wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 16, 2023 – 10:01 PM EDT

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

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

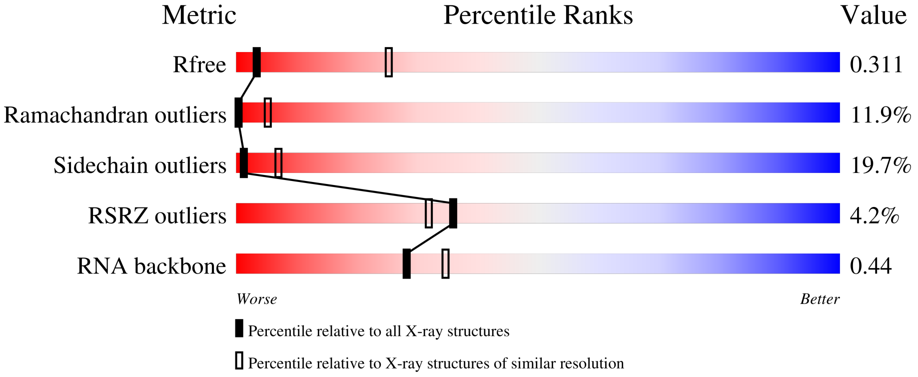
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

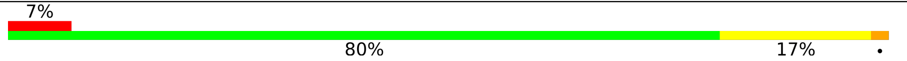
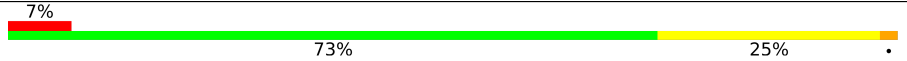
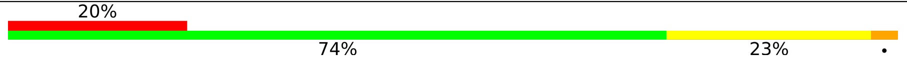
The reported resolution of this entry is 3.50 Å.

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}	130704	1659 (3.60-3.40)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)
RNA backbone	3102	1002 (4.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 <=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	
1	CB	235	
2	AC	207	
2	CC	207	
3	AD	208	

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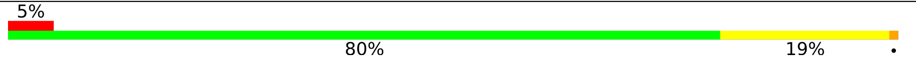
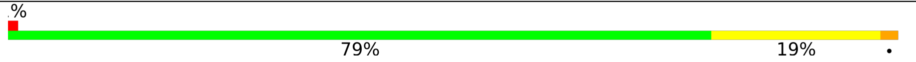
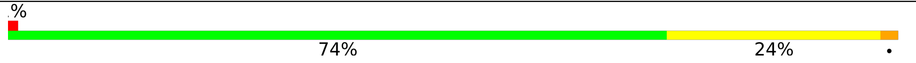
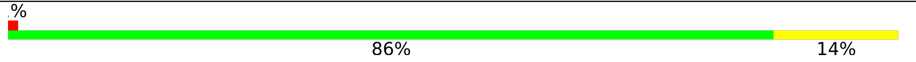
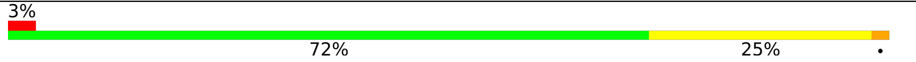
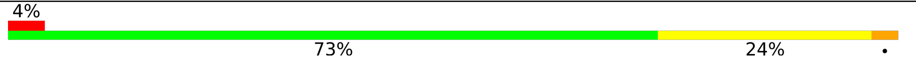
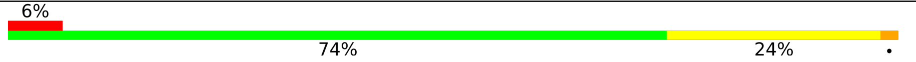
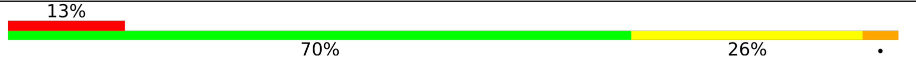
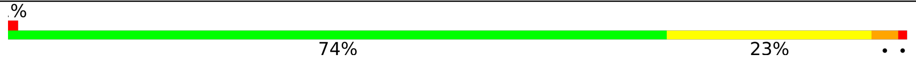
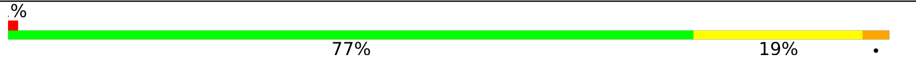
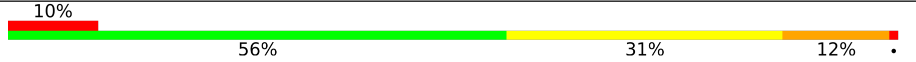
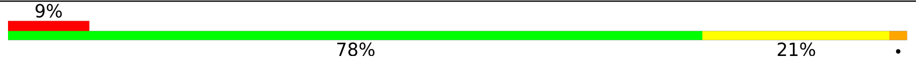
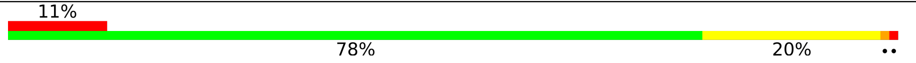
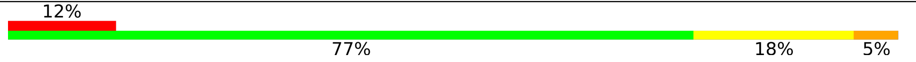
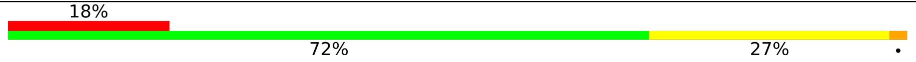
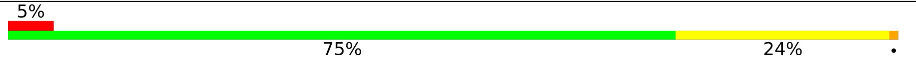
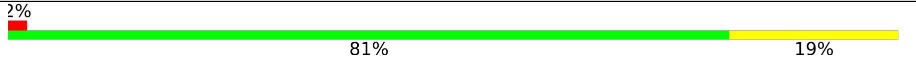
Mol	Chain	Length	Quality of chain
3	CD	208	
4	AE	151	
4	CE	151	
5	AF	101	
5	CF	101	
6	AG	155	
6	CG	155	
7	AH	138	
7	CH	138	
8	AI	127	
8	CI	127	
9	AJ	99	
9	CJ	99	
10	AK	119	
10	CK	119	
11	AL	125	
11	CL	125	
12	AM	125	
12	CM	125	
13	AN	60	
13	CN	60	
14	AO	88	
14	CO	88	
15	AP	84	
15	CP	84	

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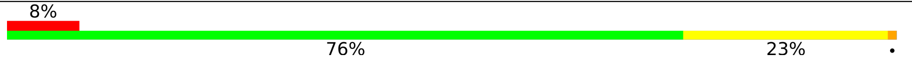
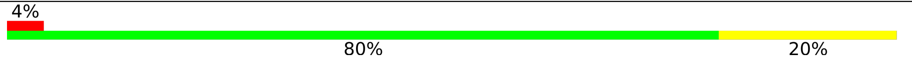
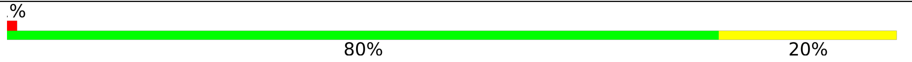
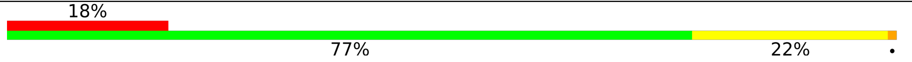
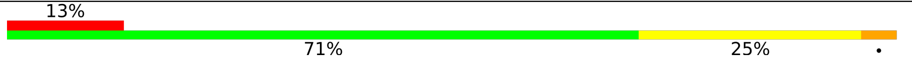
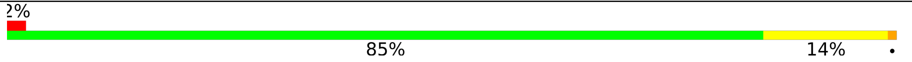
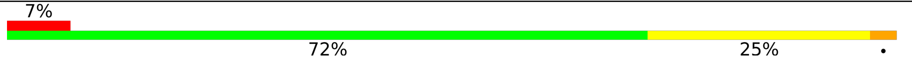
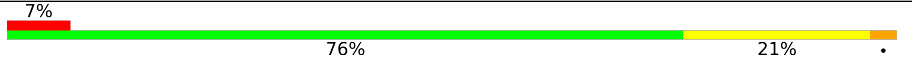
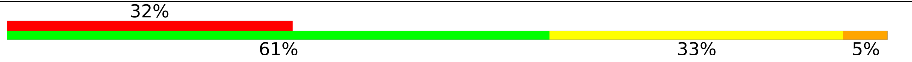
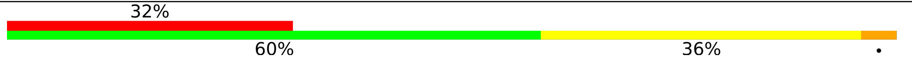
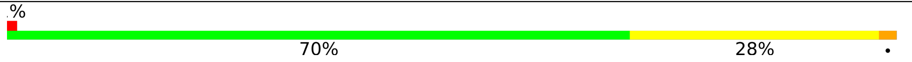
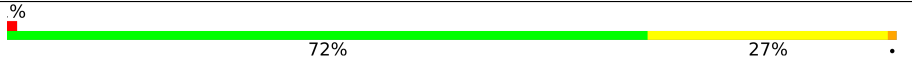
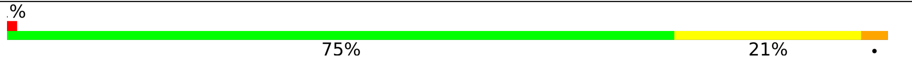
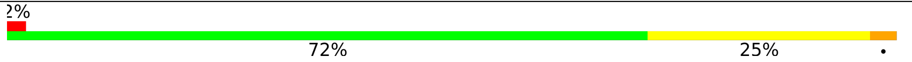
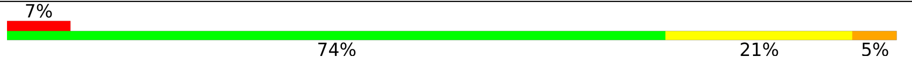
Mol	Chain	Length	Quality of chain
16	AQ	100	
16	CQ	100	
17	AR	70	
17	CR	70	
18	AS	79	
18	CS	79	
19	AT	99	
19	CT	99	
20	AY	687	
20	CY	687	
21	AA	1511	
21	CA	1511	
22	AW	77	
22	CW	77	
23	AV	23	
23	CV	23	
24	AU	6	
24	CU	6	
25	BC	228	
25	DC	228	
26	BD	275	
26	DD	275	
27	BE	205	
27	DE	205	
28	BF	208	

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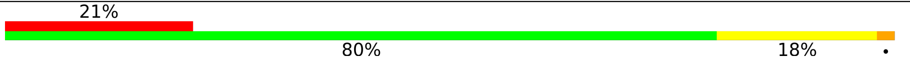
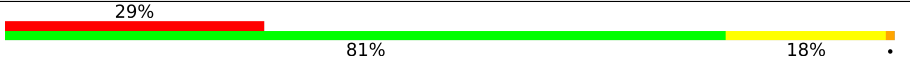
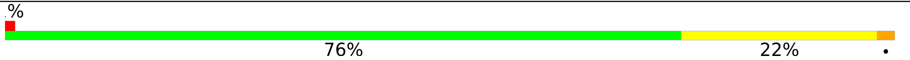
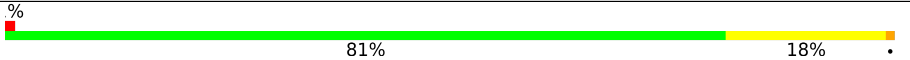
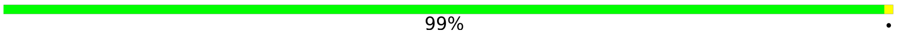
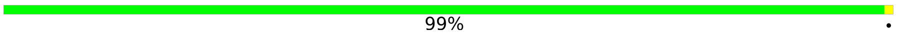
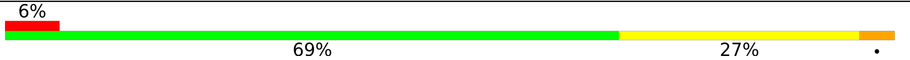
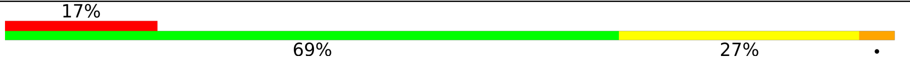
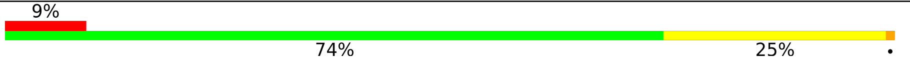
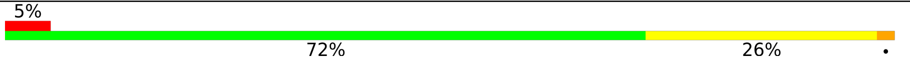
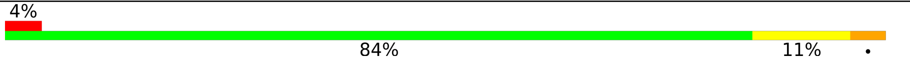
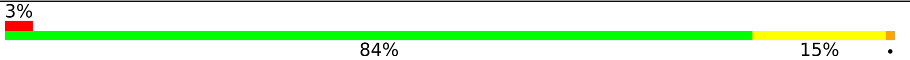
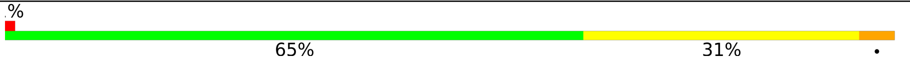
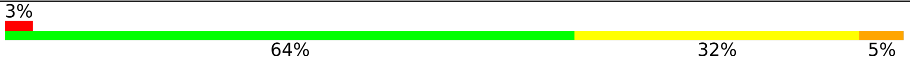
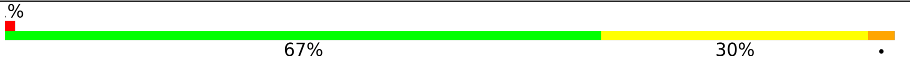
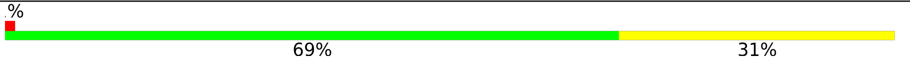
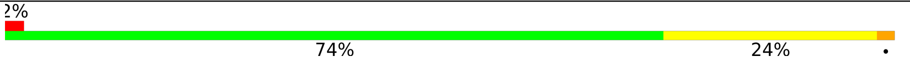
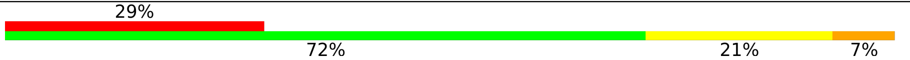
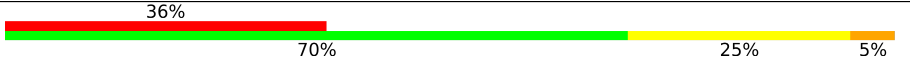
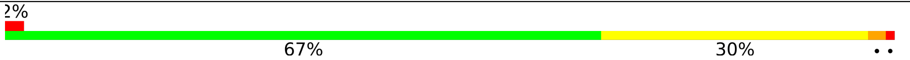
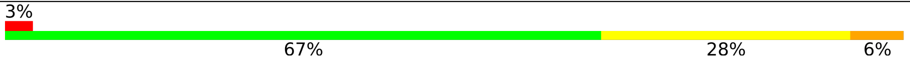
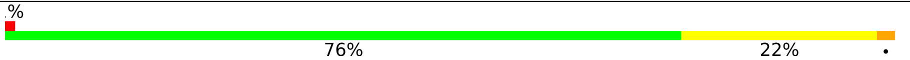
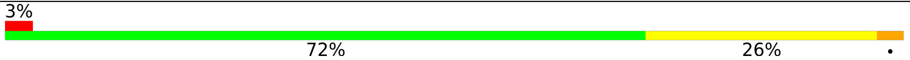
Mol	Chain	Length	Quality of chain
28	DF	208	 5% 76% 22% •
29	BG	181	 21% 80% 18% •
29	DG	181	 29% 81% 18% •
30	BH	167	 % 76% 22% •
30	DH	167	 % 81% 18% •
31	BJ	170	 99% •
31	DJ	170	 99% •
32	BK	140	 6% 69% 27% •
32	DK	140	 17% 69% 27% •
33	BN	138	 9% 74% 25% •
33	DN	138	 5% 72% 26% •
34	BO	122	 4% 84% 11% •
34	DO	122	 3% 84% 15% •
35	BP	146	 % 65% 31% •
35	DP	146	 3% 64% 32% 5%
36	BQ	141	 % 67% 30% •
36	DQ	141	 % 69% 31%
37	BR	117	 2% 74% 24% •
37	DR	117	 75% 24% •
38	BS	99	 29% 72% 21% 7%
38	DS	99	 36% 70% 25% 5%
39	BT	138	 2% 67% 30% • •
39	DT	138	 3% 67% 28% 6%
40	BU	117	 % 76% 22% •
40	DU	117	 3% 72% 26% •

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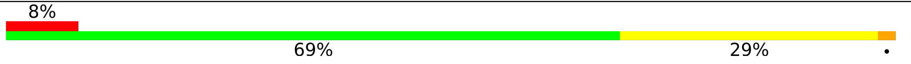
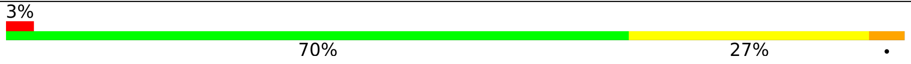
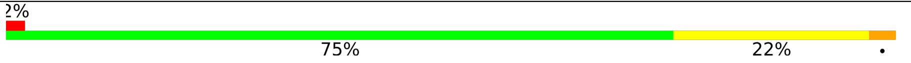
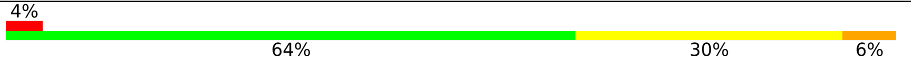
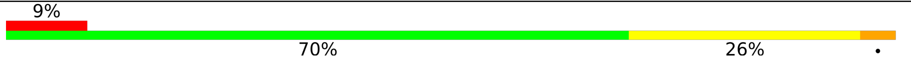
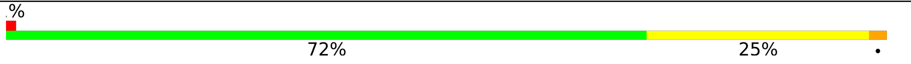
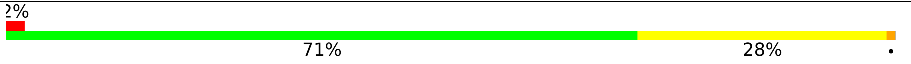
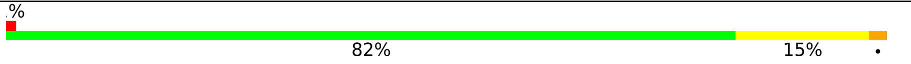
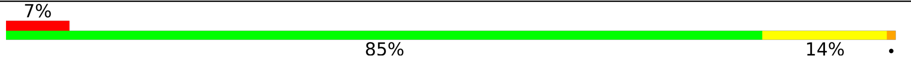
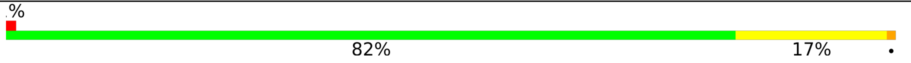
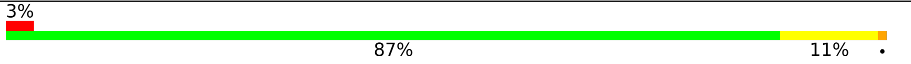
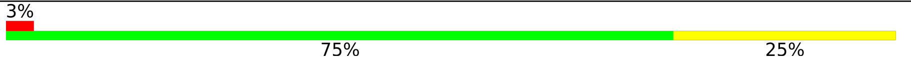
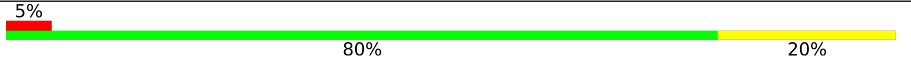
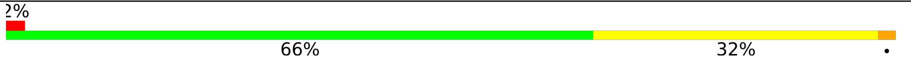
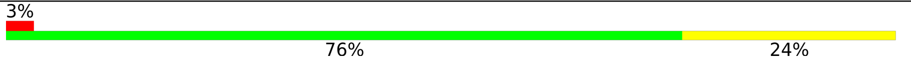
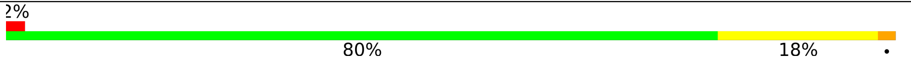
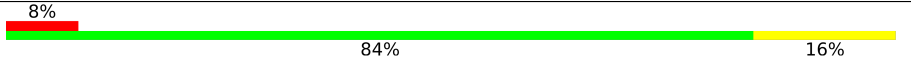
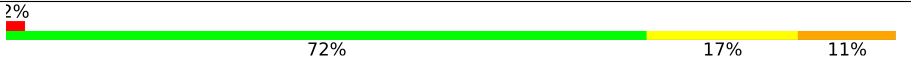
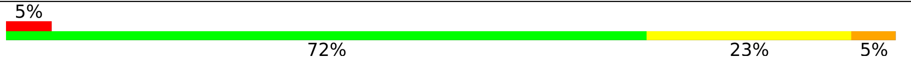
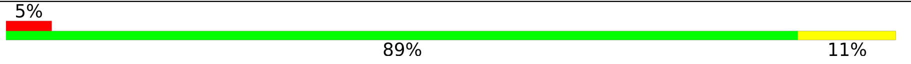
Mol	Chain	Length	Quality of chain
41	BV	101	
41	DV	101	
42	BW	113	
42	DW	113	
43	BX	93	
43	DX	93	
44	BY	107	
44	DY	107	
45	BZ	185	
45	DZ	185	
46	B0	84	
46	D0	84	
47	B2	71	
47	D2	71	
48	B3	60	
48	D3	60	
49	B5	59	
49	D5	59	
50	B6	50	
50	D6	50	
51	B7	49	
51	D7	49	
52	B8	64	
52	D8	64	
53	B9	37	

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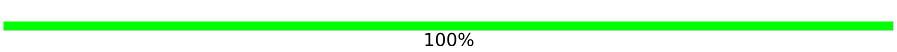
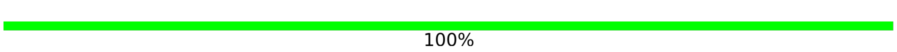
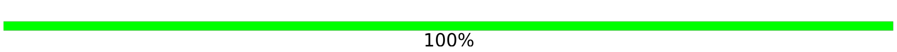
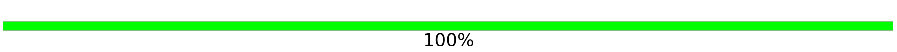
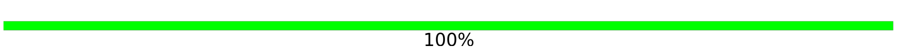
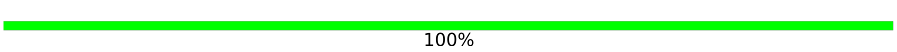
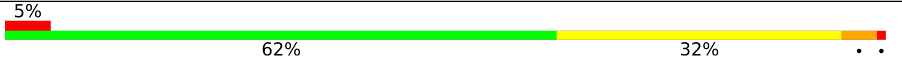
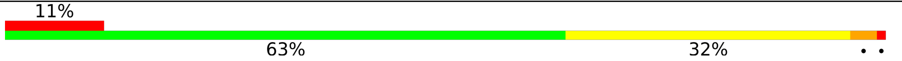
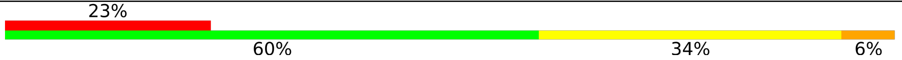
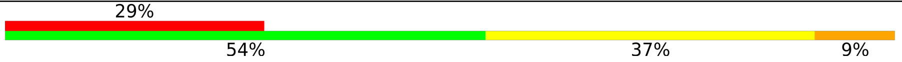
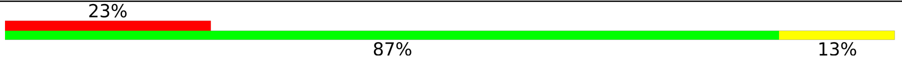
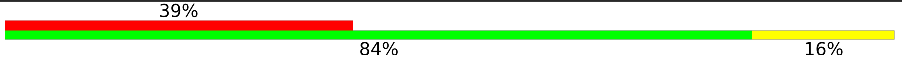
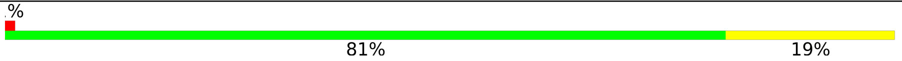
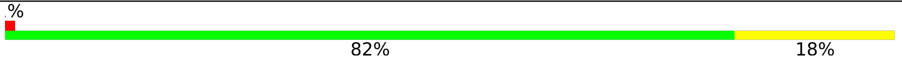
Mol	Chain	Length	Quality of chain
53	D9	37	
54	Bf	31	
54	Bg	31	
54	Df	31	
54	Dg	31	
55	Bh	30	
55	Dh	30	
56	B1	93	
56	D1	93	
57	B4	35	
57	D4	35	
58	Be	102	
58	De	102	
59	BA	2879	
59	DA	2879	
60	BB	119	
60	DB	119	

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 1910 1218 342 345 5	0	0	0
1	CB	235	Total C N O S 1910 1218 342 345 5	0	0	0

- 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 1621 1022 315 283 1	0	0	0
2	CC	207	Total C N O S 1621 1022 315 283 1	0	0	0

- 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 1703 1066 339 291 7	0	0	0
3	CD	208	Total C N O S 1703 1066 339 291 7	0	0	0

- 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 1156 729 218 205 4	0	0	0
4	CE	151	Total C N O S 1156 729 218 205 4	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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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 32474	C 14455	N 6015	O 10494	P 1510	0	0	0
21	CA	1511	Total 32474	C 14455	N 6015	O 10494	P 1510	0	0	0

- Molecule 22 is a RNA chain called transfer RNA.

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

- Molecule 23 is a RNA chain called messenger RNA.

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

- Molecule 24 is a protein called VIOMYCIN.

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

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

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

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

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 2145 1353 428 361 3	0	0	0
26	DD	275	Total C N O S 2145 1353 428 361 3	0	0	0

- 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 1569 991 300 272 6	0	0	0
27	DE	205	Total C N O S 1569 991 300 272 6	0	0	0

- 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 1628 1037 304 284 3	0	0	0
28	DF	208	Total C N O S 1628 1037 304 284 3	0	0	0

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 1474	C 942	N 268	O 260	S 4	0	0	0
29	DG	181	Total 1474	C 942	N 268	O 260	S 4	0	0	0

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 1274	C 806	N 238	O 229	S 1	0	0	0
30	DH	167	Total 1274	C 806	N 238	O 229	S 1	0	0	0

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

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

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

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

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

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

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

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

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
			Total	C	N	O	S			
35	BP	146	1114	692	227	193	2	0	0	0
35	DP	146	1114	692	227	193	2	0	0	0

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

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

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 960	C 599	N 202	O 159	0	0	0
37	DR	117	Total 960	C 599	N 202	O 159	0	0	0

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

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

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

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

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 964	C 610	N 202	O 151	S 1	0	0	0

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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
			Total	C	N	O	S			
46	B0	84	662	410	140	111	1	0	0	0
46	D0	84	662	410	140	111	1	0	0	0

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
			Total	C	N	O	S			
47	B2	71	598	370	121	106	1	0	0	0
47	D2	71	598	370	121	106	1	0	0	0

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

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

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

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

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 433 270 88 71 4	0	0	0
50	D6	50	Total C N O S 433 270 88 71 4	0	0	0

- 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 430 263 108 57 2	0	0	0
51	D7	49	Total C N O S 430 263 108 57 2	0	0	0

- 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 517 331 102 82 2	0	0	0
52	D8	64	Total C N O S 517 331 102 82 2	0	0	0

- 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 307 188 68 47 4	0	0	0
53	D9	37	Total C N O S 307 188 68 47 4	0	0	0

- 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 156 93 31 32	0	0	0
54	Bg	31	Total C N O 156 93 31 32	0	0	0
54	Df	31	Total C N O 156 93 31 32	0	0	0
54	Dg	31	Total C N O 156 93 31 32	0	0	0

- 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 151 90 30 31	0	0	0
55	Dh	30	Total C N O 151 90 30 31	0	0	0

- 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 732 460 145 126 1	0	0	0
56	D1	93	Total C N O S 732 460 145 126 1	0	0	0

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 271 174 44 50 3	0	0	0
57	D4	35	Total C N O S 271 174 44 50 3	0	0	0

- 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 686 430 119 137	0	0	0
58	De	102	Total C N O 686 430 119 137	0	0	0

- 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 61997 27594 11582 19943 2878	0	0	0

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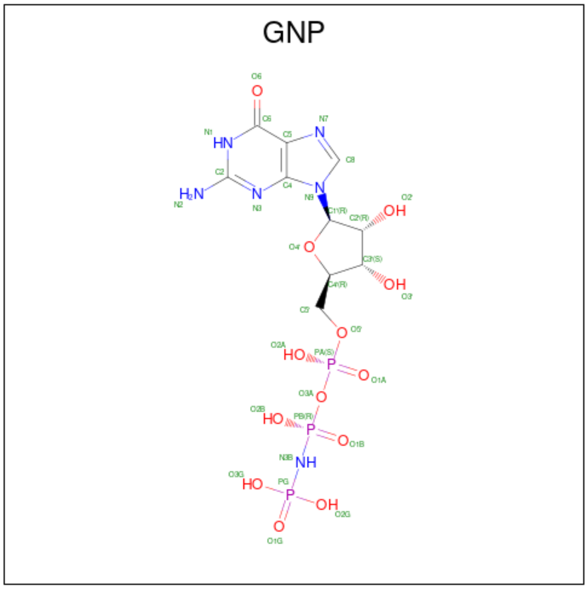
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	DA	2879	Total 61997	C 27594	N 11582	O 19943	P 2878	0	0	0

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

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

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



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

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

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

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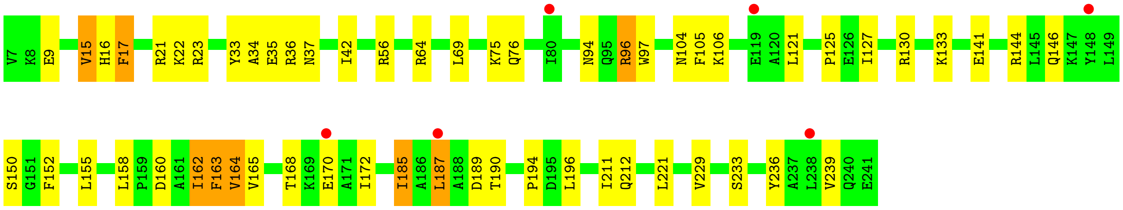
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
62	CY	1	1	1	0	0

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.

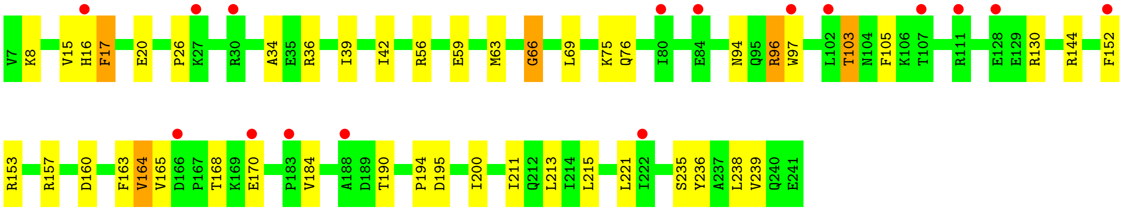
- Molecule 1: 30S ribosomal protein S2

Chain AB:



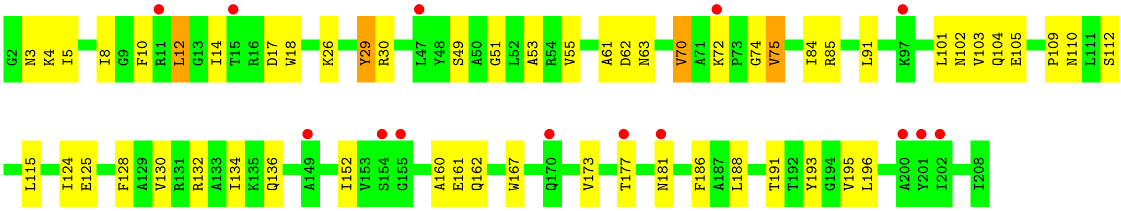
- Molecule 1: 30S ribosomal protein S2

Chain CB:



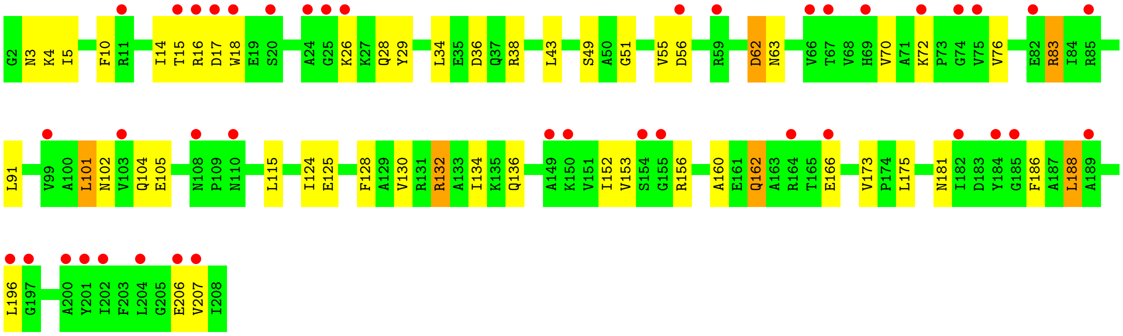
- Molecule 2: 30S ribosomal protein S3

Chain AC:



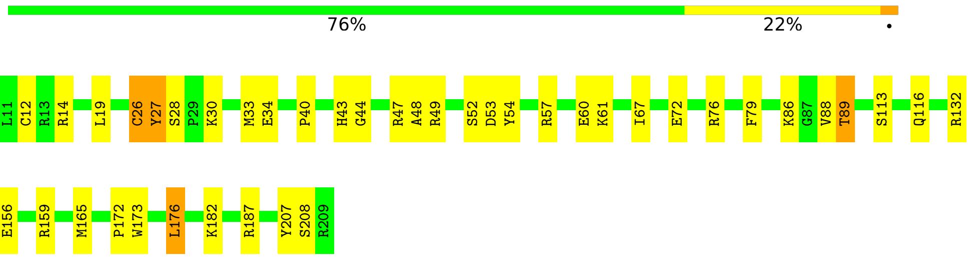
- Molecule 2: 30S ribosomal protein S3

Chain CC:



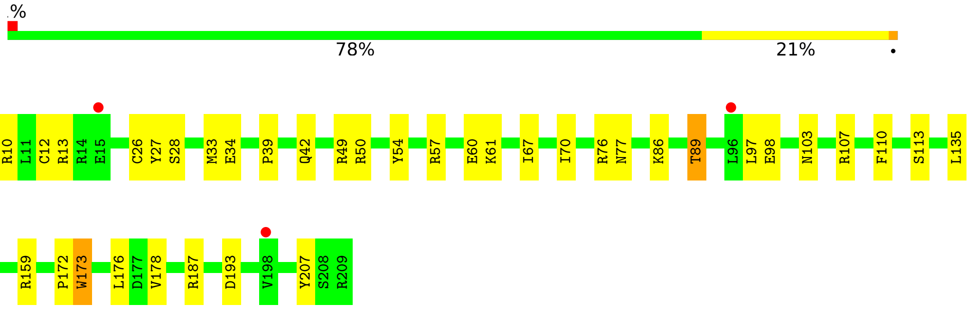
- Molecule 3: 30S ribosomal protein S4

Chain AD:



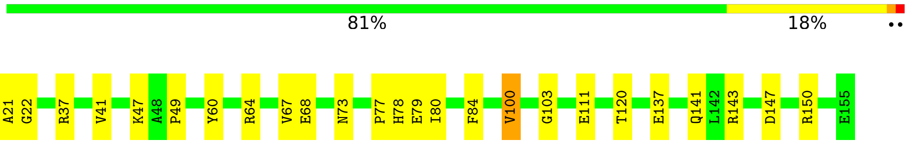
- Molecule 3: 30S ribosomal protein S4

Chain CD:



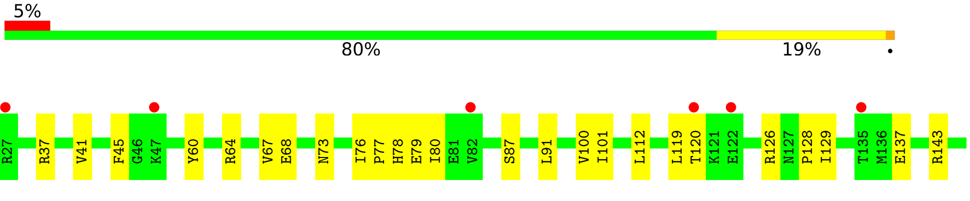
- Molecule 4: 30S ribosomal protein S5

Chain AE:



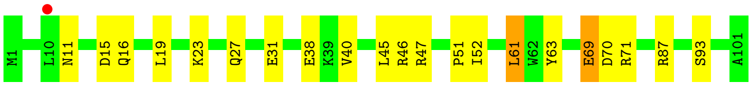
- Molecule 4: 30S ribosomal protein S5

Chain CE:



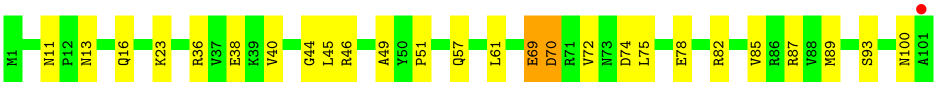
- Molecule 5: 30S ribosomal protein S6

Chain AF:



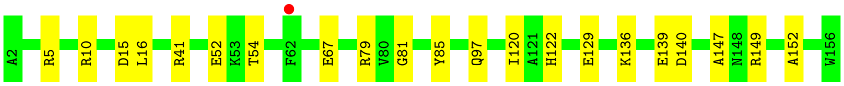
- Molecule 5: 30S ribosomal protein S6

Chain CF:



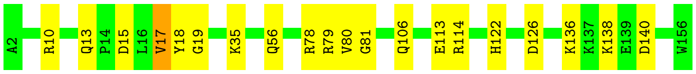
- Molecule 6: 30S ribosomal protein S7

Chain AG:



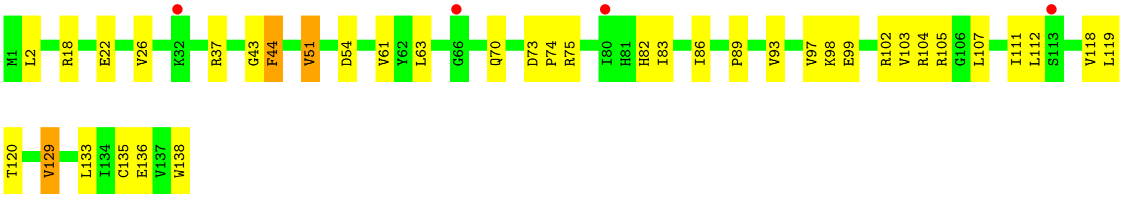
- Molecule 6: 30S ribosomal protein S7

Chain CG:



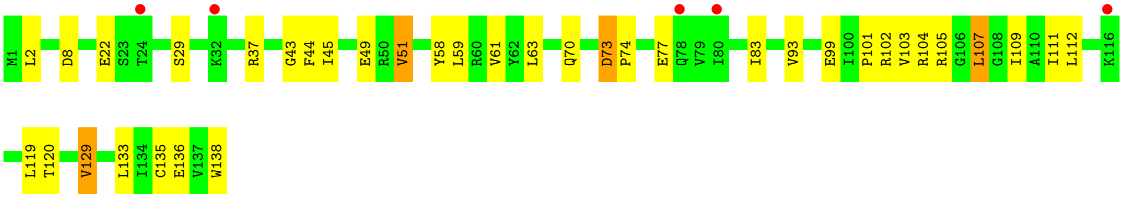
- Molecule 7: 30S ribosomal protein S8

Chain AH:

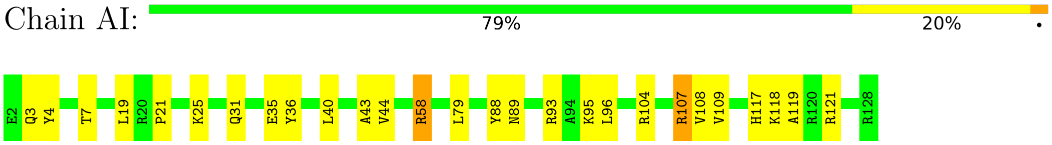


- Molecule 7: 30S ribosomal protein S8

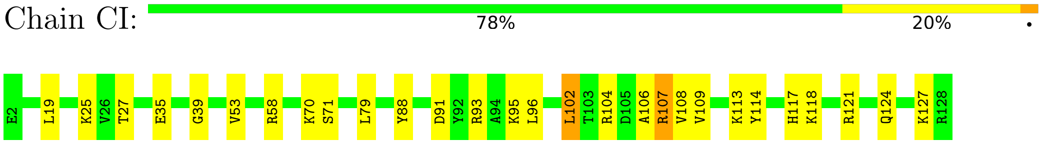
Chain CH:



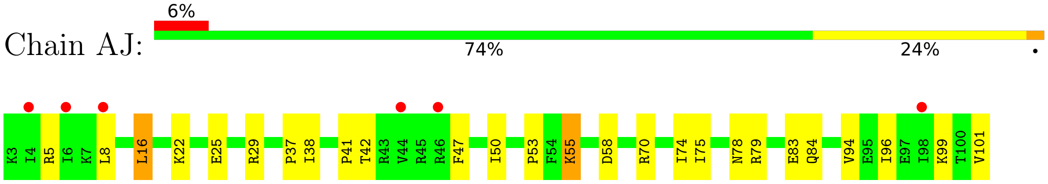
- Molecule 8: 30S ribosomal protein S9



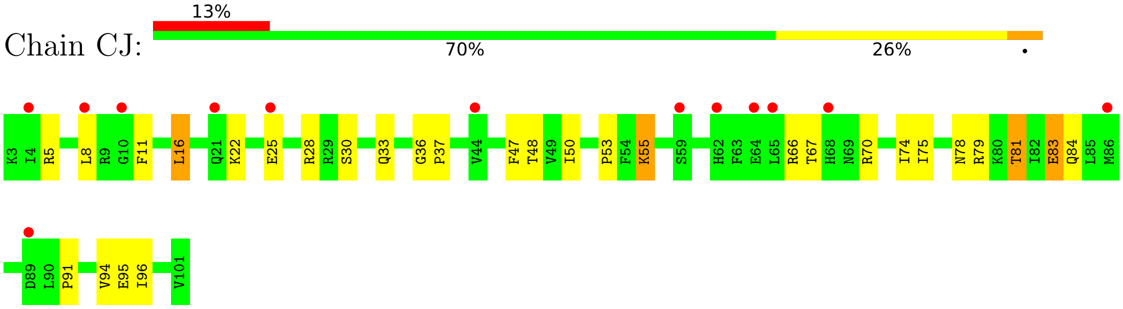
- Molecule 8: 30S ribosomal protein S9



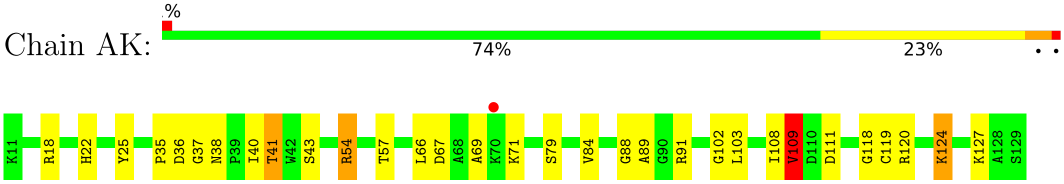
- Molecule 9: 30S ribosomal protein S10



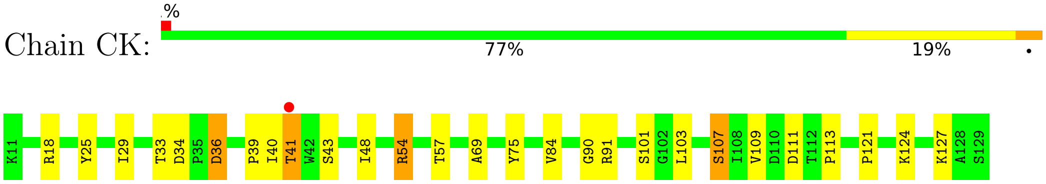
- Molecule 9: 30S ribosomal protein S10



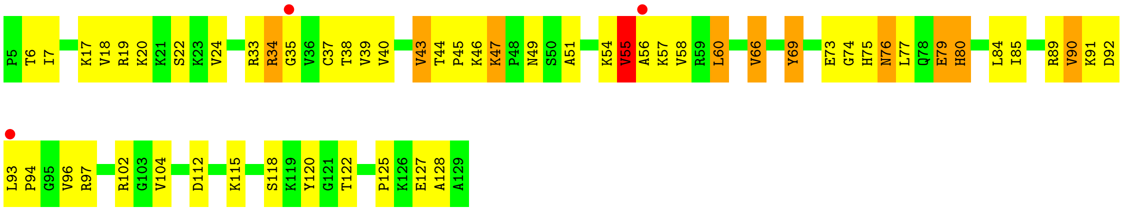
- Molecule 10: 30S ribosomal protein S11



- Molecule 10: 30S ribosomal protein S11

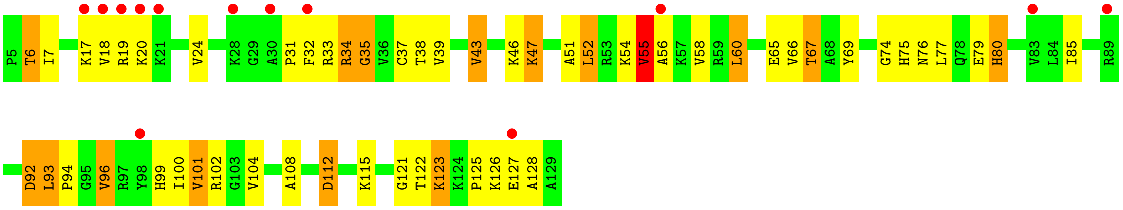


- Molecule 11: 30S ribosomal protein S12



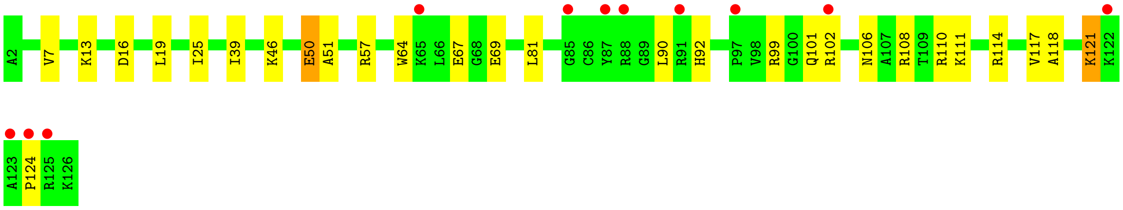
- Molecule 11: 30S ribosomal protein S12

Chain CL:



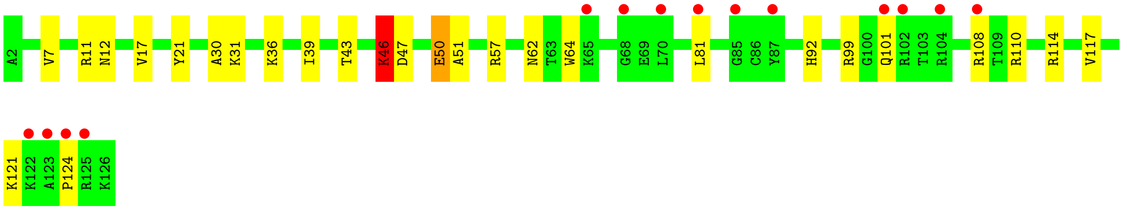
- Molecule 12: 30S ribosomal protein S13

Chain AM:



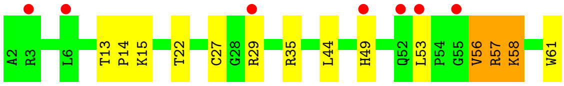
- Molecule 12: 30S ribosomal protein S13

Chain CM:



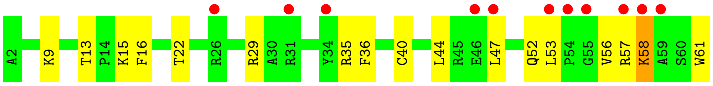
- Molecule 13: 30S ribosomal protein S14 type Z

Chain AN:



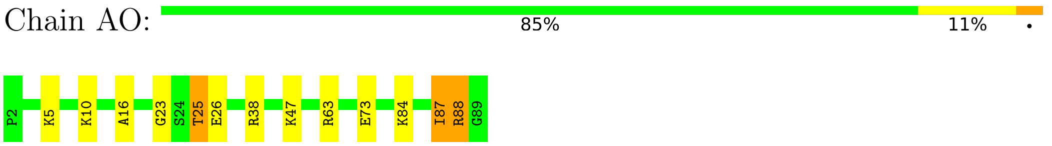
- Molecule 13: 30S ribosomal protein S14 type Z

Chain CN:



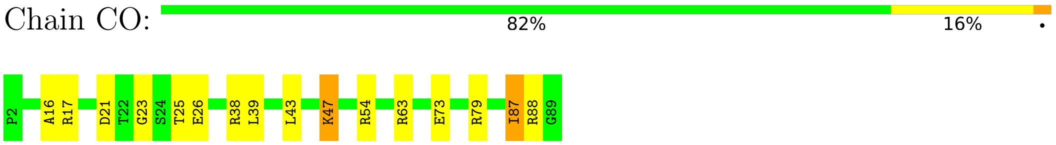
- Molecule 14: 30S ribosomal protein S15

Chain AO:



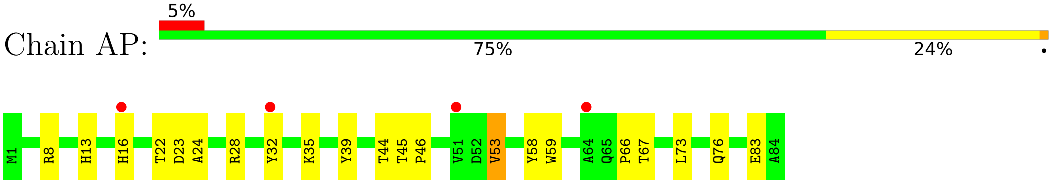
- Molecule 14: 30S ribosomal protein S15

Chain CO:



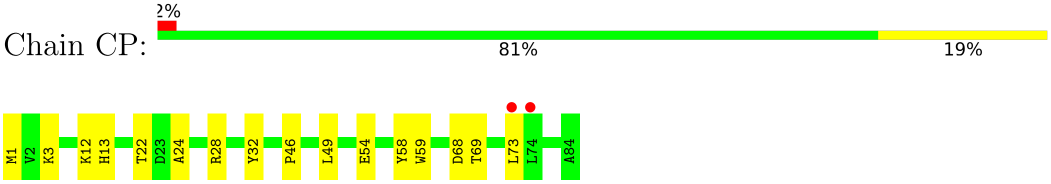
- Molecule 15: 30S ribosomal protein S16

Chain AP:



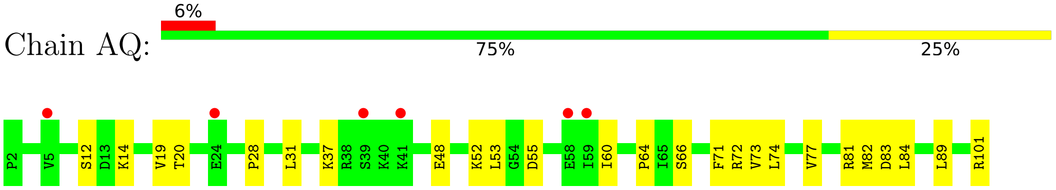
- Molecule 15: 30S ribosomal protein S16

Chain CP:



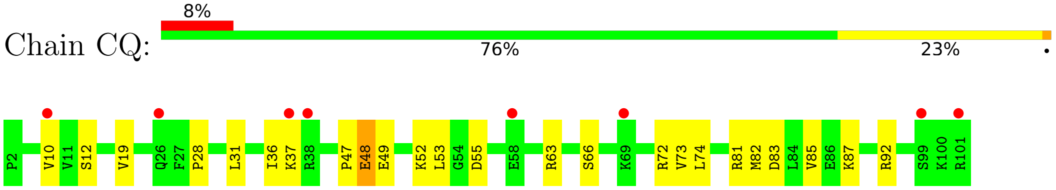
- Molecule 16: 30S ribosomal protein S17

Chain AQ:

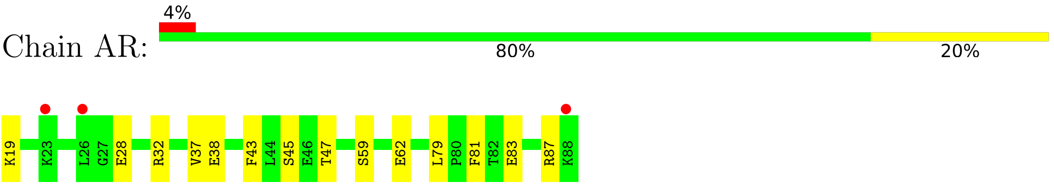


- Molecule 16: 30S ribosomal protein S17

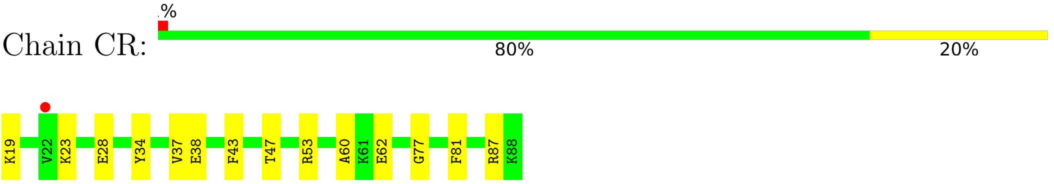
Chain CQ:



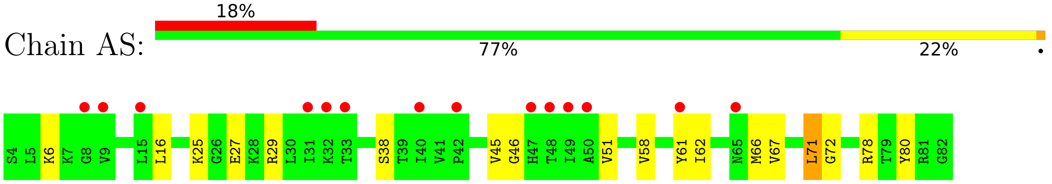
- Molecule 17: 30S ribosomal protein S18



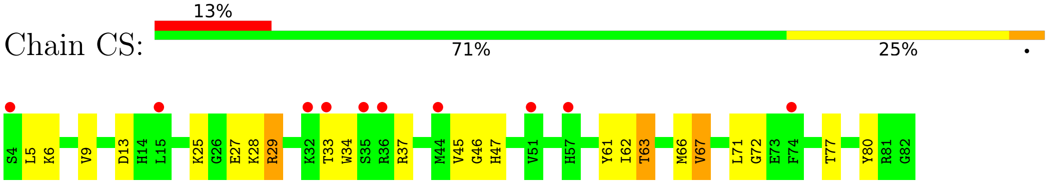
- Molecule 17: 30S ribosomal protein S18



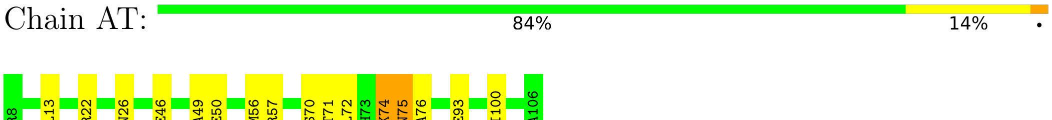
- Molecule 18: 30S ribosomal protein S19



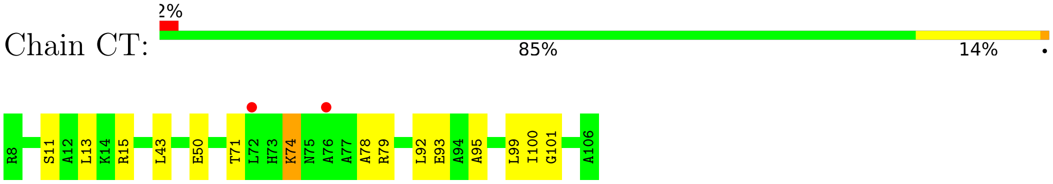
- Molecule 18: 30S ribosomal protein S19



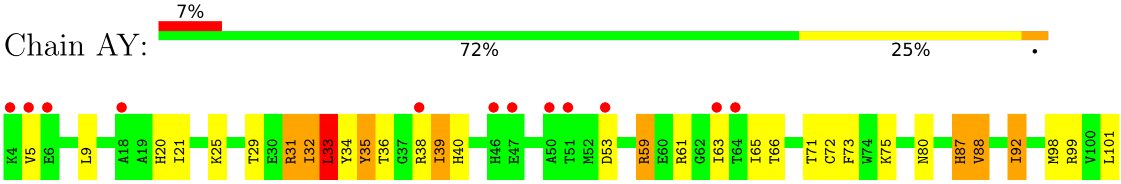
- Molecule 19: 30S ribosomal protein S20

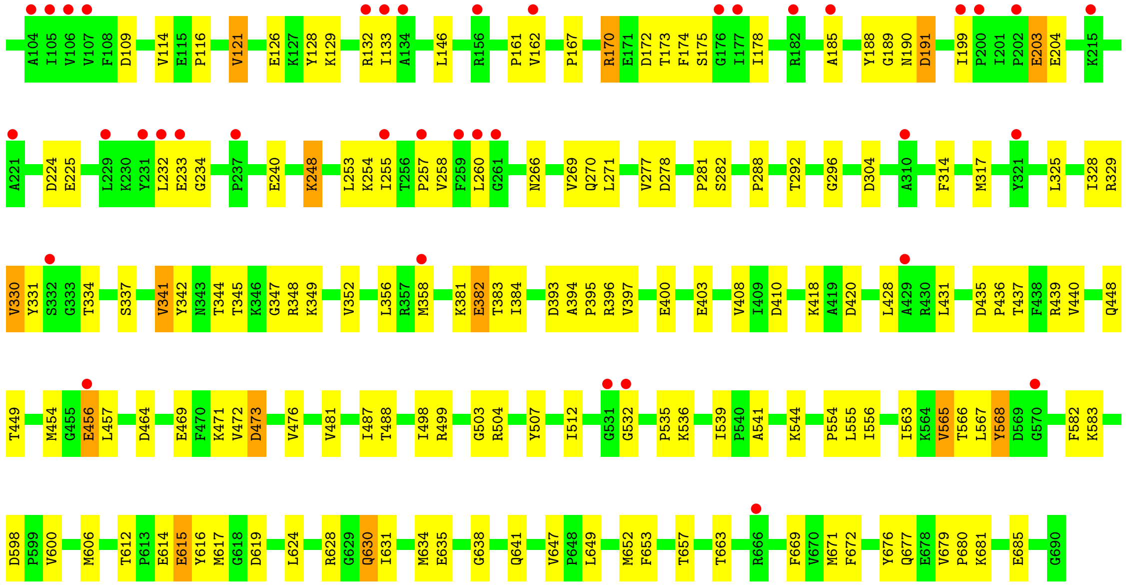


- Molecule 19: 30S ribosomal protein S20



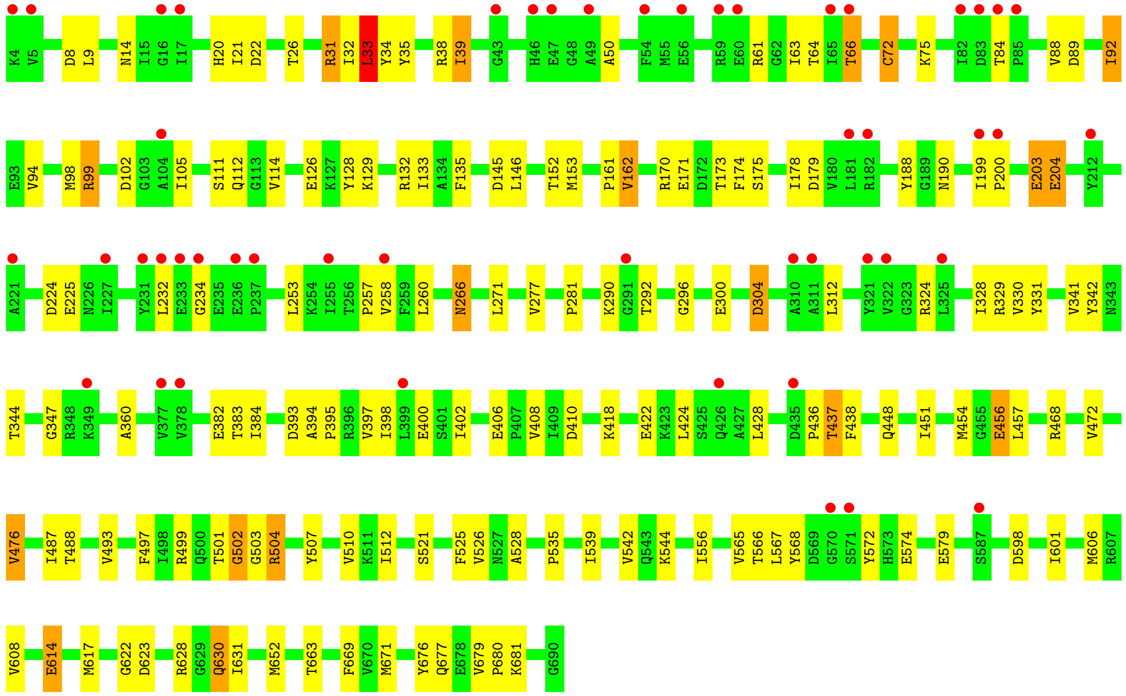
- Molecule 20: Elongation factor G





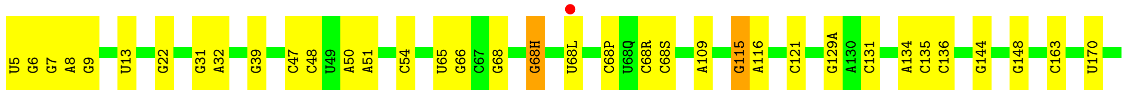
- Molecule 20: Elongation factor G

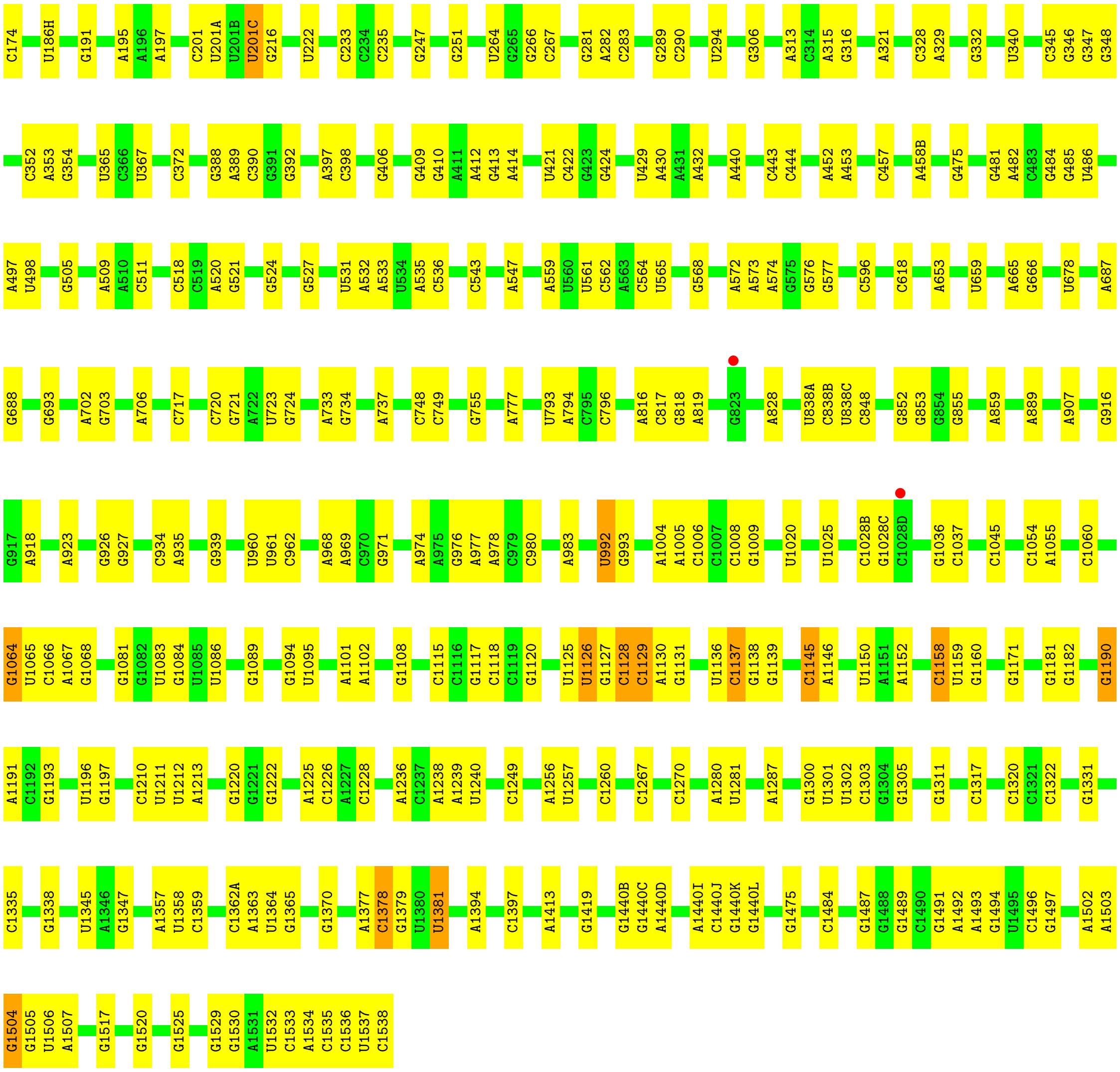
Chain CY:



- Molecule 21: ribosomal RNA 16S

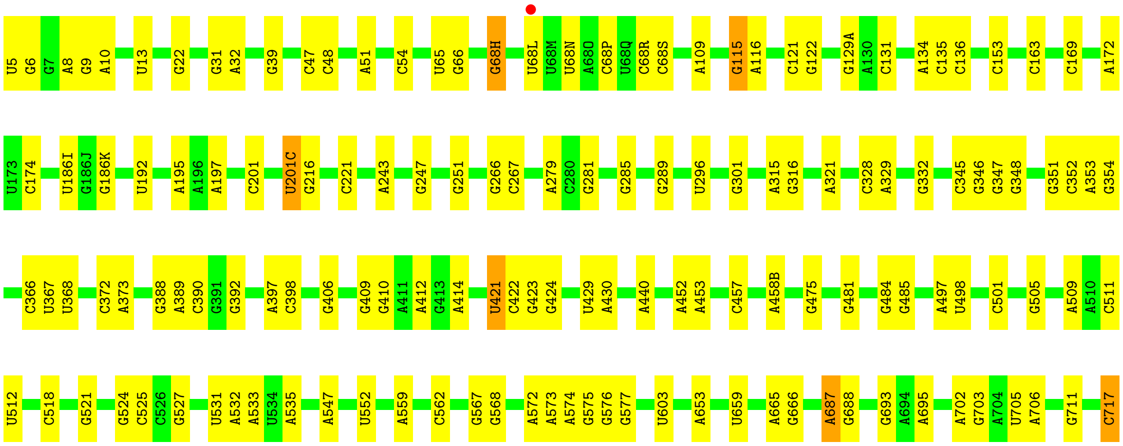
Chain AA:

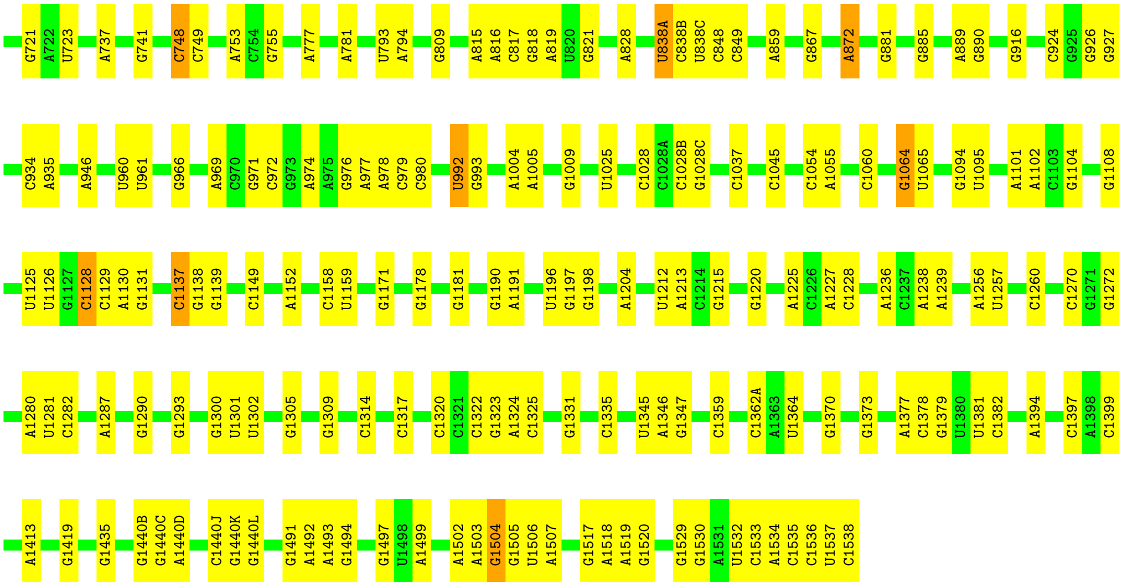




- Molecule 21: ribosomal RNA 16S

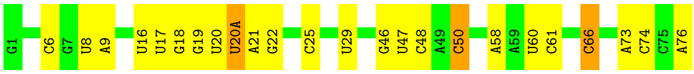
Chain CA:





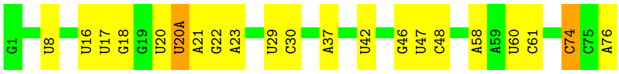
- Molecule 22: transfer RNA

Chain AW:



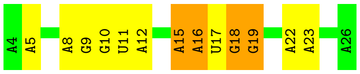
- Molecule 22: transfer RNA

Chain CW:



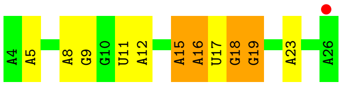
- Molecule 23: messenger RNA

Chain AV:



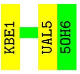
- Molecule 23: messenger RNA

Chain CV:



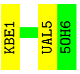
- Molecule 24: VIOMYCIN

Chain AU:



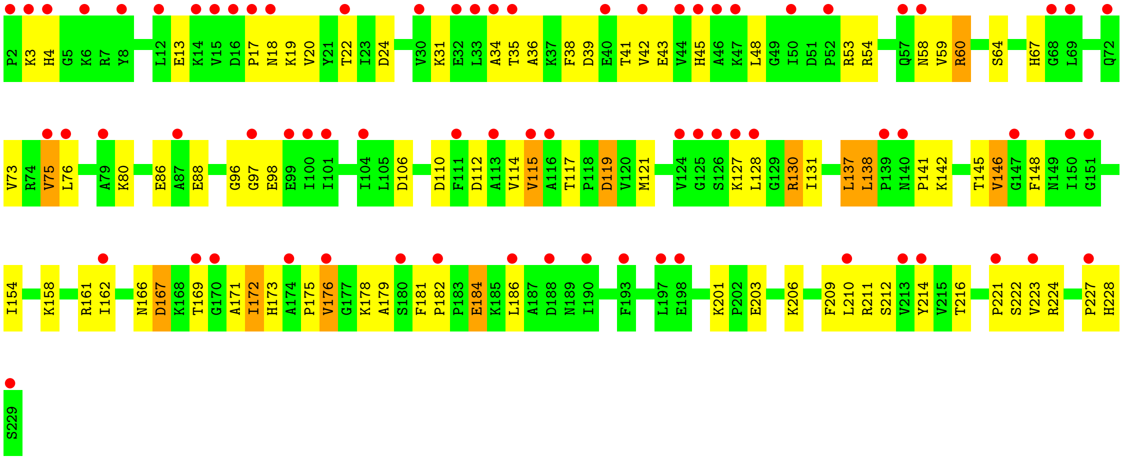
- Molecule 24: VIOMYCIN

Chain CU:



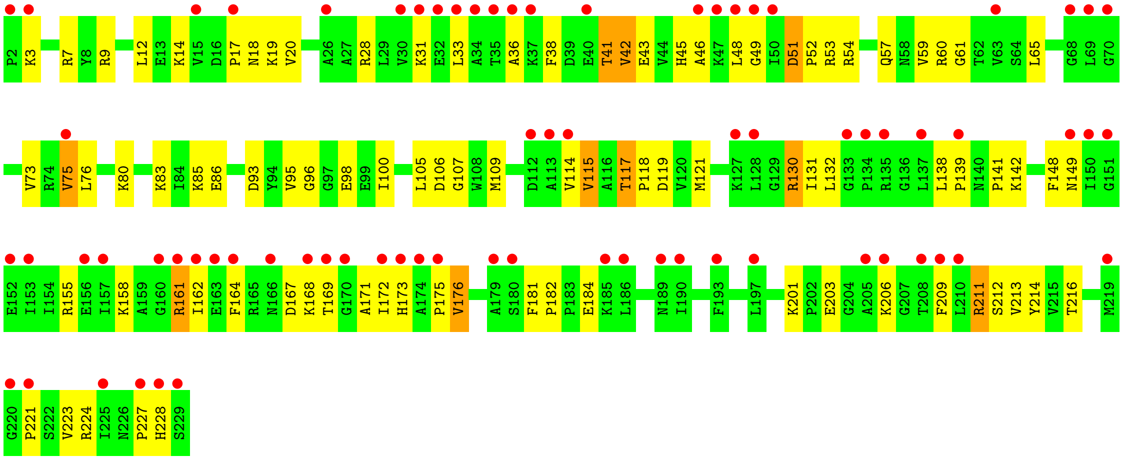
- Molecule 25: 50S ribosomal protein L1

Chain BC:



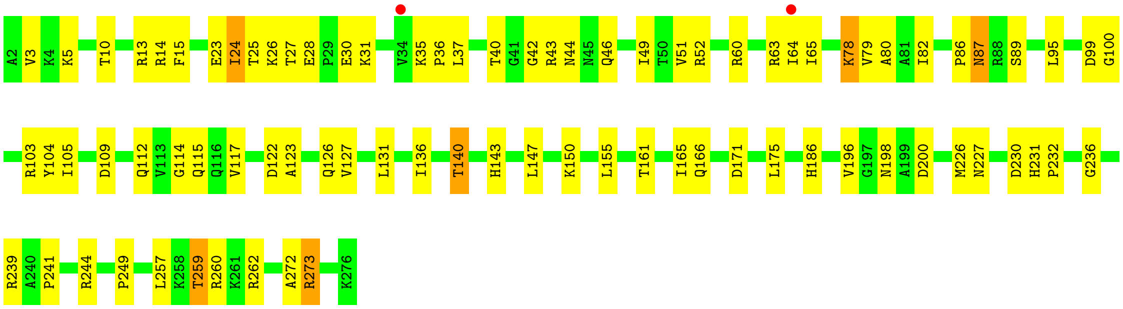
- Molecule 25: 50S ribosomal protein L1

Chain DC:



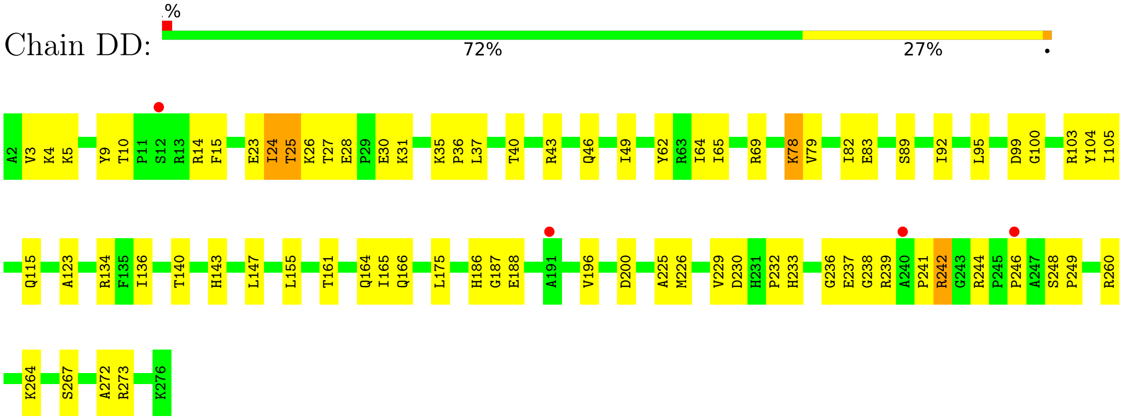
- Molecule 26: 50S ribosomal protein L2

Chain BD:



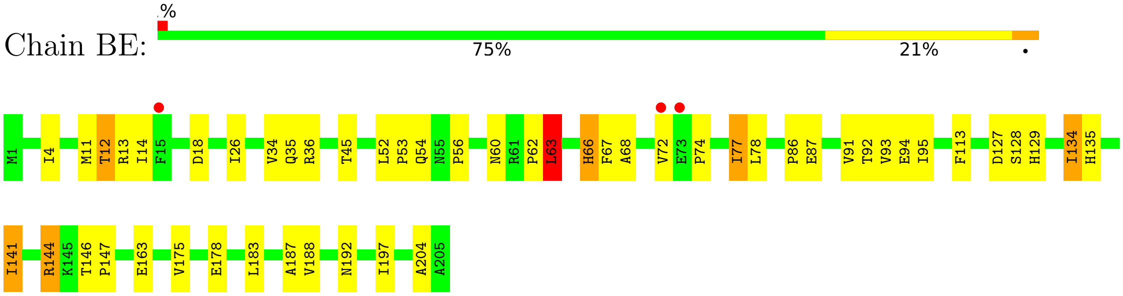
- Molecule 26: 50S ribosomal protein L2

Chain DD:



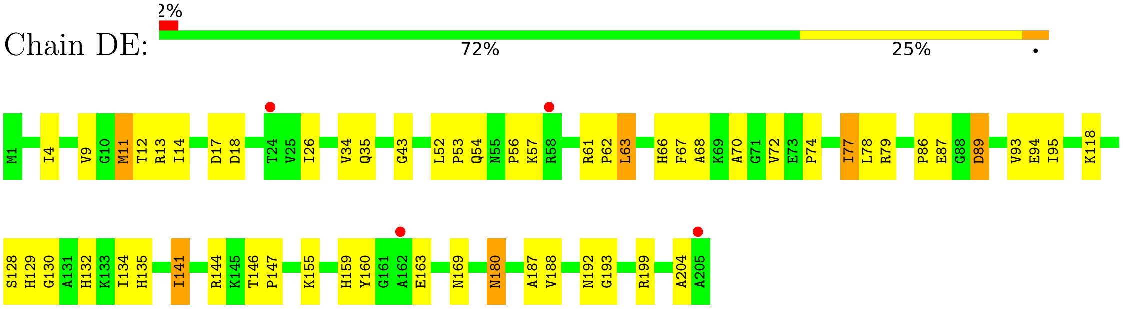
- Molecule 27: 50S ribosomal protein L3

Chain BE:



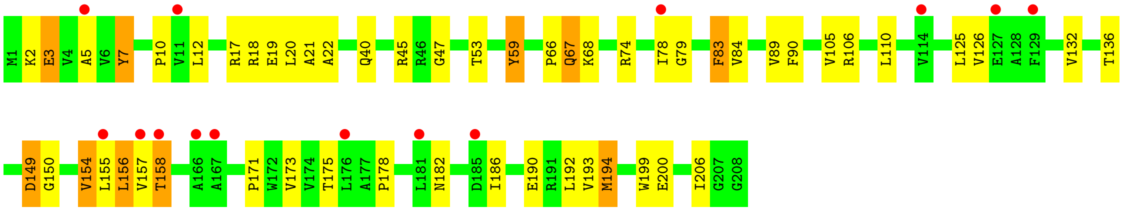
- Molecule 27: 50S ribosomal protein L3

Chain DE:



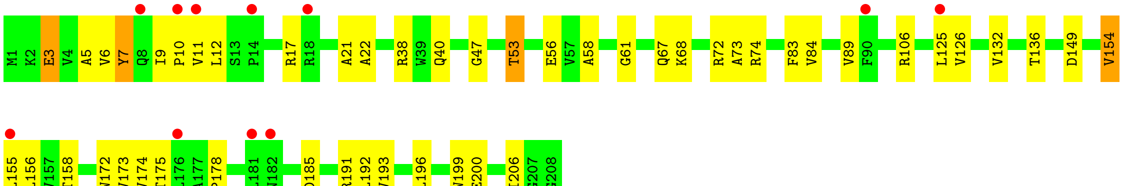
- Molecule 28: 50S ribosomal protein L4

Chain BF:



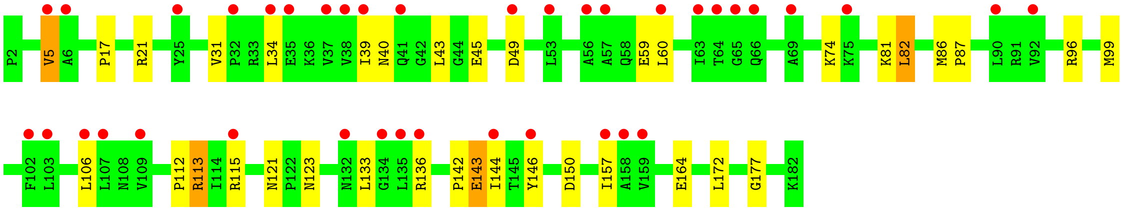
- Molecule 28: 50S ribosomal protein L4

Chain DF:



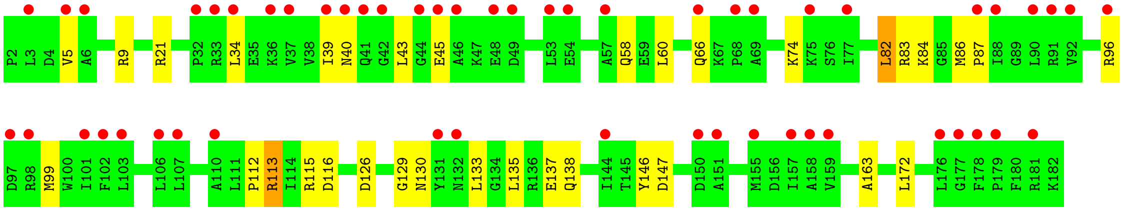
- Molecule 29: 50S ribosomal protein L5

Chain BG:



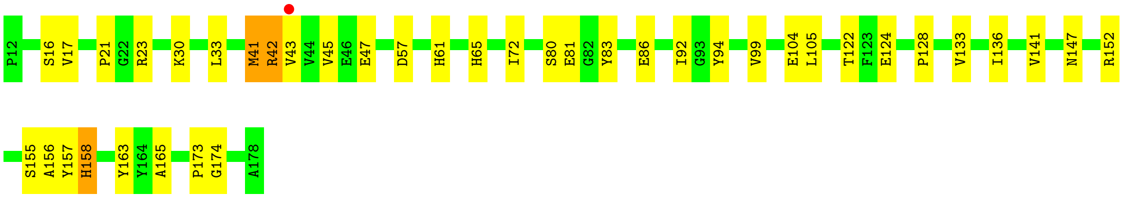
- Molecule 29: 50S ribosomal protein L5

Chain DG:



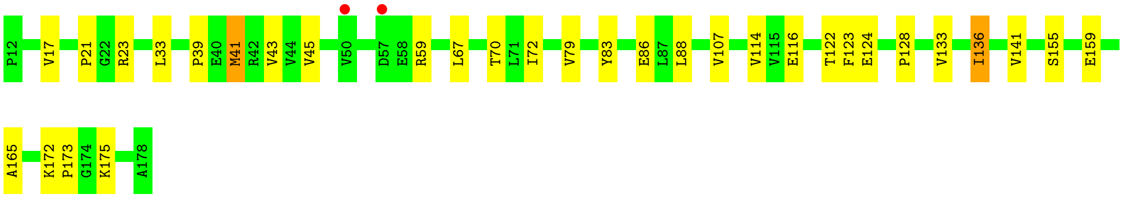
- Molecule 30: 50S ribosomal protein L6

Chain BH:



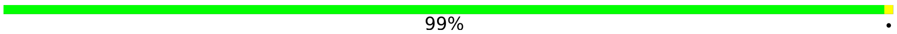
- Molecule 30: 50S ribosomal protein L6

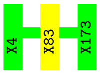
Chain DH:



- Molecule 31: 50S RIBOSOMAL PROTEIN L10

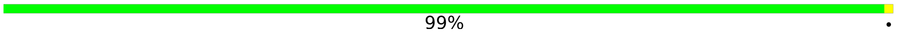
Chain BJ:

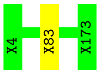




- Molecule 31: 50S RIBOSOMAL PROTEIN L10

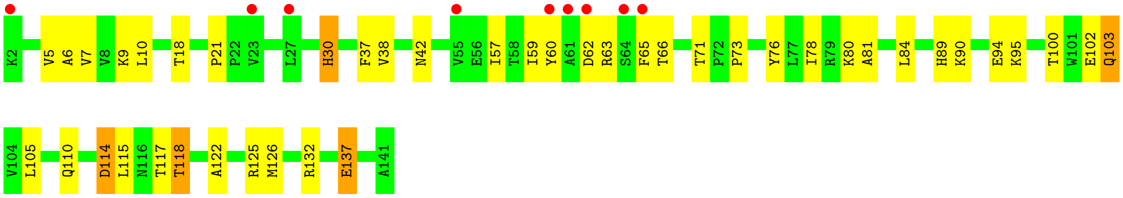
Chain DJ:





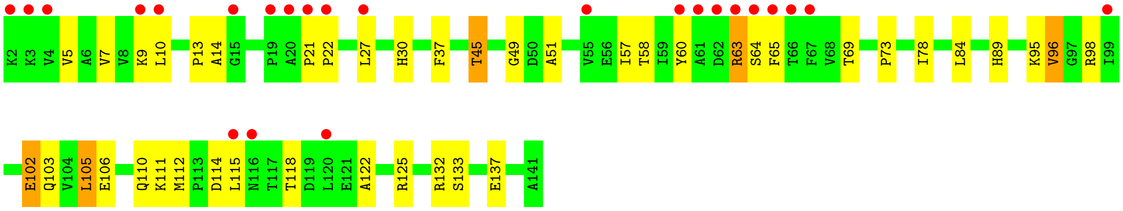
- Molecule 32: 50S ribosomal protein L11

Chain BK:



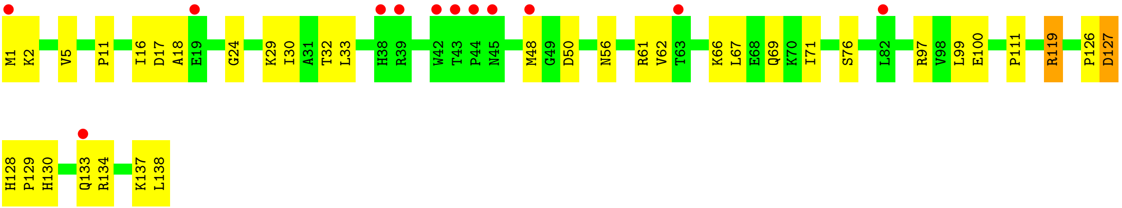
- Molecule 32: 50S ribosomal protein L11

Chain DK:



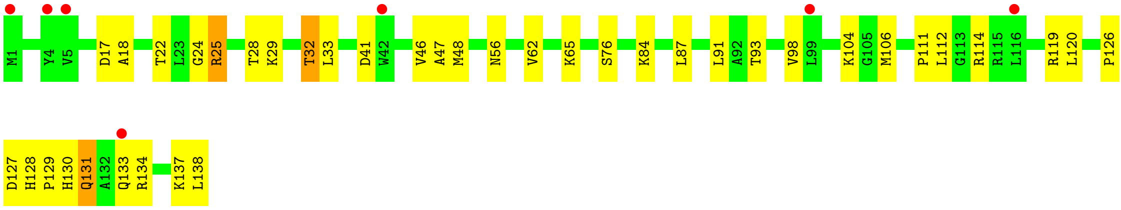
- Molecule 33: 50S ribosomal protein L13

Chain BN:



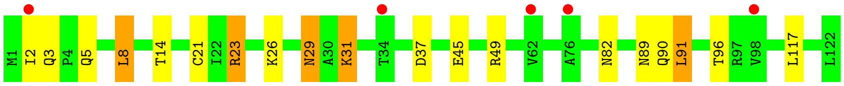
- Molecule 33: 50S ribosomal protein L13

Chain DN:



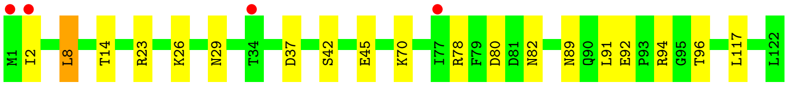
- Molecule 34: 50S ribosomal protein L14

Chain BO:



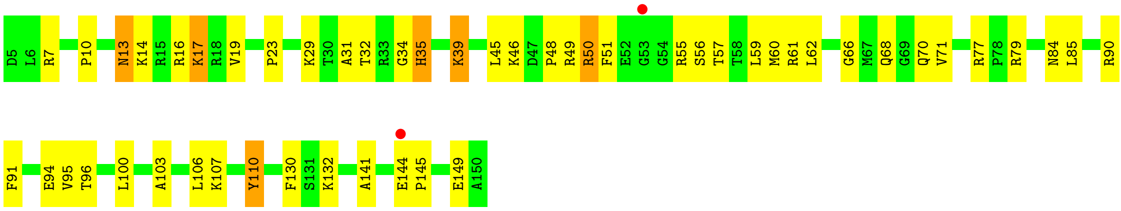
- Molecule 34: 50S ribosomal protein L14

Chain DO:



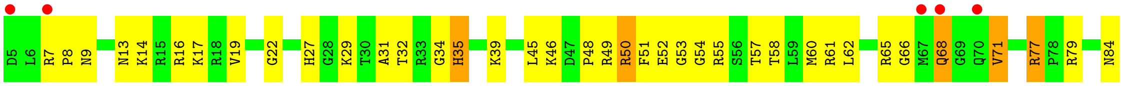
- Molecule 35: 50S ribosomal protein L15

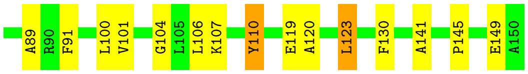
Chain BP:



- Molecule 35: 50S ribosomal protein L15

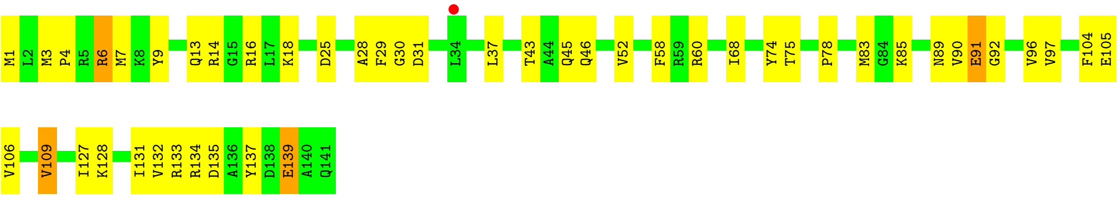
Chain DP:





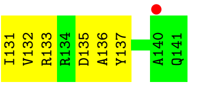
- Molecule 36: 50S ribosomal protein L16

Chain BQ:



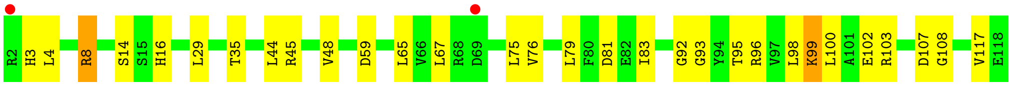
- Molecule 36: 50S ribosomal protein L16

Chain DQ:



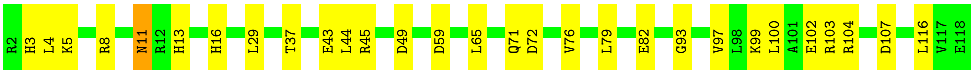
- Molecule 37: 50S ribosomal protein L17

Chain BR:



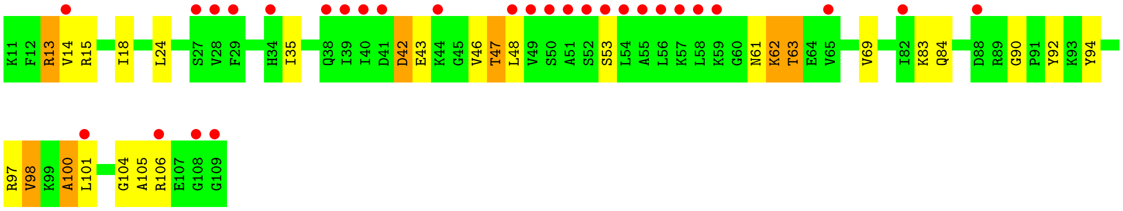
- Molecule 37: 50S ribosomal protein L17

Chain DR:



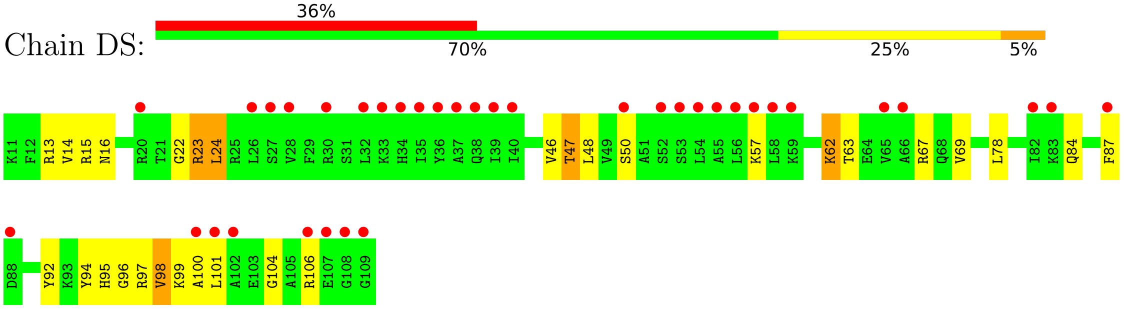
- Molecule 38: 50S ribosomal protein L18

Chain BS:



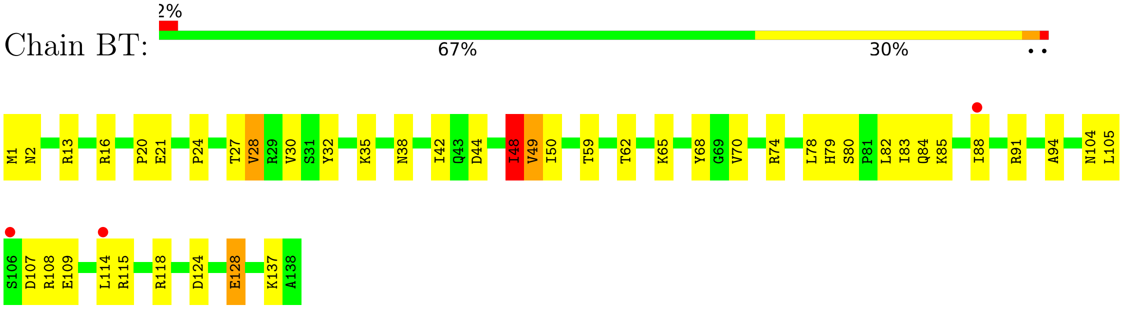
- Molecule 38: 50S ribosomal protein L18

Chain DS:



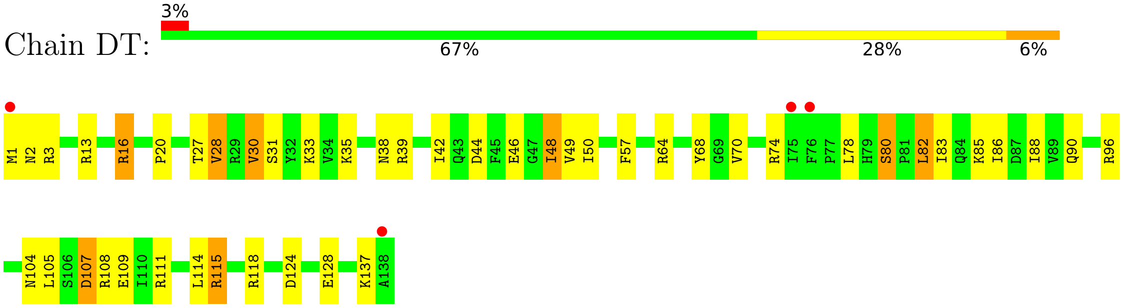
- Molecule 39: 50S ribosomal protein L19

Chain BT:



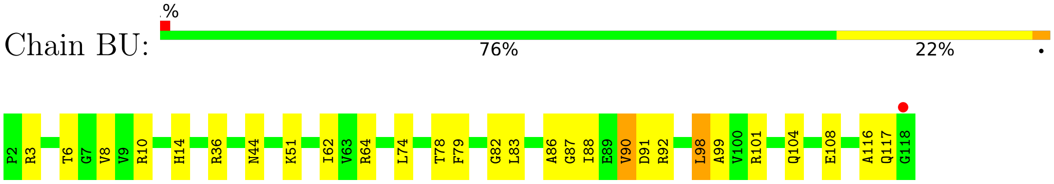
- Molecule 39: 50S ribosomal protein L19

Chain DT:



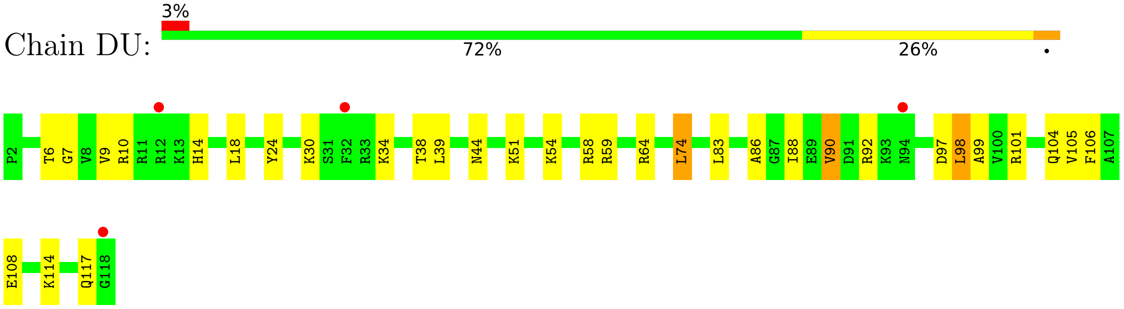
- Molecule 40: 50S ribosomal protein L20

Chain BU:



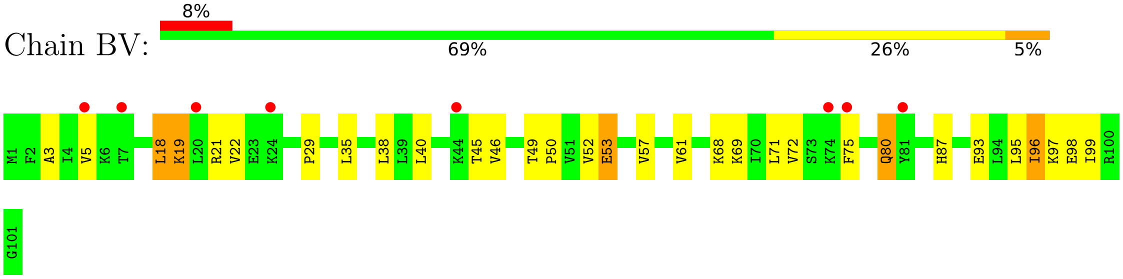
- Molecule 40: 50S ribosomal protein L20

Chain DU:



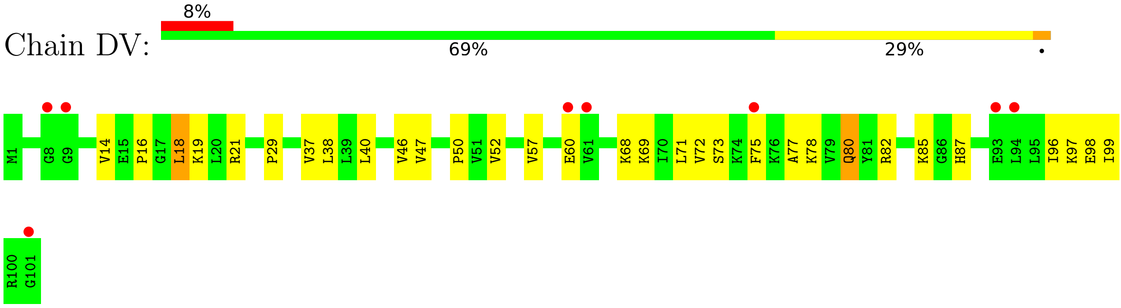
- Molecule 41: 50S ribosomal protein L21

Chain BV:



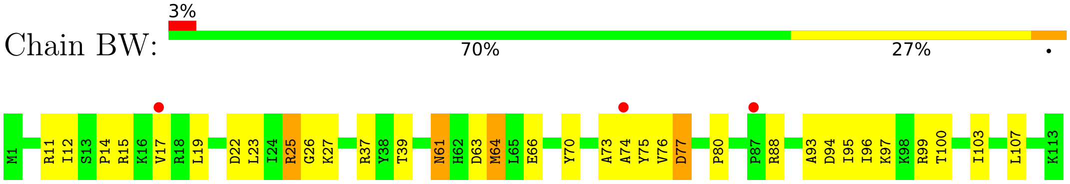
- Molecule 41: 50S ribosomal protein L21

Chain DV:



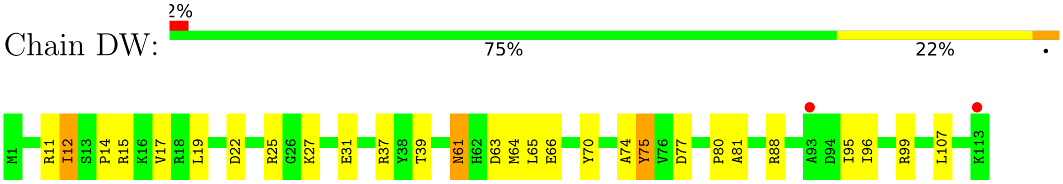
- Molecule 42: 50S ribosomal protein L22

Chain BW:



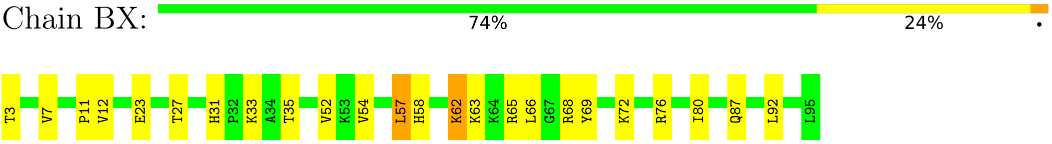
- Molecule 42: 50S ribosomal protein L22

Chain DW:



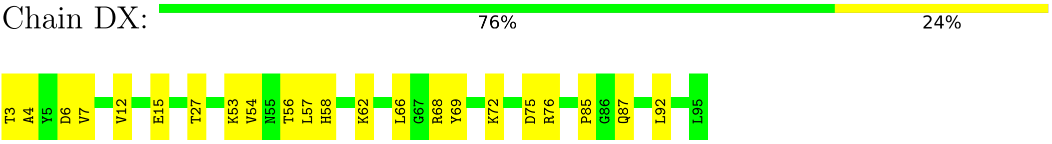
- Molecule 43: 50S ribosomal protein L23

Chain BX:



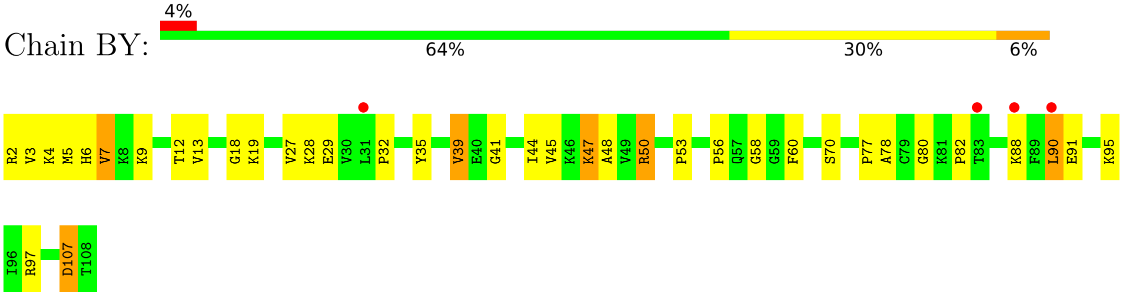
- Molecule 43: 50S ribosomal protein L23

Chain DX:



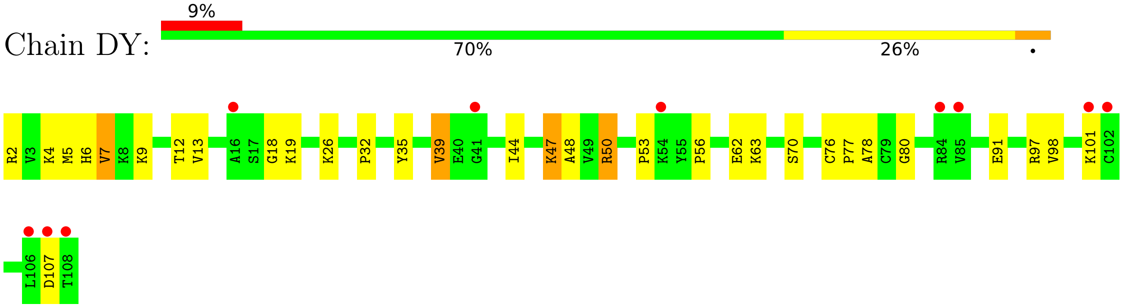
- Molecule 44: 50S ribosomal protein L24

Chain BY:



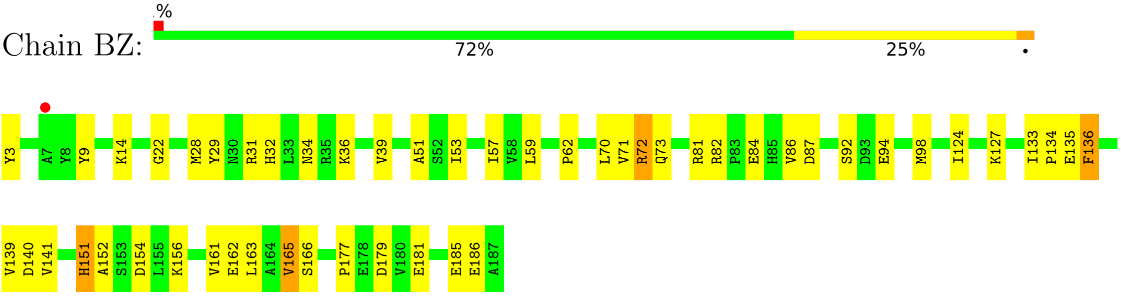
- Molecule 44: 50S ribosomal protein L24

Chain DY:



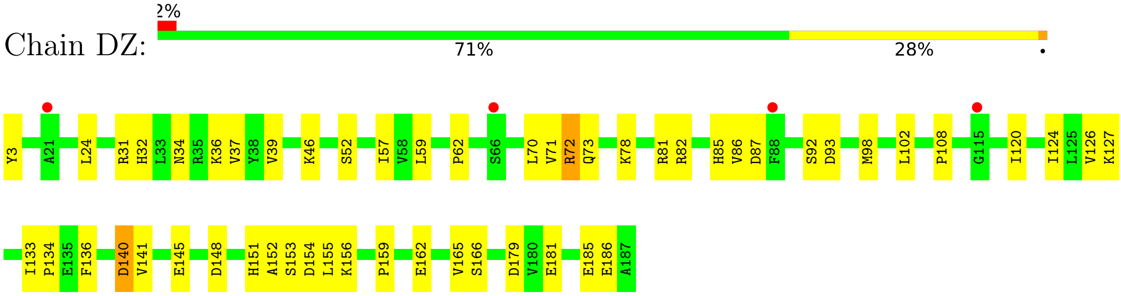
- Molecule 45: 50S ribosomal protein L25

Chain BZ:



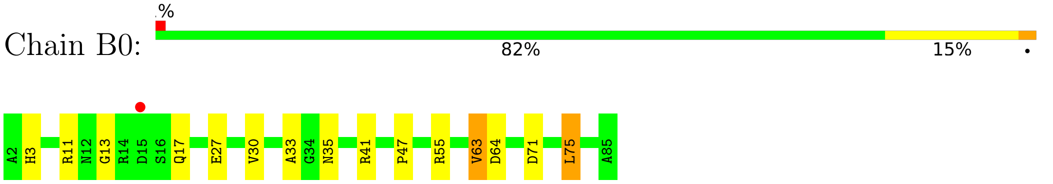
- Molecule 45: 50S ribosomal protein L25

Chain DZ:



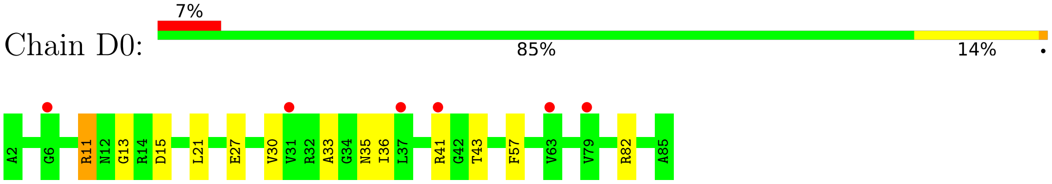
- Molecule 46: 50S ribosomal protein L27

Chain B0:



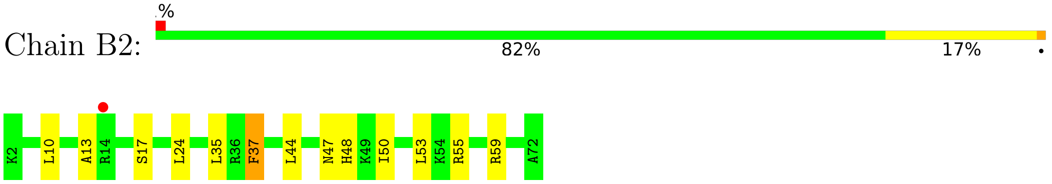
- Molecule 46: 50S ribosomal protein L27

Chain D0:



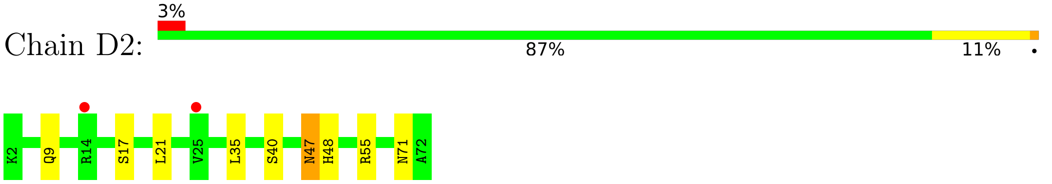
- Molecule 47: 50S ribosomal protein L29

Chain B2:



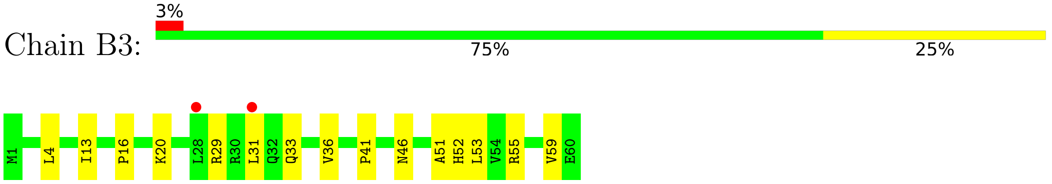
- Molecule 47: 50S ribosomal protein L29

Chain D2:



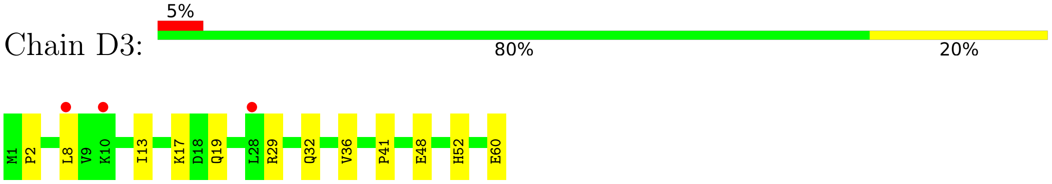
- Molecule 48: 50S ribosomal protein L30

Chain B3:



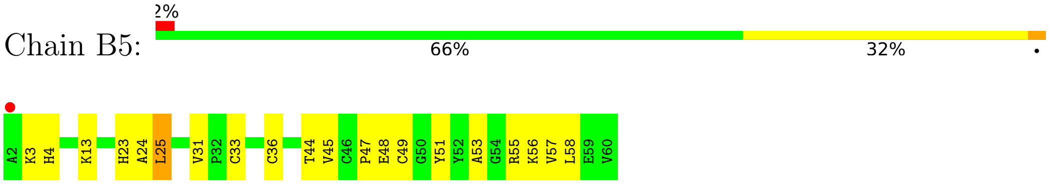
- Molecule 48: 50S ribosomal protein L30

Chain D3:



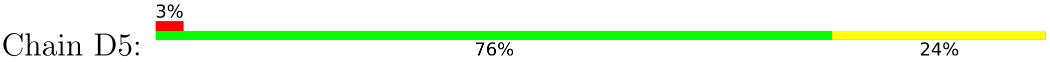
- Molecule 49: 50S ribosomal protein L32

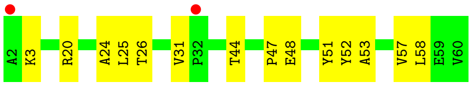
Chain B5:



- Molecule 49: 50S ribosomal protein L32

Chain D5:



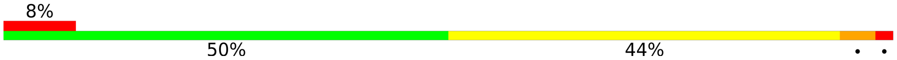


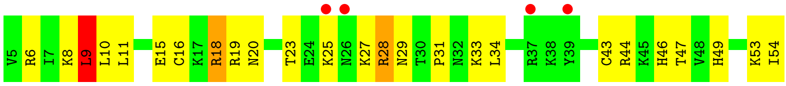
- Molecule 50: 50S ribosomal protein L33

Chain B6:

- Molecule 50: 50S ribosomal protein L33

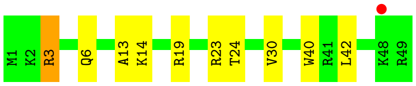
Chain D6:





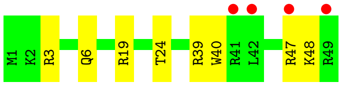
- Molecule 51: 50S ribosomal protein L34

Chain B7:



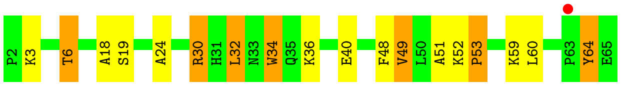
- Molecule 51: 50S ribosomal protein L34

Chain D7:



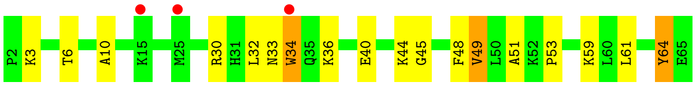
- Molecule 52: 50S ribosomal protein L35

Chain B8:



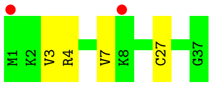
- Molecule 52: 50S ribosomal protein L35

Chain D8:



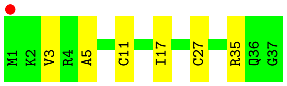
- Molecule 53: 50S ribosomal protein L36

Chain B9:



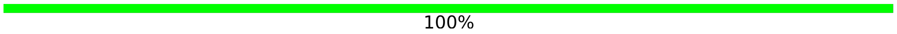
- Molecule 53: 50S ribosomal protein L36

Chain D9:



- Molecule 54: 50S RIBOSOMAL PROTEIN L7/L12

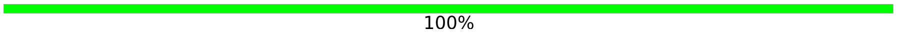
Chain Bf:



There are no outlier residues recorded for this chain.

- Molecule 54: 50S RIBOSOMAL PROTEIN L7/L12

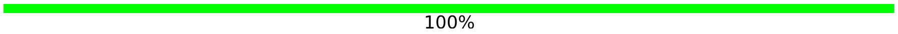
Chain Bg:



There are no outlier residues recorded for this chain.

- Molecule 54: 50S RIBOSOMAL PROTEIN L7/L12

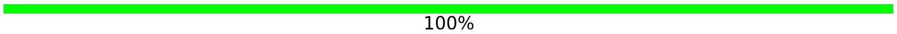
Chain Df:



There are no outlier residues recorded for this chain.

- Molecule 54: 50S RIBOSOMAL PROTEIN L7/L12

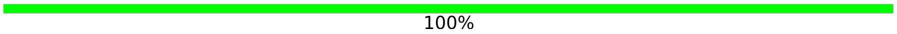
Chain Dg:



There are no outlier residues recorded for this chain.

- Molecule 55: 50S RIBOSOMAL PROTEIN L7/L12

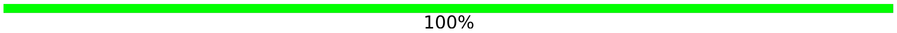
Chain Bh:



There are no outlier residues recorded for this chain.

- Molecule 55: 50S RIBOSOMAL PROTEIN L7/L12

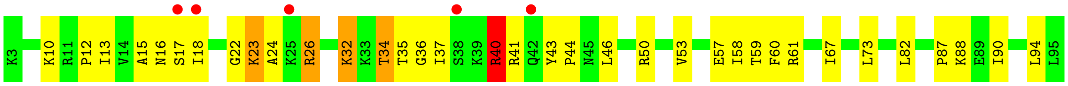
Chain Dh:



There are no outlier residues recorded for this chain.

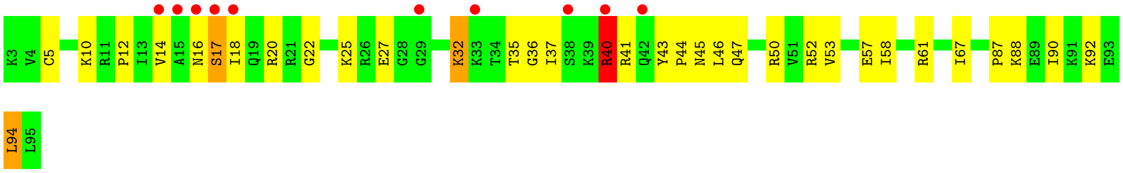
- Molecule 56: 50S ribosomal protein L28

Chain B1:



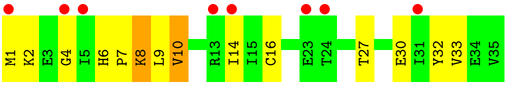
- Molecule 56: 50S ribosomal protein L28

Chain D1:



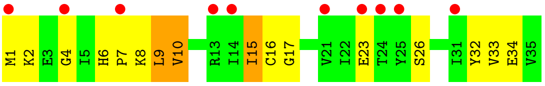
- Molecule 57: 50S ribosomal protein L31

Chain B4:



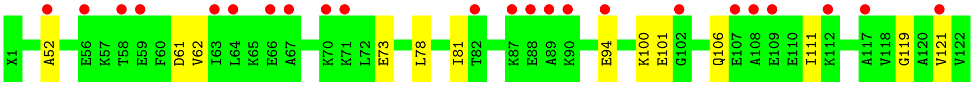
- Molecule 57: 50S ribosomal protein L31

Chain D4:



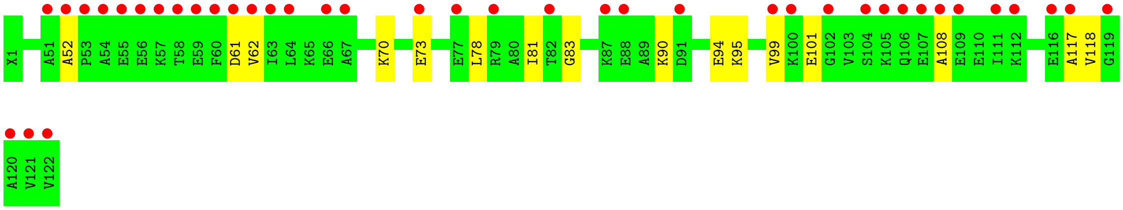
- Molecule 58: 50S ribosomal protein L7/L12

Chain Be:



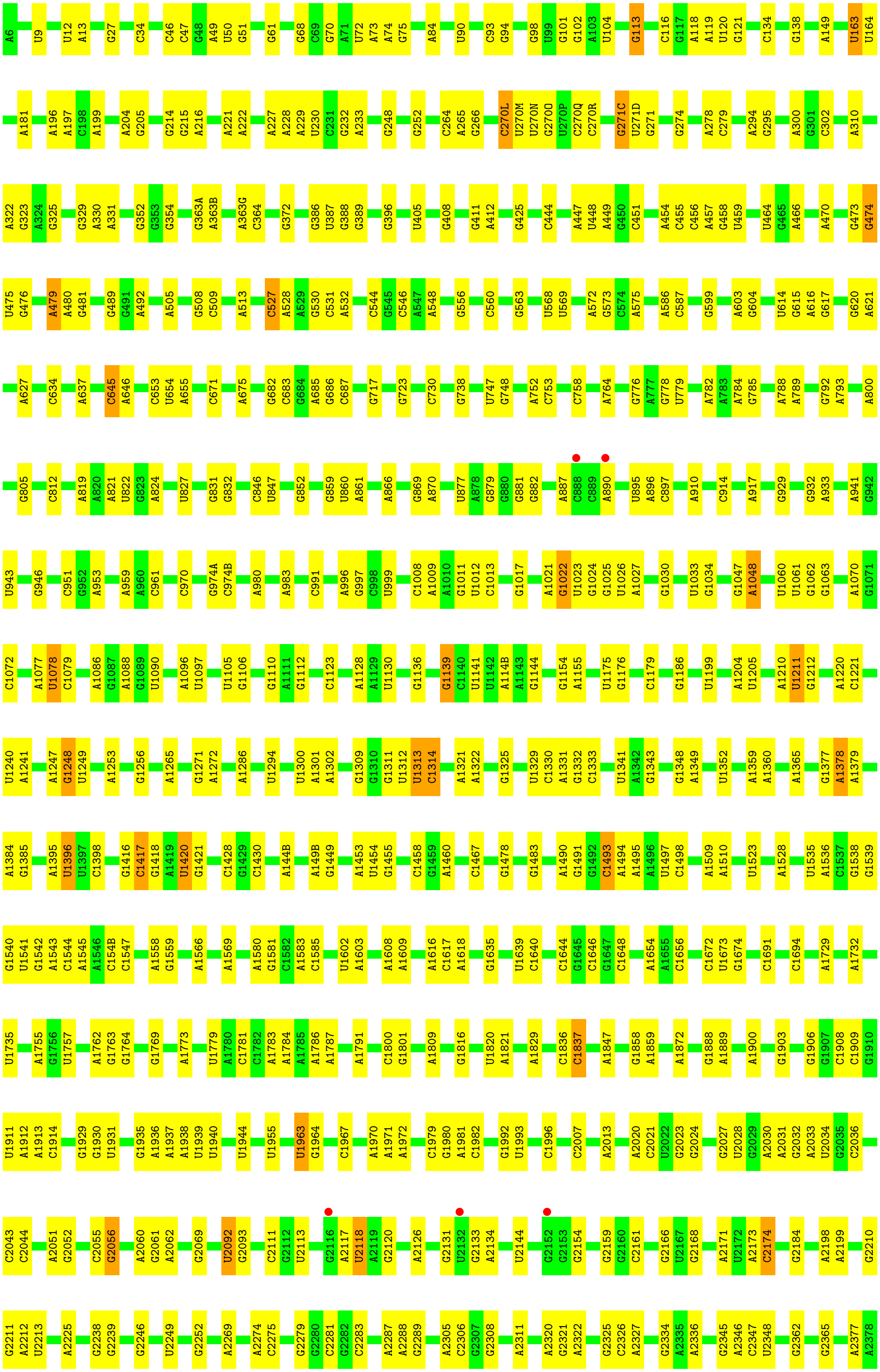
- Molecule 58: 50S ribosomal protein L7/L12

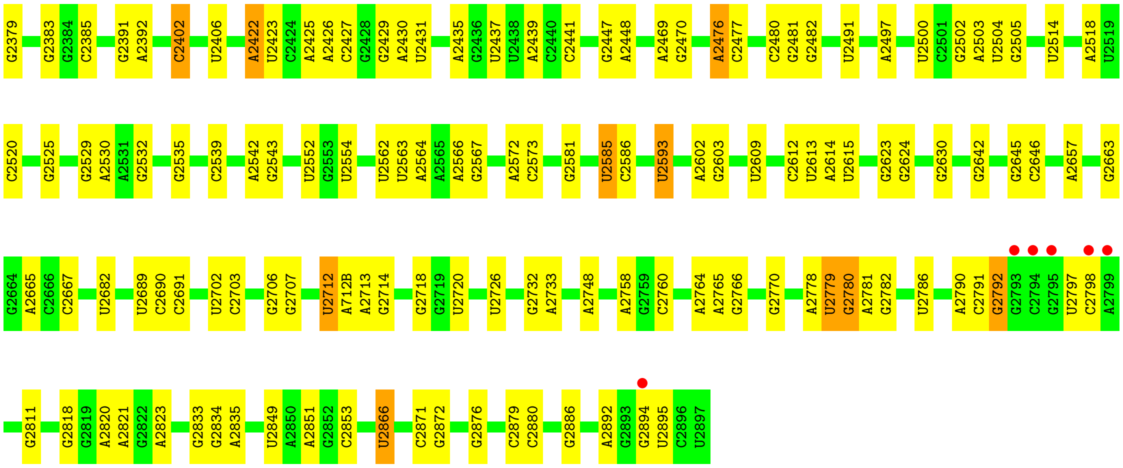
Chain De:



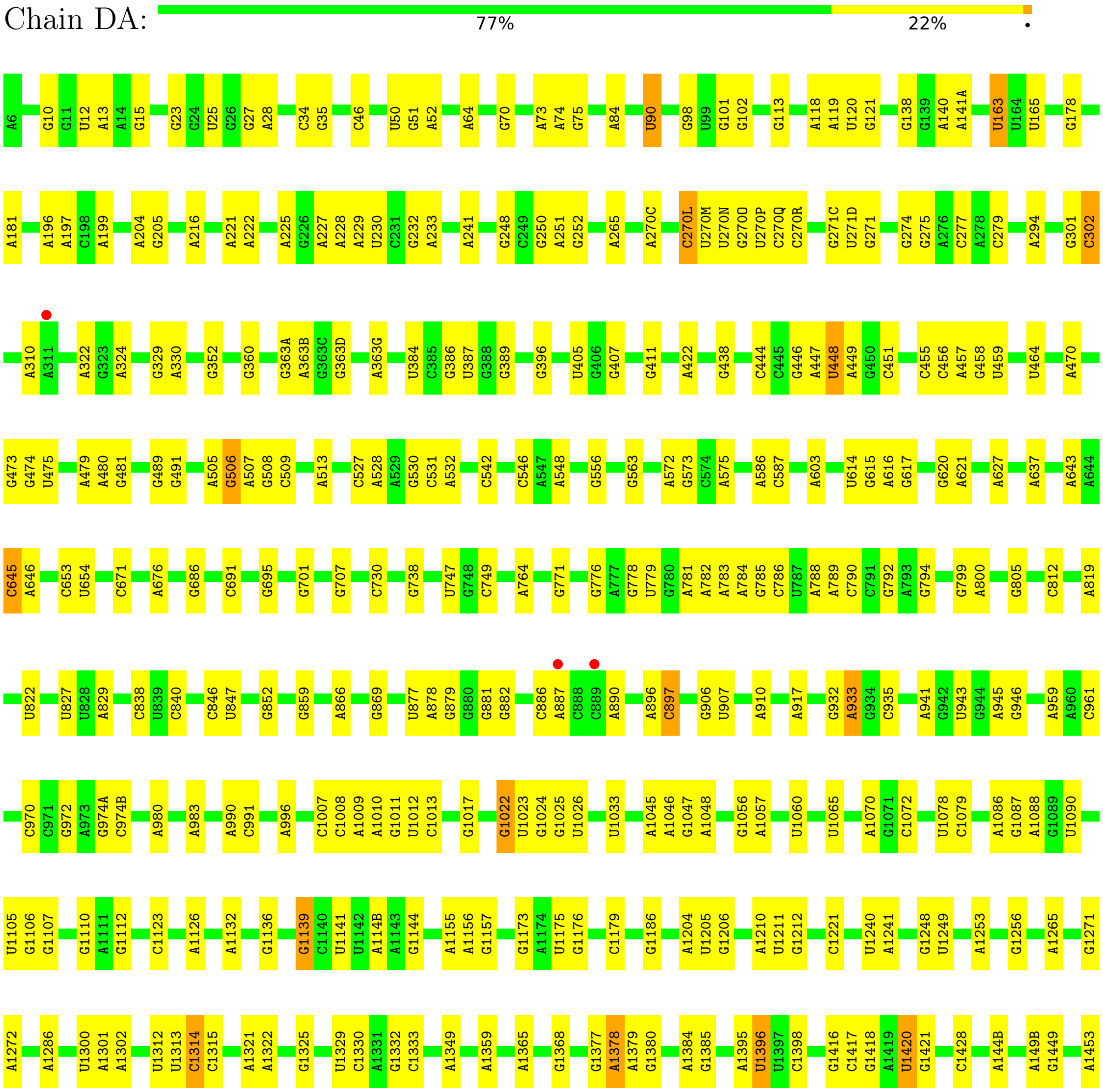
- Molecule 59: 23S ribosomal RNA

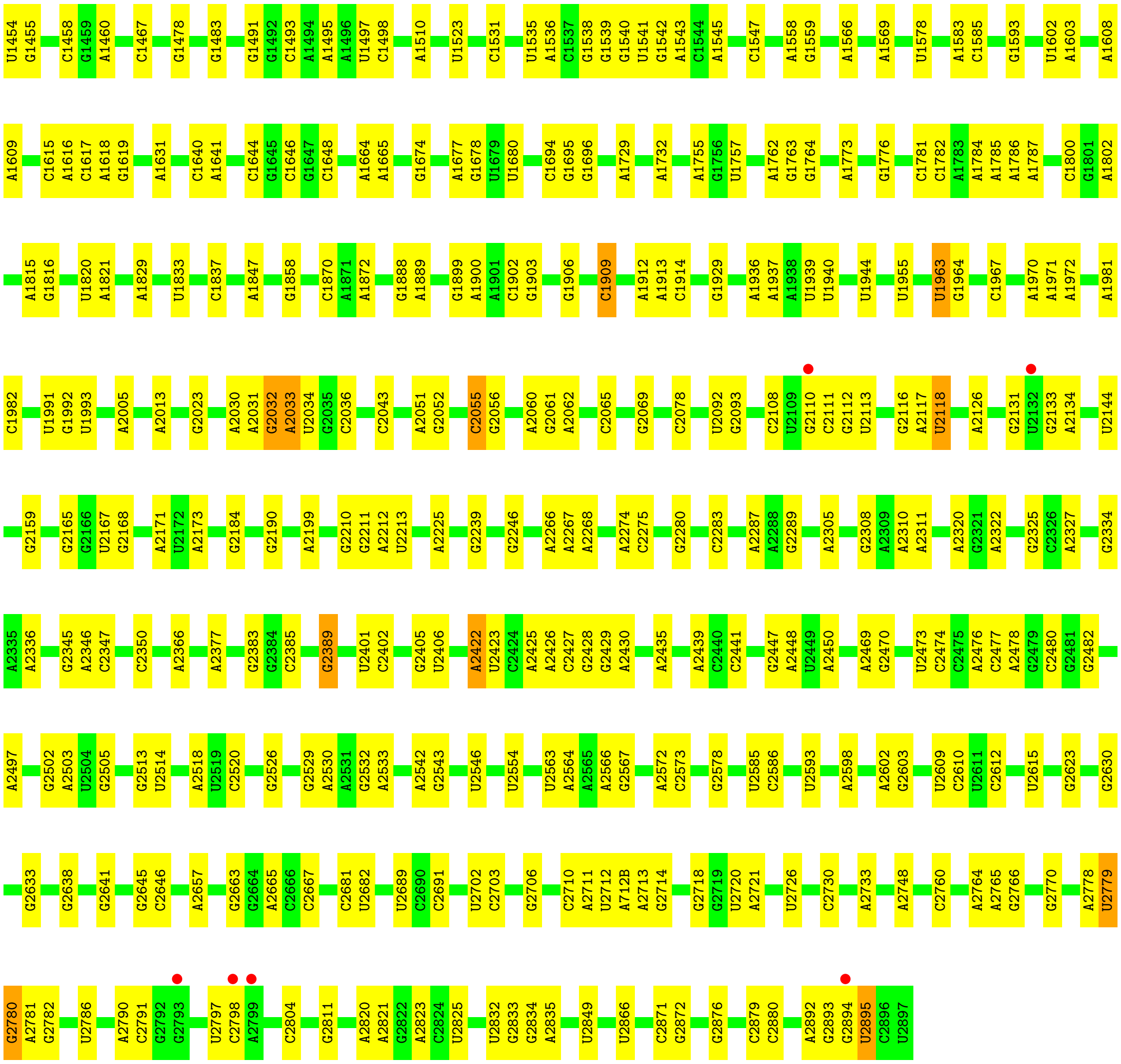
Chain BA:


A6 U9 U12 A13 G27 C34 C46 C47 G48 A49 U50 G51 G61 G68 C69 G70 A71 U72 A73 A74 G75 A84 U90 C93 G94 G98 U99 G101 G102 A103 U104 G113 C116 G117 A118 A119 U120 G121 C134 G138 A149 U163 U164
A181 A196 A197 C198 A199 A204 G205 G214 G215 A216 A221 A222 A227 A228 A229 U230 C231 G232 A233 G248 G252 C264 A265 G266 C270L U270M U270N G270O U270P C270Q C270R G271C U271D G271 G274 A278 C279 A294 G295 A300 G301 C302 A310
A322 G323 A324 G325 G329 A330 A331 G352 G353 G354 G363A A363B A363G C364 G372 G386 U387 G388 G389 G396 U405 G408 G411 A412 G425 C444 A447 U448 A449 G450 C451 A454 C455 C456 A457 G458 U459 U464 G465 A466 A470 G473 G474
U475 G476 A479 A480 G481 G489 G491 A492 A505 G508 C509 A513 C527 A528 A529 G530 C531 A532 C544 G545 C546 A547 A548 G556 C560 G563 U568 U569 A572 G573 C574 A575 A586 C587 G599 A603 G604 U614 G615 A616 G617 G620 A621
A627 C634 A637 C645 A646 C653 U654 A655 C671 A675 G682 C683 G684 A685 G686 C687 G717 G723 C730 G738 U747 G748 A752 C753 C758 A764 G776 A777 G778 U779 A782 A783 A784 G785 A788 A789 G792 A793 A800
G805 C812 A819 A820 A821 U822 G823 A824 U827 G831 G832 C846 U847 G852 G859 U860 A861 A866 G869 A870 U877 A878 G879 G880 G881 G882 A887 C888 C889 A890 U895 A896 C897 A910 C914 A917 G929 G932 A933 A941 G942
U943 G946 C951 G952 A953 A959 A960 C961 C970 G974A C974B A980 A983 C991 A996 G997 C998 U999 C1008 A1009 A1010 G1011 U1012 C1013 G1017 A1021 G1022 U1023 G1024 G1025 U1026 A1027 G1030 U1033 G1034 G1047 A1048 U1060 U1061 G1062 G1063 A1070 G1071
C1072 A1077 U1078 C1079 A1086 G1087 A1088 G1089 U1090 A1096 U1097 U1105 G1106 G1110 A1111 G1112 C1123 A1128 A1129 U1130 G1136 G1139 C1140 U1141 U1142 A114B A1143 G1144 G1154 A1155 U1175 G1176 C1179 G1186 U1199 A1204 U1205 A1210 U1211 G1212 A1220 C1221
U1240 A1241 A1247 G1248 U1249 A1253 G1256 A1265 G1271 A1272 A1286 U1294 U1300 A1301 A1302 G1309 G1310 G1311 U1312 U1313 C1314 A1321 A1322 G1325 U1329 C1330 A1331 G1332 C1333 U1341 A1342 G1343 G1348 A1349 U1352 A1359 A1360 A1365 G1377 A1378 A1379
A1384 G1385 A1395 U1396 U1397 C1398 G1416 C1417 G1418 A1419 U1420 G1421 C1428 G1429 C1430 A144B A149B G1449 A1453 U1454 G1455 C1458 G1459 A1460 C1467 G1478 G1483 A1490 G1491 G1492 C1493 A1494 A1495 A1496 U1497 C1498 A1509 A1510 U1523 A1528 U1535 A1536 C1537 G1538 G1539
G1540 U1541 G1542 A1543 C1544 A1545 A1546 C154B C1547 A1558 G1559 A1566 A1569 A1580 G1581 C1582 A1583 C1585 U1602 A1603 A1608 A1609 A1616 C1617 A1618 G1635 U1639 C1640 C1644 G1645 C1646 G1647 C1648 A1654 A1655 C1656 C1672 U1673 G1674 C1691 C1694 A1729 A1732
U1735 A1755 G1756 U1757 A1762 G1763 G1764 G1769 A1773 U1779 A1780 C1781 C1782 A1783 A1784 A1785 A1786 A1787 A1791 C1800 G1801 A1809 G1816 U1820 A1821 A1829 C1836 C1837 A1847 G1858 A1859 A1872 G1888 A1889 A1900 G1903 G1906 G1907 C1908 C1909 G1910
U1911 A1912 A1913 C1914 G1929 G1930 U1931 G1935 A1936 A1937 A1938 U1939 U1940 U1944 U1955 U1963 G1964 C1967 A1970 A1971 A1972 C1979 G1980 A1981 C1982 G1992 U1993 C1996 C2007 A2013 A2020 C2021 U2022 G2023 G2024 G2027 U2028 G2029 A2030 A2031 G2032 A2033 U2034 G2035 C2036
C2043 C2044 A2051 G2052 C2055 G2056 A2060 G2061 A2062 G2069 U2092 G2093 C2111 G2112 U2113 G2116 A2117 U2118 A2119 G2120 A2126 G2131 U2132 G2133 A2134 U2144 G2152 G2153 G2154 G2159 G2160 C2161 G2166 U2167 G2168 A2171 U2172 A2173 C2174 G2184 A2198 A2199 G2210
G2211 A2212 U2213 A2225 G2238 G2239 G2246 U2249 G2252 A2269 A2274 C2275 G2279 G2280 C2281 G2282 C2283 A2287 A2288 G2289 A2305 C2306 G2307 G2308 A2311 A2320 G2321 A2322 G2325 C2326 A2327 G2334 A2335 A2336 G2345 A2346 C2347 U2348 G2362 G2365 A2377 A2378



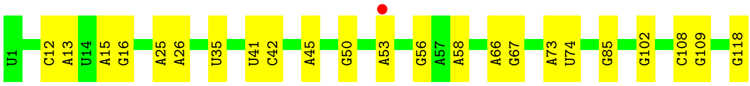
- Molecule 59: 23S ribosomal RNA





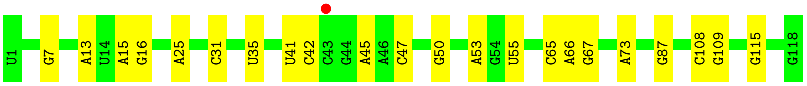
- Molecule 60: 5S ribosomal RNA

Chain BB:



- Molecule 60: 5S ribosomal RNA

Chain DB:



4 Data and refinement statistics

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

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

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MG, KBE, 5OH, UAL, 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	0.42	0/1945	0.73	4/2621 (0.2%)
1	CB	0.40	0/1945	0.69	1/2621 (0.0%)
2	AC	0.35	0/1645	0.60	0/2216
2	CC	0.33	0/1645	0.58	1/2216 (0.0%)
3	AD	0.37	0/1733	0.60	0/2318
3	CD	0.34	0/1733	0.61	0/2318
4	AE	0.35	0/1172	0.63	1/1576 (0.1%)
4	CE	0.34	0/1172	0.63	1/1576 (0.1%)
5	AF	0.38	0/856	0.67	2/1154 (0.2%)
5	CF	0.35	0/856	0.64	1/1154 (0.1%)
6	AG	0.34	0/1276	0.58	0/1709
6	CG	0.35	0/1276	0.58	0/1709
7	AH	0.34	0/1136	0.58	0/1527
7	CH	0.33	0/1136	0.57	0/1527
8	AI	0.36	0/1029	0.63	1/1378 (0.1%)
8	CI	0.36	0/1029	0.61	1/1378 (0.1%)
9	AJ	0.37	0/815	0.64	1/1095 (0.1%)
9	CJ	0.33	0/815	0.65	1/1095 (0.1%)
10	AK	0.40	0/900	0.65	0/1213
10	CK	0.37	0/900	0.63	0/1213
11	AL	0.47	0/992	0.89	3/1327 (0.2%)
11	CL	0.47	0/992	0.88	4/1327 (0.3%)
12	AM	0.33	0/1008	0.61	0/1347
12	CM	0.32	0/1008	0.58	0/1347
13	AN	0.37	0/501	0.57	0/664
13	CN	0.35	0/501	0.57	0/664
14	AO	0.39	0/745	0.62	0/992
14	CO	0.35	0/745	0.59	0/992
15	AP	0.34	0/722	0.58	0/970
15	CP	0.33	0/722	0.56	0/970
16	AQ	0.45	0/848	0.75	0/1131
16	CQ	0.42	0/848	0.71	0/1131

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

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

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

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

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

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

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

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

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

There are no chirality outliers.

5 of 44 planarity outliers are listed below:

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

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

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

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

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

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

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

5 of 1578 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

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

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

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

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

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

Mol	Chain	Res	Type
35	DP	39	LYS
37	DR	44	LEU
35	DP	32	THR
45	DZ	136	PHE
35	BP	110	TYR

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

Mol	Chain	Res	Type
37	DR	23	ASN
38	DS	38	GLN
45	DZ	118	GLN
34	BO	90	GLN
32	BK	30	HIS

5.3.3 RNA ⓘ

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

5 of 2031 RNA backbone outliers are listed below:

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

5 of 87 RNA pucker outliers are listed below:

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

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

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

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

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

All (4) bond angle outliers are listed below:

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

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
61	GNP	CY	701	62	29,34,34	1.55	4 (13%)	33,54,54	2.68	13 (39%)
61	GNP	AY	701	62	29,34,34	1.55	4 (13%)	33,54,54	2.68	13 (39%)

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 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	AY	701	GNP	PG-O1G	4.78	1.53	1.46
61	CY	701	GNP	PG-O1G	4.75	1.53	1.46
61	CY	701	GNP	C6-N1	3.61	1.39	1.33
61	AY	701	GNP	C6-N1	3.60	1.39	1.33
61	AY	701	GNP	PB-O3A	-2.39	1.56	1.59

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
61	AY	701	GNP	C5-C6-N1	-8.59	111.69	123.43
61	CY	701	GNP	C5-C6-N1	-8.56	111.72	123.43
61	AY	701	GNP	C2-N1-C6	5.79	125.14	115.93
61	CY	701	GNP	C2-N1-C6	5.77	125.10	115.93
61	AY	701	GNP	C2-N3-C4	-4.79	109.88	115.36

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

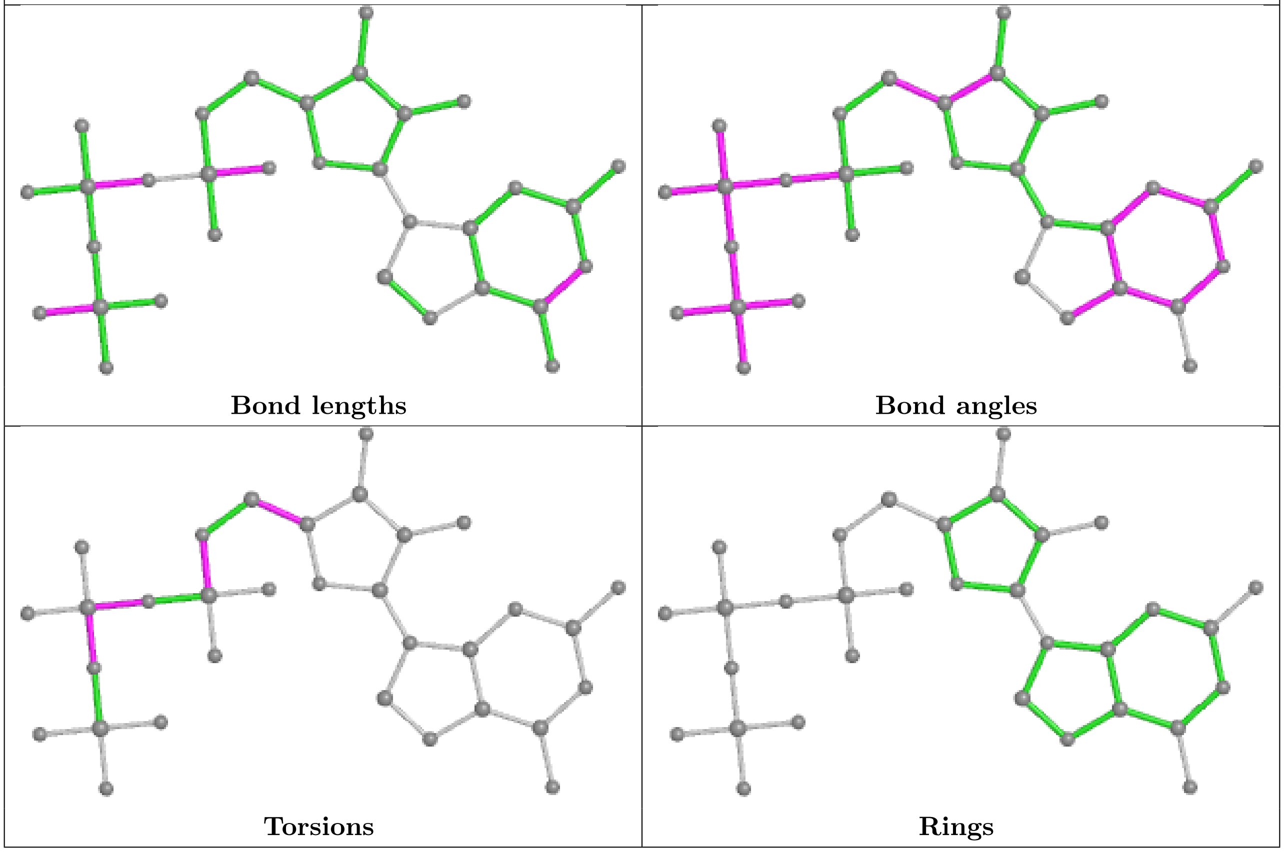
Mol	Chain	Res	Type	Atoms
61	AY	701	GNP	PG-N3B-PB-O1B
61	AY	701	GNP	PG-N3B-PB-O3A
61	AY	701	GNP	PA-O3A-PB-O1B
61	AY	701	GNP	PA-O3A-PB-O2B
61	AY	701	GNP	C5'-O5'-PA-O3A

There are no ring outliers.

No monomer is involved in short contacts.

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

Ligand GNP CY 701



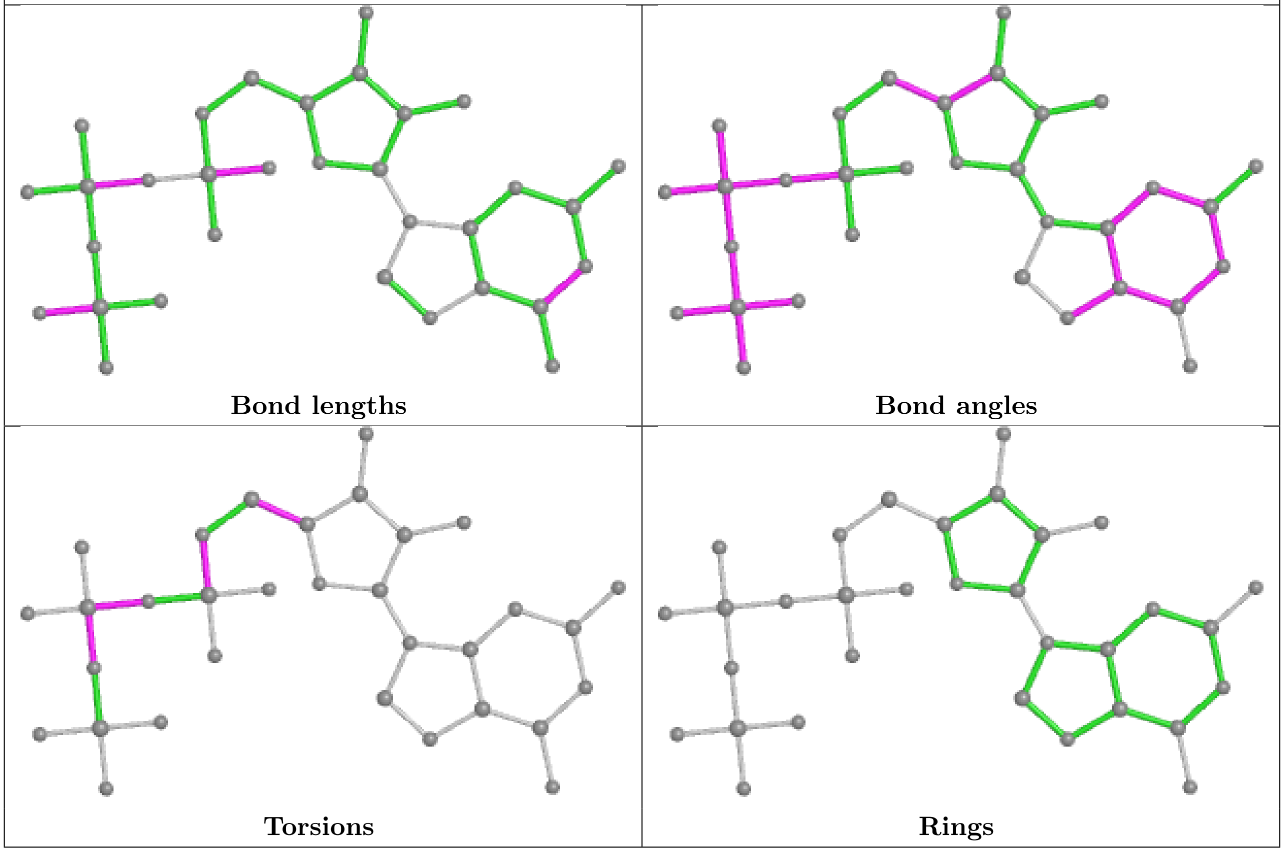
Bond lengths

Bond angles

Torsions

Rings

Ligand GNP AY 701



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
58	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%)	-0.08	6 (2%) 56 49	30, 75, 127, 171	0
1	CB	235/235 (100%)	0.41	16 (6%) 17 16	34, 86, 153, 201	0
2	AC	207/207 (100%)	0.28	14 (6%) 17 16	27, 59, 115, 156	0
2	CC	207/207 (100%)	1.01	41 (19%) 1 1	23, 74, 130, 190	0
3	AD	208/208 (100%)	-0.57	0 100 100	24, 72, 124, 159	0
3	CD	208/208 (100%)	-0.29	3 (1%) 75 69	23, 85, 142, 184	0
4	AE	151/151 (100%)	-0.41	0 100 100	17, 48, 101, 156	0
4	CE	151/151 (100%)	-0.02	7 (4%) 32 28	14, 58, 106, 151	0
5	AF	101/101 (100%)	-0.47	1 (0%) 82 77	15, 50, 100, 133	0
5	CF	101/101 (100%)	-0.62	1 (0%) 82 77	29, 61, 123, 148	0
6	AG	155/155 (100%)	-0.68	1 (0%) 89 86	30, 80, 139, 199	0
6	CG	155/155 (100%)	-0.80	0 100 100	38, 82, 137, 180	0
7	AH	138/138 (100%)	-0.16	4 (2%) 51 45	28, 59, 103, 142	0
7	CH	138/138 (100%)	0.15	5 (3%) 42 38	25, 75, 121, 155	0
8	AI	127/127 (100%)	-0.76	0 100 100	0, 71, 117, 134	0
8	CI	127/127 (100%)	-0.56	0 100 100	0, 84, 149, 220	0
9	AJ	99/99 (100%)	0.15	6 (6%) 21 19	25, 62, 116, 159	0
9	CJ	99/99 (100%)	0.90	13 (13%) 3 4	31, 75, 127, 166	0
10	AK	119/119 (100%)	-0.34	1 (0%) 86 81	31, 69, 116, 157	0
10	CK	119/119 (100%)	-0.57	1 (0%) 86 81	38, 72, 133, 151	0
11	AL	125/125 (100%)	-0.12	3 (2%) 59 53	10, 66, 120, 181	0
11	CL	125/125 (100%)	0.25	13 (10%) 6 7	29, 69, 136, 170	0
12	AM	125/125 (100%)	0.06	11 (8%) 10 10	49, 86, 144, 212	0
12	CM	125/125 (100%)	0.25	14 (11%) 5 6	53, 100, 158, 223	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	AN	60/60 (100%)	0.40	7 (11%) 4 5	28, 52, 87, 120	0
13	CN	60/60 (100%)	0.93	11 (18%) 1 1	39, 69, 117, 135	0
14	AO	88/88 (100%)	-0.31	0 100 100	22, 60, 114, 139	0
14	CO	88/88 (100%)	-0.32	0 100 100	25, 68, 119, 170	0
15	AP	84/84 (100%)	0.05	4 (4%) 30 27	26, 66, 109, 117	0
15	CP	84/84 (100%)	0.05	2 (2%) 59 53	52, 81, 127, 153	0
16	AQ	100/100 (100%)	0.25	6 (6%) 21 19	0, 67, 117, 139	0
16	CQ	100/100 (100%)	0.41	8 (8%) 12 12	0, 68, 126, 150	0
17	AR	70/70 (100%)	-0.21	3 (4%) 35 31	14, 54, 120, 154	0
17	CR	70/70 (100%)	-0.29	1 (1%) 75 69	38, 63, 113, 155	0
18	AS	79/79 (100%)	0.90	14 (17%) 1 1	47, 92, 136, 169	0
18	CS	79/79 (100%)	0.62	10 (12%) 3 4	44, 99, 145, 189	0
19	AT	99/99 (100%)	-0.50	0 100 100	0, 77, 128, 159	0
19	CT	99/99 (100%)	-0.28	2 (2%) 65 60	0, 79, 131, 166	0
20	AY	687/687 (100%)	0.00	50 (7%) 15 15	23, 84, 139, 174	0
20	CY	687/687 (100%)	0.02	49 (7%) 16 15	40, 92, 149, 204	0
21	AA	1511/1511 (100%)	-0.60	3 (0%) 95 93	15, 67, 145, 258	0
21	CA	1511/1511 (100%)	-0.61	1 (0%) 95 95	18, 70, 157, 272	0
22	AW	77/77 (100%)	-0.73	0 100 100	32, 90, 174, 205	0
22	CW	77/77 (100%)	-0.74	0 100 100	39, 101, 193, 240	0
23	AV	23/23 (100%)	-0.70	0 100 100	41, 100, 156, 172	0
23	CV	23/23 (100%)	-0.27	1 (4%) 35 31	41, 118, 186, 216	0
24	AU	2/6 (33%)	-0.75	0 100 100	114, 114, 114, 114	0
24	CU	2/6 (33%)	-0.94	0 100 100	119, 119, 119, 119	0
25	BC	228/228 (100%)	1.42	73 (32%) 0 0	81, 124, 178, 222	0
25	DC	228/228 (100%)	1.57	74 (32%) 0 0	102, 162, 214, 247	0
26	BD	275/275 (100%)	-0.49	2 (0%) 87 83	11, 47, 102, 126	0
26	DD	275/275 (100%)	-0.45	4 (1%) 73 68	23, 54, 107, 147	0
27	BE	205/205 (100%)	-0.37	3 (1%) 73 68	19, 55, 101, 193	0
27	DE	205/205 (100%)	-0.20	4 (1%) 65 60	12, 60, 120, 175	0
28	BF	208/208 (100%)	-0.02	14 (6%) 17 16	16, 69, 131, 178	0

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

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

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
60	BB	119/119 (100%)	-0.57	1 (0%) 86 81	36, 102, 157, 192	0
60	DB	119/119 (100%)	-0.44	1 (0%) 86 81	33, 108, 159, 193	0
All	All	22726/23318 (97%)	-0.23	953 (4%) 36 32	0, 72, 150, 308	0

The worst 5 of 953 RSRZ outliers are listed below:

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

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

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

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

6.3 Carbohydrates ⓘ

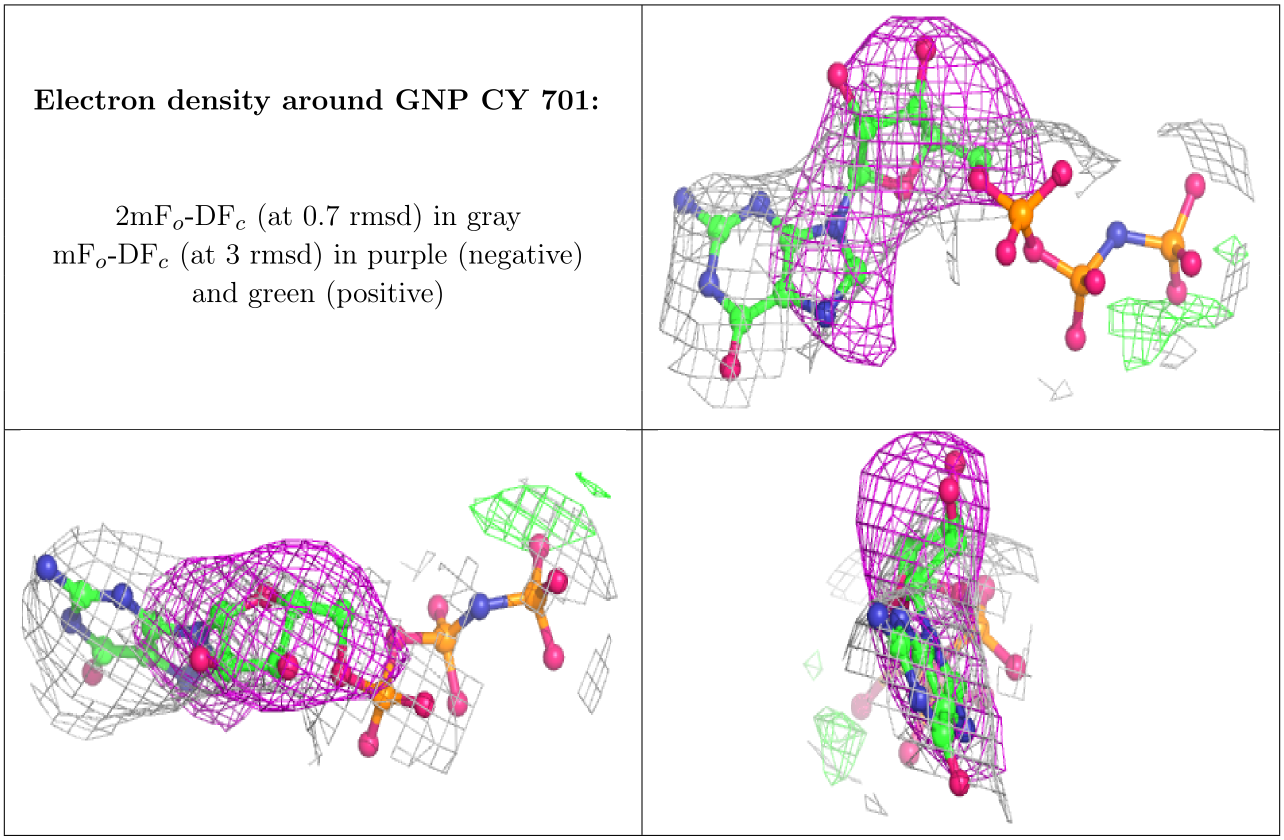
There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

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

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

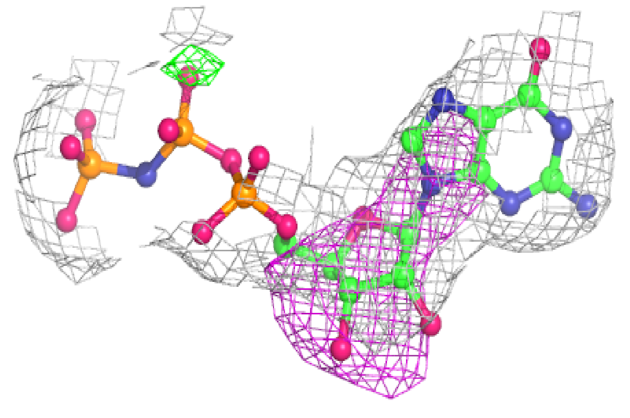


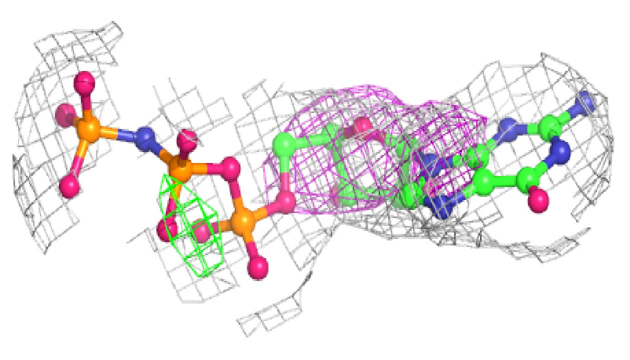
Electron density around GNP CY 701:

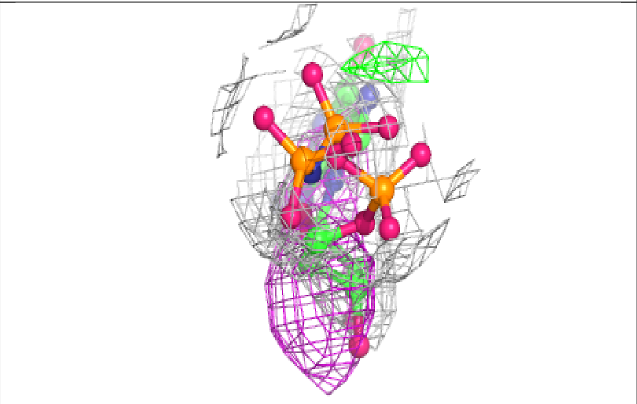
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around GNP AY 701:

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







6.5 Other polymers

There are no such residues in this entry.