	36 (86%)	6 (14%)	3	19
52	B8	54/54 (100%)	42 (78%)	12 (22%)	1	5
52	D8	54/54 (100%)	44 (82%)	10 (18%)	1	8
53	B9	34/34 (100%)	32 (94%)	2 (6%)	19	53
53	D9	34/34 (100%)	30 (88%)	4 (12%)	5	25
56	B1	78/78 (100%)	58 (74%)	20 (26%)	0	3
56	D1	78/78 (100%)	58 (74%)	20 (26%)	0	3
57	B4	31/31 (100%)	22 (71%)	9 (29%)	0	3
57	D4	31/31 (100%)	21 (68%)	10 (32%)	0	2
58	Be	54/54 (100%)	46 (85%)	8 (15%)	3	17
58	De	54/54 (100%)	46 (85%)	8 (15%)	3	17
All	All	11174/11174 (100%)	8972 (80%)	2202 (20%)	1	7

5 of 2202 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
45	BZ	124	ILE
4	CE	73	ASN
43	DX	68	ARG
47	B2	53	LEU
58	Be	106	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 68 such sidechains are listed below:

Mol	Chain	Res	Type
50	B6	32	ASN
16	CQ	96	GLN
41	DV	89	GLN
3	CD	161	ASN
6	CG	148	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1511/1511 (100%)	326 (21%)	19 (1%)
21	CA	1511/1511 (100%)	310 (20%)	16 (1%)
22	AW	76/77 (98%)	22 (28%)	1 (1%)
22	CW	76/77 (98%)	19 (25%)	1 (1%)
23	AV	22/23 (95%)	11 (50%)	2 (9%)
23	CV	22/23 (95%)	9 (40%)	3 (13%)
59	BA	2878/2879 (99%)	666 (23%)	21 (0%)
59	DA	2878/2879 (99%)	629 (21%)	17 (0%)
60	BB	118/119 (99%)	20 (16%)	4 (3%)
60	DB	118/119 (99%)	19 (16%)	3 (2%)
All	All	9210/9218 (99%)	2031 (22%)	87 (0%)

5 of 2031 RNA backbone outliers are listed below:

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

5 of 87 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
59	BA	2092	U
21	CA	115	G
59	DA	2092	U
59	BA	2422	A
60	BB	56	G

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	AU	2	24	3,5,6	0.33	0	1,5,7	0.99	0
24	5OH	AU	6	24	8,12,13	0.75	0	3,16,18	1.07	0
24	KBE	AU	1	24	8,8,9	0.65	0	7,8,10	1.44	1 (14%)
24	5OH	CU	6	24	8,12,13	0.76	0	3,16,18	1.07	0
24	UAL	AU	5	24	7,8,9	2.41	3 (42%)	5,9,11	1.44	1 (20%)
24	UAL	CU	5	24	7,8,9	2.41	3 (42%)	5,9,11	1.45	1 (20%)
24	DPP	CU	2	24	3,5,6	0.33	0	1,5,7	0.99	0
24	KBE	CU	1	24	8,8,9	0.64	0	7,8,10	1.45	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	AU	2	24	-	0/2/4/6	-
24	5OH	AU	6	24	-	0/2/18/20	0/1/1/1
24	KBE	AU	1	24	-	1/7/7/8	-
24	5OH	CU	6	24	-	0/2/18/20	0/1/1/1
24	UAL	AU	5	24	-	0/3/7/9	-
24	UAL	CU	5	24	-	0/3/7/9	-
24	DPP	CU	2	24	-	0/2/4/6	-
24	KBE	CU	1	24	-	1/7/7/8	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	CU	5	UAL	C-CA	4.72	1.52	1.45
24	AU	5	UAL	C-CA	4.71	1.52	1.45
24	AU	5	UAL	C1-N1	-3.32	1.35	1.40
24	CU	5	UAL	C1-N1	-3.30	1.35	1.40
24	AU	5	UAL	CB-N1	-2.14	1.30	1.35

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	CU	1	KBE	CB-CA-C	3.33	117.15	112.25
24	AU	1	KBE	CB-CA-C	3.30	117.11	112.25
24	AU	5	UAL	O-C-CA	-2.47	122.25	125.39
24	CU	5	UAL	O-C-CA	-2.47	122.25	125.39

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

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	2.74	8 (28%)	30,54,54	2.47	10 (33%)
61	GNP	CY	701	62	28,34,34	2.74	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	701	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	-8.20	1.38	1.52
61	CY	701	GNP	C5-C6	-8.17	1.38	1.52
61	AY	701	GNP	C4-N9	-8.13	1.36	1.47
61	CY	701	GNP	C4-N9	-8.12	1.36	1.47
61	AY	701	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	CY	701	GNP	C4-C5-N7	7.67	112.63	102.46
61	AY	701	GNP	C4-C5-N7	7.64	112.59	102.46
61	AY	701	GNP	C5-C6-N1	-5.27	111.69	118.19
61	CY	701	GNP	C5-C6-N1	-5.25	111.72	118.19
61	CY	701	GNP	PA-O3A-PB	-4.72	115.98	132.62

There are no chirality outliers.

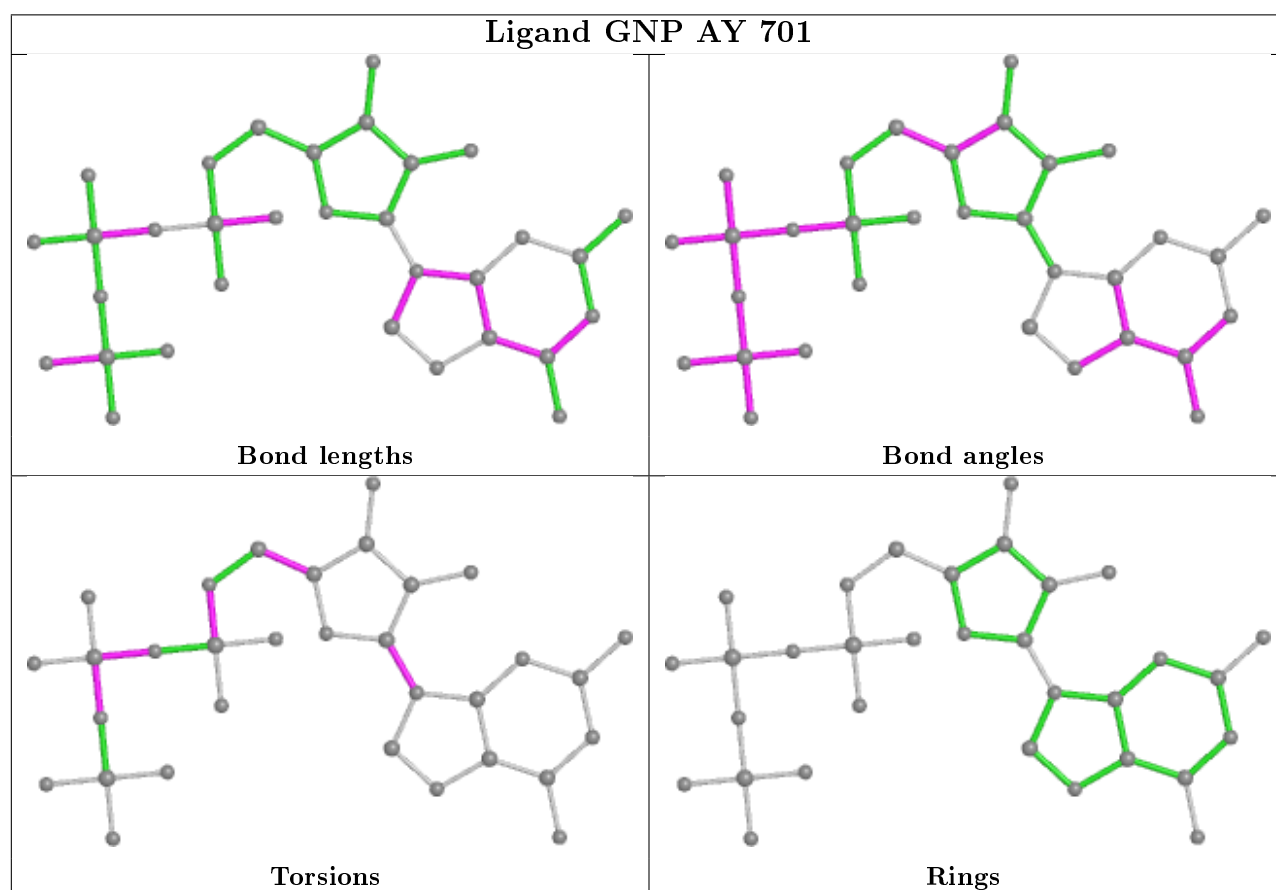
5 of 20 torsion outliers are listed below:

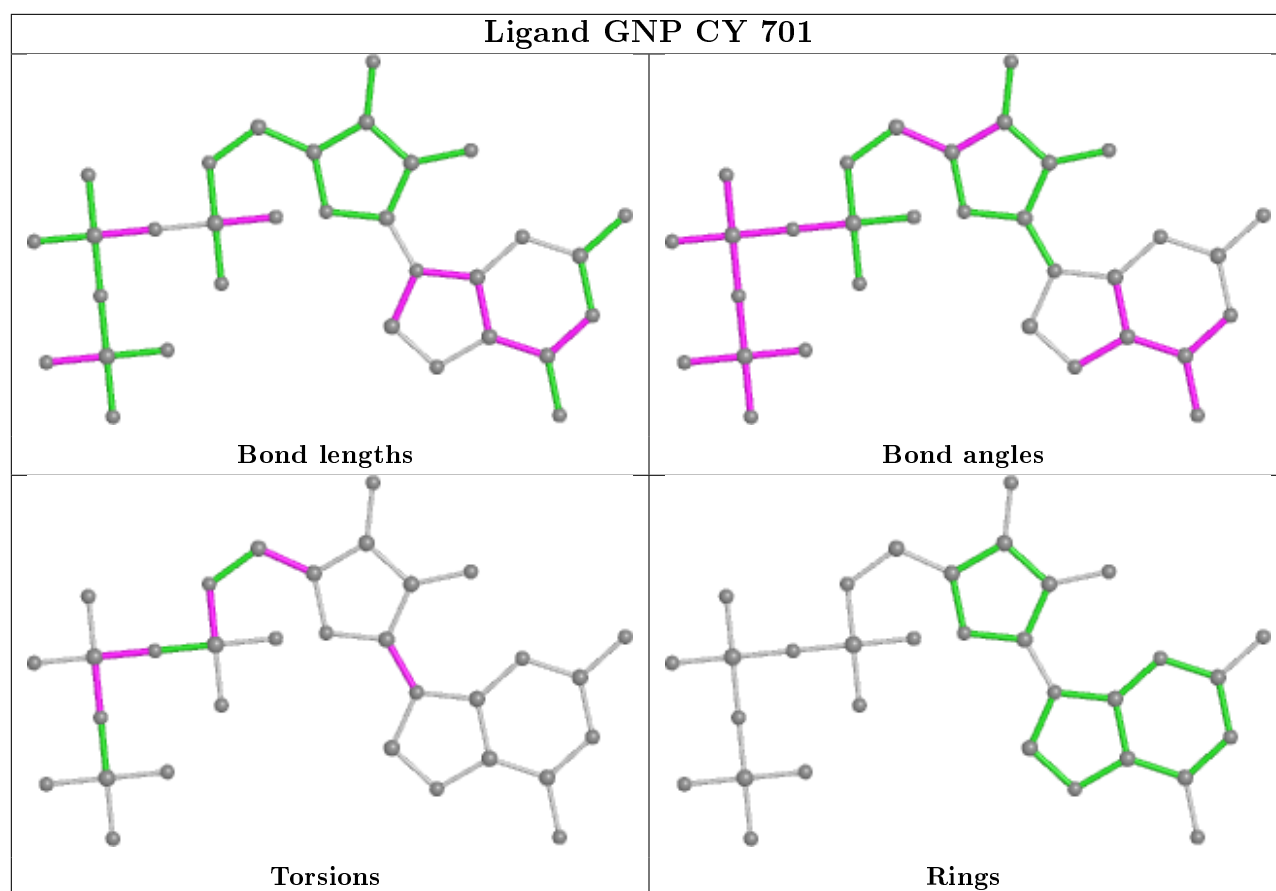
Mol	Chain	Res	Type	Atoms
61	AY	701	GNP	PG-N3B-PB-O1B
61	AY	701	GNP	PG-N3B-PB-O3A
61	AY	701	GNP	PA-O3A-PB-O1B
61	AY	701	GNP	PA-O3A-PB-O2B
61	AY	701	GNP	C5'-O5'-PA-O3A

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
58	Be	1
58	De	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	De	30:UNK	C	51:ALA	N	36.11
1	Be	30:UNK	C	51:ALA	N	35.10

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AB	235/235 (100%)	-0.08	6 (2%) 56 49	30, 75, 127, 171	0
1	CB	235/235 (100%)	0.41	16 (6%) 17 16	34, 86, 153, 201	0
2	AC	207/207 (100%)	0.28	14 (6%) 17 16	27, 59, 115, 156	0
2	CC	207/207 (100%)	1.01	41 (19%) 1 1	23, 75, 130, 190	0
3	AD	208/208 (100%)	-0.57	0 100 100	24, 72, 124, 159	0
3	CD	208/208 (100%)	-0.29	3 (1%) 75 69	23, 85, 142, 184	0
4	AE	151/151 (100%)	-0.41	0 100 100	17, 48, 101, 156	0
4	CE	151/151 (100%)	-0.02	7 (4%) 32 28	14, 58, 106, 151	0
5	AF	101/101 (100%)	-0.47	1 (0%) 82 77	15, 50, 100, 133	0
5	CF	101/101 (100%)	-0.62	1 (0%) 82 77	29, 61, 123, 148	0
6	AG	155/155 (100%)	-0.68	1 (0%) 89 86	30, 80, 139, 199	0
6	CG	155/155 (100%)	-0.80	0 100 100	38, 82, 137, 180	0
7	AH	138/138 (100%)	-0.16	4 (2%) 51 45	28, 59, 103, 142	0
7	CH	138/138 (100%)	0.15	5 (3%) 42 38	25, 75, 121, 155	0
8	AI	127/127 (100%)	-0.76	0 100 100	0, 71, 117, 134	0
8	CI	127/127 (100%)	-0.56	0 100 100	0, 84, 149, 220	0
9	AJ	99/99 (100%)	0.15	6 (6%) 21 19	25, 62, 116, 159	0
9	CJ	99/99 (100%)	0.90	13 (13%) 3 4	31, 75, 127, 166	0
10	AK	119/119 (100%)	-0.34	1 (0%) 86 81	31, 69, 116, 157	0
10	CK	119/119 (100%)	-0.57	1 (0%) 86 81	38, 72, 133, 151	0
11	AL	125/125 (100%)	-0.12	3 (2%) 59 53	10, 66, 120, 181	0
11	CL	125/125 (100%)	0.25	13 (10%) 6 7	29, 69, 136, 170	0
12	AM	125/125 (100%)	0.06	11 (8%) 10 10	49, 86, 144, 212	0
12	CM	125/125 (100%)	0.25	14 (11%) 5 6	53, 100, 158, 223	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AN	60/60 (100%)	0.40	7 (11%) 4 5	28, 52, 87, 120	0
13	CN	60/60 (100%)	0.93	11 (18%) 1 1	39, 69, 117, 135	0
14	AO	88/88 (100%)	-0.31	0 100 100	22, 60, 114, 139	0
14	CO	88/88 (100%)	-0.32	0 100 100	25, 68, 119, 170	0
15	AP	84/84 (100%)	0.05	4 (4%) 30 27	26, 66, 109, 117	0
15	CP	84/84 (100%)	0.05	2 (2%) 59 53	52, 81, 127, 153	0
16	AQ	100/100 (100%)	0.25	6 (6%) 21 19	0, 67, 117, 139	0
16	CQ	100/100 (100%)	0.41	8 (8%) 12 12	0, 68, 126, 150	0
17	AR	70/70 (100%)	-0.21	3 (4%) 35 31	14, 54, 120, 154	0
17	CR	70/70 (100%)	-0.29	1 (1%) 75 69	39, 63, 113, 155	0
18	AS	79/79 (100%)	0.90	14 (17%) 1 1	47, 92, 136, 169	0
18	CS	79/79 (100%)	0.62	10 (12%) 3 4	44, 99, 145, 189	0
19	AT	99/99 (100%)	-0.50	0 100 100	0, 77, 128, 159	0
19	CT	99/99 (100%)	-0.28	2 (2%) 65 60	0, 79, 131, 166	0
20	AY	687/687 (100%)	0.00	50 (7%) 15 15	23, 84, 139, 174	0
20	CY	687/687 (100%)	0.02	49 (7%) 16 15	40, 92, 149, 204	0
21	AA	1511/1511 (100%)	-0.60	3 (0%) 95 93	15, 67, 145, 258	0
21	CA	1511/1511 (100%)	-0.61	1 (0%) 95 95	18, 70, 157, 272	0
22	AW	77/77 (100%)	-0.73	0 100 100	32, 90, 174, 205	0
22	CW	77/77 (100%)	-0.74	0 100 100	39, 101, 193, 240	0
23	AV	23/23 (100%)	-0.70	0 100 100	41, 100, 156, 172	0
23	CV	23/23 (100%)	-0.27	1 (4%) 35 31	41, 118, 186, 216	0
24	AU	2/6 (33%)	-0.75	0 100 100	114, 114, 114, 114	0
24	CU	2/6 (33%)	-0.94	0 100 100	119, 119, 119, 119	0
25	BC	228/228 (100%)	1.42	73 (32%) 0 0	81, 124, 178, 222	0
25	DC	228/228 (100%)	1.57	74 (32%) 0 0	102, 162, 214, 247	0
26	BD	275/275 (100%)	-0.49	2 (0%) 87 83	11, 47, 102, 126	0
26	DD	275/275 (100%)	-0.45	4 (1%) 73 68	23, 54, 107, 147	0
27	BE	205/205 (100%)	-0.37	3 (1%) 73 68	19, 55, 101, 193	0
27	DE	205/205 (100%)	-0.20	4 (1%) 65 60	12, 60, 120, 175	0
28	BF	208/208 (100%)	-0.02	14 (6%) 17 16	16, 69, 131, 178	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DF	208/208 (100%)	-0.05	11 (5%) 26 24	34, 83, 176, 205	0
29	BG	181/181 (100%)	0.90	38 (20%) 1 1	41, 90, 132, 195	0
29	DG	181/181 (100%)	1.39	53 (29%) 0 0	44, 104, 159, 196	0
30	BH	167/167 (100%)	-0.46	1 (0%) 89 86	21, 68, 123, 159	0
30	DH	167/167 (100%)	-0.42	2 (1%) 79 73	36, 73, 140, 192	0
31	BJ	0/170	-	-	-	-
31	DJ	0/170	-	-	-	-
32	BK	140/140 (100%)	-0.06	9 (6%) 19 18	60, 114, 165, 206	0
32	DK	140/140 (100%)	0.43	24 (17%) 1 1	72, 142, 197, 229	0
33	BN	138/138 (100%)	0.36	12 (8%) 10 11	59, 83, 108, 111	0
33	DN	138/138 (100%)	0.25	7 (5%) 28 25	61, 89, 110, 118	0
34	BO	122/122 (100%)	-0.06	5 (4%) 37 33	23, 44, 90, 158	0
34	DO	122/122 (100%)	0.06	4 (3%) 46 41	26, 47, 96, 121	0
35	BP	146/146 (100%)	-0.45	2 (1%) 75 69	23, 71, 132, 167	0
35	DP	146/146 (100%)	-0.32	5 (3%) 45 40	19, 88, 140, 212	0
36	BQ	141/141 (100%)	-0.56	1 (0%) 87 83	32, 53, 103, 155	0
36	DQ	141/141 (100%)	-0.64	1 (0%) 87 83	34, 58, 126, 178	0
37	BR	117/117 (100%)	-0.14	2 (1%) 70 64	22, 57, 106, 123	0
37	DR	117/117 (100%)	-0.18	0 100 100	34, 67, 108, 138	0
38	BS	99/99 (100%)	1.23	29 (29%) 0 0	41, 104, 177, 190	0
38	DS	99/99 (100%)	1.66	36 (36%) 0 0	44, 114, 168, 203	0
39	BT	138/138 (100%)	-0.27	3 (2%) 62 56	23, 68, 126, 162	0
39	DT	138/138 (100%)	-0.28	4 (2%) 51 45	25, 71, 133, 177	0
40	BU	117/117 (100%)	-0.11	1 (0%) 84 79	20, 45, 102, 140	0
40	DU	117/117 (100%)	0.09	4 (3%) 45 40	29, 54, 89, 222	0
41	BV	101/101 (100%)	0.29	8 (7%) 12 13	22, 58, 105, 172	0
41	DV	101/101 (100%)	0.10	8 (7%) 12 13	28, 60, 114, 177	0
42	BW	113/113 (100%)	-0.19	3 (2%) 54 48	14, 43, 101, 135	0
42	DW	113/113 (100%)	0.02	2 (1%) 68 62	11, 60, 133, 215	0
43	BX	93/93 (100%)	-0.50	0 100 100	16, 55, 107, 137	0
43	DX	93/93 (100%)	-0.69	0 100 100	16, 66, 134, 180	0
44	BY	107/107 (100%)	-0.12	4 (3%) 41 37	38, 88, 141, 193	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	DY	107/107 (100%)	0.19	10 (9%) 8 9	45, 96, 167, 200	0
45	BZ	185/185 (100%)	-0.57	1 (0%) 91 88	36, 70, 124, 167	0
45	DZ	185/185 (100%)	-0.58	4 (2%) 62 56	48, 82, 136, 193	0
46	B0	84/84 (100%)	-0.36	1 (1%) 79 73	24, 65, 112, 142	0
46	D0	84/84 (100%)	0.28	6 (7%) 16 15	47, 77, 140, 162	0
47	B2	71/71 (100%)	-0.30	1 (1%) 75 69	34, 64, 118, 140	0
47	D2	71/71 (100%)	-0.20	2 (2%) 53 47	33, 85, 127, 141	0
48	B3	60/60 (100%)	-0.03	2 (3%) 46 41	28, 61, 116, 135	0
48	D3	60/60 (100%)	0.07	3 (5%) 28 25	32, 73, 137, 160	0
49	B5	59/59 (100%)	-0.28	1 (1%) 70 64	22, 55, 125, 138	0
49	D5	59/59 (100%)	-0.08	2 (3%) 45 40	29, 75, 130, 161	0
50	B6	50/50 (100%)	-0.57	0 100 100	36, 74, 120, 139	0
50	D6	50/50 (100%)	0.15	4 (8%) 12 12	49, 81, 143, 164	0
51	B7	49/49 (100%)	-0.36	1 (2%) 65 60	43, 53, 102, 126	0
51	D7	49/49 (100%)	-0.30	4 (8%) 11 12	34, 61, 112, 165	0
52	B8	64/64 (100%)	-0.42	1 (1%) 72 66	22, 66, 108, 137	0
52	D8	64/64 (100%)	-0.14	3 (4%) 31 28	33, 70, 118, 139	0
53	B9	37/37 (100%)	-0.02	2 (5%) 25 23	39, 60, 122, 134	0
53	D9	37/37 (100%)	-0.42	1 (2%) 54 48	46, 60, 134, 159	0
54	Bf	0/31	-	-	-	-
54	Bg	0/31	-	-	-	-
54	Df	0/31	-	-	-	-
54	Dg	0/31	-	-	-	-
55	Bh	0/30	-	-	-	-
55	Dh	0/30	-	-	-	-
56	B1	93/93 (100%)	-0.16	5 (5%) 25 23	22, 78, 160, 236	0
56	D1	93/93 (100%)	0.18	10 (10%) 5 6	41, 89, 159, 194	0
57	B4	35/35 (100%)	1.25	8 (22%) 0 0	67, 116, 167, 189	0
57	D4	35/35 (100%)	1.54	10 (28%) 0 0	73, 136, 168, 196	0
58	Be	72/102 (70%)	1.53	23 (31%) 0 0	77, 113, 160, 174	0
58	De	72/102 (70%)	2.84	40 (55%) 0 0	87, 141, 192, 236	0
59	BA	2879/2879 (100%)	-0.59	11 (0%) 92 90	9, 59, 146, 260	0
59	DA	2879/2879 (100%)	-0.58	9 (0%) 94 91	5, 63, 160, 308	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
60	BB	119/119 (100%)	-0.57	1 (0%) 86 81	36, 103, 157, 192	0
60	DB	119/119 (100%)	-0.44	1 (0%) 86 81	33, 108, 159, 193	0
All	All	22726/23318 (97%)	-0.23	953 (4%) 36 32	0, 72, 150, 308	0

The worst 5 of 953 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
58	De	59	GLU	13.9
32	DK	62	ASP	13.5
59	DA	2799	A	12.6
58	De	55	GLU	12.1
25	DC	2	PRO	11.2

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
24	KBE	CU	1	9/10	0.85	0.34	118,118,118,118	0
24	UAL	AU	5	9/10	0.88	0.16	114,114,114,114	0
24	UAL	CU	5	9/10	0.90	0.13	118,118,118,118	0
24	KBE	AU	1	9/10	0.90	0.32	114,114,114,114	0
24	DPP	CU	2	6/7	0.92	0.18	118,118,118,118	0
24	5OH	AU	6	12/13	0.93	0.29	99,101,102,102	0
24	5OH	CU	6	12/13	0.93	0.21	99,101,102,102	0
24	DPP	AU	2	6/7	0.97	0.23	114,114,114,114	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

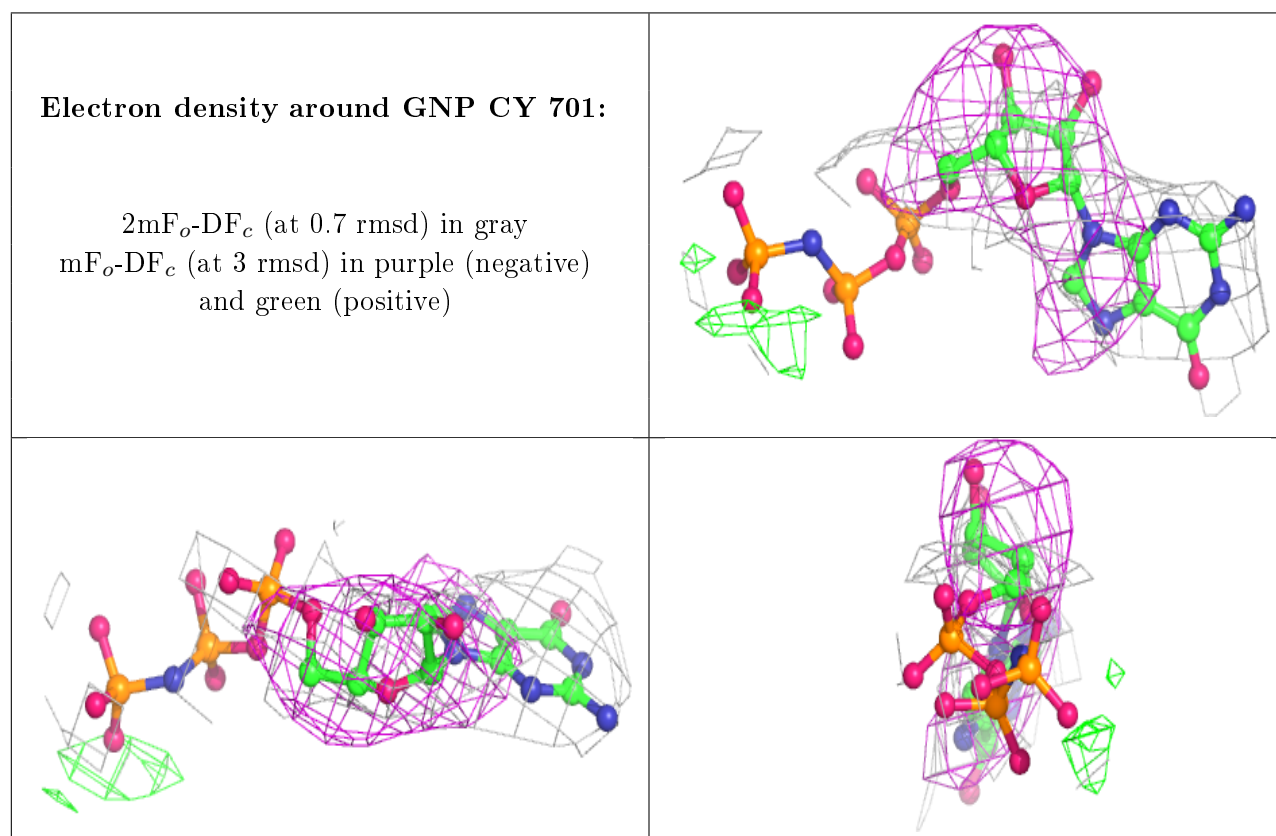
6.4 Ligands ⓘ

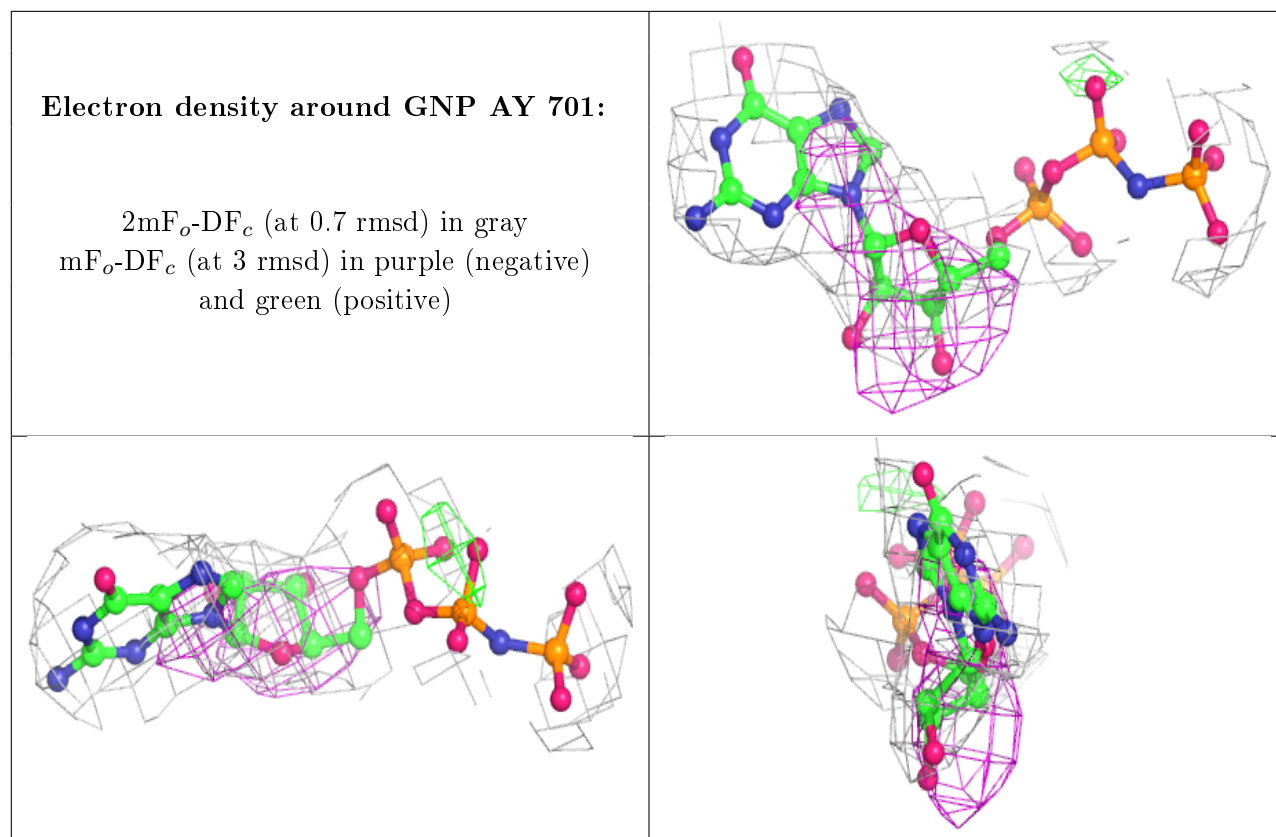
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
61	GNP	CY	701	32/32	0.91	0.23	58,71,81,83	0
61	GNP	AY	701	32/32	0.92	0.22	58,71,81,83	0
62	MG	CY	702	1/1	0.97	0.11	135,135,135,135	0
62	MG	AY	702	1/1	0.98	0.11	88,88,88,88	0

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





6.5 Other polymers [i](#)

There are no such residues in this entry.