



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 29, 2025 – 07:50 PM EDT

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

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0rc1
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

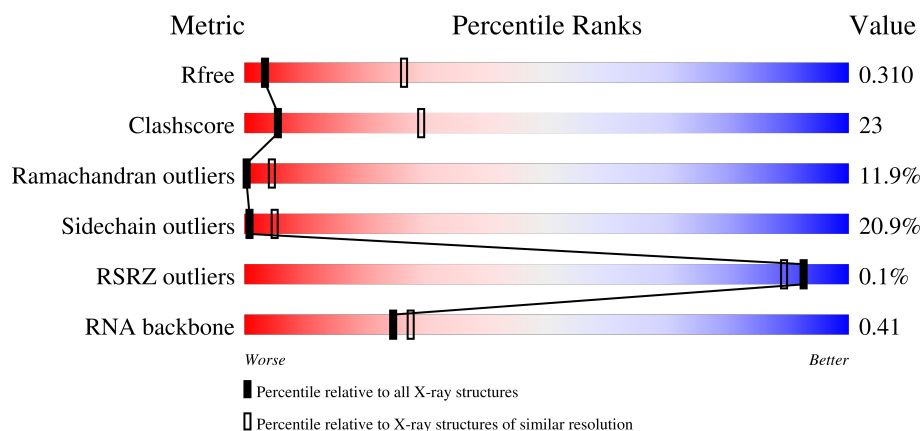
1 Overall quality at a glance

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.




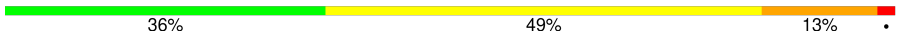
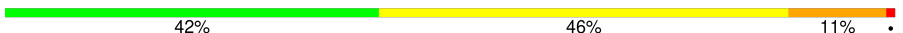


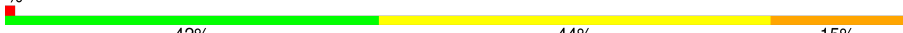
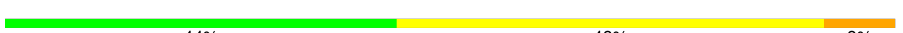




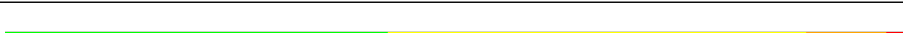













Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1094 (3.56-3.44)
Clashscore	180529	1045 (3.54-3.46)
Ramachandran outliers	177936	1032 (3.54-3.46)
Sidechain outliers	177891	1033 (3.54-3.46)
RSRZ outliers	164620	1093 (3.56-3.44)
RNA backbone	3690	1089 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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



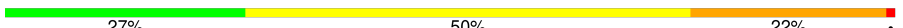

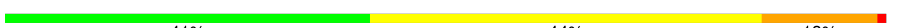
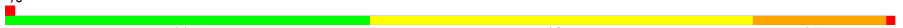







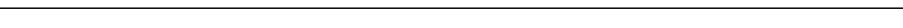



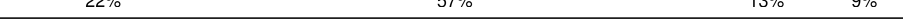
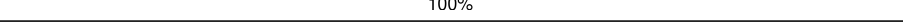






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Mol	Chain	Length	Quality of chain
3	AD	208	
3	CD	208	
4	AE	151	
4	CE	151	
5	AF	101	
5	CF	101	
6	AG	155	
6	CG	155	
7	AH	138	
7	CH	138	
8	AI	127	
8	CI	127	
9	AJ	99	
9	CJ	99	
10	AK	119	
10	CK	119	
11	AL	125	
11	CL	125	
12	AM	125	
12	CM	125	
13	AN	60	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


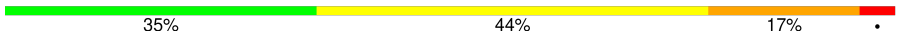
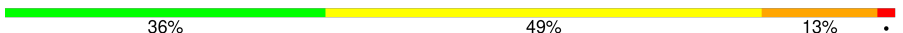


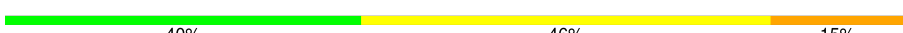





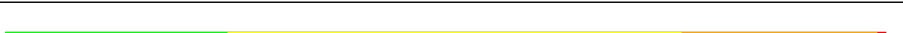



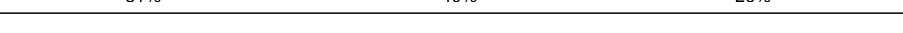
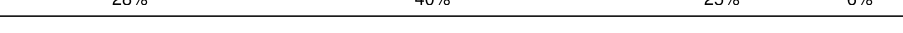
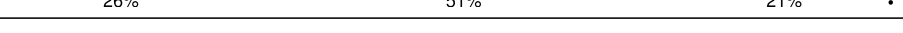



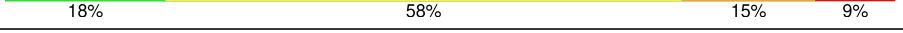

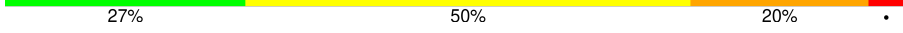

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Mol	Chain	Length	Quality of chain
15	CP	84	
16	AQ	100	
16	CQ	100	
17	AR	70	
17	CR	70	
18	AS	79	
18	CS	79	
19	AT	99	
19	CT	99	
20	AY	687	
20	CY	687	
21	AA	1511	
21	CA	1511	
22	AW	77	
22	CW	77	
23	AV	23	
23	CV	23	
24	AU	6	
24	CU	6	
25	BC	228	
25	DC	228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



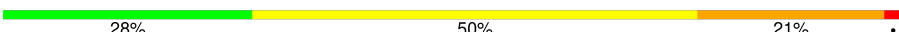

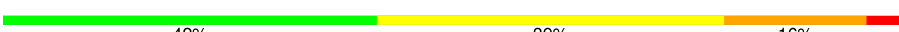
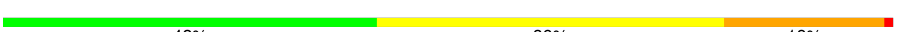
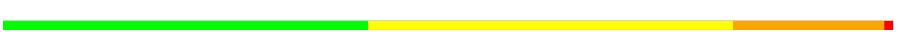





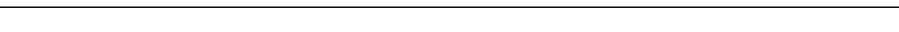

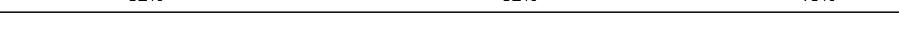

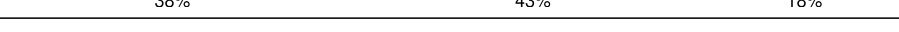







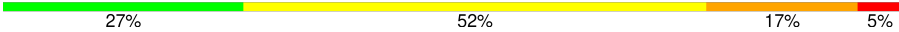
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Mol	Chain	Length	Quality of chain
28	BF	208	
28	DF	208	
29	BG	181	
29	DG	181	
30	BH	167	
30	DH	167	
31	BJ	170	
31	DJ	170	
32	BK	140	
32	DK	140	
33	BN	138	
33	DN	138	
34	BO	122	
34	DO	122	
35	BP	146	
35	DP	146	
36	BQ	141	
36	DQ	141	
37	BR	117	
37	DR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



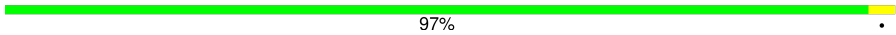



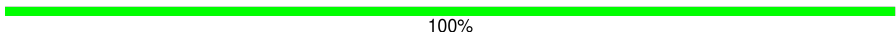

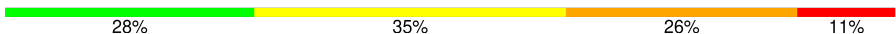

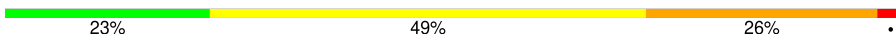
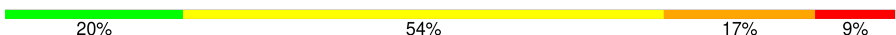






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Mol	Chain	Length	Quality of chain
40	DU	117	 41% 42% 15% .
41	BV	101	 30% 50% 16% .
41	DV	101	 28% 50% 21% .
42	BW	113	 34% 48% 16% .
42	DW	113	 42% 39% 16% .
43	BX	93	 42% 39% 18% .
43	DX	93	 41% 41% 17% .
44	BY	107	 27% 49% 21% .
44	DY	107	 36% 39% 21% .
45	BZ	185	 38% 44% 16% .
45	DZ	185	 34% 48% 15% .
46	B0	84	 35% 55% 11%
46	D0	84	 40% 52% 6% .
47	B2	71	 32% 52% 15%
47	D2	71	 44% 44% 11% .
48	B3	60	 38% 43% 18%
48	D3	60	 37% 48% 15%
49	B5	59	 34% 51% 14% .
49	D5	59	 42% 47% 10%
50	B6	50	 20% 52% 22% 6%
50	D6	50	 16% 46% 34% .
51	B7	49	 39% 47% 14%
51	D7	49	 45% 43% 12%
52	B8	64	 27% 52% 17% 5%
52	D8	64	 33% 48% 12% 6%

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Mol	Chain	Length	Quality of chain
53	B9	37	
53	D9	37	
54	Bf	31	
54	Bg	31	
54	Df	31	
54	Dg	31	
55	Bh	30	
55	Dh	30	
56	B1	93	
56	D1	93	
57	B4	35	
57	D4	35	
58	Be	102	
58	De	102	
59	BA	2879	
59	DA	2879	
60	BB	119	
60	DB	119	

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

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

2 Entry composition

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 20 is a protein called Elongation factor G.

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

- Molecule 22 is a RNA chain called transfer RNA.

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

- Molecule 23 is a RNA chain called messenger RNA.

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

- Molecule 24 is a protein called VIOMYCIN.

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

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

There are 10 discrepancies between the modelled and reference sequences:

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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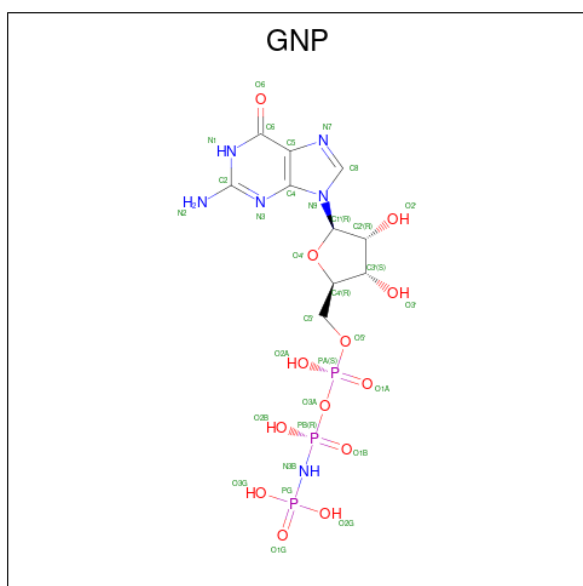
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	DA	2879	Total	C	N	O	P	0	0	0
			61997	27594	11582	19943	2878			

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

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

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



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

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

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

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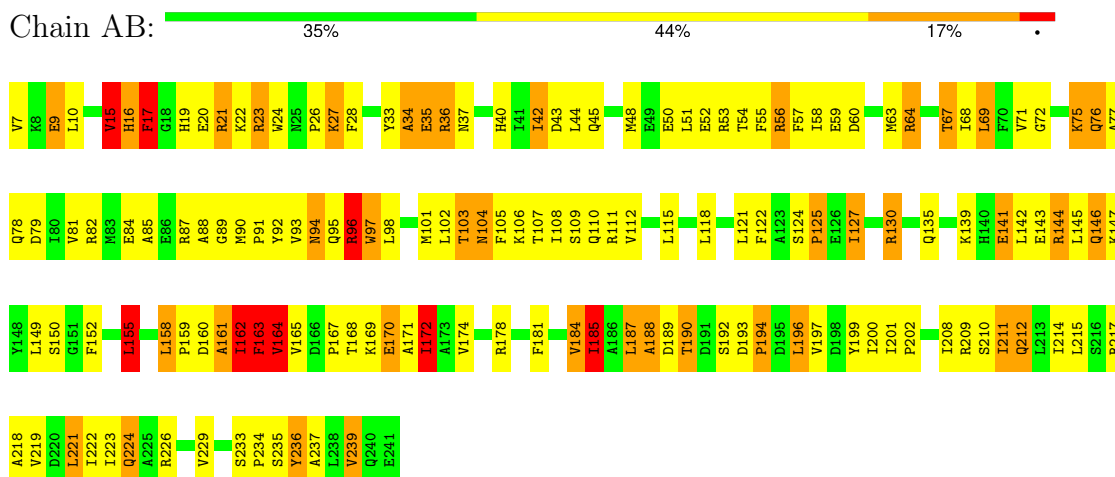
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	CY	1	Total	Mg	0	0
			1	1		

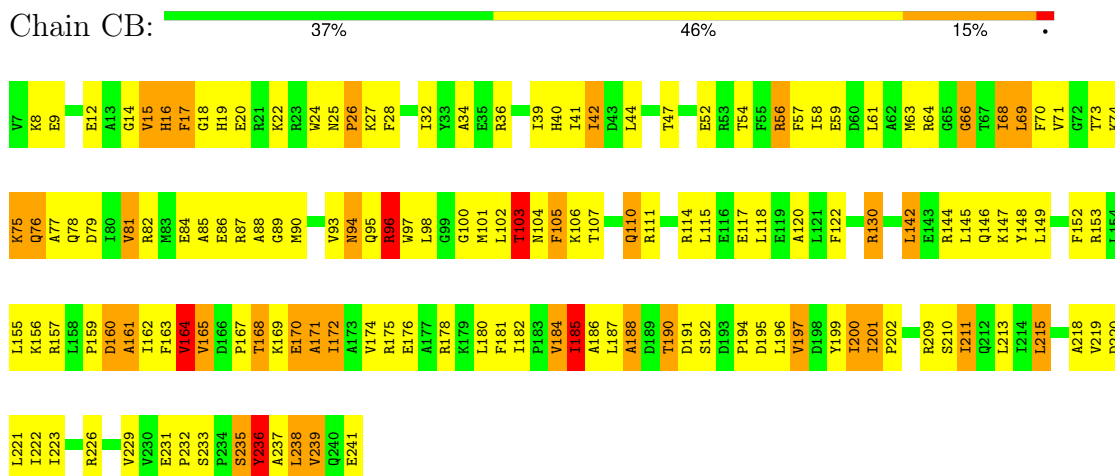
3 Residue-property plots

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

• Molecule 1: 30S ribosomal protein S2

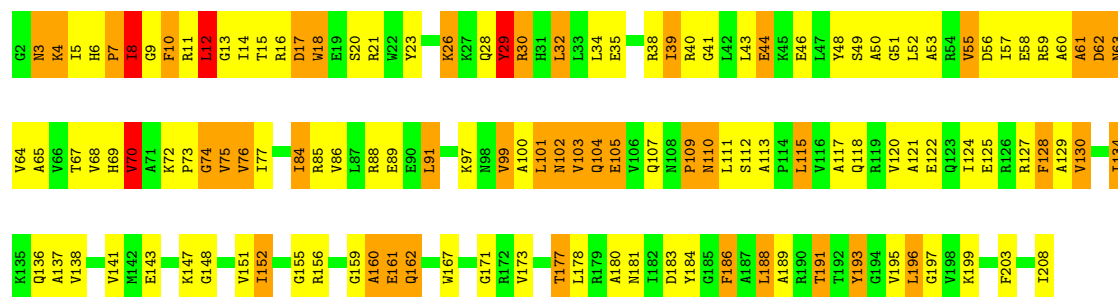


• Molecule 1: 30S ribosomal protein S2



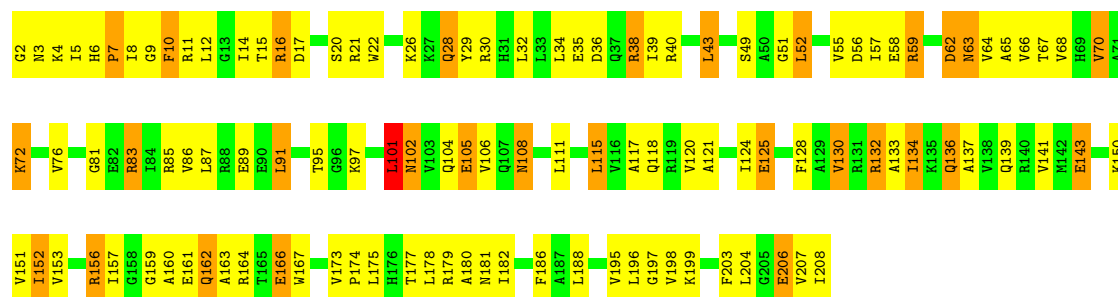
• Molecule 2: 30S ribosomal protein S3





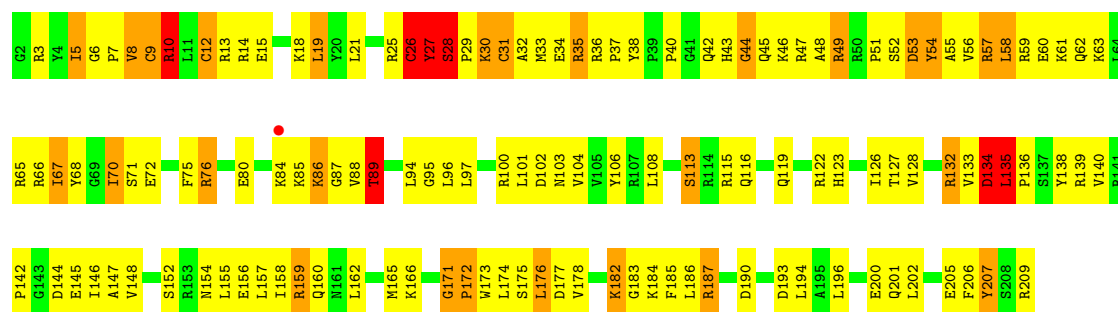
• Molecule 2: 30S ribosomal protein S3

Chain CC: 44% 42% 14%



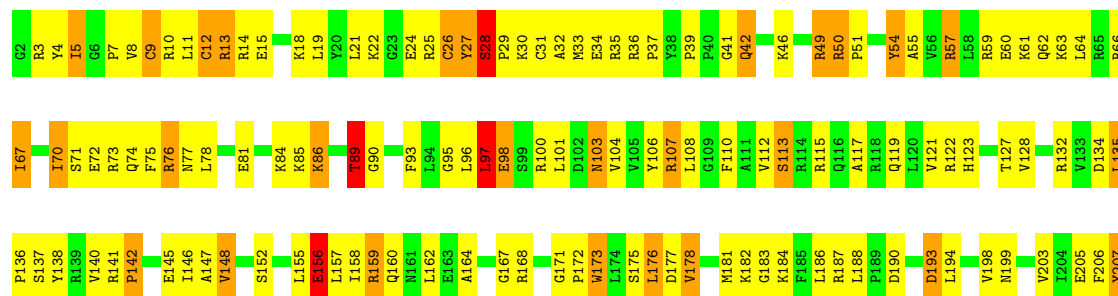
• Molecule 3: 30S ribosomal protein S4

Chain AD: 35% 49% 13%



• Molecule 3: 30S ribosomal protein S4

Chain CD: 36% 49% 13%



S208
R209

- Molecule 4: 30S ribosomal protein S5

Chain AE:  42% 46% 11%

P5 F6 I11 I12 I13 I14 I15 I16 I17 I18 I19 I20 I21 I22 I23 I24 I25 I26 I27 I28 L31 L32 V33 V34 G35 D36 R37 R38 Q38 R39 R40 V41 R47 A48 P49 E50 V51 P52 Y60 R64 V67 E68 V69 N73 G74 T75 T76 P77 H78 E79 I80 E83 F84

G85 A86 S87 K88 I89 V90 L91 K92 P93 A94 A95 Q96 P97 Q98 T98 G99 F96 G23 I101 A102 G103 A104 V105 Q106 R107 T108 I109 L110 E111 L112 V115 T116 D117 I118 T119 S125 R126 N127 P128 I131 T135 M136 E137 A138 L139 R140 Q141 L142 R143 T144 K145 A146 D147 V148 R149 L151

R152 K153 G154 E155

- Molecule 4: 30S ribosomal protein S5

Chain CE:  52% 34% 15%

D5 F6 E7 I11 I12 I13 T16 M19 Q20 A21 R25 F26 G27 F28 G29 A30 L31 D36 R37 R40 V41 F45 G46 E50 V51 P52 A58 G59 Y60 R64 V67 E68 N73 I76 H78 E79 I80 E81 V82 S87 K88 L91 R92 P93 A94

G97 T98 V100 I101 A102 G103 A104 V105 Q106 R107 L112 A113 G114 D117 T118 L119 T120 K121 E122 L123 R126 N127 P128 T129 I131 A132 A134 T135 M136 E137 L142 R143 T144 K145 A146 D147 V148 E149 K153 G154 E155

- Molecule 5: 30S ribosomal protein S6

Chain AF:  40% 44% 16%

M1 R2 E5 V6 M11 L14 D15 Q16 S17 Q18 L19 A20 E22 K23 E24 I25 I26 Q27 R28 A29 I30 E31 N32 A35 E38 K39 V40 E41 E42 L43 G44 L45 R46 R47 Y50 P51 I52 A53 F60 L61 W62 Y63 Q64 V65 E66 E69 D70 R71 V72 L75

A76 R77 E78 L79 R80 I81 R82 R86 R87 V88 M89 V90 V91 S93 Q94 E95 P96 F97 L98 A99 N100 A101

- Molecule 5: 30S ribosomal protein S6

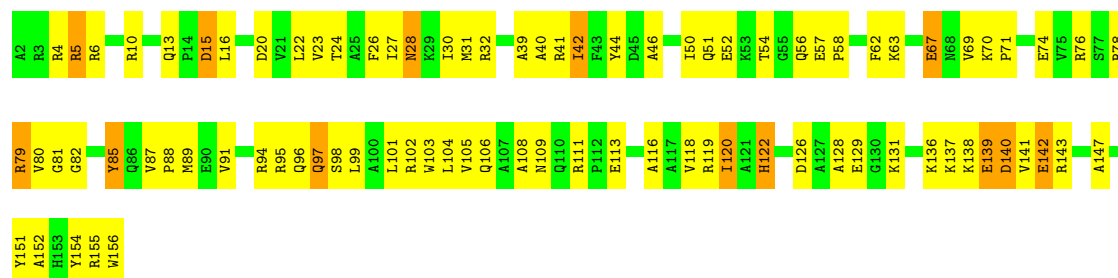
Chain CF:  42% 44% 15%

M1 R2 E5 V6 M11 L14 D15 Q16 S17 Q18 L21 E22 K23 E24 R28 A35 R36 V37 E38 K39 V40 G44 L45 R46 R47 L48 A49 Y50 P51 I52 A53 P56 Q57 G58 Y59 F60 L61 W62 Y63 Q64 V65 E66 E69 D70 R71 V72 N73

D74 L75 A76 R79 R80 I81 R82 R86 R87 V88 M89 V90 V91 S93 Q94 E95 P96 A99 N100 A101

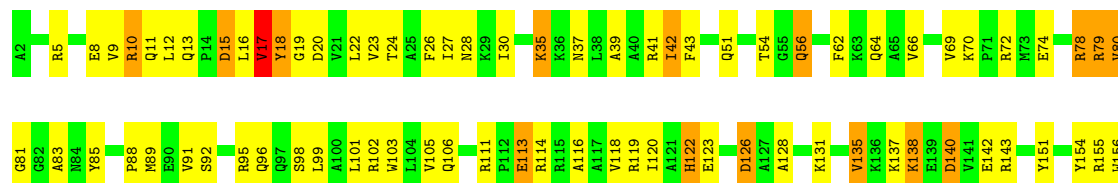
- Molecule 6: 30S ribosomal protein S7

Chain AG:  44% 48% 8%



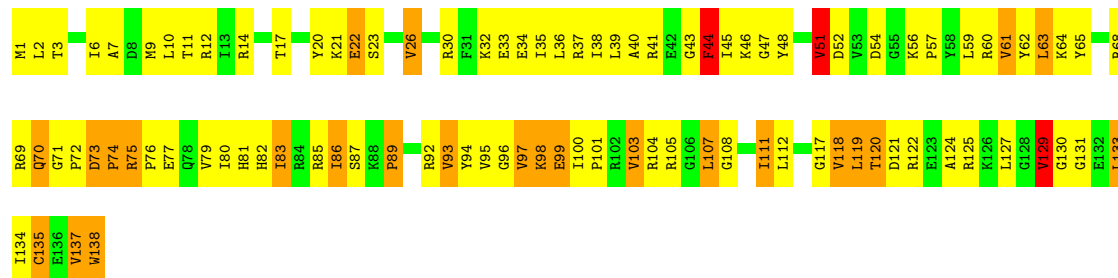
• Molecule 6: 30S ribosomal protein S7

Chain CG: 50% 39% 10% .



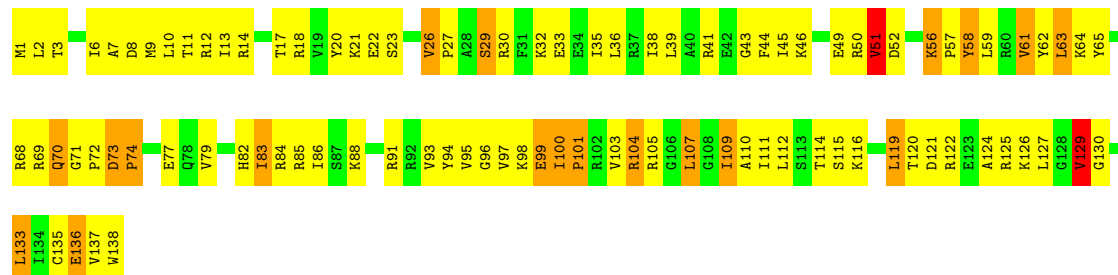
• Molecule 7: 30S ribosomal protein S8

Chain AH: 29% 51% 18% .



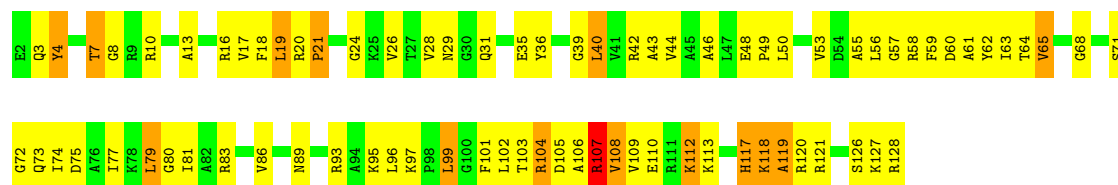
• Molecule 7: 30S ribosomal protein S8

Chain CH: 30% 55% 14% .



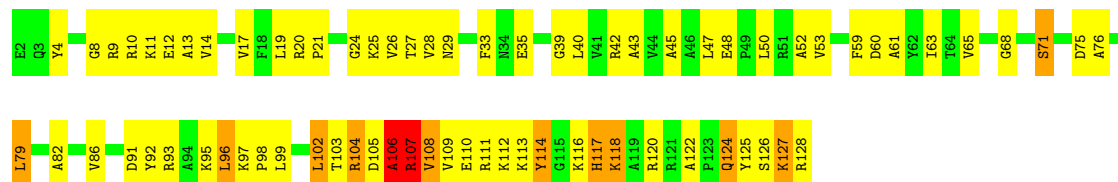
• Molecule 8: 30S ribosomal protein S9

Chain AI: 39% 50% 11% .



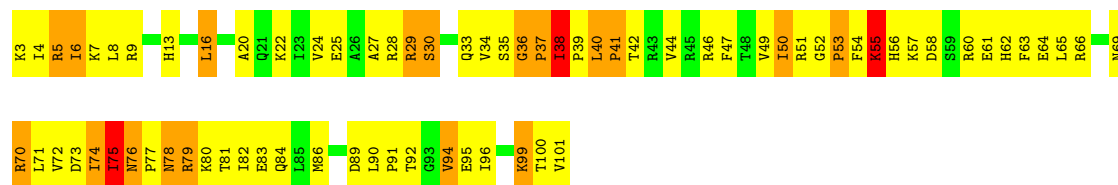
• Molecule 8: 30S ribosomal protein S9

Chain CI: 43% 47% 9% .



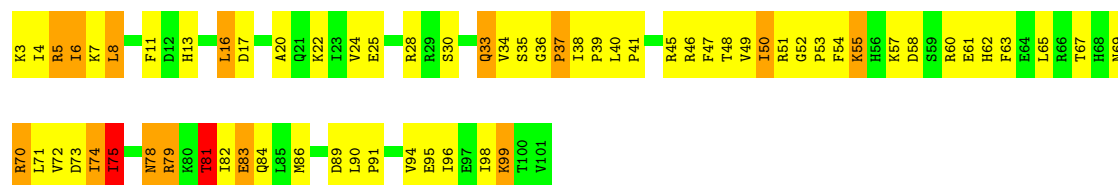
• Molecule 9: 30S ribosomal protein S10

Chain AJ: 25% 54% 18% .



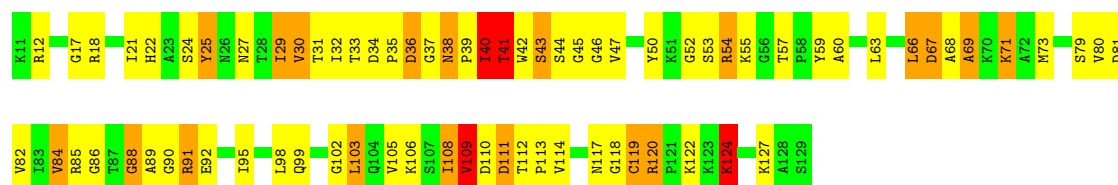
• Molecule 9: 30S ribosomal protein S10

Chain CJ: 33% 51% 14% .



• Molecule 10: 30S ribosomal protein S11

Chain AK: 37% 44% 16% .

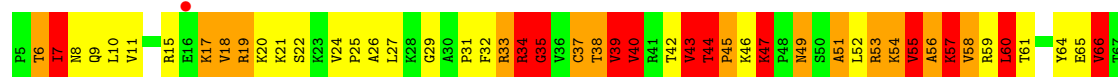
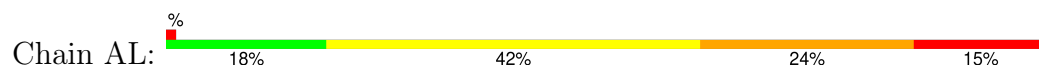


• Molecule 10: 30S ribosomal protein S11

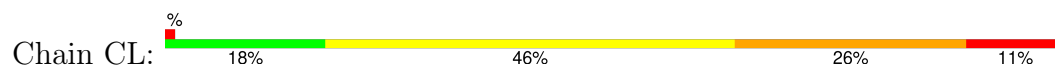
Chain CK: 2% 45% 39% 15% .



• Molecule 11: 30S ribosomal protein S12



• Molecule 11: 30S ribosomal protein S12



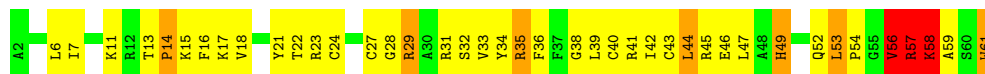
• Molecule 12: 30S ribosomal protein S13



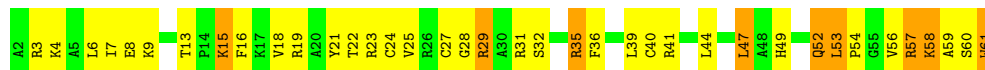
• Molecule 12: 30S ribosomal protein S13



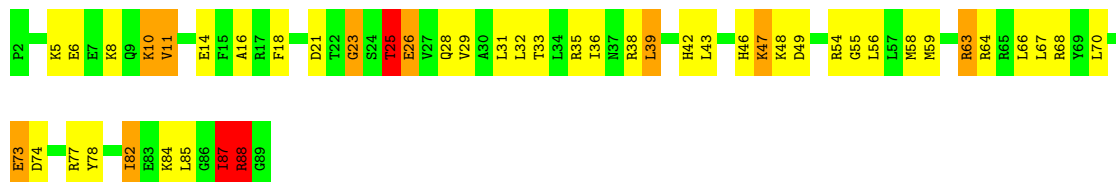
• Molecule 13: 30S ribosomal protein S14 type Z

Chain AN:  32% 52% 12% 5%

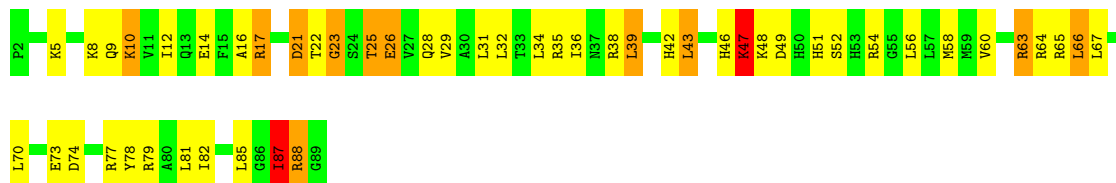
• Molecule 13: 30S ribosomal protein S14 type Z

Chain CN:  37% 48% 15%

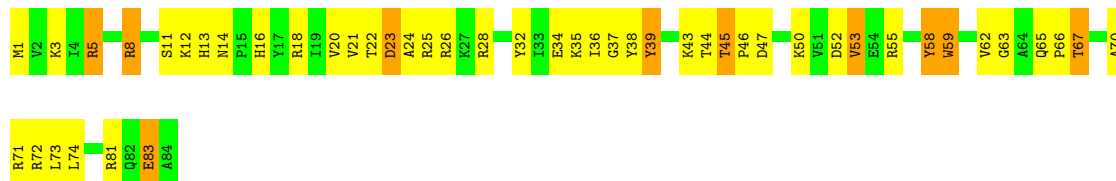
• Molecule 14: 30S ribosomal protein S15

Chain AO:  47% 40% 10% 3%

• Molecule 14: 30S ribosomal protein S15

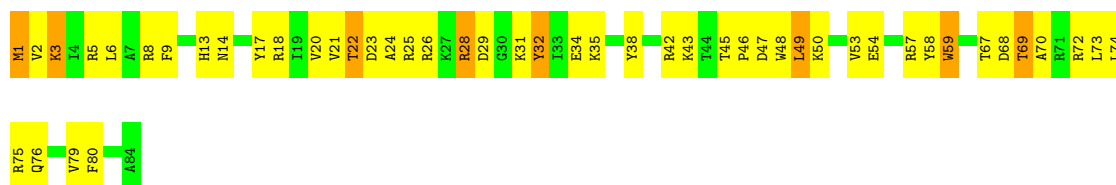
Chain CO:  43% 42% 13% 2%

• Molecule 15: 30S ribosomal protein S16

Chain AP:  43% 45% 12%

• Molecule 15: 30S ribosomal protein S16

Chain CP:  42% 49% 10%



- Molecule 16: 30S ribosomal protein S17



- Molecule 16: 30S ribosomal protein S17



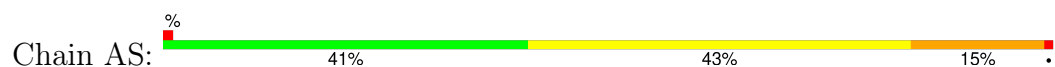
- Molecule 17: 30S ribosomal protein S18

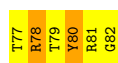


- Molecule 17: 30S ribosomal protein S18



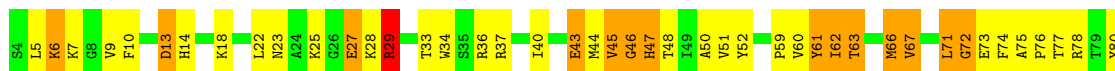
- Molecule 18: 30S ribosomal protein S19





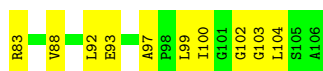
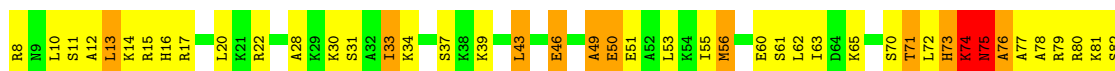
• Molecule 18: 30S ribosomal protein S19

Chain CS: 42% 39% 18% .



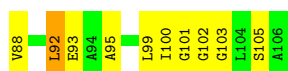
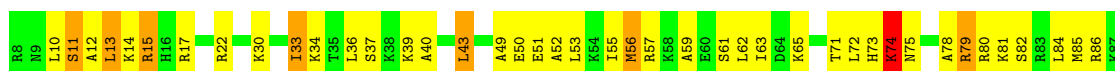
• Molecule 19: 30S ribosomal protein S20

Chain AT: 45% 42% 10% .



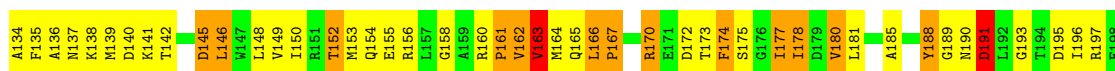
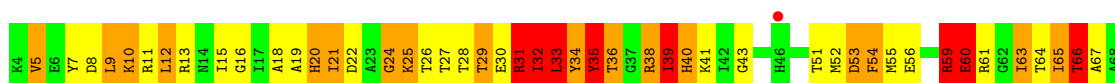
• Molecule 19: 30S ribosomal protein S20

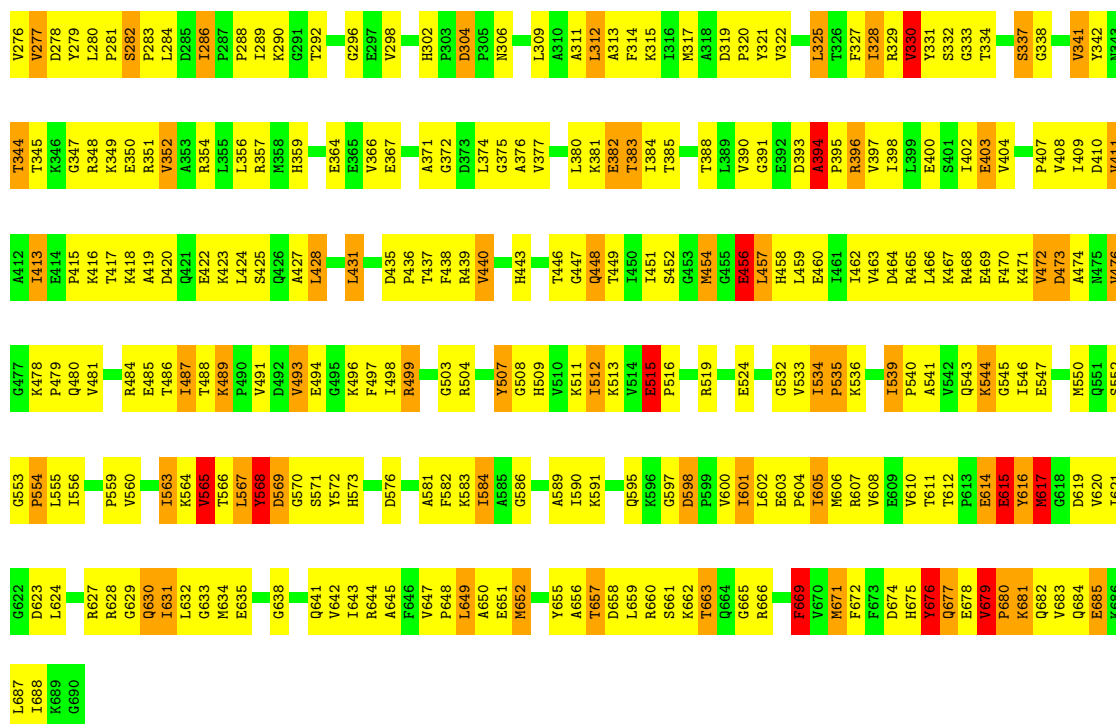
Chain CT: 47% 43% 8% .



• Molecule 20: Elongation factor G

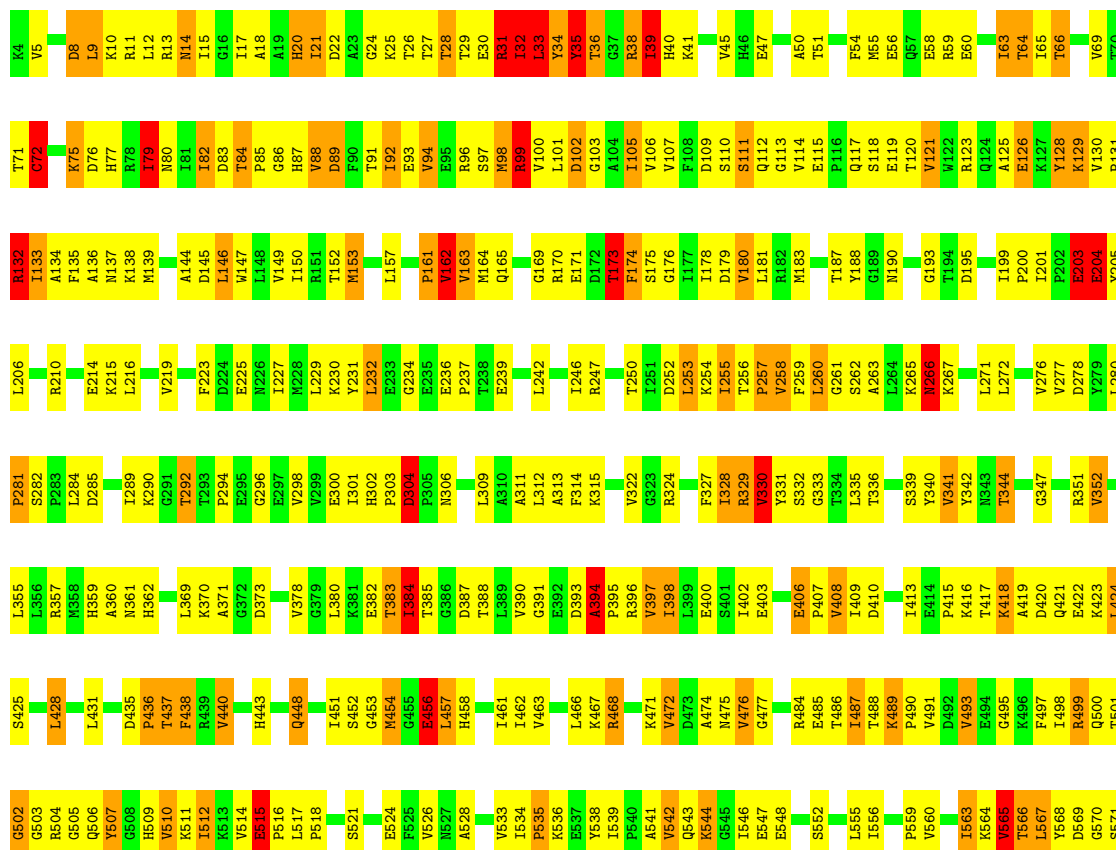
Chain AY: 33% 47% 16% .





● Molecule 20: Elongation factor G

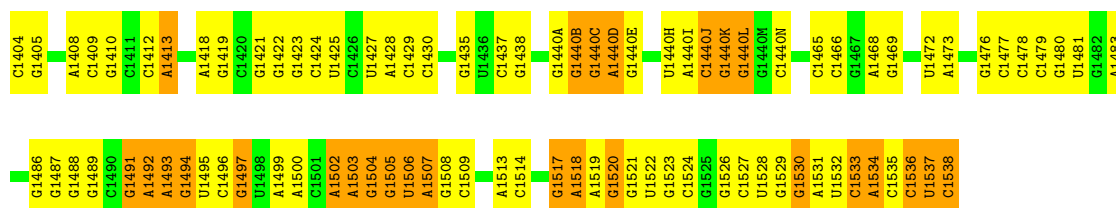
Chain CY: 37% 45% 14% ●



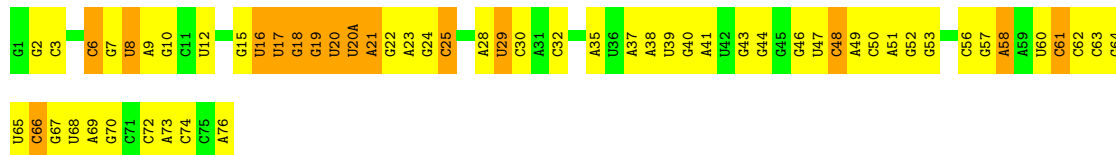




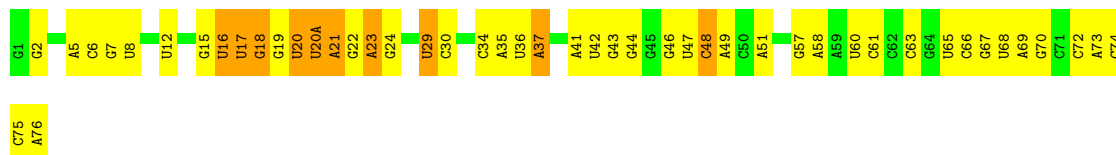
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U1341	C295	C442	A532	C443	A533	U603	C880	U757	G829	A907	G976	G1131	U1212	U1278	U1341
G1342	U296	C444	A534	C445	U534	G604	C887	G758	U833	A908	A977	G1134	A1213	A1278	G1342
G1343	G297	G604	U535	G445	G605	U605	G888	C762	C834	A909	A978	U1135	C1214	A1279	G1343
U1344	A298	G446	C536	G445	G606	U606	G889	C763	U835	C910	C979	U1136	G1215	U1281	U1344
A1345	G299	G447	G537	G446	G607	U607	C890	C764	G836	U911	C980	U1137	C1217	U1282	U1345
G1346	A300	A448	G538	G448	A608	A609	G891	C765	G837	C912	U981	U1138	C1218	G1283	G1346
G1347	G301	A452	G541	A453	G542	A610	U692	A766	G838	G916	C985	G1139	C1219	G1284	G1347
U1348	G302	A454	G543	A455	G544	G612	U693	A767	U838A	G917	A986	C1140	G1220	A1285	U1348
A1349	G305	A457	G545	A458	G546	C613	A694	A768	C838B	A918	U992	C1141	G1221	A1286	A1349
A1350	G306	C457	G547	C458	G548	C614	A695	C769	U838C	A919	U993	G1142	G1222	A1287	A1350
U1351	G307	C459	G549	C460	G550	A615	A696	C770	C848	U920	A994	G1143	G1223	A1288	U1351
C1352	C308	C461	G551	C462	G552	A616	U697	G771	C849	U921	C995	U1144	G1224	A1289	C1352
G1353	C309	C463	G553	C464	G554	G617	C701	G772	U850	G922	U999	G1145	A1225	G1290	G1353
U1354	G310	C465	G555	C466	G556	C620	A702	G773	G851	A923	A1000	C1063	A1226	G1291	G1354
C1355	C311	C467	G557	C468	G558	A621	G703	G774	G852	C924	A1001	U1085	A1227	U1292	U1355
U1356	C312	C469	G559	C470	G560	U628	A704	G775	U853	C925	G1002	G1088	C1228	U1293	C1356
A1357	A313	C471	G561	C472	G562	U634	G705	G776	A854	G926	G1003	U1089	A1229	G1294	C1357
U1358	C314	C473	G563	C474	G564	U635	A706	G777	A855	U927	G1004	C1090	A1230	G1295	U1358
C1359	A315	C475	G565	C476	G566	U636	G707	G778	A856	C928	A1005	U1091	G1231	G1296	C1359
U1360	G316	C477	G567	C478	G568	U637	G708	G779	C857	G929	U1006	A1080	G1232	C1298	U1360
G1361	C321	C479	G569	C480	G570	U638	A709	G780	U858	C933	C1007	A1157	U1233	G1299	G1361
U1362	G322	C481	G571	C482	G572	U639	G710	G781	A859	G934	C1008	C1086	U1234	G1300	C1362
C1363	C323	C483	G573	C484	G574	U640	G711	G782	A860	C935	C1009	U1088	A1235	U1301	U1363
U1364	U323	C485	G575	C486	G576	U641	A712	G783	C858	A936	G1010	U1089	A1236	U1302	U1364
G1365	G324	C487	G577	C488	G578	U642	G713	G784	C859	U937	C1011	U1090	A1237	U1303	G1365
C1366	A325	C489	G579	C490	G580	U643	G714	G785	C860	A938	G1012	U1091	C1237	G1304	C1366
G1367	G326	C491	G581	C492	G582	U644	A715	G786	C861	U939	U1017	U1092	A1238	U1305	G1367
C1368	C327	C493	G583	C494	G584	U645	A716	G787	C862	C940	G1013	G1089	A1239	A1306	C1368
U1369	A328	C495	G585	C496	G586	U646	C717	G788	U863	C941	G1014	G1171	G1240	G1307	G1369
G1370	C329	C497	G587	C498	G588	U647	G718	G789	A871	G942	A1015	C1172	G1241	U1372	U1370
U1371	A330	C499	G589	C500	G590	U648	A719	G790	A872	U943	A1016	G1173	A1245	G1373	U1371
C1372	G331	C501	G591	C502	G592	U649	G720	G791	A873	U944	C1017	G1174	C1246	A1374	C1372
U1373	C332	C503	G593	C504	G594	U650	G721	G792	C874	G945	C1018	G1175	A1247	U1375	U1373
G1374	G333	C505	G595	C506	G596	U651	G722	G793	C875	A946	C1019	G1176	A1248	U1376	G1374
U1375	A338	C507	G597	C508	G598	U652	G723	G794	C876	U947	U1020	G1177	A1249	U1377	U1375
C1376	C339	C509	G599	C510	G600	U653	G724	G795	C877	C947	G1021	G1178	A1250	G1378	C1376
U1377	U340	C511	G601	C512	G602	U654	G725	G796	C878	G948	G1022	G1179	A1251	G1379	U1377
G1378	C341	C513	G603	C514	G604	U655	G726	G797	C879	U950	G1023	G1180	A1252	U1380	G1378
U1379	C342	C515	G605	C516	G606	U656	G727	G798	C880	G951	G1024	G1181	A1253	A1381	U1379
C1380	C343	C517	G607	C518	G608	U657	G728	G799	C881	U952	G1025	G1182	A1254	C1382	C1380
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G1382	G346	C521	G611	C522	G612	U659	G730	G801	C883	G954	G1027	G1184	G1255	C1321	G1382
C1383	C347	C523	G613	C524	G614	U660	G731	G802	U884	U955	G1028	G1185	A1256	C1322	C1383
U1384	U421	C525	G615	C526	G616	U661	G732	G803	U885	U956	C1028A	G1186	A1257	C1323	U1384
G1385	C422	C527	G617	C528	G618	U662	G733	G804	G886	U957	C1028B	G1187	U1257	G1324	G1385
C1386	G423	C529	G619	C530	G620	U663	G734	G805	U887	U958	C1028C	G1188	G1258	A1324	C1386
G1387	G424	C531	G621	C532	G622	U664	G735	G806	U888	U959	G1028D	G1189	G1259	C1325	G1387
U1391	U427	C533	G623	C534	G624	U665	G736	G807	U889	U960	C1028E	G1190	C1260	C1326	U1391
C1392	C435	C535	G625	C536	G626	U666	G737	G808	U890	U961	G1028F	G1191	A1261	C1327	C1392
U1393	U437	C537	G627	C538	G628	U667	G738	G809	U891	C962	G1028G	G1192	C1262	C1328	U1393
A1394	A360	C539	G629	C540	G630	U668	G739	G810	U892	G963	G1028H	G1193	C1263	A1329	U1394
C1395	G361	C541	G631	C542	G632	U669	G740	G811	U893	C964	G1028I	G1194	C1264	U1330	C1395
G1396	C362	C543	G633	C544	G634	U670	G741	G812	U894	C965	G1028J	G1195	G1265	G1331	G1396
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C1398	U438	C547	G637	C548	G638	U672	G743	G814	U896	C967	G1028L	G1197	A1267	G1333	U1397
G1399	A441	C549	G639	C550	G640	U673	G744	G815	U897	C968	G1028M	G1198	C1267	A1334	A1398
C1400	U439	C551	G641	C552	G642	U674	G745	G816	U898	C969	G1028N	G1199	C1268	G1335	C1399
U1401	A363	C553	G643	C554	G644	U675	G746	G817	U899	C970	G1028O	G1200	C1269	U1269	C1400
G1402	C355	C555	G645	C556	G646	U676	G747	G818	U900	C971	G1028P	G1201	C1270	G1401	G1402
C1403	U437	C557	G647	C558	G648	U677	G748	G819	A901	C972	G1028Q	G1202	C1271	G1402	C1403
U438	A364	C559	G649	C560	G650	U678	G749	G820	G902	C973	G1028R	G1203	C1272	G1338	U438
A440	G362	C561	G651	C562	G652	U679	G750	G821	G903	A974	G1028S	G1204	C1273	A1339	A440



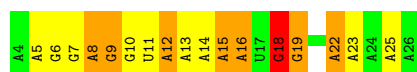
- Molecule 22: transfer RNA



- Molecule 22: transfer RNA



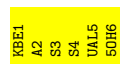
- Molecule 23: messenger RNA



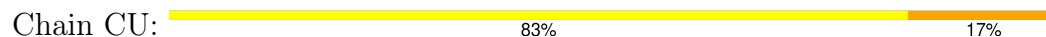
- Molecule 23: messenger RNA



- Molecule 24: VIOMYCIN



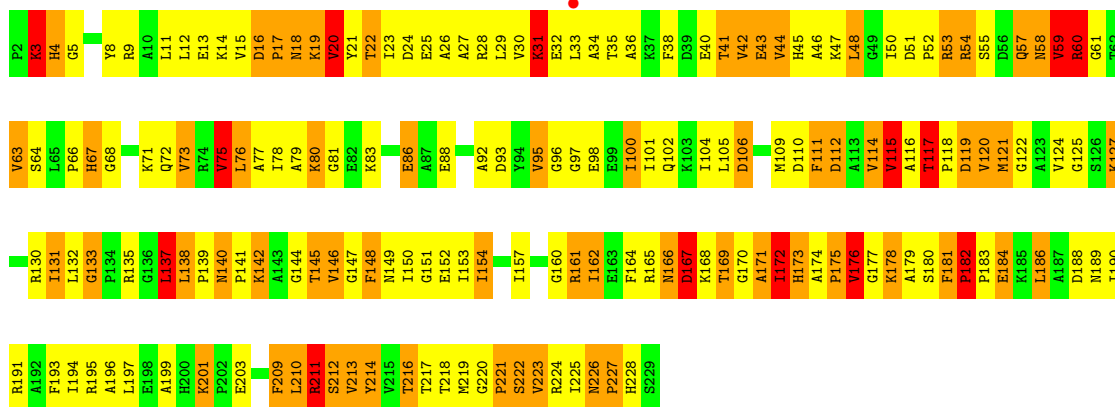
- Molecule 24: VIOMYCIN



KBEL
A2
S3
S4
UAI5
50H6

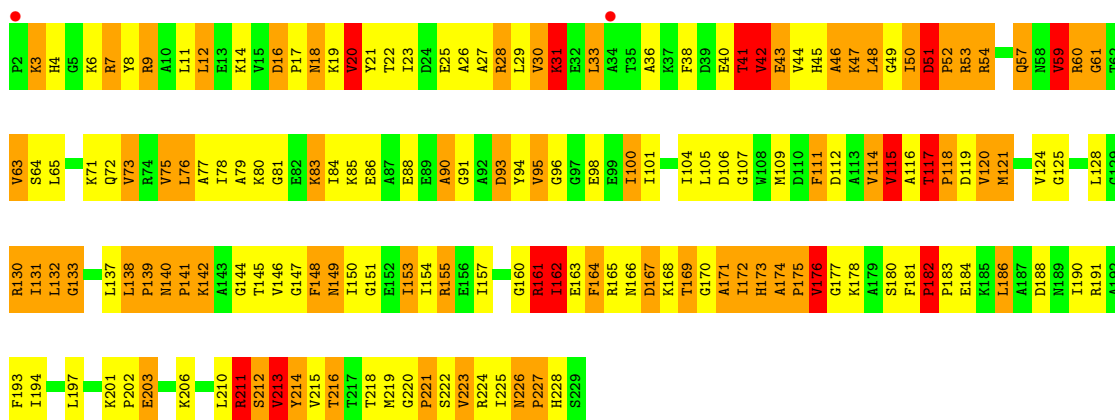
• Molecule 25: 50S ribosomal protein L1

Chain BC: 22% 44% 28% 6%



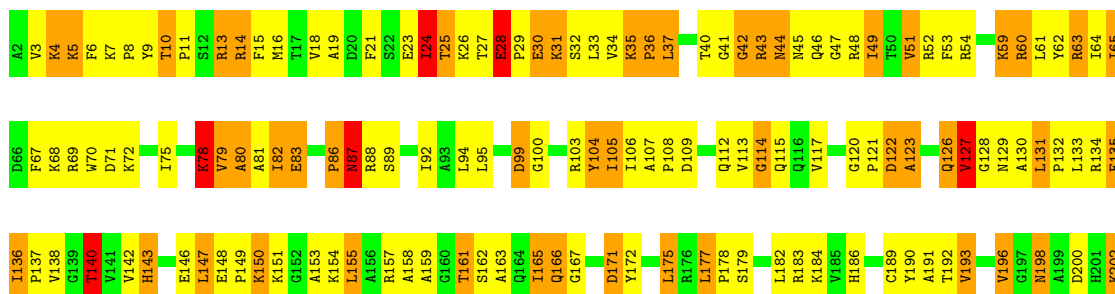
• Molecule 25: 50S ribosomal protein L1

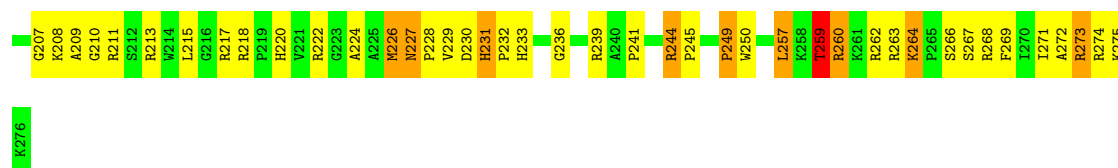
Chain DC: 27% 39% 28% 6%



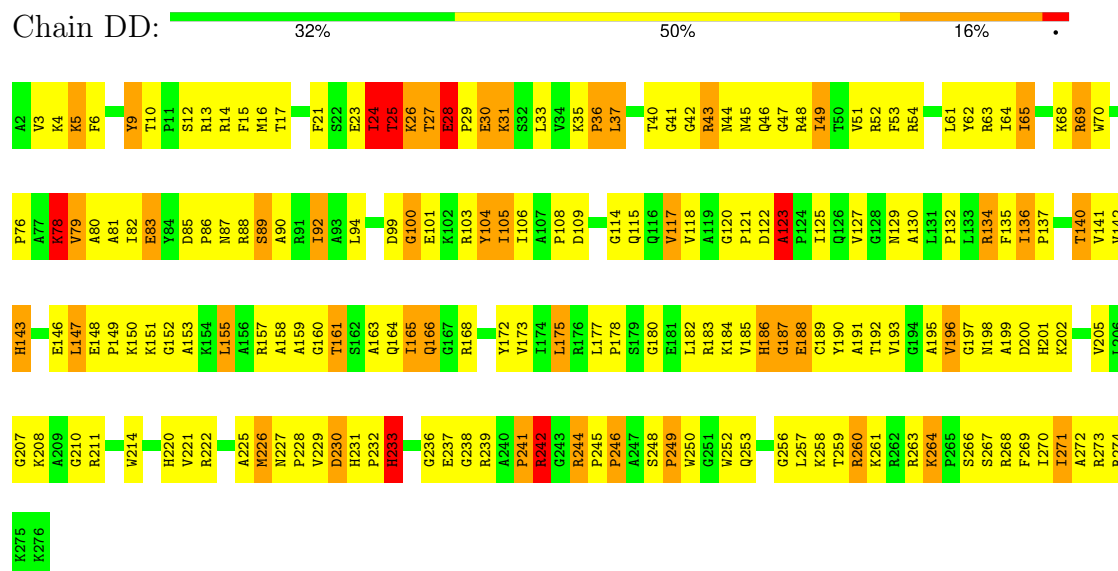
• Molecule 26: 50S ribosomal protein L2

Chain BD: 33% 44% 21% 6%

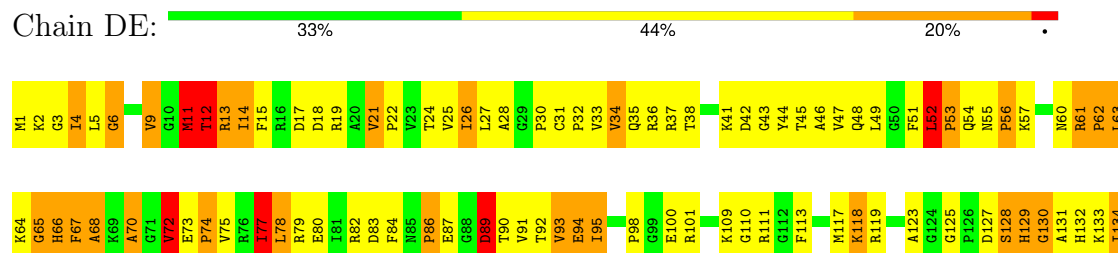
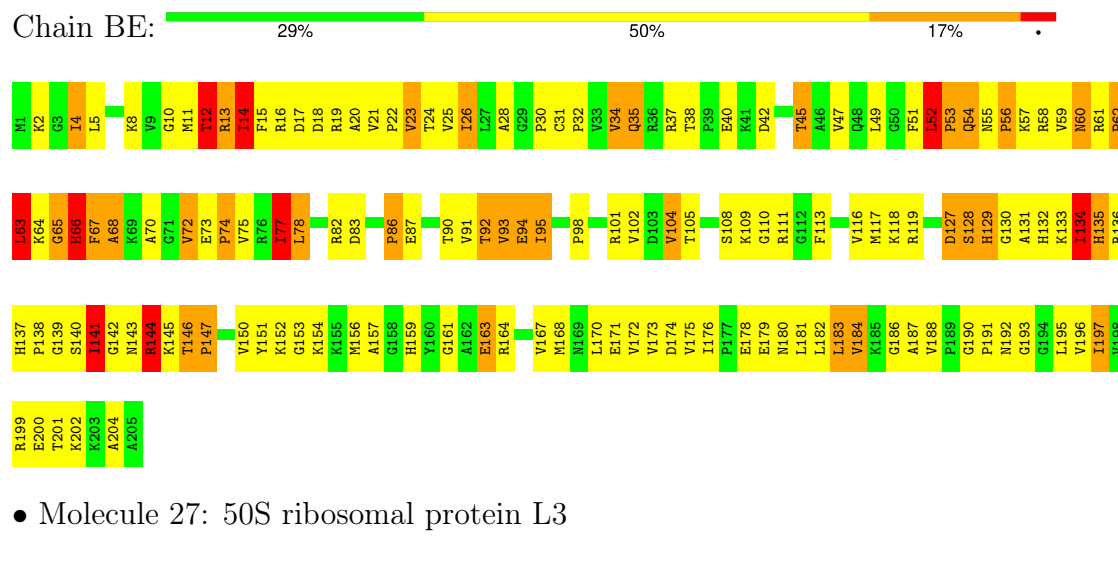




- Molecule 26: 50S ribosomal protein L2



- Molecule 27: 50S ribosomal protein L3

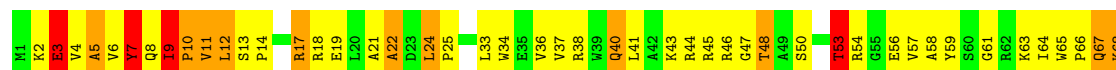




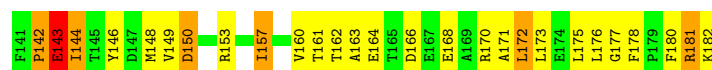
• Molecule 28: 50S ribosomal protein L4



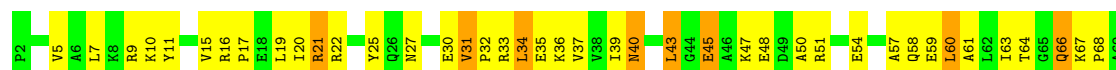
• Molecule 28: 50S ribosomal protein L4

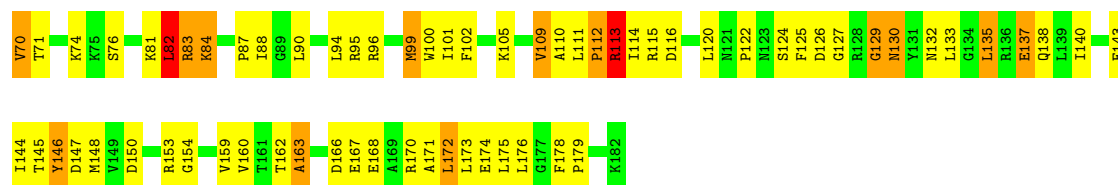


• Molecule 29: 50S ribosomal protein L5



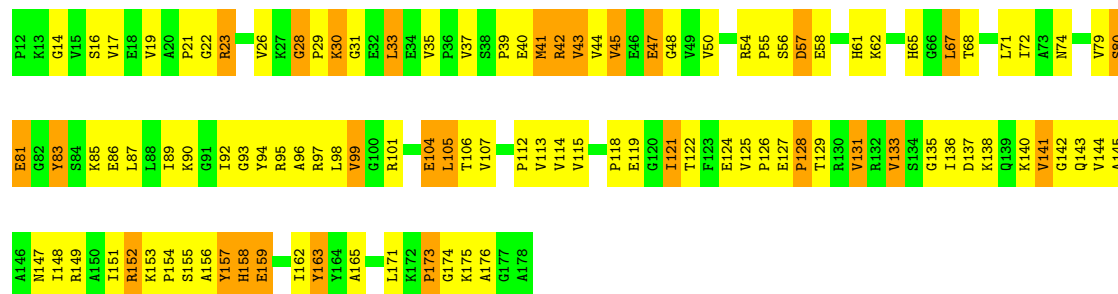
• Molecule 29: 50S ribosomal protein L5





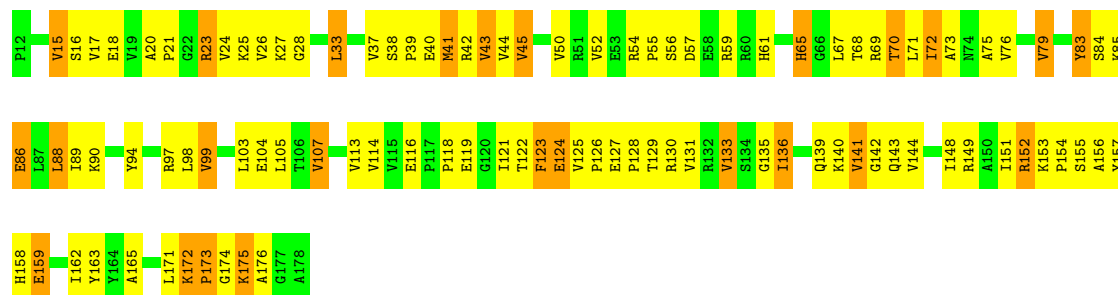
- Molecule 30: 50S ribosomal protein L6

Chain BH: 37% 47% 17%



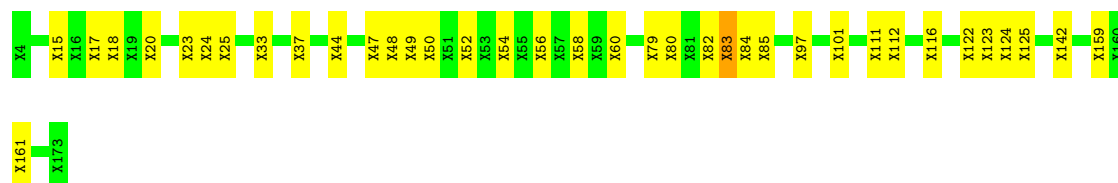
- Molecule 30: 50S ribosomal protein L6

Chain DH: 40% 46% 15%



- Molecule 31: 50S RIBOSOMAL PROTEIN L10

Chain BJ: 78% 21%



- Molecule 31: 50S RIBOSOMAL PROTEIN L10

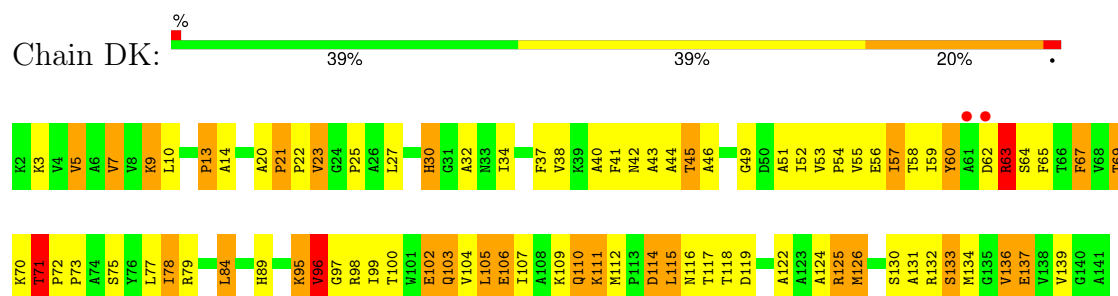
Chain DJ: 81% 19%



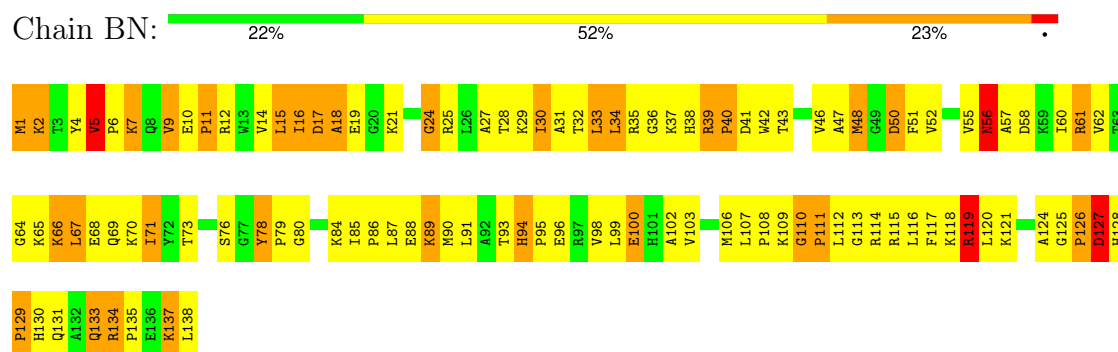
• Molecule 32: 50S ribosomal protein L11



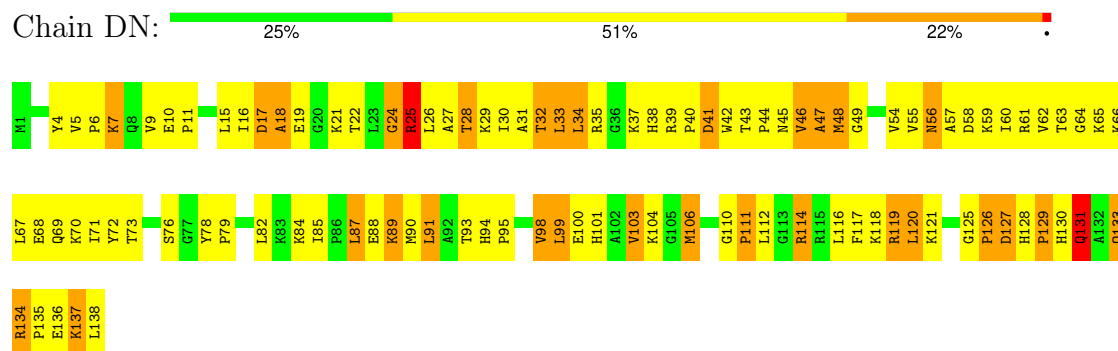
• Molecule 32: 50S ribosomal protein L11



• Molecule 33: 50S ribosomal protein L13

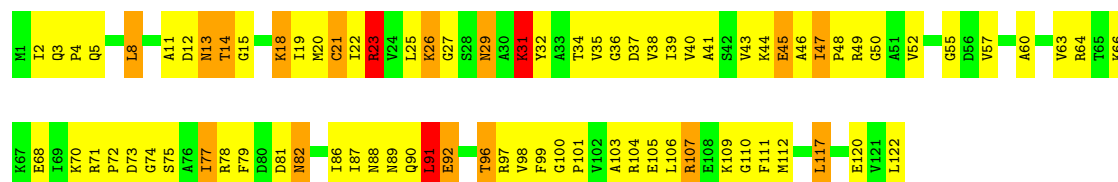


• Molecule 33: 50S ribosomal protein L13

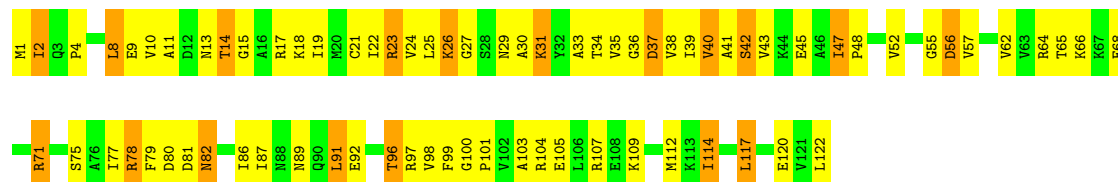


• Molecule 34: 50S ribosomal protein L14

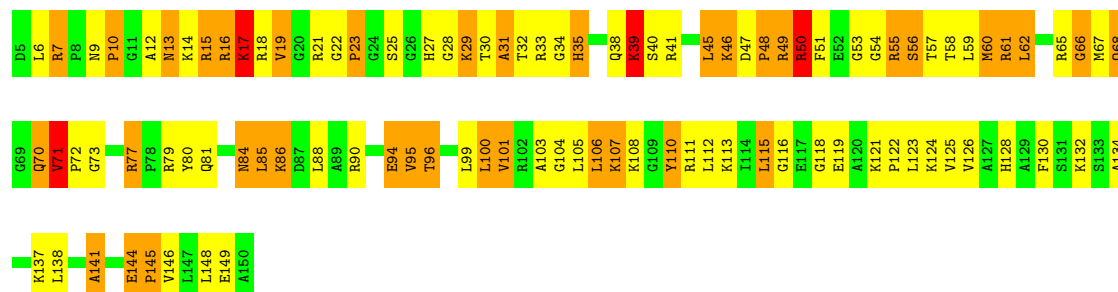




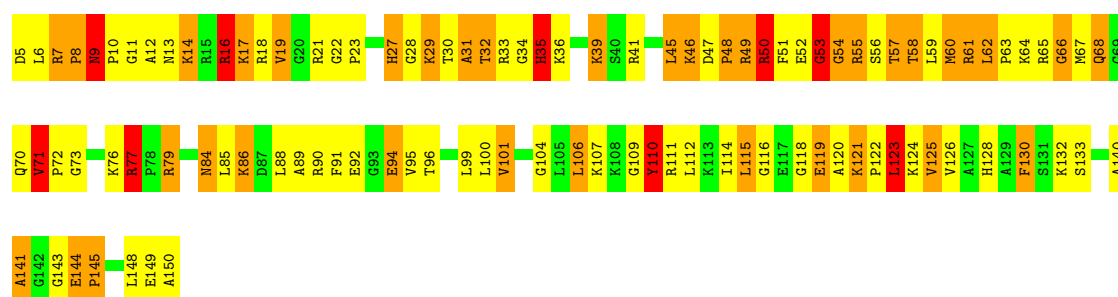
• Molecule 34: 50S ribosomal protein L14



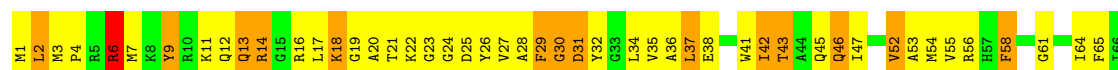
• Molecule 35: 50S ribosomal protein L15

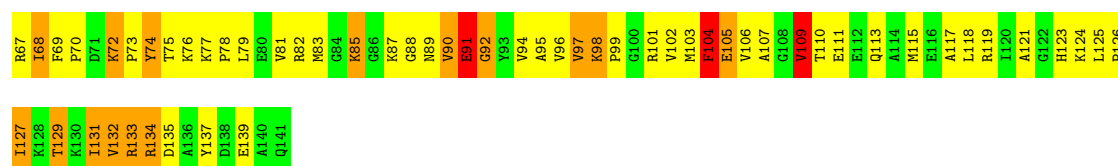


• Molecule 35: 50S ribosomal protein L15

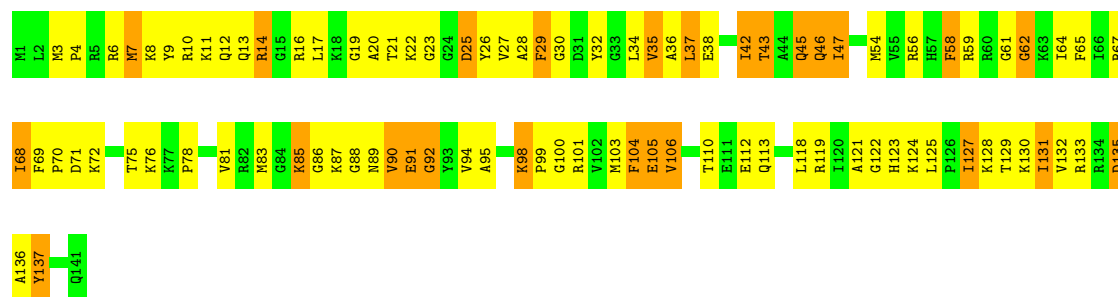


• Molecule 36: 50S ribosomal protein L16

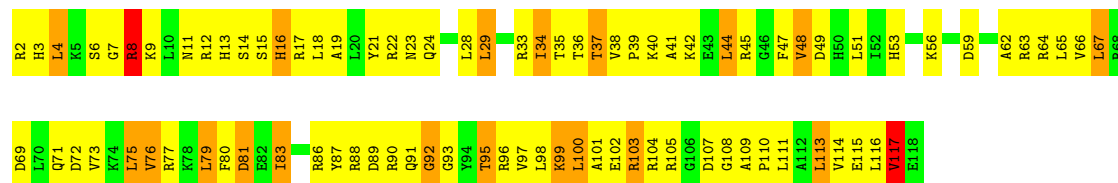




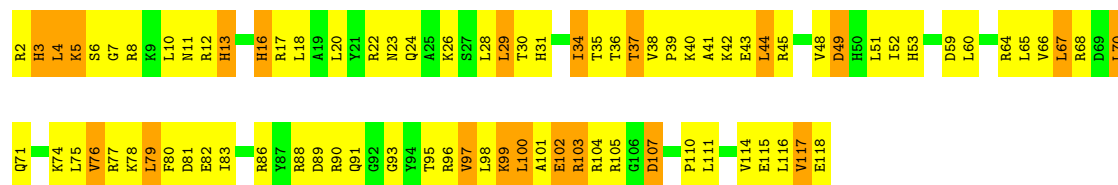
- Molecule 36: 50S ribosomal protein L16



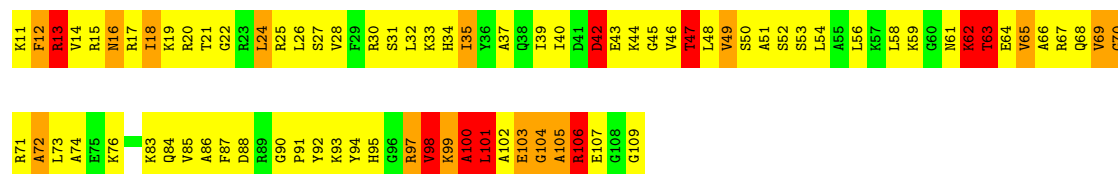
- Molecule 37: 50S ribosomal protein L17



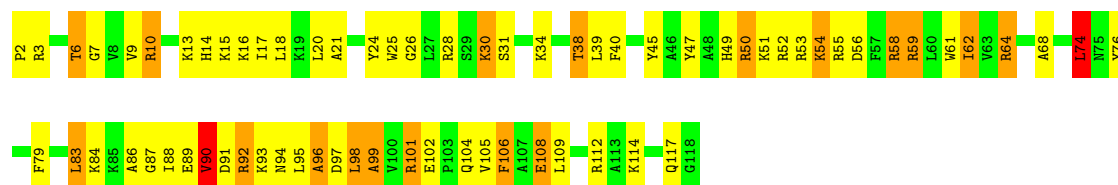
- Molecule 37: 50S ribosomal protein L17



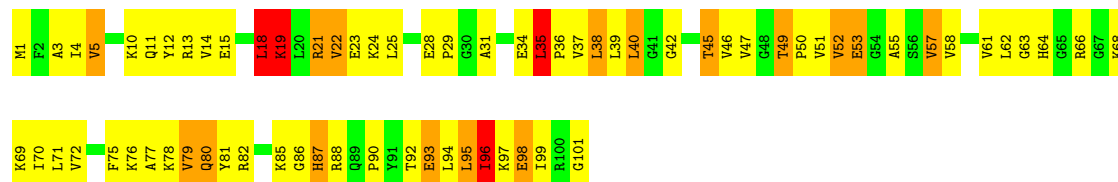
- Molecule 38: 50S ribosomal protein L18



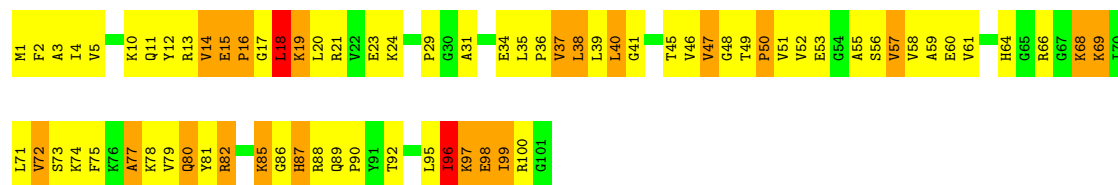
- Molecule 38: 50S ribosomal protein L18



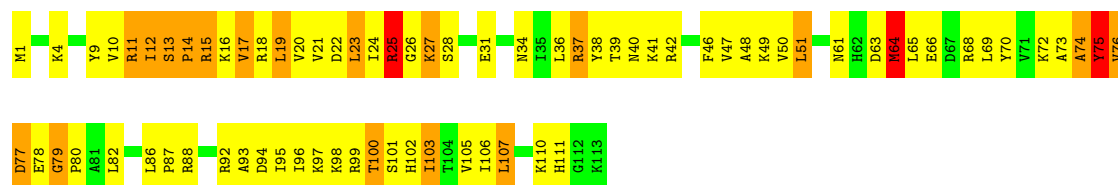
• Molecule 41: 50S ribosomal protein L21



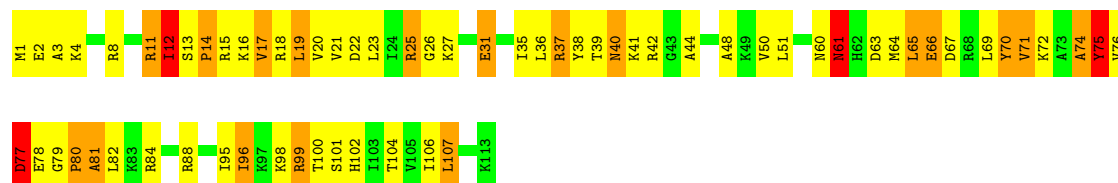
• Molecule 41: 50S ribosomal protein L21



• Molecule 42: 50S ribosomal protein L22

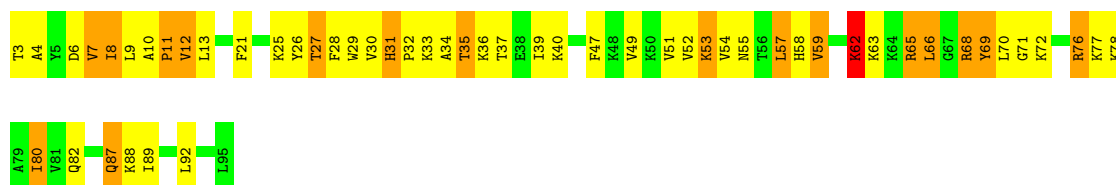


• Molecule 42: 50S ribosomal protein L22

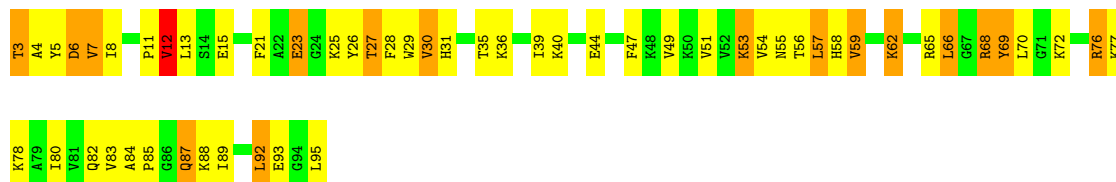


• Molecule 43: 50S ribosomal protein L23

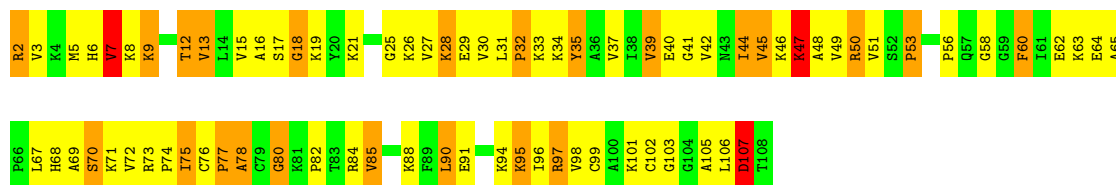




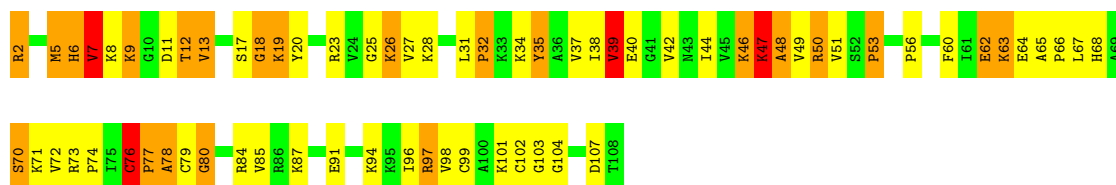
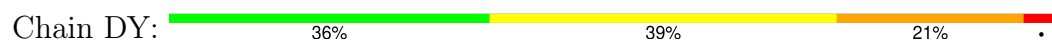
• Molecule 43: 50S ribosomal protein L23



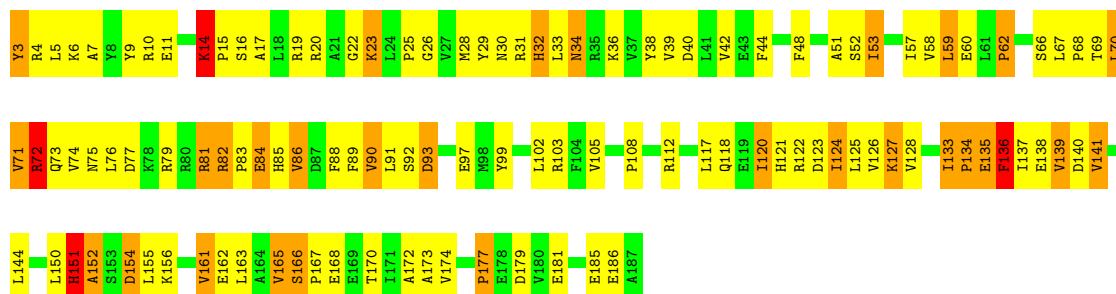
• Molecule 44: 50S ribosomal protein L24



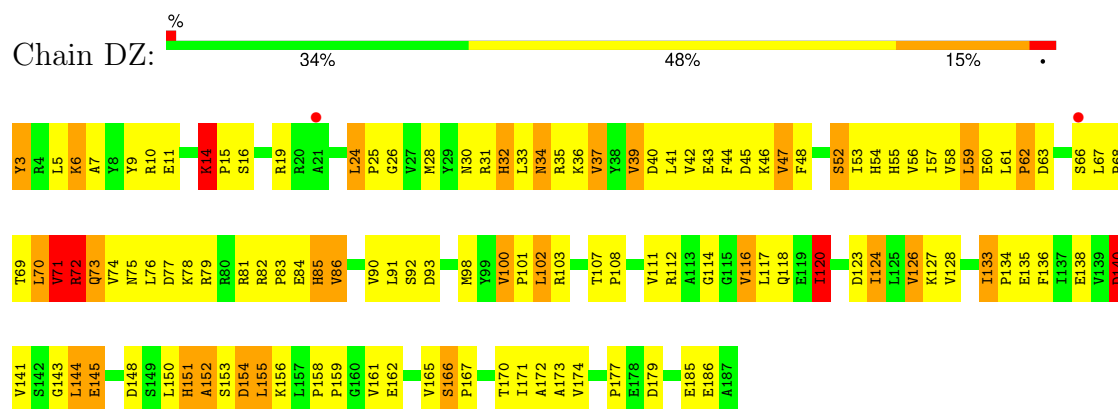
• Molecule 44: 50S ribosomal protein L24



• Molecule 45: 50S ribosomal protein L25



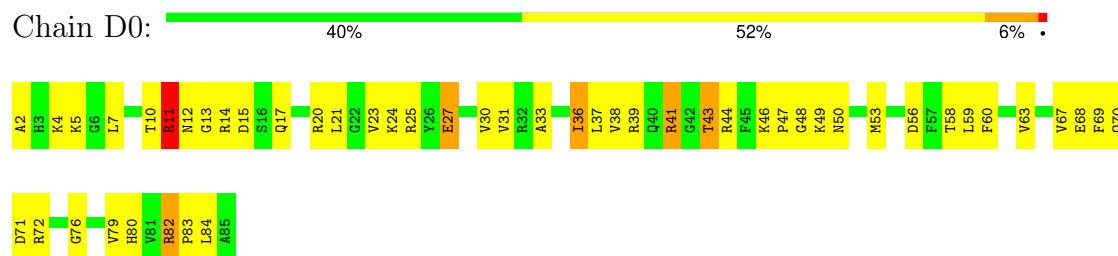
• Molecule 45: 50S ribosomal protein L25



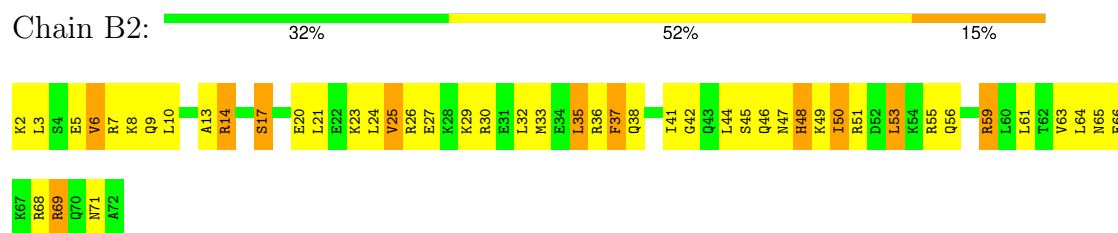
• Molecule 46: 50S ribosomal protein L27



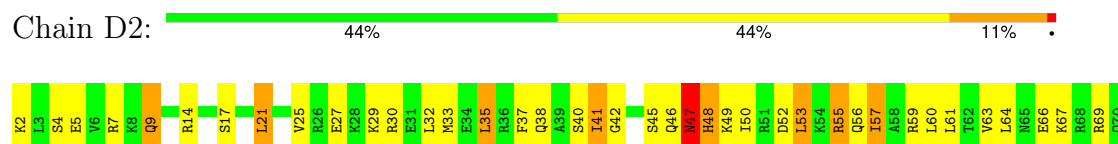
• Molecule 46: 50S ribosomal protein L27



• Molecule 47: 50S ribosomal protein L29



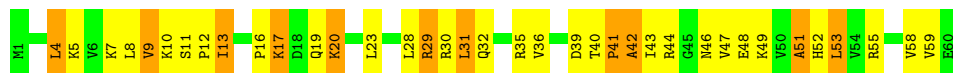
• Molecule 47: 50S ribosomal protein L29





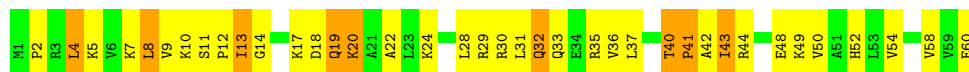
- Molecule 48: 50S ribosomal protein L30

Chain B3: 38% 43% 18%



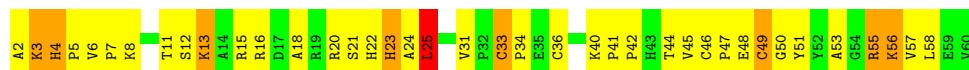
- Molecule 48: 50S ribosomal protein L30

Chain D3: 37% 48% 15%



- Molecule 49: 50S ribosomal protein L32

Chain B5: 34% 51% 14%



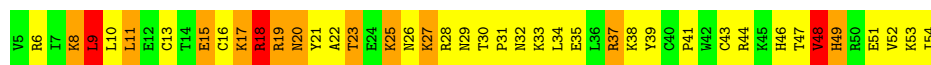
- Molecule 49: 50S ribosomal protein L32

Chain D5: 42% 47% 10%



- Molecule 50: 50S ribosomal protein L33

Chain B6: 20% 52% 22% 6%



- Molecule 50: 50S ribosomal protein L33

Chain D6: 16% 46% 34%

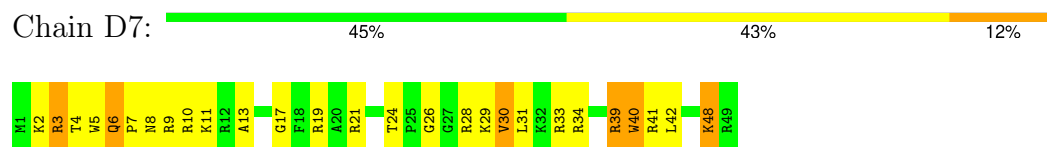


- Molecule 51: 50S ribosomal protein L34

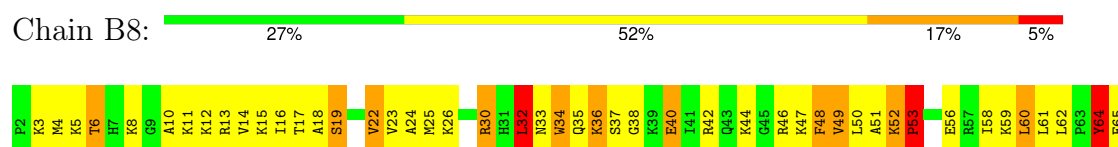
Chain B7: 39% 47% 14%



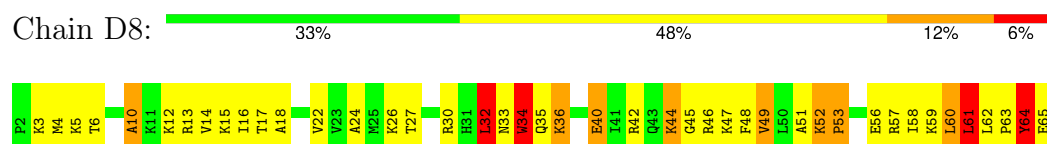
- Molecule 51: 50S ribosomal protein L34



- Molecule 52: 50S ribosomal protein L35



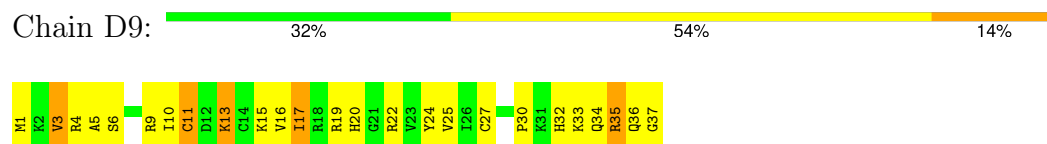
- Molecule 52: 50S ribosomal protein L35



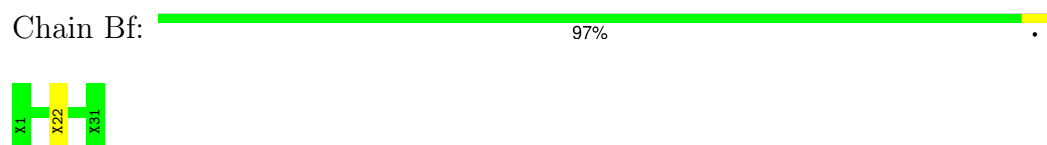
- Molecule 53: 50S ribosomal protein L36



- Molecule 53: 50S ribosomal protein L36



- Molecule 54: 50S RIBOSOMAL PROTEIN L7/L12




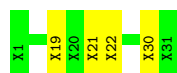
- Molecule 54: 50S RIBOSOMAL PROTEIN L7/L12



There are no outlier residues recorded for this chain.

- Molecule 54: 50S RIBOSOMAL PROTEIN L7/L12

Chain Df:  87% 13%



- Molecule 54: 50S RIBOSOMAL PROTEIN L7/L12

Chain Dg:  100%

There are no outlier residues recorded for this chain.

- Molecule 55: 50S RIBOSOMAL PROTEIN L7/L12

Chain Bh:  100%

There are no outlier residues recorded for this chain.

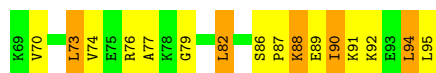
- Molecule 55: 50S RIBOSOMAL PROTEIN L7/L12

Chain Dh:  90% 10%




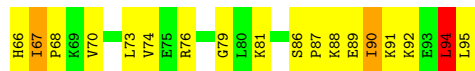
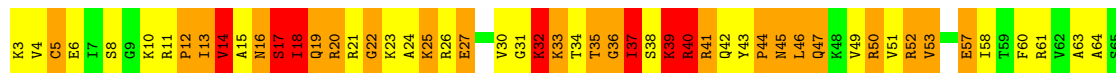
- Molecule 56: 50S ribosomal protein L28

Chain B1:  28% 35% 26% 11%



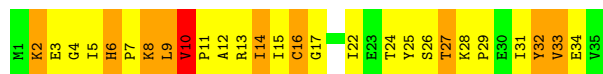
- Molecule 56: 50S ribosomal protein L28

Chain D1:  25% 42% 25% 9%

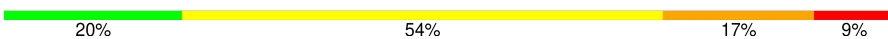


- Molecule 57: 50S ribosomal protein L31

Chain B4:  23% 49% 26% 2%



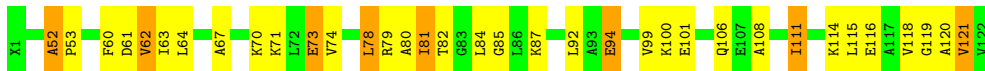
- Molecule 57: 50S ribosomal protein L31

Chain D4: 



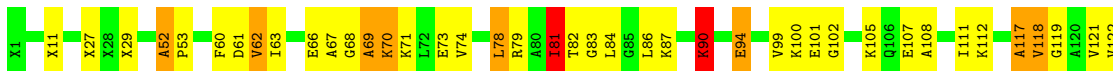
- Molecule 58: 50S ribosomal protein L7/L12

Chain Be: 

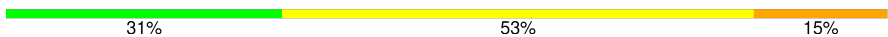


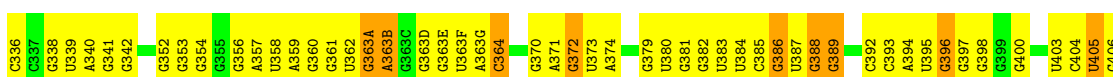
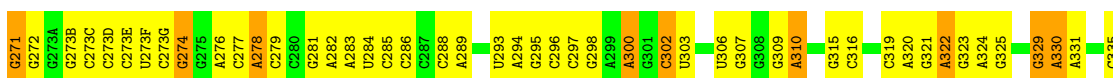
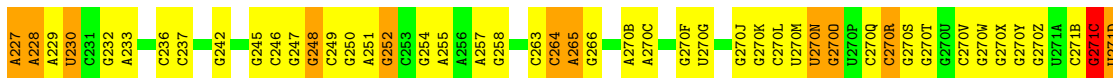
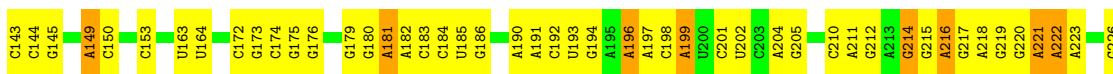
- Molecule 58: 50S ribosomal protein L7/L12

Chain De: 



- Molecule 59: 23S ribosomal RNA

Chain BA: 

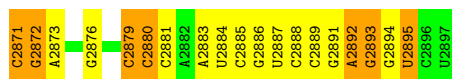


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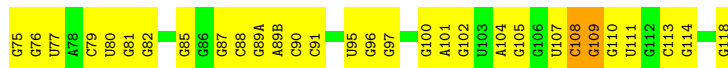
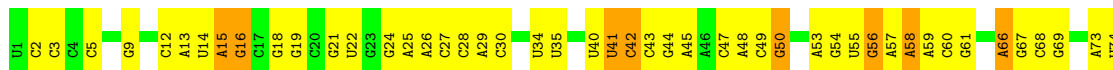
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C1712	G1635	C1558	G1488	G1422	A1353	A1286	G1215	G1143	A1077	G1002	G940	A872	G805	G729
	A1637	G1559	G1491	G1423	A1354	U1287	G1216	G1144	U1078	C1005	G942	G874	G806	C730
U1727	C1638	C1565	G1492	G1424	G1355	U1288	C1217	A1148	C1080	C1006	U943	U877	U807	C731
G1728	U1639	A1566	C1493	A1427	G1356	C1291	C1221	G1149	U1081	C1007	G944	A878	G808	C732
A1729	C1640	A1567	A1494	C1428	U1357	U1292	C1224	C1152	U1082	C1008	A945	U879	G809	A734
	A1641	A1568	A1495	C1429	G1358	C1293	A1225	C1153	A1083	A1009	G946	C879	C812	G738
G1732	G1642	G1569	A1496	C1430	A1359	U1294	A1226	G1154	U1084	A1010	G948	G880	C813	G739
	G1643	A1570	C1498	U1431	G1360	U1295	A1227	A1155	A1085	A1011	G949	G881	C814	G740
G1750	C1644		C1499	C1432	G1361	G1296		A1156	A1086	C1012	G950	G882	C815	U740
C1751	G1645	C1577	G1500	U1433	C1362		C1280	A1157	G1087	U1013	C951	C884	C816	G741
	G1647	U1578	C1501	A1434	C1363	U1300	G1231	G1158	A1088	U1014	C952	C885	G817	G742
A1755	C1648		C1502	G1435	A1365	A1301	G1232	U1159	C1089	G1015	A953	C886	G818	G743
G1756		G1581	C1505	G1436	A1366	A1302	C1233	G1160	U1090	G1016	G954	A887	A819	G744
U1757	G1651	A1582	C1506	G1437	G1369	C1303	U1234	G1161	C1091	G1017	G954	C888	A820	U747
	A1652	A1583		U1438	G1372		G1235	G1162		U1018	C955	C889	A821	G748
A1762	G1653	C1585		U1439	U1372	C1306	A1236	G1163	U1094	A1020	A957	A890	U822	C749
G1763	A1654	G1586	A1510	G1440	A1373	G1309	G1237	G1164	U1095	A1021	U958	G892	U826	U757
G1764	A1655	A1587	A1511	G1441	A1374	G1310	G1238	G1165	A1096	G1022	A959	C893	U827	C758
	C1656	C1588	G1512	G1442	G1374	U1311	A1240	C1166	U1097	U1023	A960	C894	U828	
G1770	C1657	U1513	U1514		C1375	U1312	U1241	U1167	U1101	G1024	C961	U895	A829	A761
C1771	C1658	C1590	C1515	A1448	C1376	U1313	A1242	G1170	C1102	U1025	C964	A896	A829	
G1772	A1591	C1515		C1445	G1377	U1314	A1243	G1171	C1103	U1026	C965	C897	G830	U762
A1773	C1592	U1516	G1517	G1446	A1378	C1315	G1244	G1173	C1104	A1028	G966	A900	G831	G763
	G1593	G1517	G1517	G1447	A1379	U1316	A1245	G1174	U1105	A1029	C967	A901	G836	G765
U1775	A1664	G1594	G1522	G1448	G1380	A1317	A1246	U1175	G1106	G1030	G968	C902	C837	C766
G1776	A1665	G1595		A1498	G1380		A1247	G1176	G1107	U1033	U969	C903	C838	U767
	C1666	A1596	U1523	G1449	A1384	C1320	G1248	A1177	U1108	U1033	C970	C904	U839	G768
U1779	G1667	U1524	G1524		G1385	A1321	U1249	G1178	C1109	G1036	G972	U905	C840	
A1780	A1668	C1599	G1525	A1463	C1386	U1322	G1250	C1179	G1110	G1037	A973	G906	A841	G771
C1781	A1669	G1600	G1526	U1454	C1387	A1323	C1251	A1111	G1112	U1037	C974	C908	G843	A774
C1782	G1670	U1601	G1527	G1455		G1324	G1252	G1184	U1113	A1045	C974B	A909	G843	
A1783	U1671	U1602	A1528	C1458	U1394	G1325	A1253	G1185	U1113	A1045	G974B	A910	C846	G775
G1784		A1603	G1529	G1459	U1395	U1326	A1254	G1186	G1114	A1046	G975	A911	U847	G776
A1785	G1674	C1604	G1530	A1460	U1397	C1327	U1255	G1187	C1115	G1047	C976	C912	G848	A777
A1786	C1675	C1605	C1531	G1461	C1398	G1328	G1256	U1199	G1125	A1048	G977	G913	U849	G778
A1787	A1676	G1606	C1532	C1462	C1399	U1329	A1257	G1190	C1116	C1049	G978	C914	C849	U779
C1788	C1677	C1607	C1533	C1463	G1400	C1330	C1258	G1190		A1050	G979	C915	G852	G780
A1789	G1678	A1608	G1534	C1464	G1401	C1331	C1259	G1193	C1119	G1051	A980	C916	A781	A782
C1790		U1535	U1536	C1465	C1402	G1332	G1260	G1193	C1120	G1055	A983	A917	G853	A783
A1791	G1681	A1610	A1536	G1466	C1403	C1333	C1261	C1196	G1122	G1056	A984	C917	G854	A784
	G1682	C1611	C1537	G1467	C1404	U1334	A1262	U1197	C1123	A1057	C985	A918	G855	G785
G1792	C1683	C1612	G1538	C1468	C1405	U1335	U1263	U1198	C1124	G1058	C986	G919	G856	C786
C1793		G1615	G1539	C1469	U1406	A1336	G1264	U1199	G1125	G1059	G987	G921	U858	U787
U1794	A1690	A1616	U1541	G1470	C1407	G1337	A1265	C1200	A1126	U1060	A990	C923	U860	A789
C1795	C1691	C1617	G1542	A1471	C1408	G1338	G1266	C1201	A1127	U1061	C991	C924	A861	C790
U1796		A1618	A1543		C1409	G1339	U1267	C1202		G1062	C992	C925	A862	C791
C1797	U1692	G1619	C1544	C1476	G1410	U1340	A1268	G1203	A1132	G1063	G993	G929	A863	G792
	G1693	G1619	A1545	A1477	C1411	U1341	A1269	A1204	U1133	C1064	G994	G930	G864	A793
C1800	G1694	G1620	A1546	G1478	A1412	A1342	C1270	U1205	C1135	U1065	C995	U931	C865	C795
G1801	G1695	U1621	A1546	G1479	G1413	G1343	G1271	G1206	G1136	U1066	A996	G932	A866	G796
A1802	C1622	C1548	C1480	G1479	G1414	G1344	A1272	C1207	G1137	A1067	G997	A933	C867	
A1803	G1623	C1547	C1480	G1479	G1414	C1345	A1272		G1138				U868	
C1804	A1698	G1624	C1548	U1481	U1415	C1345	A1272		G1138	A1070			G869	G799
		G1624	C1548	U1481	U1415	C1345	A1272		G1138	A1070			G869	G799
U1805		G1624	C1548	U1481	U1415	C1345	A1272		G1138	A1070			G869	G799
C1806		G1624	C1548	U1481	U1415	C1345	A1272		G1138	A1070			G869	G799





• Molecule 60: 5S ribosomal RNA

Chain BB: 35% 56% 8%



• Molecule 60: 5S ribosomal RNA

Chain DB: 43% 46% 11%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	306.01Å 673.49Å 351.98Å 90.00° 92.69° 90.00°	Depositor
Resolution (Å)	40.00 – 3.50 40.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.50) 75.0 (40.00-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 3.49Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.262 , 0.309 0.270 , 0.310	Depositor DCC
R_{free} test set	38171 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	80.5	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 362.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.26$, $\langle L^2 \rangle = 0.11$	Xtriage
Estimated twinning fraction	0.247 for h,-k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	308422	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: UAL, 5OH, KBE, MG, DPP, GNP

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

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

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

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

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

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

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

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

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

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

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

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

There are no chirality outliers.

5 of 44 planarity outliers are listed below:

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

5.2 Too-close contacts [i](#)

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

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

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

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

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

The worst 5 of 12013 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:CW:37:A:C2	23:CV:16:A:C2	1.85	1.57
20:AY:33:LEU:HD21	20:AY:34:TYR:CE2	1.42	1.54
29:DG:112:PRO:CA	29:DG:112:PRO:C	1.88	1.45
29:BG:112:PRO:CA	29:BG:112:PRO:C	1.87	1.45
20:AY:33:LEU:HD21	20:AY:34:TYR:CD2	1.54	1.43

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

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

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

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

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

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

5 of 1578 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AB	203/203 (100%)	161 (79%)	42 (21%)	1	5
1	CB	203/203 (100%)	170 (84%)	33 (16%)	2	11
2	AC	161/161 (100%)	119 (74%)	42 (26%)	0	3
2	CC	161/161 (100%)	123 (76%)	38 (24%)	0	3
3	AD	180/180 (100%)	147 (82%)	33 (18%)	1	7
3	CD	180/180 (100%)	147 (82%)	33 (18%)	1	7
4	AE	116/116 (100%)	100 (86%)	16 (14%)	3	17
4	CE	116/116 (100%)	92 (79%)	24 (21%)	1	5
5	AF	90/90 (100%)	74 (82%)	16 (18%)	1	8
5	CF	90/90 (100%)	76 (84%)	14 (16%)	2	13
6	AG	126/126 (100%)	107 (85%)	19 (15%)	2	14
6	CG	126/126 (100%)	109 (86%)	17 (14%)	3	18
7	AH	119/119 (100%)	96 (81%)	23 (19%)	1	6
7	CH	119/119 (100%)	92 (77%)	27 (23%)	0	4
8	AI	98/98 (100%)	84 (86%)	14 (14%)	2	16
8	CI	98/98 (100%)	80 (82%)	18 (18%)	1	7
9	AJ	89/89 (100%)	68 (76%)	21 (24%)	0	3
9	CJ	89/89 (100%)	67 (75%)	22 (25%)	0	3
10	AK	90/90 (100%)	72 (80%)	18 (20%)	1	6
10	CK	90/90 (100%)	74 (82%)	16 (18%)	1	8
11	AL	104/104 (100%)	71 (68%)	33 (32%)	0	2
11	CL	104/104 (100%)	76 (73%)	28 (27%)	0	2
12	AM	100/100 (100%)	85 (85%)	15 (15%)	2	14
12	CM	100/100 (100%)	83 (83%)	17 (17%)	1	10
13	AN	49/49 (100%)	39 (80%)	10 (20%)	1	5
13	CN	49/49 (100%)	37 (76%)	12 (24%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	AO	79/79 (100%)	68 (86%)	11 (14%)	3	17
14	CO	79/79 (100%)	64 (81%)	15 (19%)	1	6
15	AP	72/72 (100%)	61 (85%)	11 (15%)	2	14
15	CP	72/72 (100%)	62 (86%)	10 (14%)	3	17
16	AQ	95/95 (100%)	80 (84%)	15 (16%)	2	13
16	CQ	95/95 (100%)	79 (83%)	16 (17%)	1	10
17	AR	61/61 (100%)	54 (88%)	7 (12%)	4	22
17	CR	61/61 (100%)	50 (82%)	11 (18%)	1	7
18	AS	69/69 (100%)	55 (80%)	14 (20%)	1	5
18	CS	69/69 (100%)	50 (72%)	19 (28%)	0	2
19	AT	76/76 (100%)	65 (86%)	11 (14%)	2	15
19	CT	76/76 (100%)	65 (86%)	11 (14%)	2	15
20	AY	579/579 (100%)	447 (77%)	132 (23%)	0	4
20	CY	579/579 (100%)	468 (81%)	111 (19%)	1	6
24	AU	2/2 (100%)	2 (100%)	0	100	100
24	CU	2/2 (100%)	2 (100%)	0	100	100
25	BC	180/180 (100%)	127 (71%)	53 (29%)	0	2
25	DC	180/180 (100%)	126 (70%)	54 (30%)	0	2
26	BD	217/217 (100%)	162 (75%)	55 (25%)	0	3
26	DD	217/217 (100%)	172 (79%)	45 (21%)	1	5
27	BE	165/165 (100%)	133 (81%)	32 (19%)	1	6
27	DE	165/165 (100%)	135 (82%)	30 (18%)	1	7
28	BF	165/165 (100%)	131 (79%)	34 (21%)	1	5
28	DF	165/165 (100%)	132 (80%)	33 (20%)	1	6
29	BG	155/155 (100%)	130 (84%)	25 (16%)	2	12
29	DG	155/155 (100%)	129 (83%)	26 (17%)	1	10
30	BH	136/136 (100%)	111 (82%)	25 (18%)	1	7
30	DH	136/136 (100%)	113 (83%)	23 (17%)	1	10
32	BK	105/105 (100%)	70 (67%)	35 (33%)	0	1
32	DK	105/105 (100%)	73 (70%)	32 (30%)	0	2
33	BN	117/117 (100%)	92 (79%)	25 (21%)	1	4

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

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

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

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

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

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

5.3.3 RNA ⓘ

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

5 of 2032 RNA backbone outliers are listed below:

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

5 of 87 RNA pucker outliers are listed below:

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

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

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

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

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

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

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

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

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

All (4) bond angle outliers are listed below:

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

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

5 monomers are involved in 13 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
61	GNP	CY	701	62	29,34,34	1.80	7 (24%)	33,54,54	2.79	14 (42%)
61	GNP	AY	701	62	29,34,34	1.81	7 (24%)	33,54,54	2.80	14 (42%)

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	CY	701	62	-	7/14/38/38	0/3/3/3
61	GNP	AY	701	62	-	7/14/38/38	0/3/3/3

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	AY	701	GNP	PG-O1G	4.99	1.53	1.46
61	CY	701	GNP	PG-O1G	4.96	1.53	1.46
61	CY	701	GNP	PA-O3A	-4.30	1.54	1.59
61	AY	701	GNP	PA-O3A	-4.29	1.54	1.59
61	CY	701	GNP	C6-N1	3.69	1.39	1.33

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	AY	701	GNP	C5-C6-N1	-8.78	111.69	123.42
61	CY	701	GNP	C5-C6-N1	-8.75	111.72	123.42
61	AY	701	GNP	C2-N1-C6	6.60	125.14	115.96
61	CY	701	GNP	C2-N1-C6	6.57	125.10	115.96
61	AY	701	GNP	C2-N3-C4	-5.20	109.88	115.48

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

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

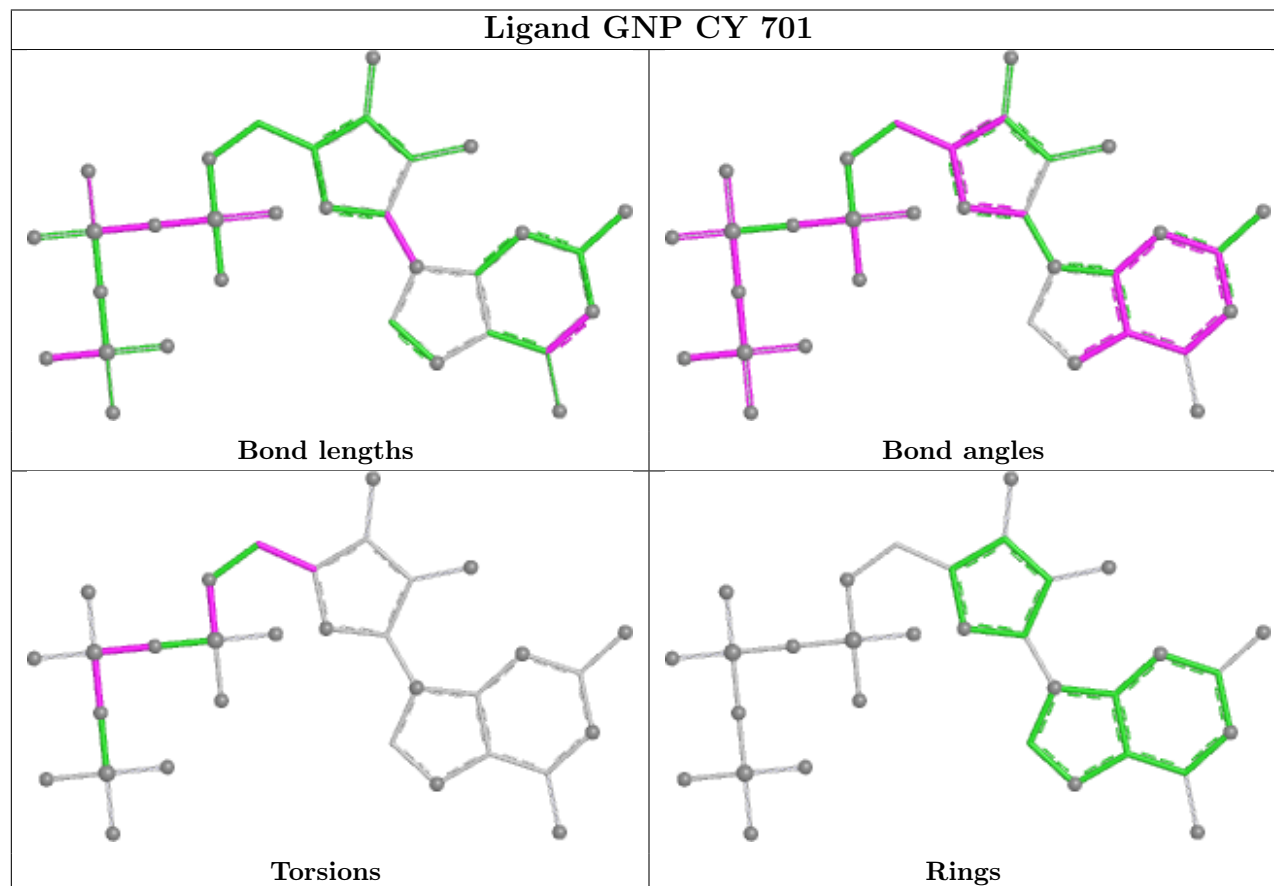
There are no ring outliers.

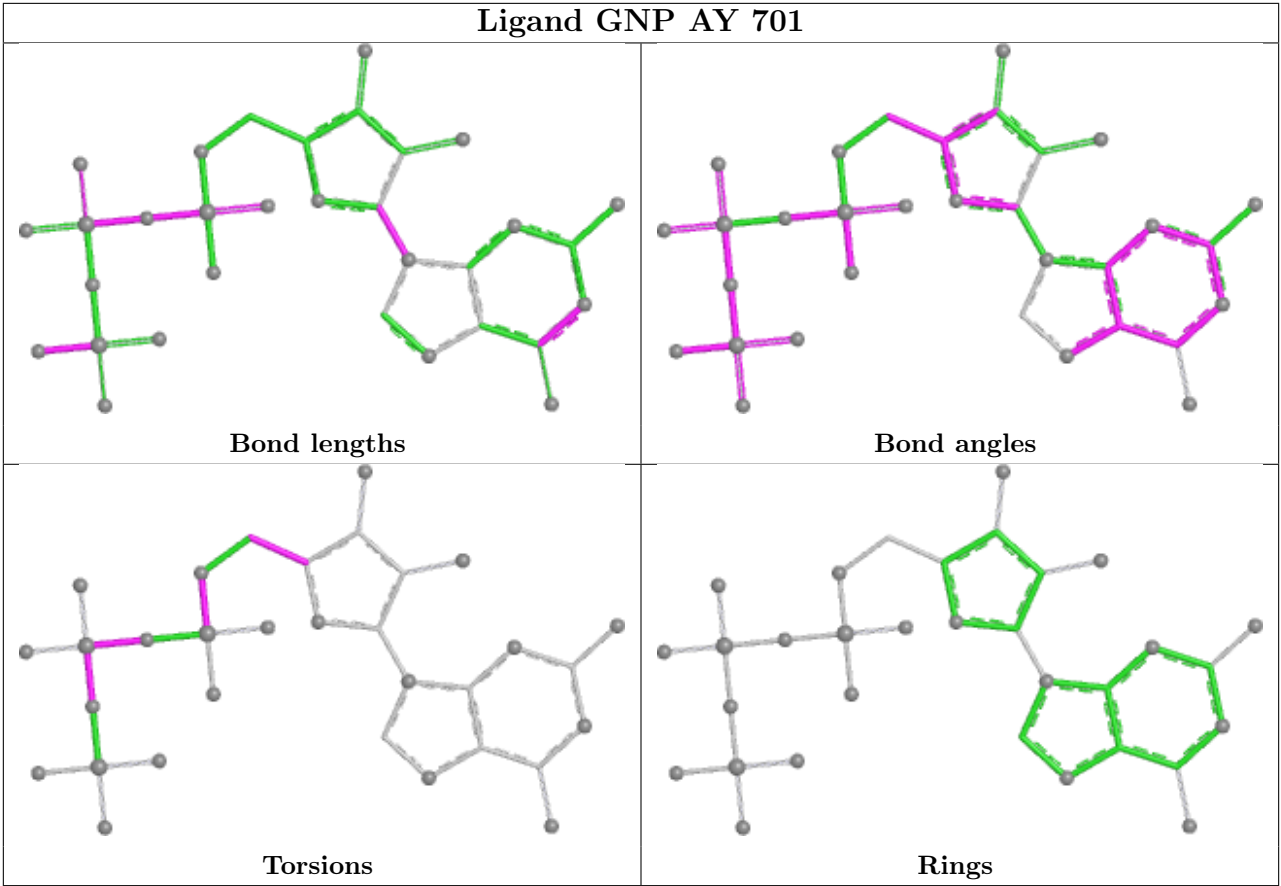
2 monomers are involved in 51 short contacts:

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

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

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





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
58	De	1
58	Be	1

All chain breaks are listed below:

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

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AB	235/235 (100%)	-1.51	0 100 100	30, 75, 127, 171	0
1	CB	235/235 (100%)	-1.44	0 100 100	34, 86, 153, 201	0
2	AC	207/207 (100%)	-1.40	0 100 100	27, 59, 115, 156	0
2	CC	207/207 (100%)	-1.47	0 100 100	23, 74, 130, 190	0
3	AD	208/208 (100%)	-1.40	1 (0%) 87 75	24, 72, 124, 159	0
3	CD	208/208 (100%)	-1.33	0 100 100	23, 85, 142, 184	0
4	AE	151/151 (100%)	-1.42	0 100 100	17, 48, 101, 156	0
4	CE	151/151 (100%)	-1.28	0 100 100	14, 58, 106, 151	0
5	AF	101/101 (100%)	-1.53	0 100 100	15, 50, 100, 133	0
5	CF	101/101 (100%)	-1.42	1 (0%) 79 61	29, 61, 123, 148	0
6	AG	155/155 (100%)	-1.39	0 100 100	30, 80, 139, 199	0
6	CG	155/155 (100%)	-1.24	0 100 100	38, 82, 137, 180	0
7	AH	138/138 (100%)	-1.41	0 100 100	28, 59, 103, 142	0
7	CH	138/138 (100%)	-1.37	0 100 100	25, 75, 121, 155	0
8	AI	127/127 (100%)	-1.39	0 100 100	0, 71, 117, 134	0
8	CI	127/127 (100%)	-1.20	0 100 100	0, 84, 149, 220	0
9	AJ	99/99 (100%)	-1.41	0 100 100	25, 62, 116, 159	0
9	CJ	99/99 (100%)	-1.35	0 100 100	31, 75, 127, 166	0
10	AK	119/119 (100%)	-1.32	0 100 100	31, 69, 116, 157	0
10	CK	119/119 (100%)	-1.22	2 (1%) 69 49	38, 72, 133, 151	0
11	AL	125/125 (100%)	-1.31	1 (0%) 82 67	10, 66, 120, 181	0
11	CL	125/125 (100%)	-1.12	1 (0%) 82 67	29, 69, 136, 170	0
12	AM	125/125 (100%)	-1.16	0 100 100	49, 86, 144, 212	0
12	CM	125/125 (100%)	-1.01	0 100 100	53, 100, 158, 223	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AN	60/60 (100%)	-1.32	0 100 100	28, 52, 87, 120	0
13	CN	60/60 (100%)	-1.40	0 100 100	39, 69, 117, 135	0
14	AO	88/88 (100%)	-1.54	0 100 100	22, 60, 114, 139	0
14	CO	88/88 (100%)	-1.50	0 100 100	25, 68, 119, 170	0
15	AP	84/84 (100%)	-1.39	0 100 100	26, 66, 109, 117	0
15	CP	84/84 (100%)	-1.28	0 100 100	52, 81, 127, 153	0
16	AQ	100/100 (100%)	-1.32	0 100 100	0, 67, 117, 139	0
16	CQ	100/100 (100%)	-1.34	0 100 100	0, 68, 126, 150	0
17	AR	70/70 (100%)	-1.61	0 100 100	14, 54, 120, 154	0
17	CR	70/70 (100%)	-1.38	0 100 100	38, 63, 113, 155	0
18	AS	79/79 (100%)	-1.27	1 (1%) 74 56	47, 92, 136, 169	0
18	CS	79/79 (100%)	-1.32	0 100 100	44, 99, 145, 189	0
19	AT	99/99 (100%)	-1.43	0 100 100	0, 77, 128, 159	0
19	CT	99/99 (100%)	-1.25	0 100 100	0, 79, 131, 166	0
20	AY	687/687 (100%)	-1.33	1 (0%) 92 89	23, 84, 139, 174	0
20	CY	687/687 (100%)	-1.32	0 100 100	40, 92, 149, 204	0
21	AA	1511/1511 (100%)	-1.70	1 (0%) 92 89	15, 67, 145, 258	0
21	CA	1511/1511 (100%)	-1.66	0 100 100	18, 70, 157, 272	0
22	AW	77/77 (100%)	-1.73	0 100 100	32, 90, 174, 205	0
22	CW	77/77 (100%)	-1.71	0 100 100	39, 101, 193, 240	0
23	AV	23/23 (100%)	-1.28	0 100 100	41, 100, 156, 172	0
23	CV	23/23 (100%)	-0.97	0 100 100	41, 118, 186, 216	0
24	AU	2/6 (33%)	-1.46	0 100 100	114, 114, 114, 114	0
24	CU	2/6 (33%)	-1.38	0 100 100	119, 119, 119, 119	0
25	BC	228/228 (100%)	-1.37	1 (0%) 89 79	81, 124, 178, 222	0
25	DC	228/228 (100%)	-1.25	2 (0%) 81 64	102, 162, 214, 247	0
26	BD	275/275 (100%)	-1.31	0 100 100	11, 47, 102, 126	0
26	DD	275/275 (100%)	-1.28	0 100 100	23, 54, 107, 147	0
27	BE	205/205 (100%)	-1.35	0 100 100	19, 55, 101, 193	0
27	DE	205/205 (100%)	-1.27	0 100 100	12, 60, 120, 175	0
28	BF	208/208 (100%)	-1.30	0 100 100	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%)	-1.19	0 100 100	34, 83, 176, 205	0
29	BG	181/181 (100%)	-1.35	0 100 100	41, 90, 132, 195	0
29	DG	181/181 (100%)	-1.40	0 100 100	44, 104, 159, 196	0
30	BH	167/167 (100%)	-1.47	0 100 100	21, 68, 123, 159	0
30	DH	167/167 (100%)	-1.45	0 100 100	36, 72, 140, 192	0
31	BJ	0/170	-	-	-	-
31	DJ	0/170	-	-	-	-
32	BK	140/140 (100%)	-1.29	1 (0%) 84 69	60, 114, 165, 206	0
32	DK	140/140 (100%)	-1.06	2 (1%) 73 53	72, 142, 197, 229	0
33	BN	138/138 (100%)	-1.19	0 100 100	59, 83, 108, 111	0
33	DN	138/138 (100%)	-1.16	0 100 100	61, 89, 110, 118	0
34	BO	122/122 (100%)	-1.48	0 100 100	23, 44, 90, 158	0
34	DO	122/122 (100%)	-1.46	0 100 100	26, 47, 96, 121	0
35	BP	146/146 (100%)	-1.23	0 100 100	23, 71, 132, 167	0
35	DP	146/146 (100%)	-1.06	0 100 100	19, 88, 140, 212	0
36	BQ	141/141 (100%)	-1.31	0 100 100	32, 53, 103, 155	0
36	DQ	141/141 (100%)	-1.27	0 100 100	34, 58, 126, 178	0
37	BR	117/117 (100%)	-1.37	0 100 100	22, 57, 106, 123	0
37	DR	117/117 (100%)	-1.32	0 100 100	34, 67, 108, 138	0
38	BS	99/99 (100%)	-1.24	0 100 100	41, 104, 177, 190	0
38	DS	99/99 (100%)	-1.23	0 100 100	44, 114, 168, 203	0
39	BT	138/138 (100%)	-1.33	0 100 100	23, 68, 126, 162	0
39	DT	138/138 (100%)	-1.27	0 100 100	25, 71, 133, 177	0
40	BU	117/117 (100%)	-1.45	0 100 100	20, 45, 102, 140	0
40	DU	117/117 (100%)	-1.34	0 100 100	29, 54, 89, 222	0
41	BV	101/101 (100%)	-1.29	0 100 100	22, 58, 105, 172	0
41	DV	101/101 (100%)	-1.23	0 100 100	28, 60, 114, 177	0
42	BW	113/113 (100%)	-1.43	0 100 100	14, 43, 101, 135	0
42	DW	113/113 (100%)	-1.39	0 100 100	11, 60, 133, 215	0
43	BX	93/93 (100%)	-1.32	0 100 100	16, 55, 107, 137	0
43	DX	93/93 (100%)	-1.38	0 100 100	16, 66, 134, 180	0
44	BY	107/107 (100%)	-1.21	0 100 100	38, 88, 141, 193	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	DY	107/107 (100%)	-1.12	0 100 100	45, 96, 167, 200	0
45	BZ	185/185 (100%)	-1.49	0 100 100	36, 70, 124, 167	0
45	DZ	185/185 (100%)	-1.28	2 (1%) 77 59	48, 82, 136, 193	0
46	B0	84/84 (100%)	-1.17	0 100 100	24, 65, 112, 142	0
46	D0	84/84 (100%)	-1.22	0 100 100	47, 77, 140, 162	0
47	B2	71/71 (100%)	-1.59	0 100 100	34, 64, 118, 140	0
47	D2	71/71 (100%)	-1.39	0 100 100	33, 85, 127, 141	0
48	B3	60/60 (100%)	-1.42	0 100 100	28, 61, 116, 135	0
48	D3	60/60 (100%)	-1.27	0 100 100	32, 73, 137, 160	0
49	B5	59/59 (100%)	-1.47	0 100 100	22, 55, 125, 138	0
49	D5	59/59 (100%)	-1.31	0 100 100	29, 75, 130, 161	0
50	B6	50/50 (100%)	-1.32	0 100 100	36, 74, 120, 139	0
50	D6	50/50 (100%)	-1.21	0 100 100	49, 81, 143, 164	0
51	B7	49/49 (100%)	-1.15	0 100 100	43, 53, 102, 126	0
51	D7	49/49 (100%)	-1.29	0 100 100	34, 61, 112, 165	0
52	B8	64/64 (100%)	-1.19	0 100 100	22, 66, 108, 137	0
52	D8	64/64 (100%)	-1.26	0 100 100	33, 70, 118, 139	0
53	B9	37/37 (100%)	-1.17	0 100 100	39, 60, 122, 134	0
53	D9	37/37 (100%)	-1.25	0 100 100	46, 60, 134, 159	0
54	Bf	0/31	-	-	-	-
54	Bg	0/31	-	-	-	-
54	Df	0/31	-	-	-	-
54	Dg	0/31	-	-	-	-
55	Bh	0/30	-	-	-	-
55	Dh	0/30	-	-	-	-
56	B1	93/93 (100%)	-1.21	0 100 100	22, 78, 160, 236	0
56	D1	93/93 (100%)	-1.06	0 100 100	41, 89, 159, 194	0
57	B4	35/35 (100%)	-1.48	0 100 100	67, 116, 167, 189	0
57	D4	35/35 (100%)	-1.36	0 100 100	73, 136, 168, 196	0
58	Be	72/102 (70%)	-1.39	0 100 100	77, 113, 160, 174	0
58	De	72/102 (70%)	-1.19	0 100 100	87, 141, 192, 236	0
59	BA	2879/2879 (100%)	-1.73	0 100 100	9, 59, 146, 260	0
59	DA	2879/2879 (100%)	-1.66	0 100 100	5, 63, 160, 308	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
60	BB	119/119 (100%)	-1.63	0 100 100	36, 102, 157, 192	0
60	DB	119/119 (100%)	-1.76	0 100 100	33, 108, 159, 193	0
All	All	22726/23318 (97%)	-1.47	17 (0%) 92 89	0, 72, 150, 308	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
45	DZ	21	ALA	3.3
32	DK	61	ALA	3.2
32	DK	62	ASP	3.0
3	AD	84	LYS	2.9
25	DC	2	PRO	2.8

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

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

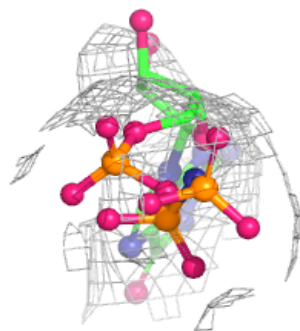
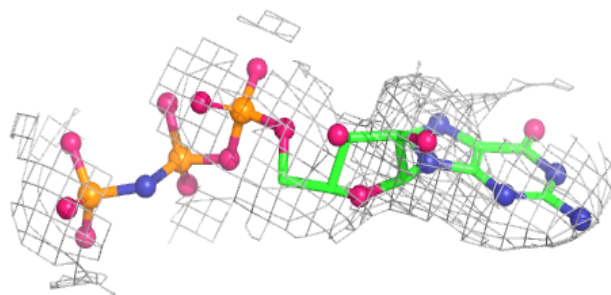
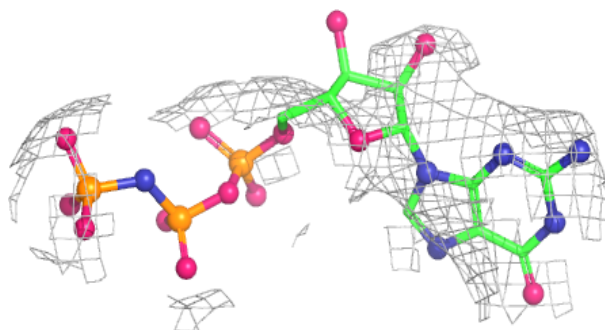
labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

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

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

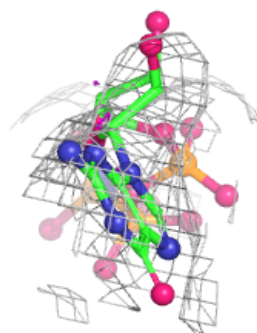
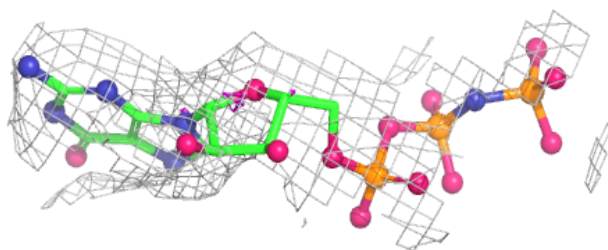
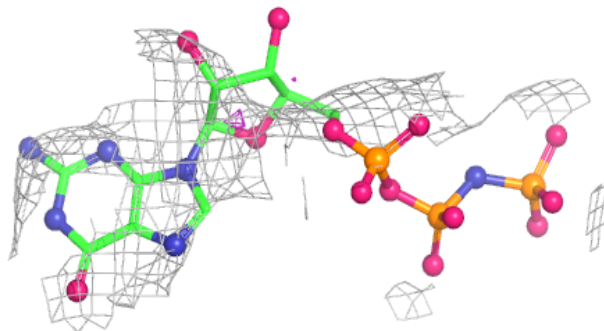
Electron density around GNP AY 701:

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



Electron density around GNP CY 701:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.