wwPDB X-ray Structure Validation Summary Report (i)

Jun 1, 2020 – 11:21 am BST

PDB ID	:	4V9P
Title	:	Control of ribosomal subunit rotation by elongation factor G
Authors	:	Pulk, A.; Cate, J.H.D.
Deposited on	:	2013-05-03
Resolution	:	2.90 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

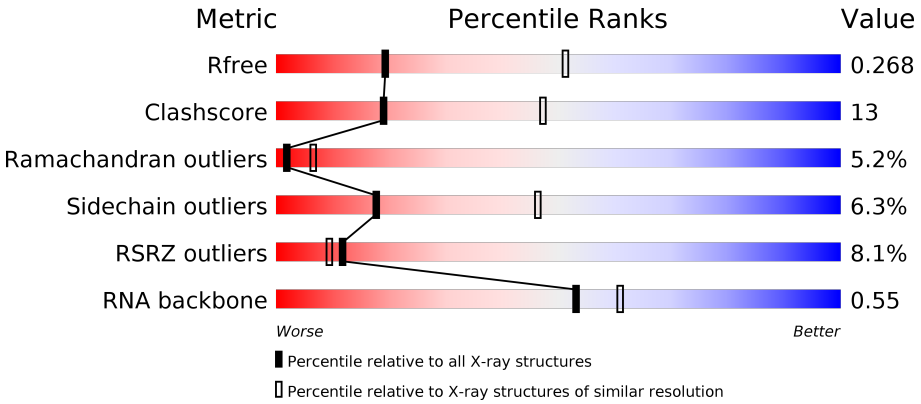
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	AA	2904	2% 47% 38% 12%
1	CA	2904	2% 52% 33% 11%
1	EA	2904	2% 50% 34% 12%
1	GA	2904	2% 53% 32% 11%

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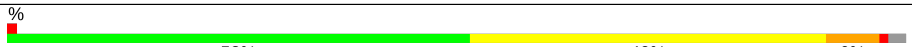
Mol	Chain	Length	Quality of chain
2	AB	120	
2	CB	120	
2	EB	120	
2	GB	120	
3	AC	273	
3	CC	273	
3	EC	273	
3	GC	273	
4	AD	209	
4	CD	209	
4	ED	209	
4	GD	209	
5	AE	201	
5	CE	201	
5	EE	201	
5	GE	201	
6	AF	179	
6	CF	179	
6	EF	179	
6	GF	179	
7	AG	177	
7	CG	177	
7	EG	177	
7	GG	177	
8	AH	50	

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Mol	Chain	Length	Quality of chain
8	CH	50	34% 56% 38% 6%
8	EH	50	28% 62% 32%
8	GH	50	30% 58% 40%
9	AI	142	41% 46% 51%
9	CI	142	51% 50% 44% 5%
9	EI	142	57% 61% 35%
9	GI	142	77% 48% 46% 6%
10	AJ	142	% 60% 30% 9%
10	CJ	142	% 58% 31% 11%
10	EJ	142	% 53% 33% 11%
10	GJ	142	4% 58% 32% 9%
11	AK	123	% 51% 39% 8%
11	CK	123	2% 47% 44% 7%
11	EK	123	2% 54% 37% 9%
11	GK	123	2% 50% 42% 7%
12	AL	144	5% 67% 28%
12	CL	144	% 63% 32%
12	EL	144	% 70% 25%
12	GL	144	10% 57% 38%
13	AM	136	% 61% 31% 6%
13	CM	136	% 63% 32% 5%
13	EM	136	% 66% 27% 6%
13	GM	136	3% 71% 26%
14	AN	127	2% 62% 30% 6%
14	CN	127	% 60% 28% 6% 6%

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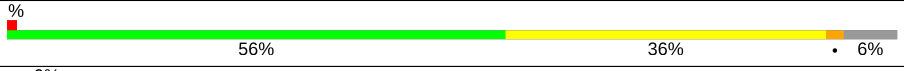
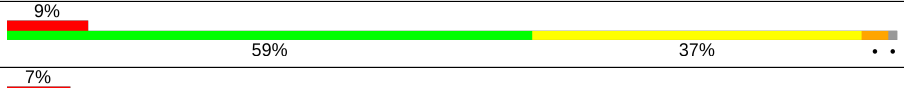
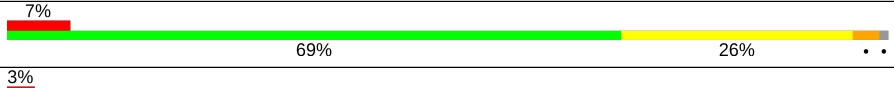
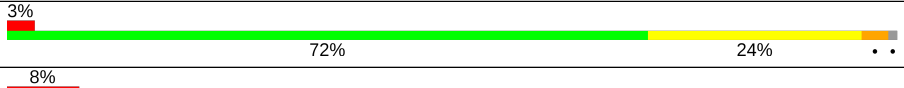
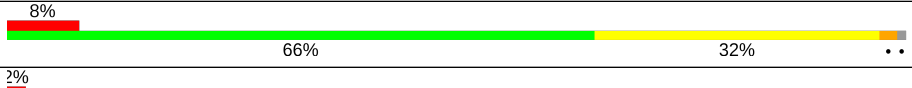
Mol	Chain	Length	Quality of chain
14	EN	127	
14	GN	127	
15	AO	117	
15	CO	117	
15	EO	117	
15	GO	117	
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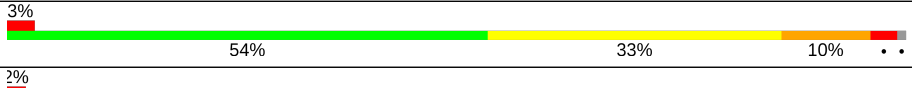
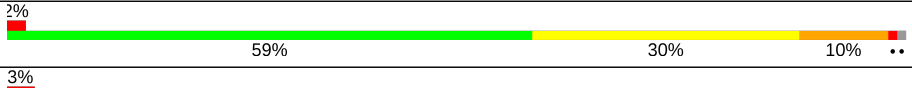
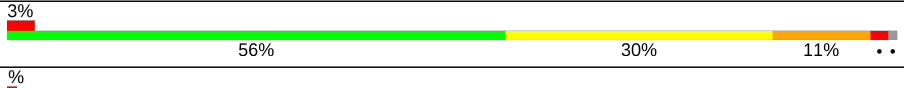
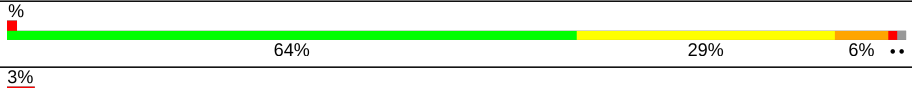
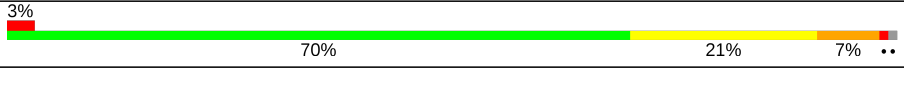
16	CP	115	
16	EP	115	
16	GP	115	
17	AQ	118	
17	CQ	118	
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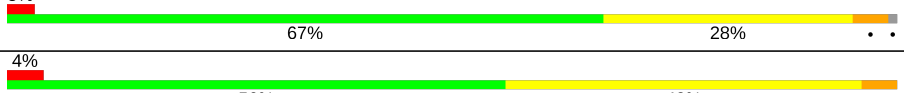
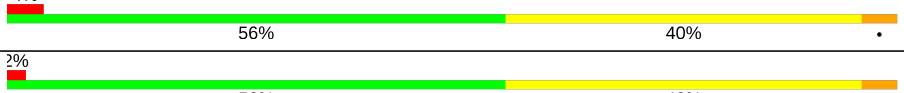
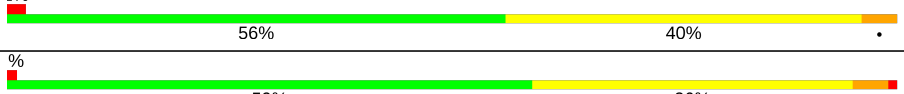
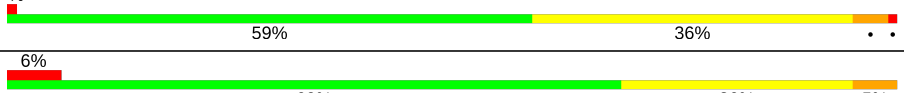
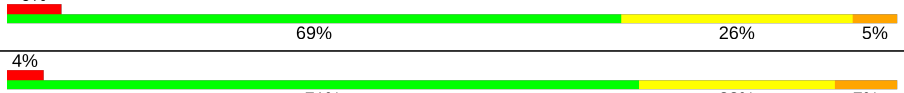
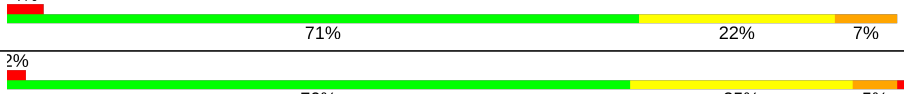
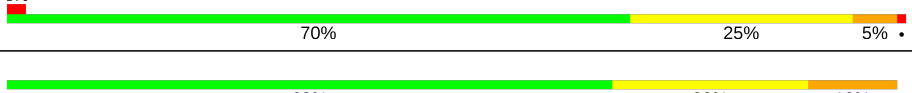
17	GQ	118	
18	AR	103	
18	CR	103	
18	ER	103	
18	GR	103	
19	AS	110	
19	CS	110	
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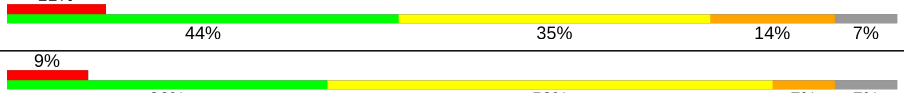
19	GS	110	
20	AT	100	
20	CT	100	
20	ET	100	

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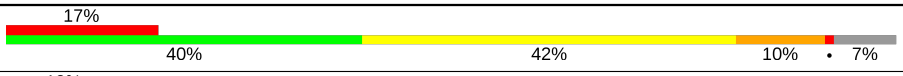
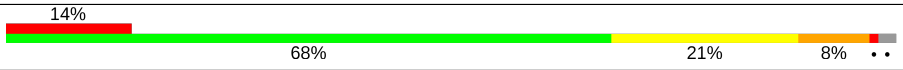
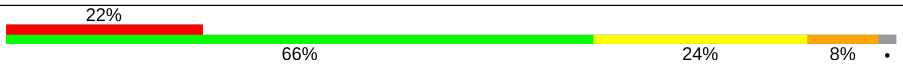
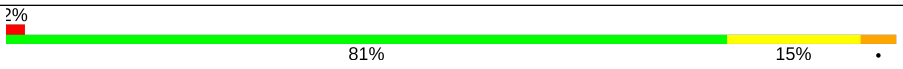
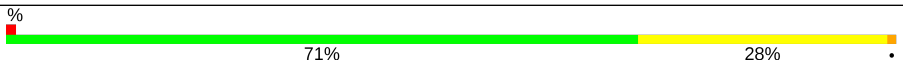
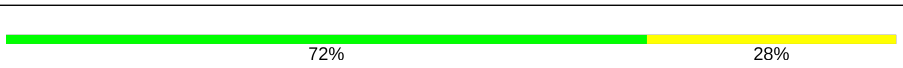
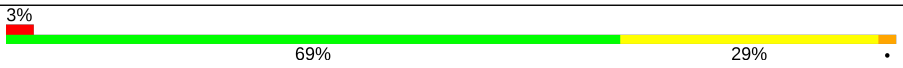
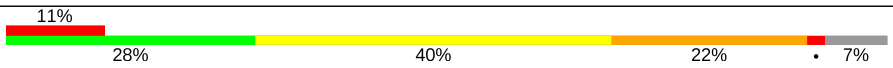
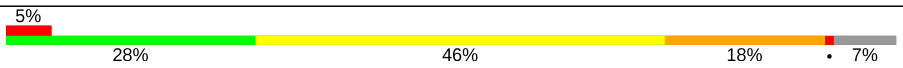
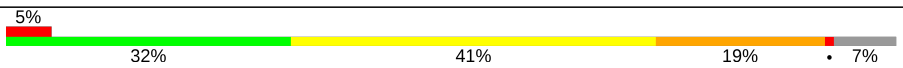
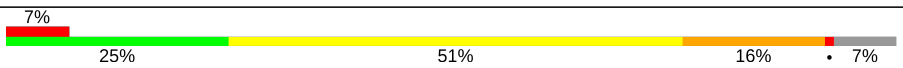
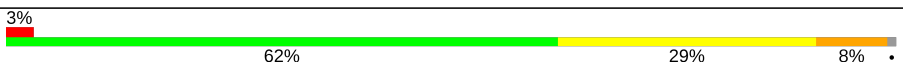
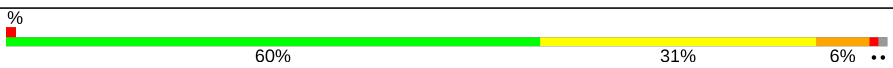
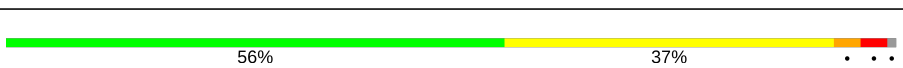
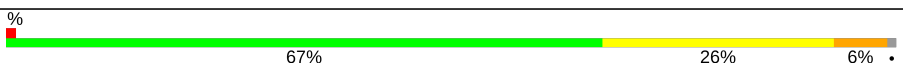
Mol	Chain	Length	Quality of chain
20	GT	100	
21	AU	104	
21	CU	104	
21	EU	104	
21	GU	104	
22	AV	94	
22	CV	94	
22	EV	94	
22	GV	94	
23	AW	85	
23	CW	85	
23	EW	85	
23	GW	85	
24	AX	78	
24	CX	78	
24	EX	78	
24	GX	78	
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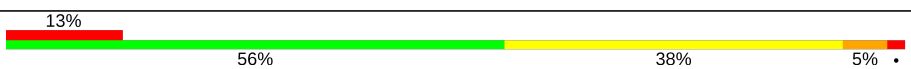
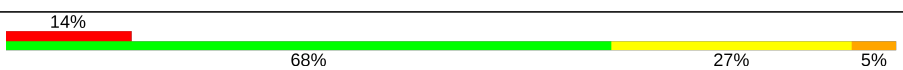
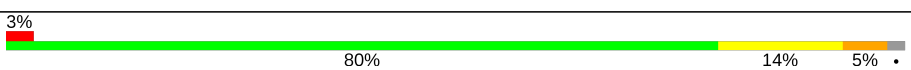
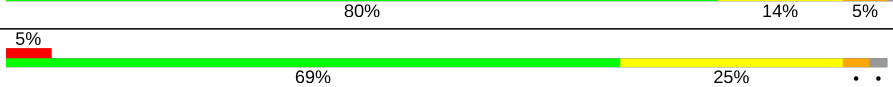
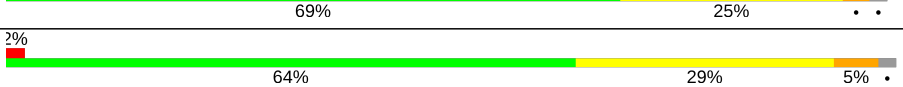
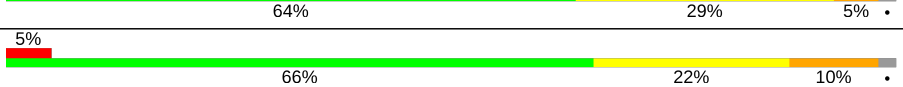
25	CY	63	
25	EY	63	
25	GY	63	
26	AZ	59	
26	CZ	59	
26	EZ	59	
26	GZ	59	

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Mol	Chain	Length	Quality of chain
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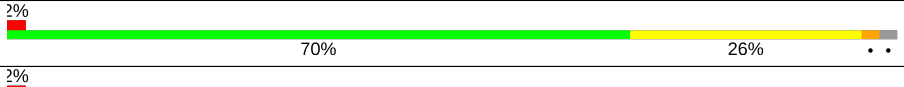
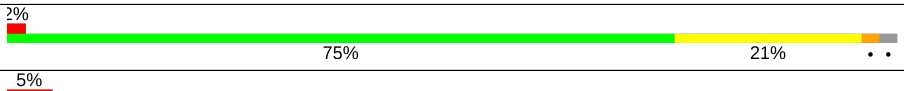
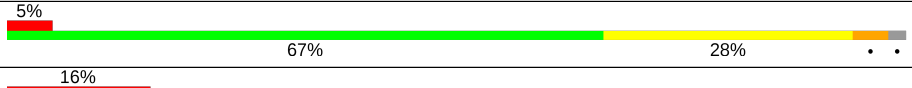
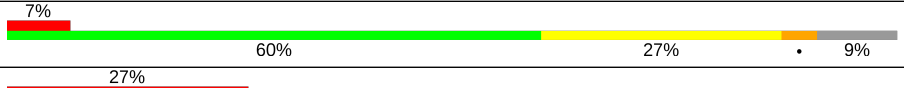
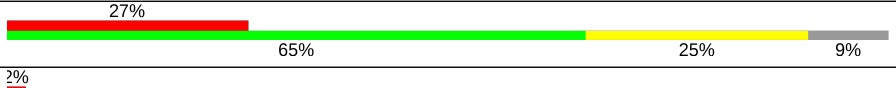
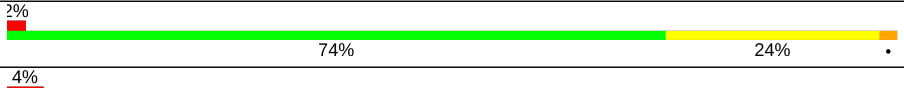
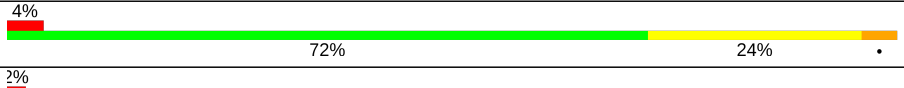
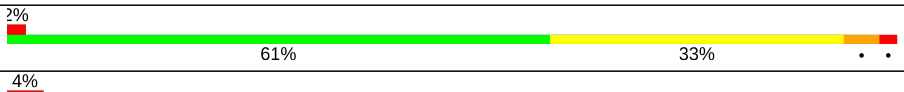
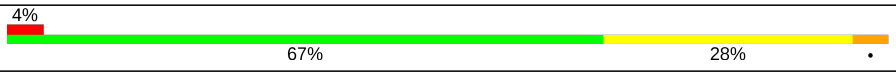
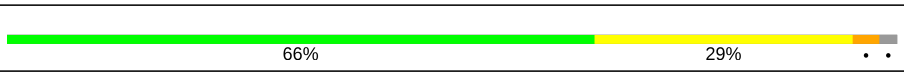
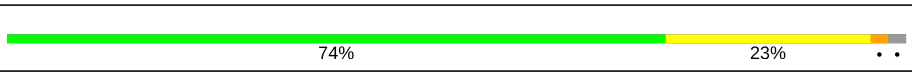
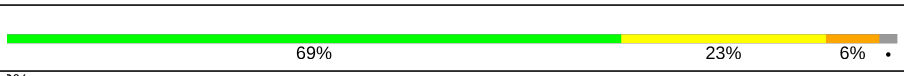
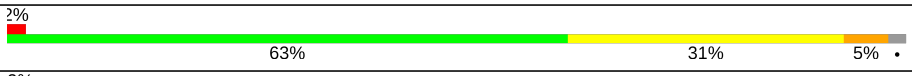
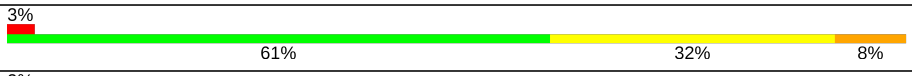
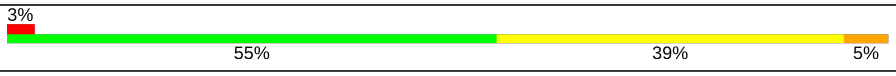
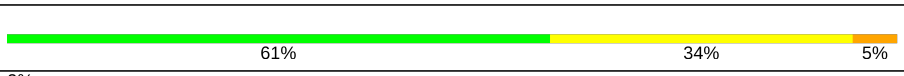
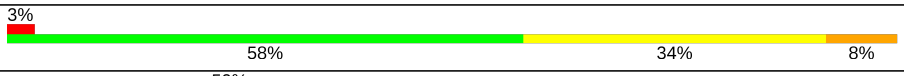
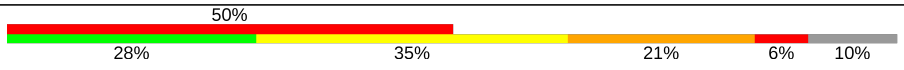
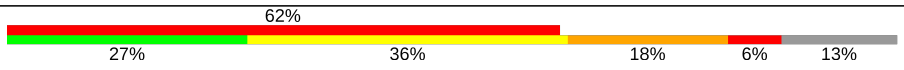
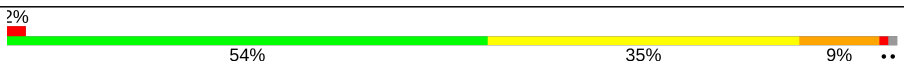
27	C0	57	
27	E0	57	
27	G0	57	
28	A1	55	
28	C1	55	
28	E1	55	
28	G1	55	
29	A2	46	
29	C2	46	
29	E2	46	
29	G2	46	
30	A3	65	
30	C3	65	
30	E3	65	
30	G3	65	
31	A4	38	
31	C4	38	
31	E4	38	
31	G4	38	
32	A5	165	
32	E5	165	
33	BA	1542	
33	DA	1542	
33	FA	1542	

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Mol	Chain	Length	Quality of chain
33	HA	1542	3% 56% 34% 8%
34	BB	241	27% 51% 35% 5% 10%
34	DB	241	28% 48% 37% 5% 10%
34	FB	241	12% 52% 34% 5% 10%
34	HB	241	19% 51% 35% 5% 10%
35	BC	233	13% 58% 28% 12%
35	DC	233	8% 60% 28% 12%
35	FC	233	62% 23% 12%
35	HC	233	5% 59% 28% 12%
36	BD	206	7% 54% 38% 7%
36	DD	206	16% 54% 36% 9%
36	FD	206	15% 54% 38% 7%
36	HD	206	11% 58% 35% 7%
37	BE	167	7% 50% 35% 10%
37	DE	167	4% 62% 25% 10%
37	FE	167	53% 34% 10%
37	HE	167	62% 24% 10%
38	BF	135	24% 29% 41% 26%
38	DF	135	11% 44% 25% 26%
38	FF	135	11% 44% 26% 26%
38	HF	135	7% 47% 24% 26%
39	BG	179	6% 62% 22% 16%
39	DG	179	4% 60% 23% 16%
39	FG	179	5% 55% 27% 16%
39	HG	179	12% 60% 24% 16%

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Mol	Chain	Length	Quality of chain
40	BH	130	12% 58% 37%
40	DH	130	11% 64% 32%
40	FH	130	2% 70% 24% 5%
40	HH	130	4% 72% 26%
41	BI	130	19% 48% 40% 9%
41	DI	130	15% 51% 42% 5%
41	FI	130	7% 60% 30% 8%
41	HI	130	27% 47% 45% 5%
42	BJ	103	38% 64% 24% 6% 5%
42	DJ	103	35% 50% 38% 6% 5%
42	FJ	103	12% 56% 32% 7% 5%
42	HJ	103	26% 58% 33% 5%
43	BK	129	22% 43% 43% 5% 9%
43	DK	129	7% 60% 29% 9%
43	FK	129	8% 57% 29% 5% 9%
43	HK	129	25% 41% 41% 9% 9%
44	BL	124	2% 54% 38% 7%
44	DL	124	4% 56% 39% 5%
44	FL	124	3% 53% 39% 6%
44	HL	124	6% 59% 35% 6%
45	BM	118	11% 66% 27%
45	DM	118	5% 70% 23%
45	FM	118	10% 64% 29%
45	HM	118	51% 53% 40%
46	BN	101	14% 58% 36% 5%

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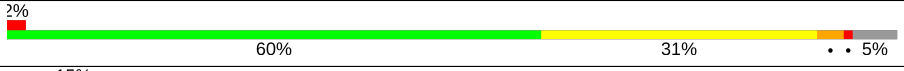
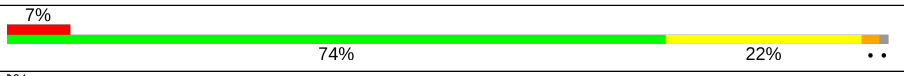
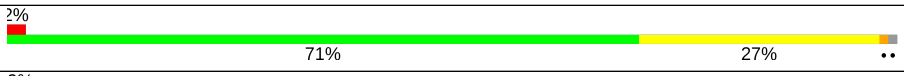
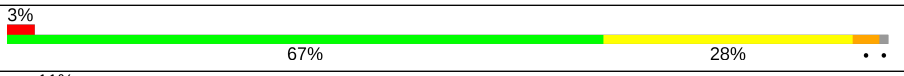
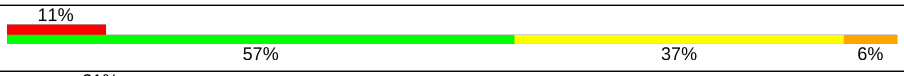
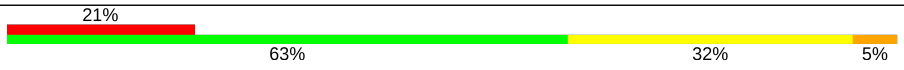
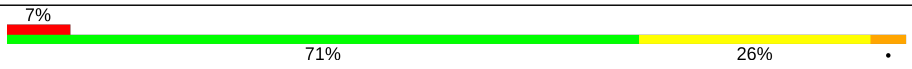
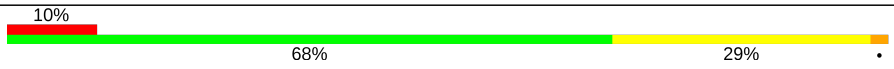
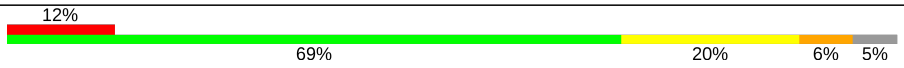
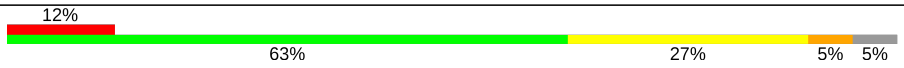
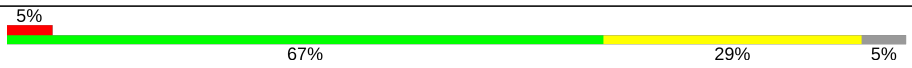
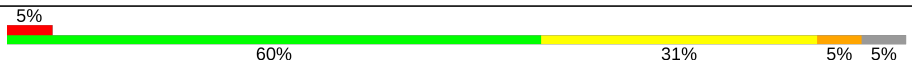
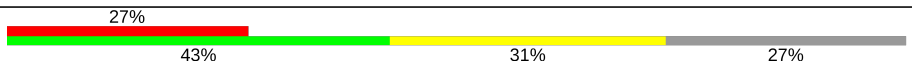
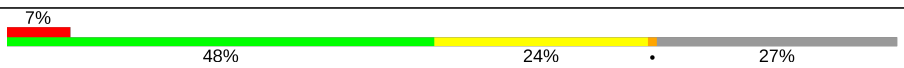
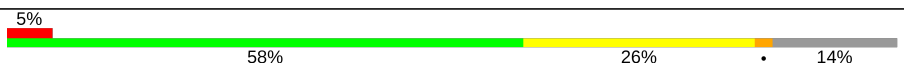
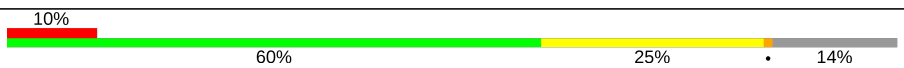
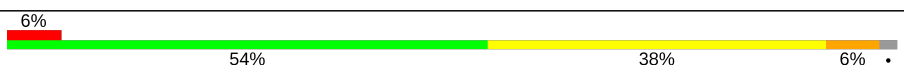
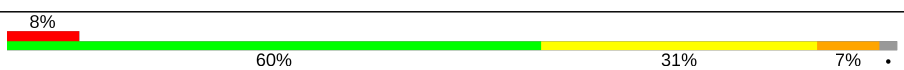
Mol	Chain	Length	Quality of chain
46	DN	101	
46	FN	101	
46	HN	101	
47	BO	89	
47	DO	89	
47	FO	89	
47	HO	89	
48	BP	82	
48	DP	82	
48	FP	82	
48	HP	82	
49	BQ	84	
49	DQ	84	
49	FQ	84	
49	HQ	84	
50	BR	75	
50	DR	75	
50	FR	75	
50	HR	75	
51	BS	92	
51	DS	92	
51	FS	92	
51	HS	92	
52	BT	87	
52	DT	87	

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Mol	Chain	Length	Quality of chain
52	FT	87	6% 60% 32% 6%
52	HT	87	7% 66% 29%
53	BU	71	48% 30% 35% 7% 28%
53	DU	71	23% 41% 27% 28%
53	FU	71	27% 39% 27% 6% 28%
53	HU	71	28% 34% 35% 28%
54	BV	704	9% 67% 27%
54	DV	704	13% 68% 25%
54	FV	704	52% 68% 26%
54	HV	704	20% 65% 27% 5%
55	BW	6	17% 17% 50% 33%
55	DW	6	17% 83% 17%
55	FW	6	33% 17% 67% 17%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	KBE	BW	1	-	-	-	X
55	UAL	BW	5	-	-	-	X
55	5OH	BW	6	-	-	-	X
55	UAL	DW	5	-	-	-	X
55	5OH	DW	6	-	-	-	X
55	KBE	FW	1	-	-	-	X
55	DPP	FW	2	-	-	-	X
55	UAL	FW	5	-	-	-	X
55	5OH	FW	6	-	-	-	X

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 590573 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 RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	2854	Total	C	N	O	P	0	0	0
			61274	27334	11279	19807	2854			
1	CA	2854	Total	C	N	O	P	0	0	0
			61274	27334	11279	19807	2854			
1	EA	2854	Total	C	N	O	P	0	0	0
			61274	27334	11279	19807	2854			
1	GA	2854	Total	C	N	O	P	0	0	0
			61274	27334	11279	19807	2854			

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			
2	CB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			
2	EB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			
2	GB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			
3	CC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			
3	EC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			
3	GC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			
4	CD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			
4	ED	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			
4	GD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			
5	CE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			
5	EE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			
5	GE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	177	Total	C	N	O	S	0	0	0
			1410	899	249	256	6			
6	CF	177	Total	C	N	O	S	0	0	0
			1410	899	249	256	6			
6	EF	177	Total	C	N	O	S	0	0	0
			1410	899	249	256	6			
6	GF	177	Total	C	N	O	S	0	0	0
			1410	899	249	256	6			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			
7	CG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			
7	EG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	GG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	50	Total	C	N	O	S	0	0	0
			384	247	68	68	1			
8	CH	50	Total	C	N	O	S	0	0	0
			384	247	68	68	1			
8	EH	50	Total	C	N	O	S	0	0	0
			384	247	68	68	1			
8	GH	50	Total	C	N	O	S	0	0	0
			384	247	68	68	1			

- Molecule 9 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			
9	CI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			
9	EI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			
9	GI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			

- Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			
10	CJ	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			
10	EJ	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			
10	GJ	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			

- Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			
11	CK	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			
11	EK	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			
11	GK	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			
12	CL	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			
12	EL	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			
12	GL	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			

- Molecule 13 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			
13	CM	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			
13	EM	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			
13	GM	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			
14	CN	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			
14	EN	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	GN	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			

- Molecule 15 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	AO	116	Total	C	N	O	0	0	0
			892	552	178	162			
15	CO	116	Total	C	N	O	0	0	0
			892	552	178	162			
15	EO	116	Total	C	N	O	0	0	0
			892	552	178	162			
15	GO	116	Total	C	N	O	0	0	0
			892	552	178	162			

- Molecule 16 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			
16	CP	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			
16	EP	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			
16	GP	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			

- Molecule 17 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	AQ	117	Total	C	N	O	0	0	0
			947	604	192	151			
17	CQ	117	Total	C	N	O	0	0	0
			947	604	192	151			
17	EQ	117	Total	C	N	O	0	0	0
			947	604	192	151			
17	GQ	117	Total	C	N	O	0	0	0
			947	604	192	151			

- Molecule 18 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AR	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			
18	CR	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			
18	ER	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			
18	GR	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			

- Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			
19	CS	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			
19	ES	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			
19	GS	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			
20	CT	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			
20	ET	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			
20	GT	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	102	Total	C	N	O	0	0	0
			779	492	146	141			
21	CU	102	Total	C	N	O	0	0	0
			779	492	146	141			
21	EU	102	Total	C	N	O	0	0	0
			779	492	146	141			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	GU	102	Total	C	N	O	0	0	0
			779	492	146	141			

- Molecule 22 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			
22	CV	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			
22	EV	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			
22	GV	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	79	Total	C	N	O	S	0	0	0
			596	367	120	108	1			
23	CW	79	Total	C	N	O	S	0	0	0
			596	367	120	108	1			
23	EW	79	Total	C	N	O	S	0	0	0
			596	367	120	108	1			
23	GW	79	Total	C	N	O	S	0	0	0
			596	367	120	108	1			

- Molecule 24 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AX	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			
24	CX	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			
24	EX	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			
24	GX	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			

- Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	AY	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			
25	CY	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			
25	EY	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			
25	GY	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			

- Molecule 26 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	AZ	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			
26	CZ	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			
26	EZ	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			
26	GZ	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	A0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			
27	C0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			
27	E0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			
27	G0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
28	A1	50	Total	C	N	O	0	0	0
			409	263	75	71			
28	C1	50	Total	C	N	O	0	0	0
			409	263	75	71			
28	E1	50	Total	C	N	O	0	0	0
			409	263	75	71			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
28	G1	50	Total	C	N	O	0	0	0
			409	263	75	71			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	A2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			
29	C2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			
29	E2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			
29	G2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	A3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			
30	C3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			
30	E3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			
30	G3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	A4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			
31	C4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			
31	E4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			
31	G4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

- Molecule 32 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	A5	148	Total	C	N	O	S	0	0	0
			1117	705	196	209	7			
32	E5	144	Total	C	N	O	S	0	0	0
			1092	691	192	202	7			

- Molecule 33 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BA	1533	Total	C	N	O	P	0	0	0
			32895	14671	6036	10655	1533			
33	DA	1533	Total	C	N	O	P	0	0	0
			32895	14671	6036	10655	1533			
33	FA	1533	Total	C	N	O	P	0	0	0
			32895	14671	6036	10655	1533			
33	HA	1533	Total	C	N	O	P	0	0	0
			32895	14671	6036	10655	1533			

- Molecule 34 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BB	218	Total	C	N	O	S	0	0	0
			1704	1081	305	311	7			
34	DB	218	Total	C	N	O	S	0	0	0
			1704	1081	305	311	7			
34	FB	218	Total	C	N	O	S	0	0	0
			1704	1081	305	311	7			
34	HB	218	Total	C	N	O	S	0	0	0
			1704	1081	305	311	7			

- Molecule 35 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BC	206	Total	C	N	O	S	0	0	0
			1624	1028	305	288	3			
35	DC	206	Total	C	N	O	S	0	0	0
			1624	1028	305	288	3			
35	FC	206	Total	C	N	O	S	0	0	0
			1624	1028	305	288	3			
35	HC	206	Total	C	N	O	S	0	0	0
			1624	1028	305	288	3			

- Molecule 36 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			
36	DD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			
36	FD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			
36	HD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			

- Molecule 37 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BE	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			
37	DE	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			
37	FE	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			
37	HE	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			

- Molecule 38 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			
38	DF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			
38	FF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			
38	HF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			

- Molecule 39 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BG	151	Total	C	N	O	S	0	0	0
			1181	735	227	215	4			
39	DG	151	Total	C	N	O	S	0	0	0
			1181	735	227	215	4			
39	FG	151	Total	C	N	O	S	0	0	0
			1181	735	227	215	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	HG	151	Total	C	N	O	S	0	0	0
			1181	735	227	215	4			

- Molecule 40 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			
40	DH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			
40	FH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			
40	HH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			

- Molecule 41 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			
41	DI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			
41	FI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			
41	HI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			

- Molecule 42 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BJ	98	Total	C	N	O	S	0	0	0
			786	493	150	142	1			
42	DJ	98	Total	C	N	O	S	0	0	0
			786	493	150	142	1			
42	FJ	98	Total	C	N	O	S	0	0	0
			786	493	150	142	1			
42	HJ	98	Total	C	N	O	S	0	0	0
			786	493	150	142	1			

- Molecule 43 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			
43	DK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			
43	FK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			
43	HK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			

- Molecule 44 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			
44	DL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			
44	FL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			
44	HL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			

- Molecule 45 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BM	114	Total	C	N	O	S	0	0	0
			883	546	178	156	3			
45	DM	114	Total	C	N	O	S	0	0	0
			883	546	178	156	3			
45	FM	114	Total	C	N	O	S	0	0	0
			883	546	178	156	3			
45	HM	114	Total	C	N	O	S	0	0	0
			883	546	178	156	3			

- Molecule 46 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			
46	DN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			
46	FN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	HN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			

- Molecule 47 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			
47	DO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			
47	FO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			
47	HO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			

- Molecule 48 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			
48	DP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			
48	FP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			
48	HP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			

- Molecule 49 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BQ	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			
49	DQ	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			
49	FQ	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			
49	HQ	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			

- Molecule 50 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
50	BR	55	Total	C	N	O	0	0	0
			455	288	86	81			
50	DR	55	Total	C	N	O	0	0	0
			455	288	86	81			
50	FR	55	Total	C	N	O	0	0	0
			455	288	86	81			
50	HR	55	Total	C	N	O	0	0	0
			455	288	86	81			

- Molecule 51 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BS	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			
51	DS	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			
51	FS	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			
51	HS	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			

- Molecule 52 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			
52	DT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			
52	FT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			
52	HT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			

- Molecule 53 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BU	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			
53	DU	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			
53	FU	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	HU	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			

- Molecule 54 is a protein called elongation factor G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	BV	689	Total	C	N	O	S	0	0	0
			5319	3345	919	1030	25			
54	DV	689	Total	C	N	O	S	0	0	0
			5319	3345	919	1030	25			
54	FV	689	Total	C	N	O	S	0	0	0
			5319	3345	919	1030	25			
54	HV	689	Total	C	N	O	S	0	0	0
			5319	3345	919	1030	25			

- Molecule 55 is a protein called Viomycin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
55	BW	6	Total	C	N	O	0	0	0
			48	25	13	10			
55	DW	6	Total	C	N	O	0	0	0
			48	25	13	10			
55	FW	6	Total	C	N	O	0	0	0
			48	25	13	10			

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	FA	41	Total	Mg	0	0
			41	41		
56	BA	40	Total	Mg	0	0
			40	40		
56	CA	134	Total	Mg	0	0
			134	134		
56	HE	1	Total	Mg	0	0
			1	1		
56	AB	4	Total	Mg	0	0
			4	4		
56	BL	1	Total	Mg	0	0
			1	1		
56	BE	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	GA	134	Total Mg 134 134	0	0
56	DU	1	Total Mg 1 1	0	0
56	EB	4	Total Mg 4 4	0	0
56	FU	1	Total Mg 1 1	0	0
56	FV	1	Total Mg 1 1	0	0
56	C4	1	Total Mg 1 1	0	0
56	AE	1	Total Mg 1 1	0	0
56	AA	130	Total Mg 130 130	0	0
56	FE	1	Total Mg 1 1	0	0
56	GB	4	Total Mg 4 4	0	0
56	DV	1	Total Mg 1 1	0	0
56	EA	133	Total Mg 133 133	0	0
56	BU	1	Total Mg 1 1	0	0
56	GC	1	Total Mg 1 1	0	0
56	AD	1	Total Mg 1 1	0	0
56	HT	1	Total Mg 1 1	0	0
56	GL	1	Total Mg 1 1	0	0
56	DA	42	Total Mg 42 42	0	0
56	EC	1	Total Mg 1 1	0	0
56	HC	1	Total Mg 1 1	0	0
56	BV	1	Total Mg 1 1	0	0

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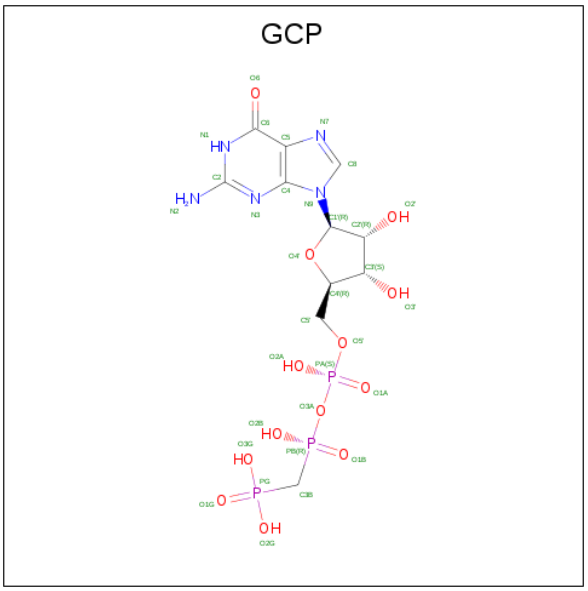
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	CB	4	Total Mg 4 4	0	0
56	GS	1	Total Mg 1 1	0	0
56	AC	3	Total Mg 3 3	0	0
56	EQ	1	Total Mg 1 1	0	0
56	ED	2	Total Mg 2 2	0	0
56	CD	1	Total Mg 1 1	0	0
56	AT	1	Total Mg 1 1	0	0
56	CE	1	Total Mg 1 1	0	0
56	A3	1	Total Mg 1 1	0	0
56	HA	40	Total Mg 40 40	0	0
56	HV	1	Total Mg 1 1	0	0

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	E4	1	Total Zn 1 1	0	0
57	G4	1	Total Zn 1 1	0	0
57	A4	1	Total Zn 1 1	0	0
57	C4	1	Total Zn 1 1	0	0

- Molecule 58 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
58	BV	1	Total	C	N	O	P	0	0
			32	11	5	13	3		
58	DV	1	Total	C	N	O	P	0	0
			32	11	5	13	3		
58	FV	1	Total	C	N	O	P	0	0
			32	11	5	13	3		
58	HV	1	Total	C	N	O	P	0	0
			32	11	5	13	3		

- Molecule 59 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	AA	608	Total	O	0	0
			608	608		
59	AB	19	Total	O	0	0
			19	19		
59	AC	10	Total	O	0	0
			10	10		
59	AD	3	Total	O	0	0
			3	3		
59	AE	1	Total	O	0	0
			1	1		
59	AJ	1	Total	O	0	0
			1	1		
59	AL	7	Total	O	0	0
			7	7		
59	AN	4	Total	O	0	0
			4	4		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	AP	1	Total O 1 1	0	0
59	AQ	1	Total O 1 1	0	0
59	AS	1	Total O 1 1	0	0
59	AU	1	Total O 1 1	0	0
59	A0	1	Total O 1 1	0	0
59	A3	1	Total O 1 1	0	0
59	A4	2	Total O 2 2	0	0
59	BA	197	Total O 197 197	0	0
59	BC	1	Total O 1 1	0	0
59	BD	1	Total O 1 1	0	0
59	BI	1	Total O 1 1	0	0
59	BK	1	Total O 1 1	0	0
59	BN	3	Total O 3 3	0	0
59	BT	2	Total O 2 2	0	0
59	BU	1	Total O 1 1	0	0
59	BV	1	Total O 1 1	0	0
59	CA	604	Total O 604 604	0	0
59	CB	20	Total O 20 20	0	0
59	CC	11	Total O 11 11	0	0
59	CD	3	Total O 3 3	0	0
59	CE	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	CF	1	Total O 1 1	0	0
59	CJ	3	Total O 3 3	0	0
59	CL	6	Total O 6 6	0	0
59	CN	4	Total O 4 4	0	0
59	CS	1	Total O 1 1	0	0
59	CT	2	Total O 2 2	0	0
59	C2	1	Total O 1 1	0	0
59	C3	1	Total O 1 1	0	0
59	C4	2	Total O 2 2	0	0
59	DA	193	Total O 193 193	0	0
59	DC	1	Total O 1 1	0	0
59	DE	2	Total O 2 2	0	0
59	DG	1	Total O 1 1	0	0
59	DK	1	Total O 1 1	0	0
59	DL	1	Total O 1 1	0	0
59	DN	6	Total O 6 6	0	0
59	DQ	1	Total O 1 1	0	0
59	DT	1	Total O 1 1	0	0
59	DU	1	Total O 1 1	0	0
59	DV	1	Total O 1 1	0	0
59	EA	617	Total O 617 617	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	EB	20	Total O 20 20	0	0
59	EC	8	Total O 8 8	0	0
59	ED	1	Total O 1 1	0	0
59	EL	4	Total O 4 4	0	0
59	EN	2	Total O 2 2	0	0
59	ER	1	Total O 1 1	0	0
59	ET	1	Total O 1 1	0	0
59	EU	1	Total O 1 1	0	0
59	E0	2	Total O 2 2	0	0
59	E3	2	Total O 2 2	0	0
59	E4	1	Total O 1 1	0	0
59	FA	198	Total O 198 198	0	0
59	FE	1	Total O 1 1	0	0
59	FK	1	Total O 1 1	0	0
59	FN	3	Total O 3 3	0	0
59	FQ	1	Total O 1 1	0	0
59	FT	4	Total O 4 4	0	0
59	FV	1	Total O 1 1	0	0
59	GA	607	Total O 607 607	0	0
59	GB	19	Total O 19 19	0	0
59	GC	9	Total O 9 9	0	0

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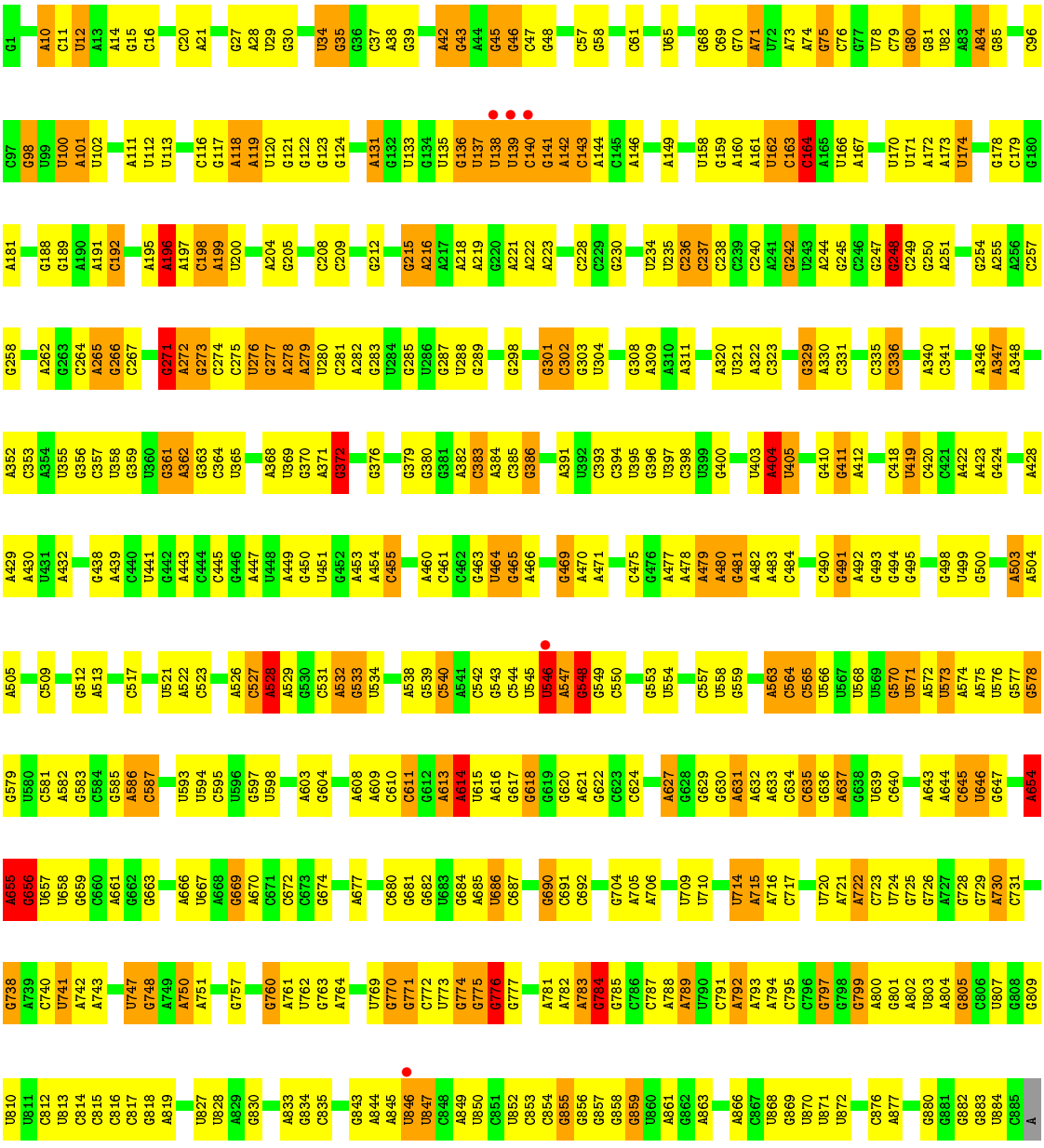
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	GD	4	Total O 4 4	0	0
59	GE	2	Total O 2 2	0	0
59	GL	4	Total O 4 4	0	0
59	GN	3	Total O 3 3	0	0
59	GQ	1	Total O 1 1	0	0
59	GR	2	Total O 2 2	0	0
59	GS	1	Total O 1 1	0	0
59	GT	1	Total O 1 1	0	0
59	GU	2	Total O 2 2	0	0
59	GV	1	Total O 1 1	0	0
59	G2	2	Total O 2 2	0	0
59	G3	1	Total O 1 1	0	0
59	G4	1	Total O 1 1	0	0
59	HA	197	Total O 197 197	0	0
59	HD	1	Total O 1 1	0	0
59	HE	3	Total O 3 3	0	0
59	HN	5	Total O 5 5	0	0
59	HT	1	Total O 1 1	0	0
59	HU	1	Total O 1 1	0	0
59	HV	1	Total O 1 1	0	0

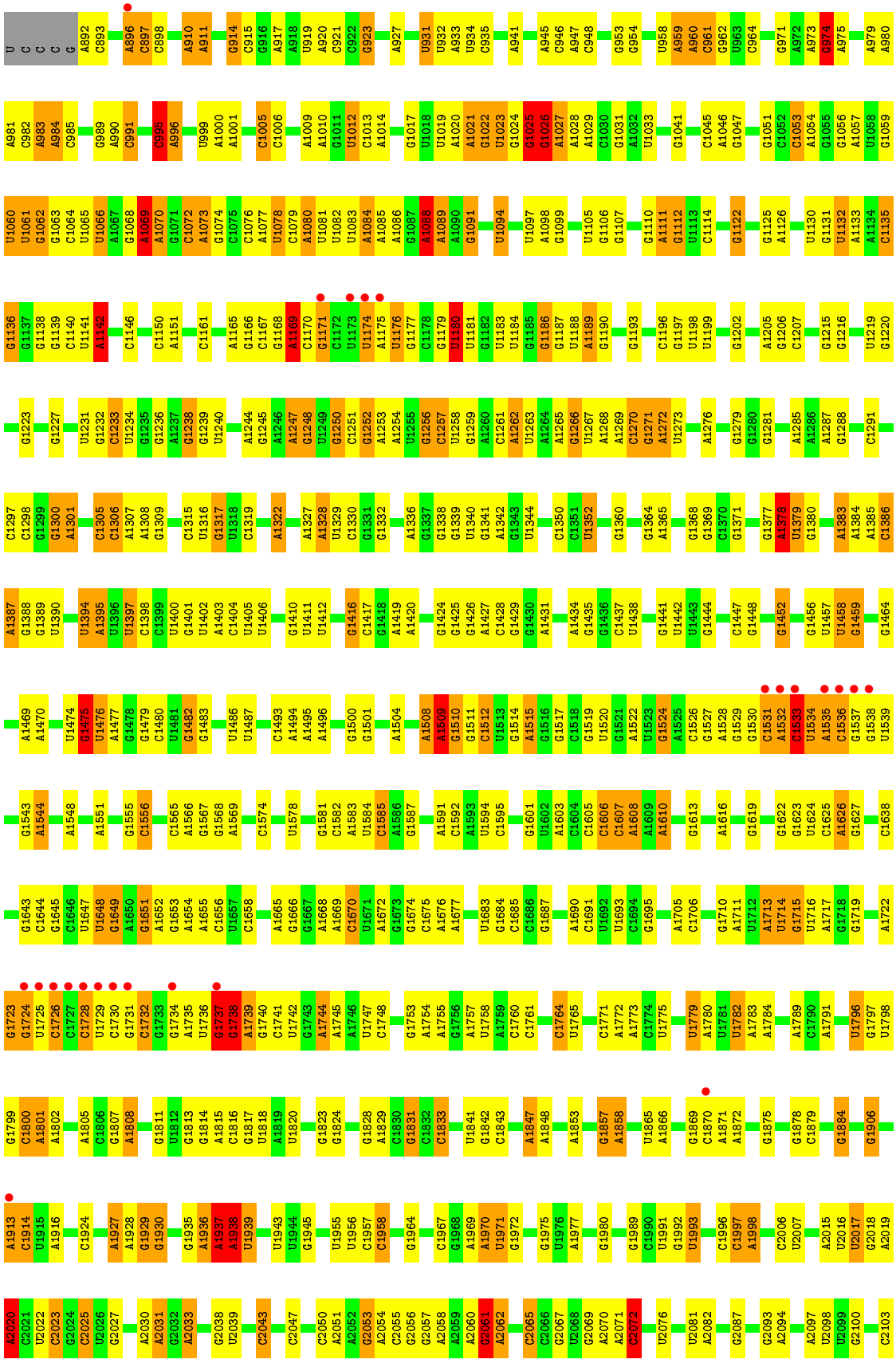
3 Residue-property plots (i)

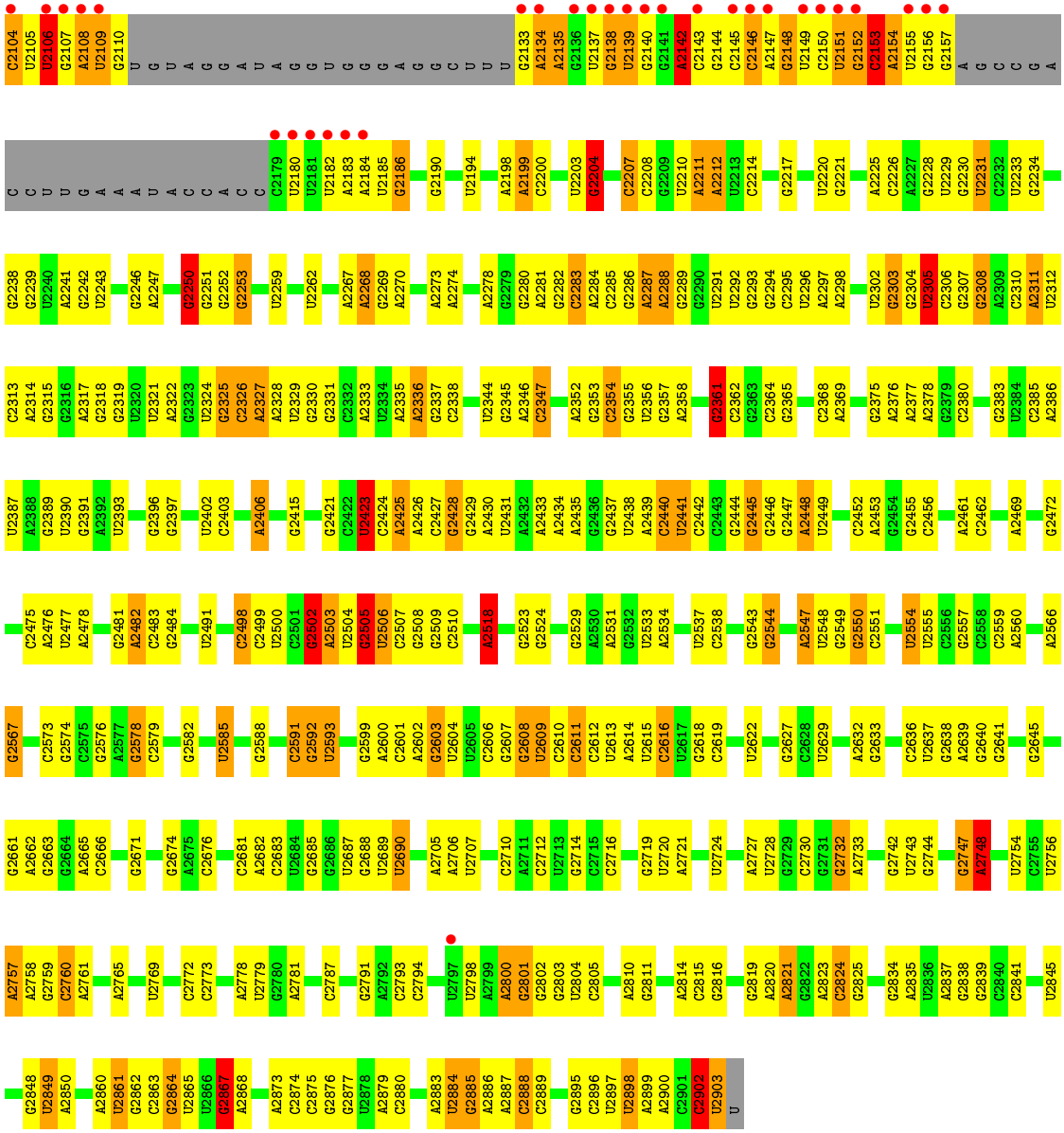
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: 23S rRNA

Chain AA:

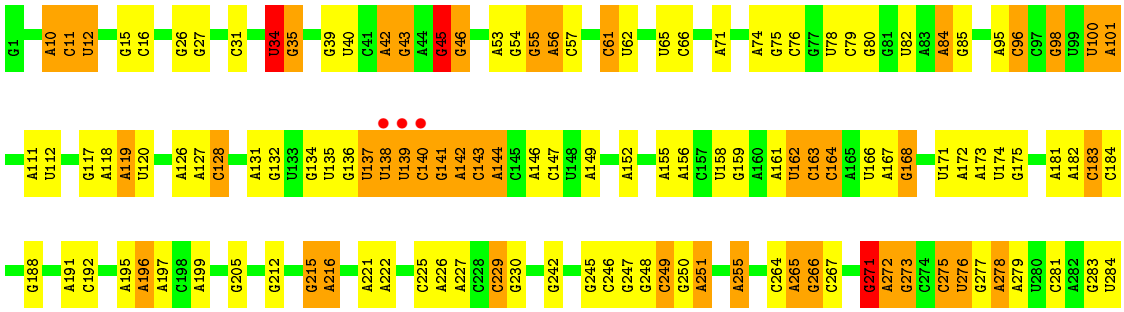


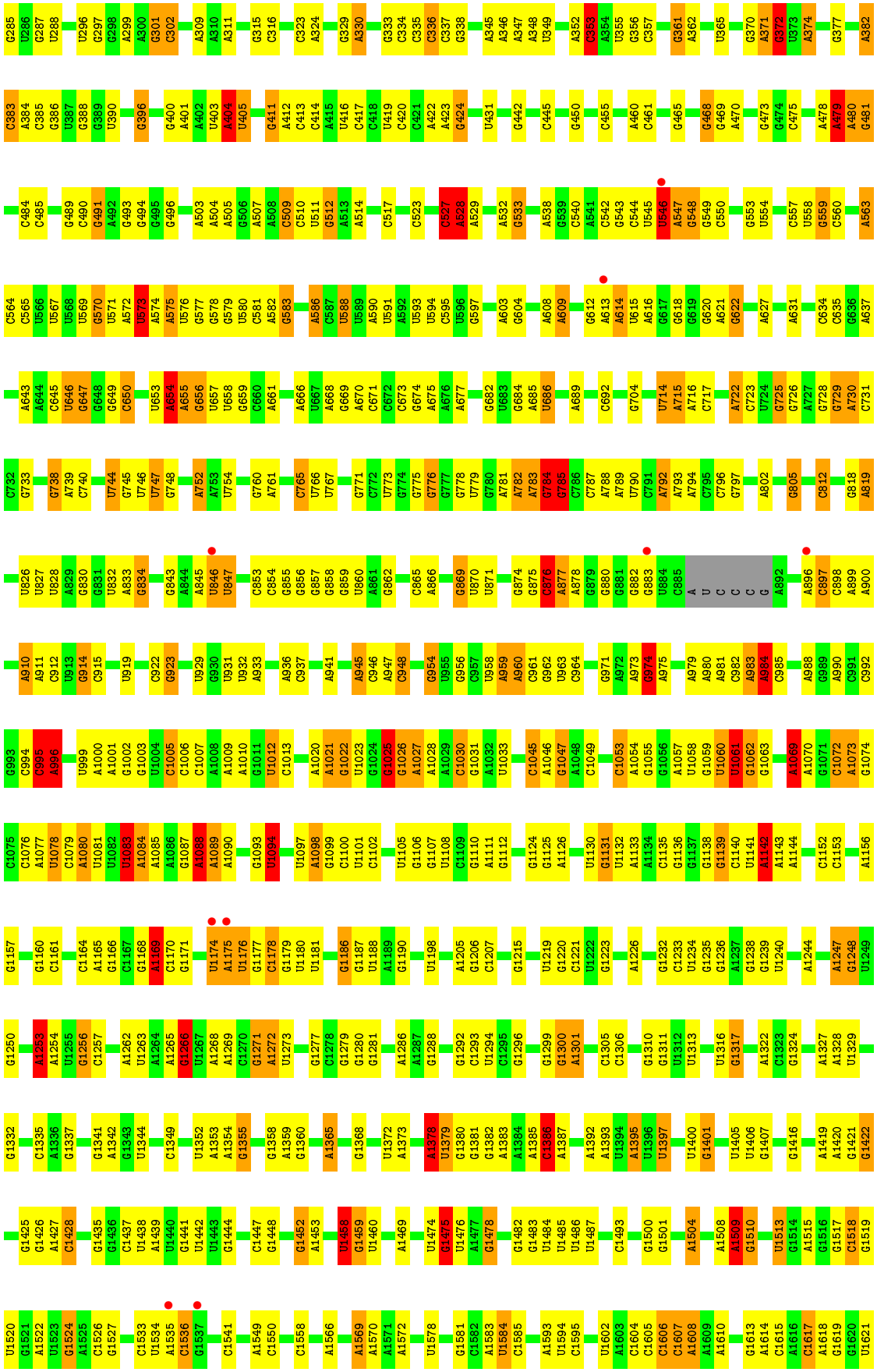

U C C C G
A892 C893 A896 C897 C898 A910 A911 G914 C915 G916 A917 A918 U919 A920 C921 C922 G923 A927 U931 U932 A933 U934 C935 A941 A945 C946 A947 C948 G953 G954 U958 A959 A960 C961 G962 U963 C964 G971 A972 A973 G974 A975 A979 A980
A981 C982 A983 A984 C985 G989 A990 C991 C995 A996 U999 A1000 A1001 C1005 C1006 A1009 A1010 G1011 U1012 C1013 A1014 G1017 U1018 U1019 A1020 A1021 G1022 U1023 G1024 G1025 G1026 A1027 A1028 A1029 C1030 G1031 A1032 U1033 G1041 C1045 A1046 G1047 G1051 C1052 C1053 A1054 G1055 C1056 A1057 U1058 G1059
U1060 U1061 G1062 G1063 C1064 U1065 U1066 A1067 G1068 A1069 A1070 G1071 C1072 A1073 G1074 C1075 C1076 A1077 U1078 C1079 A1080 U1081 U1082 U1083 A1084 A1085 A1086 G1087 A1088 A1089 A1090 G1091 U1094 U1097 A1098 G1099 U1105 G1106 G1107 G1110 A1111 G1112 U1113 C1114 G1122 G1125 A1126 G1130 G1131 U1132 A1133 A1134 C1135
G1136 G1137 G1138 G1139 C1140 U1141 A1142 C1146 C1150 A1151 C1161 A1165 G1166 C1167 G1168 A1169 C1170 G1171 C1172 U1173 U1174 A1175 U1176 G1177 C1178 G1179 U1180 U1181 G1182 U1183 U1184 G1185 G1186 G1187 U1188 A1189 G1190 G1193 C1196 G1197 U1198 U1199 G1202 A1205 G1206 C1207 G1215 G1216 U1219 G1220
G1223 G1227 U1231 G1232 C1233 U1234 G1235 G1236 A1237 G1238 G1239 U1240 A1244 G1245 A1246 A1247 G1248 U1249 G1250 C1251 G1252 A1253 A1254 U1255 G1256 C1257 U1258 G1259 A1260 C1261 A1262 U1263 A1264 A1265 G1266 U1267 A1268 A1269 C1270 G1271 A1272 U1273 A1276 G1279 G1280 G1281 A1285 A1286 A1287 G1288 C1291
C1297 C1298 G1299 G1300 A1301 C1305 C1306 A1307 A1308 G1309 C1315 U1316 G1317 U1318 C1319 A1322 A1327 A1328 U1329 C1330 G1331 G1332 A1336 G1337 G1338 G1339 U1340 G1341 A1342 G1343 U1344 C1350 G1351 U1352 G1360 G1364 A1365 G1368 G1369 C1370 G1371 G1377 A1378 U1379 G1380 A1383 A1384 A1385 C1386
A1387 G1388 G1389 U1390 U1394 A1395 U1396 U1397 C1398 C1399 U1400 G1401 U1402 A1403 C1404 U1405 U1406 G1410 U1411 U1412 G1416 C1417 G1418 A1419 A1420 G1424 G1425 G1426 A1427 C1428 G1429 G1430 A1431 A1434 G1435 G1436 C1437 U1438 G1441 U1442 U1443 G1444 C1447 G1448 G1452 G1456 U1457 U1458 G1459 G1464
A1469 A1470 U1474 G1475 U1476 A1477 G1478 G1479 C1480 U1481 G1482 G1483 U1486 U1487 C1493 A1494 A1495 A1496 G1500 G1501 A1504 A1508 A1509 G1510 G1511 C1512 U1513 G1514 A1515 G1516 G1517 G1518 G1519 U1520 G1521 A1522 U1523 G1524 A1525 C1526 G1527 A1528 G1529 G1530 C1531 A1532 G1533 U1534 A1535 C1536 G1537 G1538 U1539
G1543 A1544 A1548 A1551 G1555 C1556 C1565 A1566 G1567 G1568 A1569 C1574 U1578 G1581 C1582 A1583 U1584 C1585 A1586 G1587 A1591 C1592 A1593 U1594 C1595 G1601 U1602 A1603 C1604 C1605 C1606 C1607 A1608 A1609 A1610 G1613 A1616 G1619 G1622 G1623 U1624 C1625 A1626 G1627 C1638
G1643 C1644 G1645 C1646 U1647 U1648 G1649 A1650 G1651 A1652 G1653 A1654 A1655 C1656 U1667 C1658 A1665 G1666 G1667 A1668 A1669 C1670 U1671 A1672 G1673 G1674 C1675 A1676 A1677 U1683 G1684 C1685 C1686 G1687 A1690 C1691 U1692 U1693 C1694 G1695 A1705 C1706 G1710 A1711 U1712 A1713 U1714 G1715 U1716 A1717 G1718 G1719 A1722
G1723 G1724 U1725 C1726 C1727 C1728 U1729 C1730 G1731 C1732 G1733 G1734 A1735 U1736 G1737 G1738 A1739 G1740 C1741 U1742 G1743 A1744 A1745 A1746 U1747 C1748 G1753 A1754 A1755 G1756 A1757 U1758 A1759 C1760 C1761 C1764 U1765 C1771 A1772 A1773 C1774 U1775 U1779 A1780 U1781 U1782 A1783 A1784 A1789 C1790 A1791 U1796 G1797 U1798
G1799 C1800 A1801 A1802 A1805 C1806 G1807 A1808 G1811 U1812 G1813 G1814 A1815 C1816 G1817 U1818 A1819 U1820 G1823 G1824 G1828 A1829 C1830 G1831 C1832 C1833 U1841 G1842 C1843 A1847 A1848 A1853 G1857 A1858 U1865 A1866 G1869 C1870 A1871 A1872 G1875 G1878 C1879 G1884 G1906
A1913 C1914 U1915 A1916 C1924 A1927 A1928 G1929 G1930 G1935 A1936 A1937 A1938 U1939 U1943 U1944 G1945 U1955 U1956 C1957 C1958 G1964 C1967 G1968 A1969 A1970 U1971 G1972 G1975 U1976 A1977 G1980 G1989 C1990 U1991 U1992 U1993 C1996 C1997 A1998 C2006 U2007 A2015 U2016 U2017 G2018 A2019
A2020 C2021 U2022 C2023 G2024 C2025 U2026 G2027 A2030 A2031 G2032 A2033 G2038 U2039 C2043 C2047 C2050 A2051 A2052 G2053 A2054 C2055 G2056 G2057 A2058 A2059 A2060 G2061 A2062 C2065 C2066 G2067 U2068 G2069 A2070 A2071 C2072 U2076 U2081 A2082 G2087 G2093 A2094 A2097 U2098 U2099 G2100 C2103

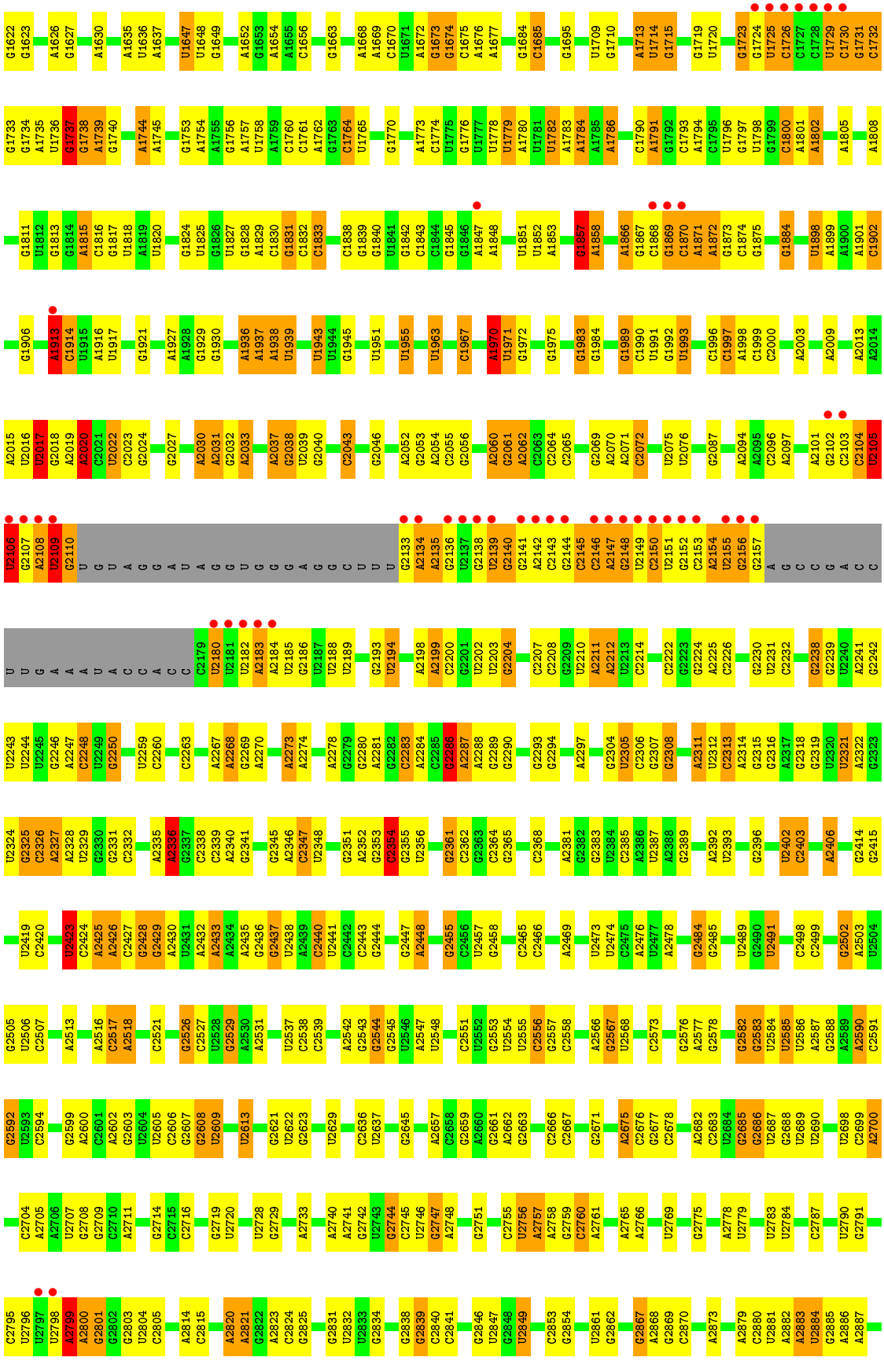


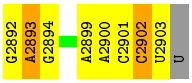
- Molecule 1: 23S rRNA

Chain CA:



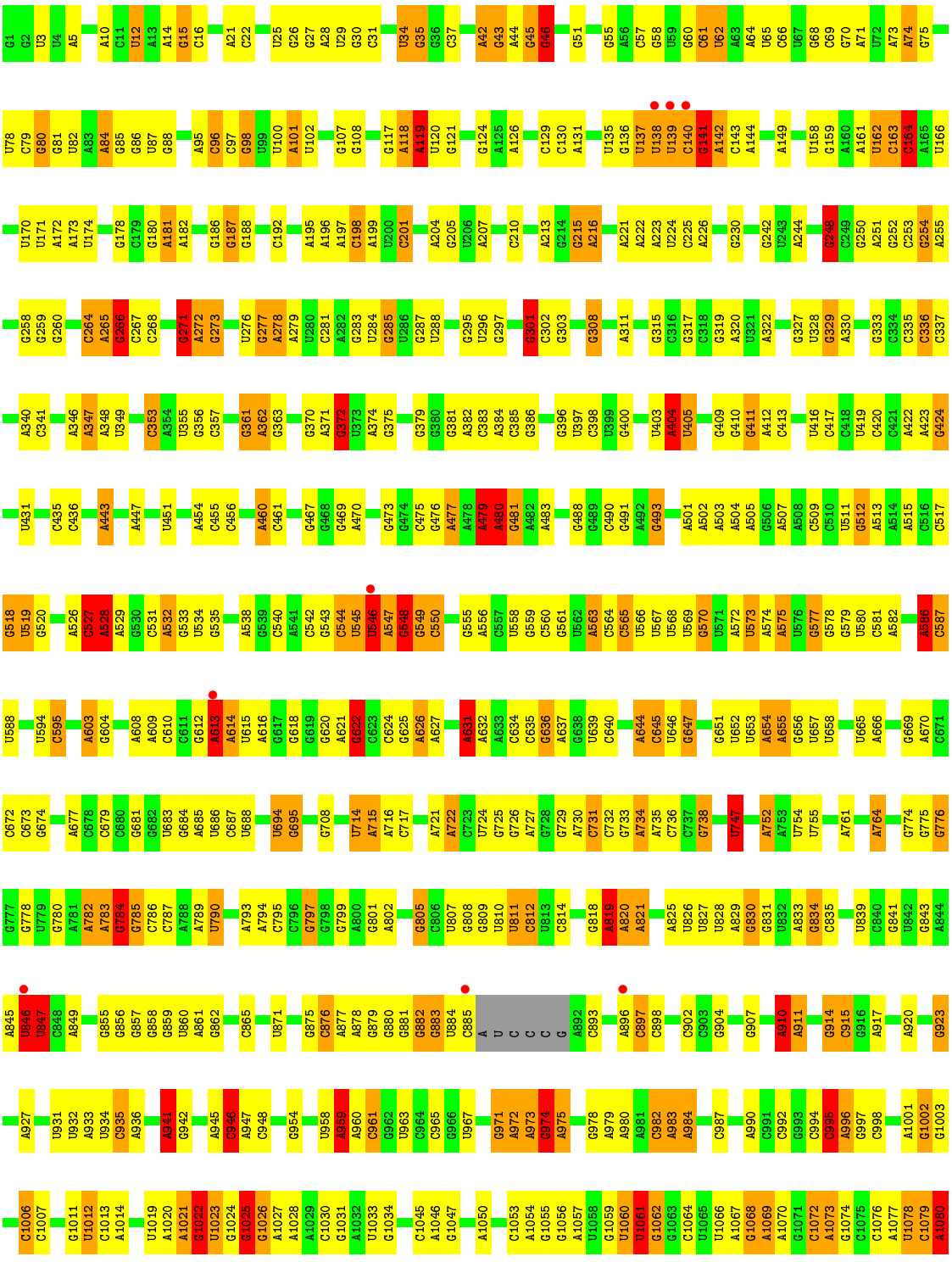


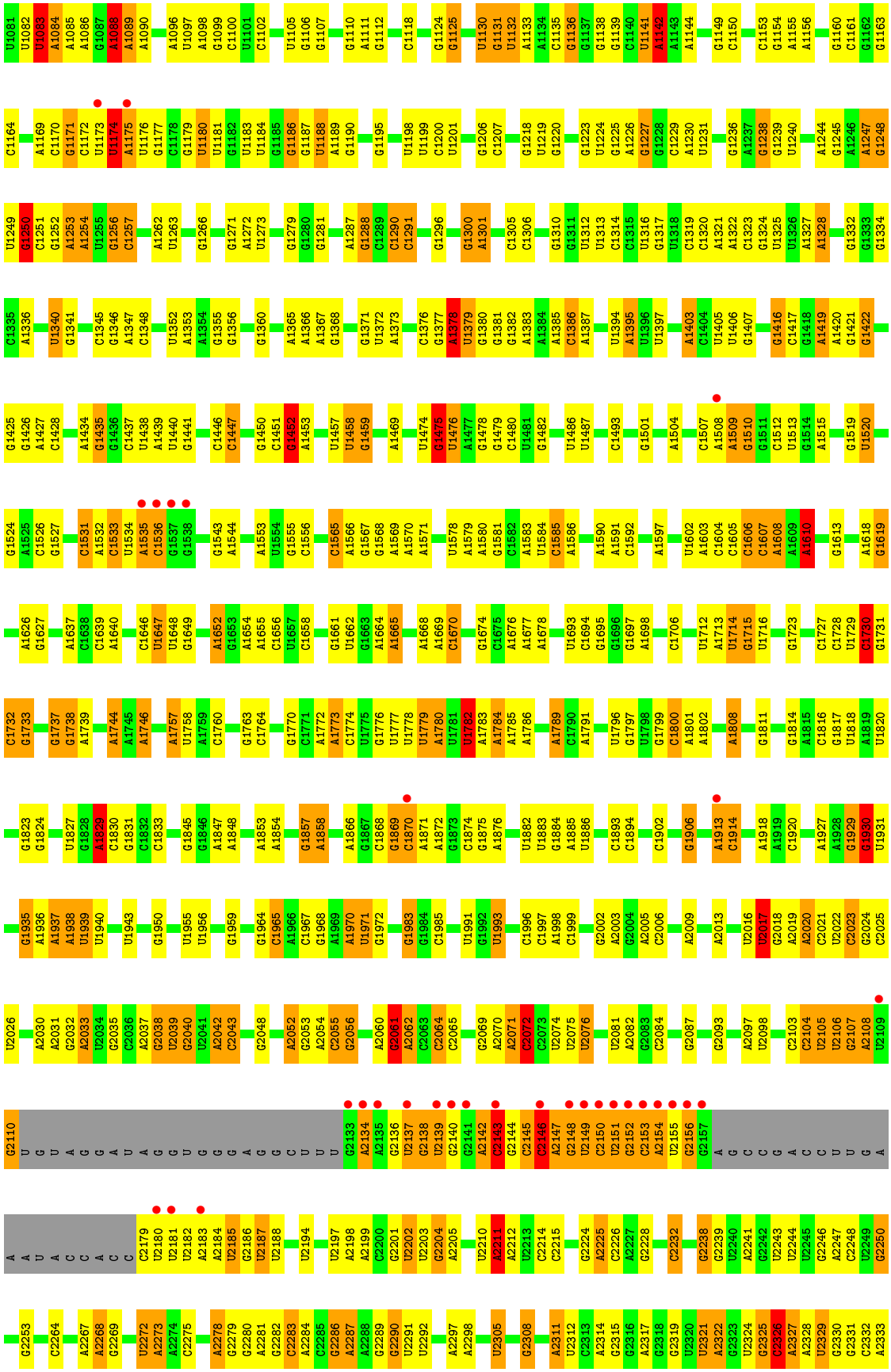


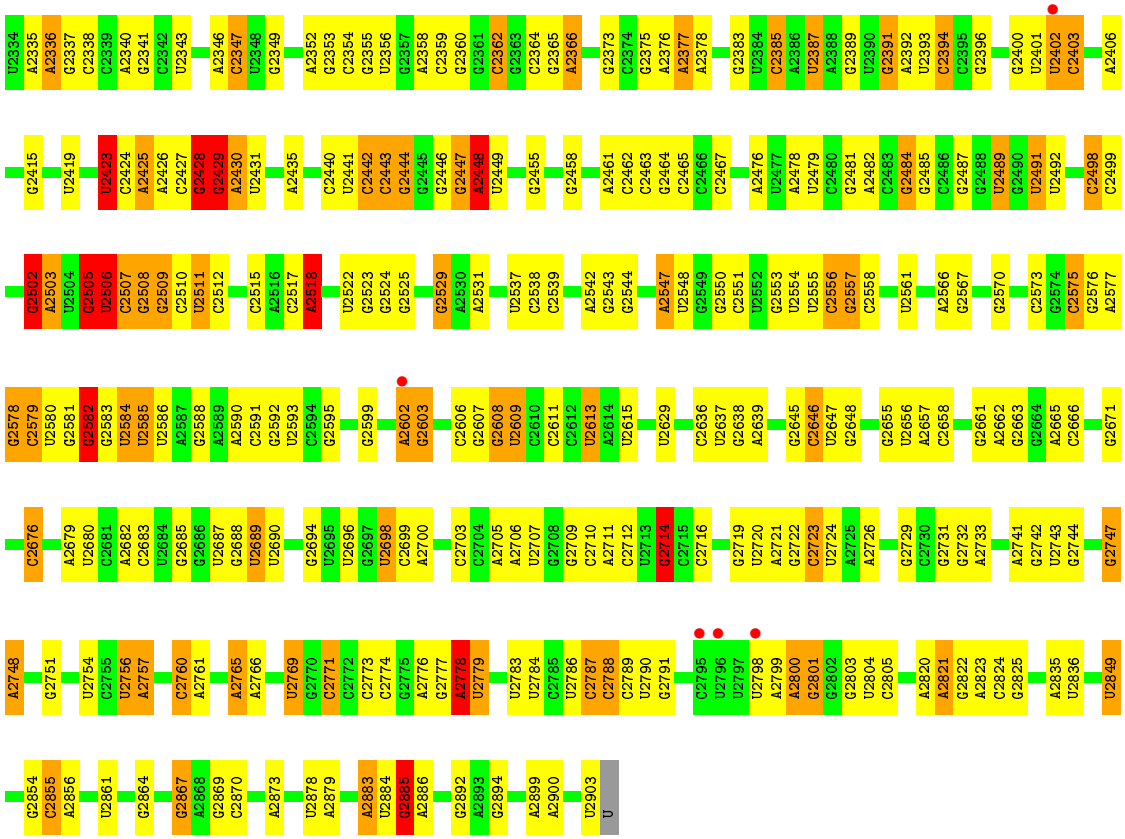


- Molecule 1: 23S rRNA

Chain EA:

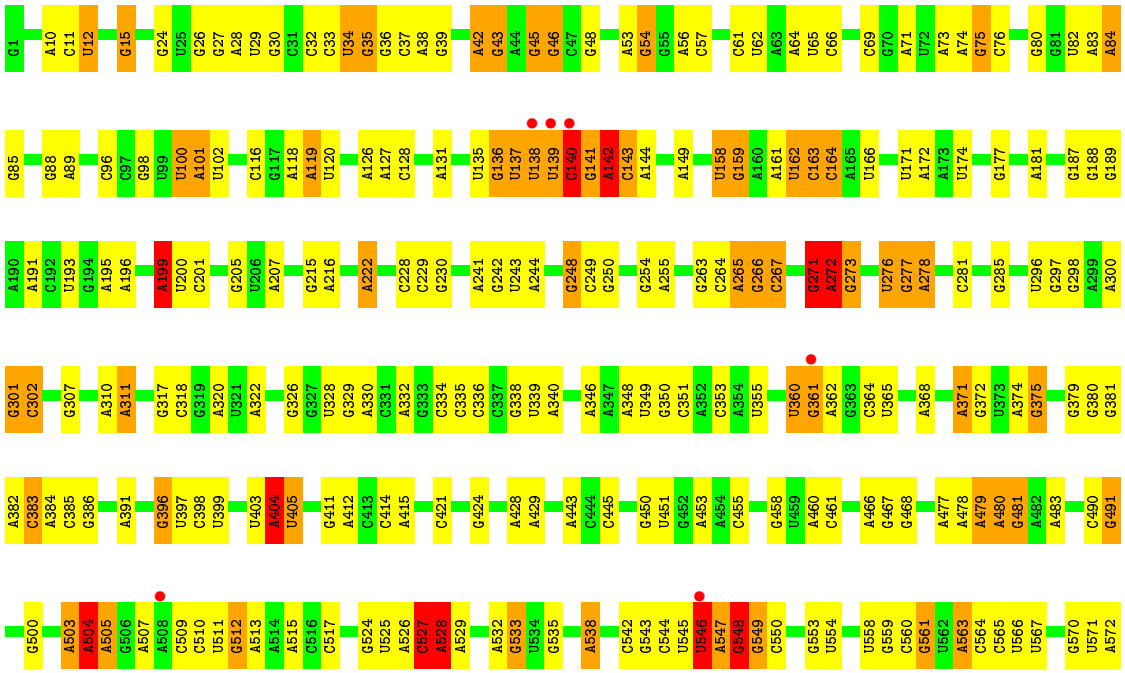


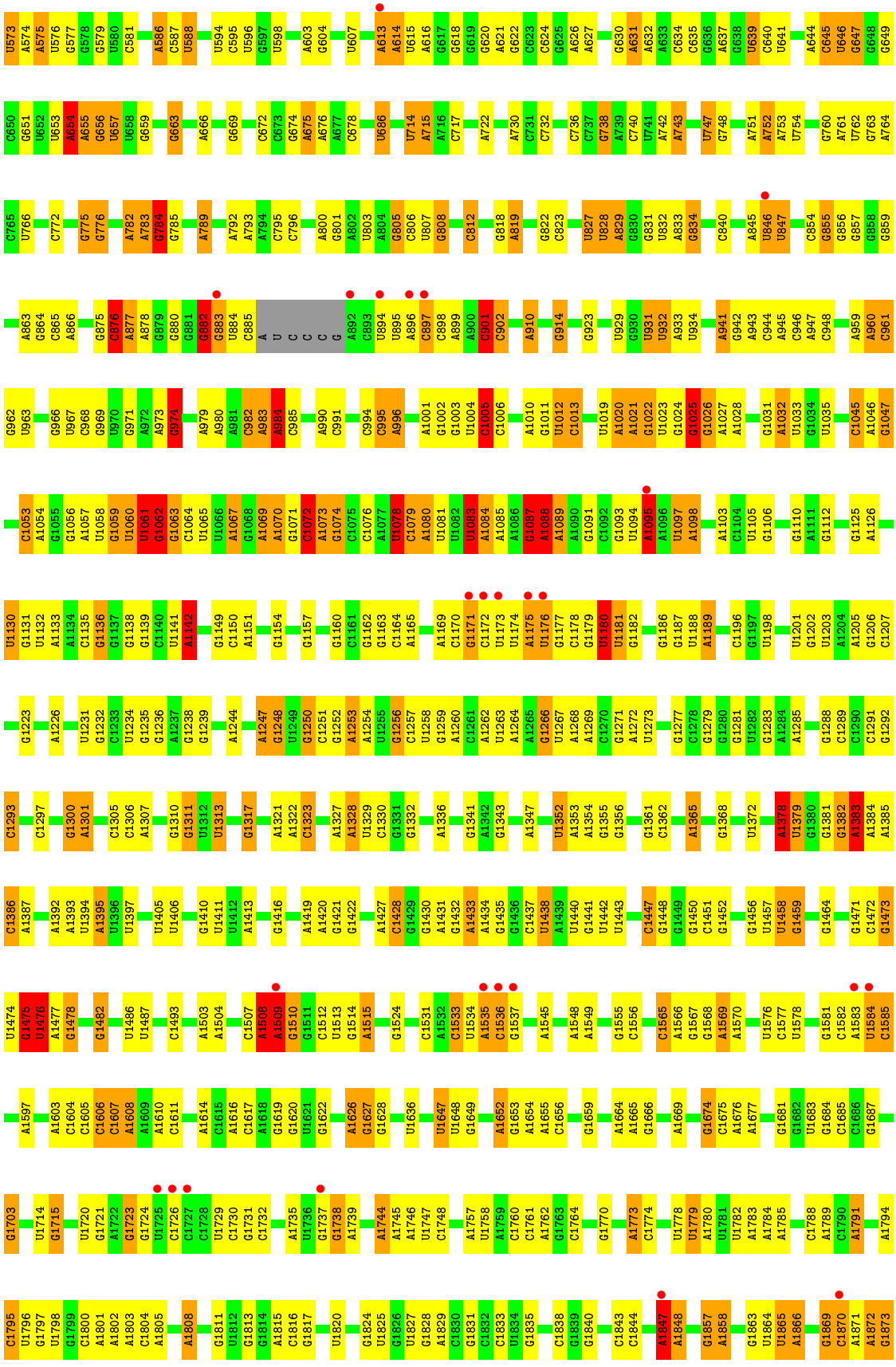


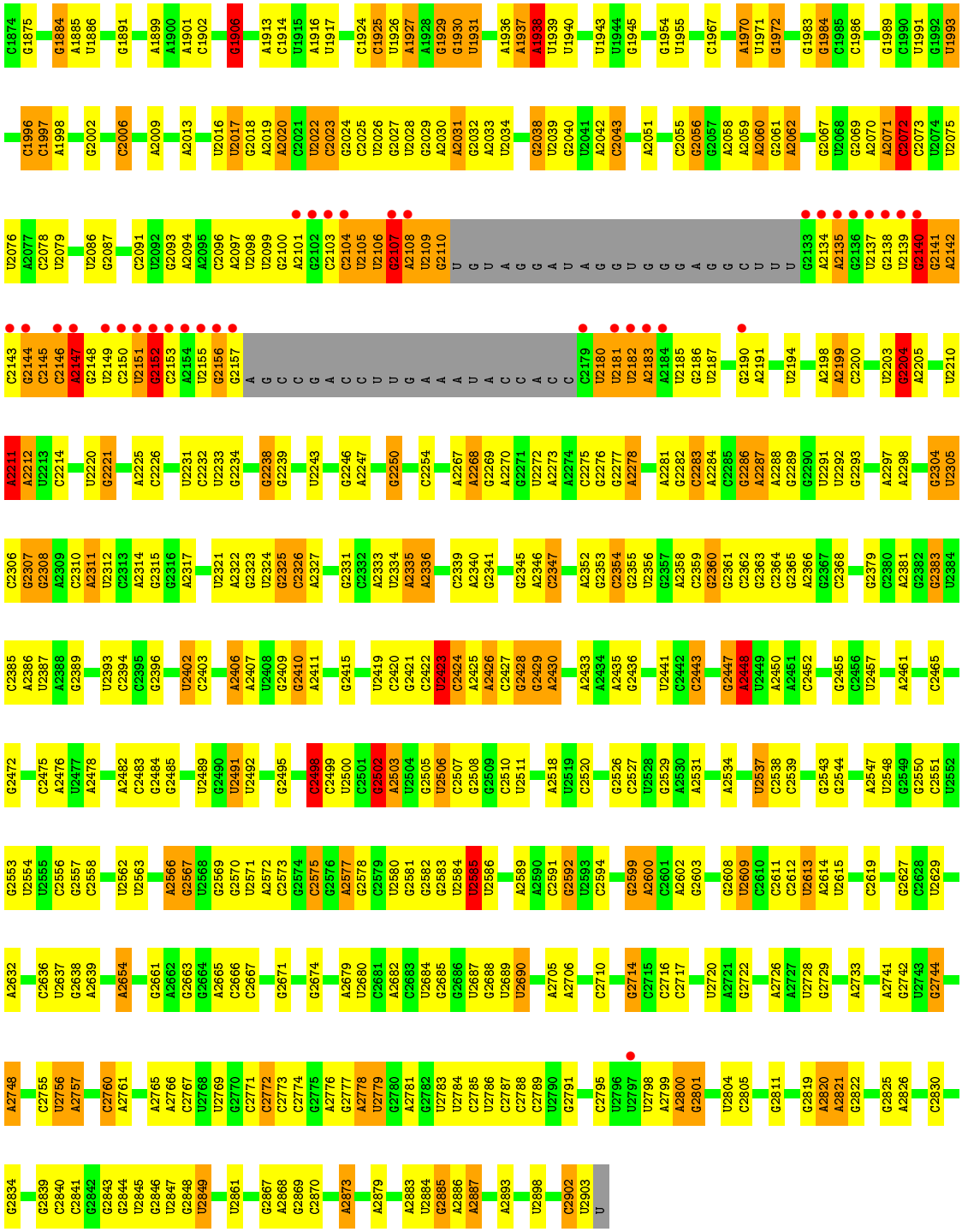


- Molecule 1: 23S rRNA

Chain GA:

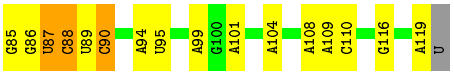






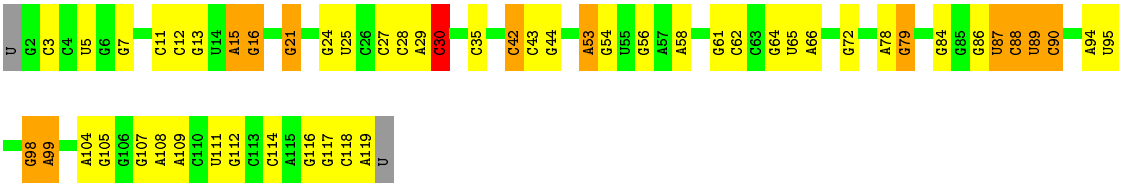
• Molecule 2: 5S rRNA

Chain AB:



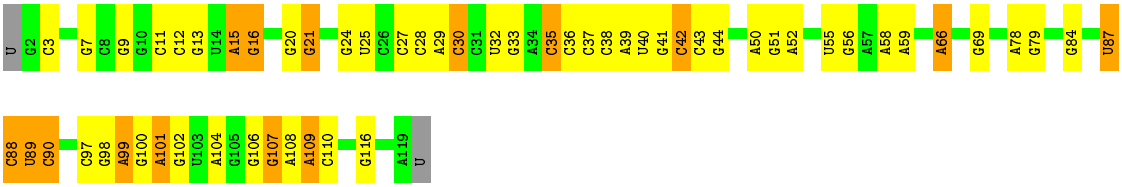
• Molecule 2: 5S rRNA

Chain CB:



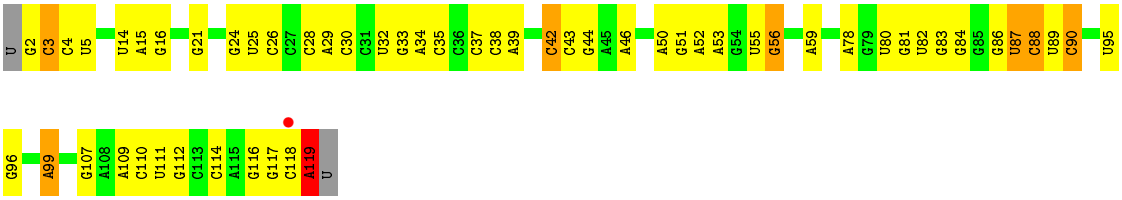
• Molecule 2: 5S rRNA

Chain EB:



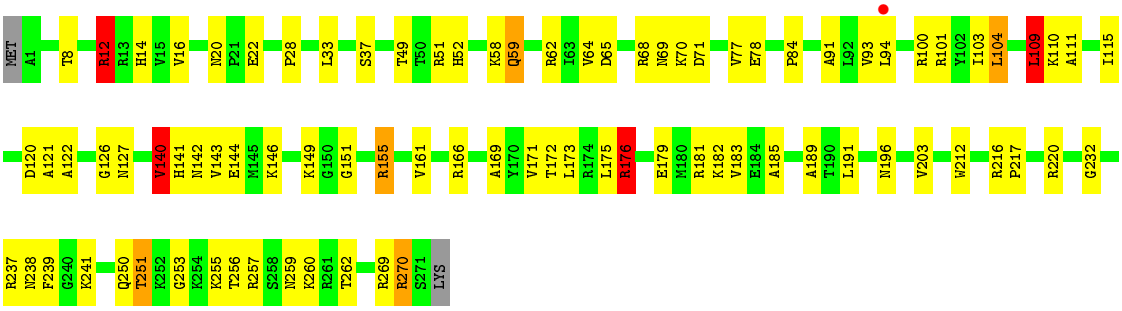
• Molecule 2: 5S rRNA

Chain GB:



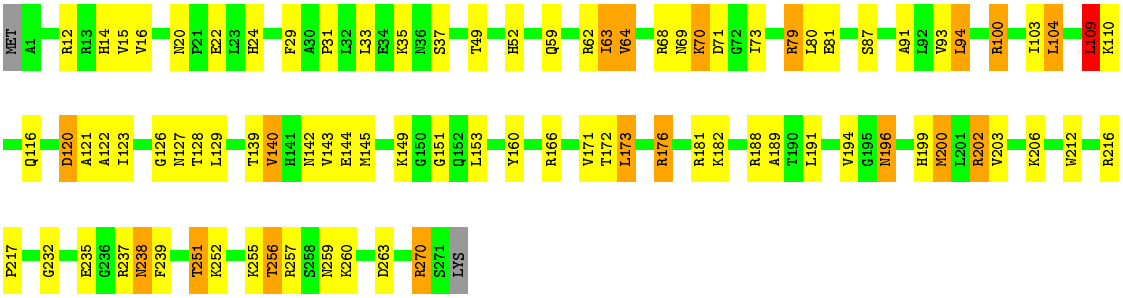
• Molecule 3: 50S ribosomal protein L2

Chain AC:

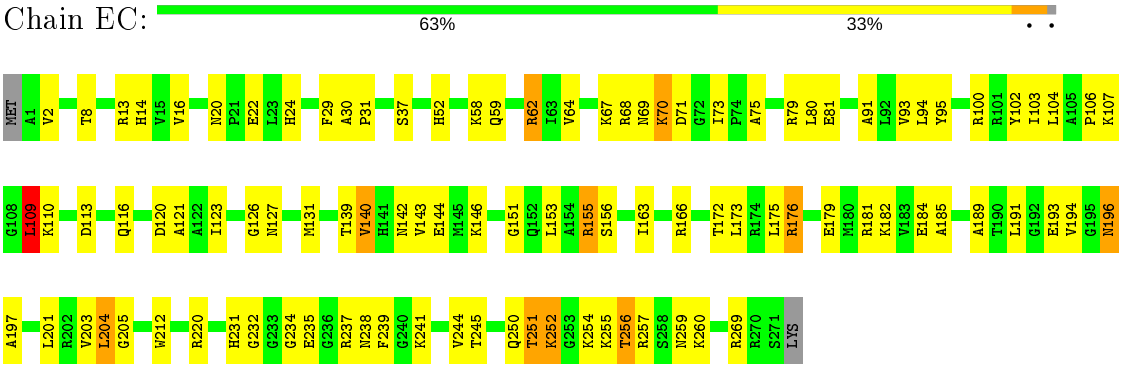


• Molecule 3: 50S ribosomal protein L2

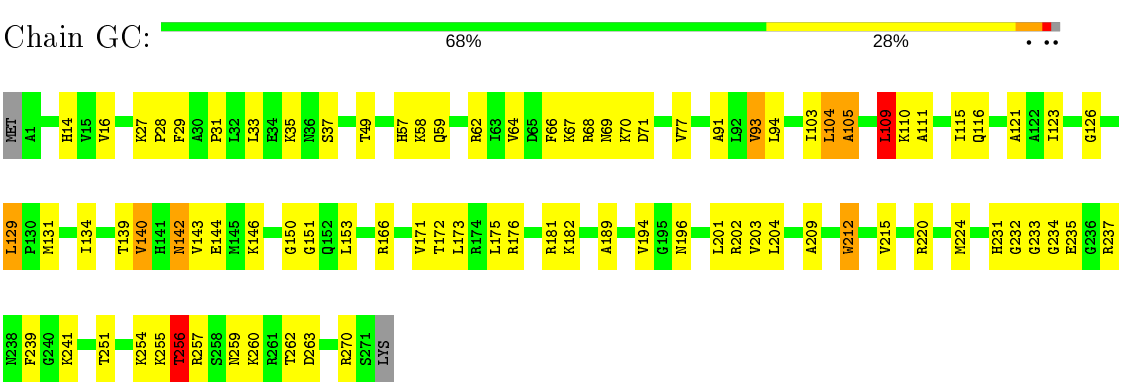
Chain CC:



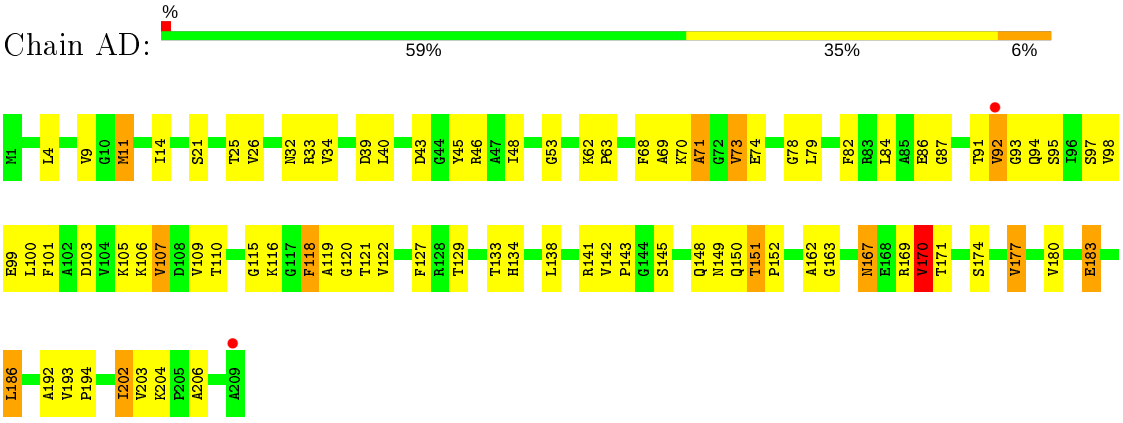
• Molecule 3: 50S ribosomal protein L2



• Molecule 3: 50S ribosomal protein L2

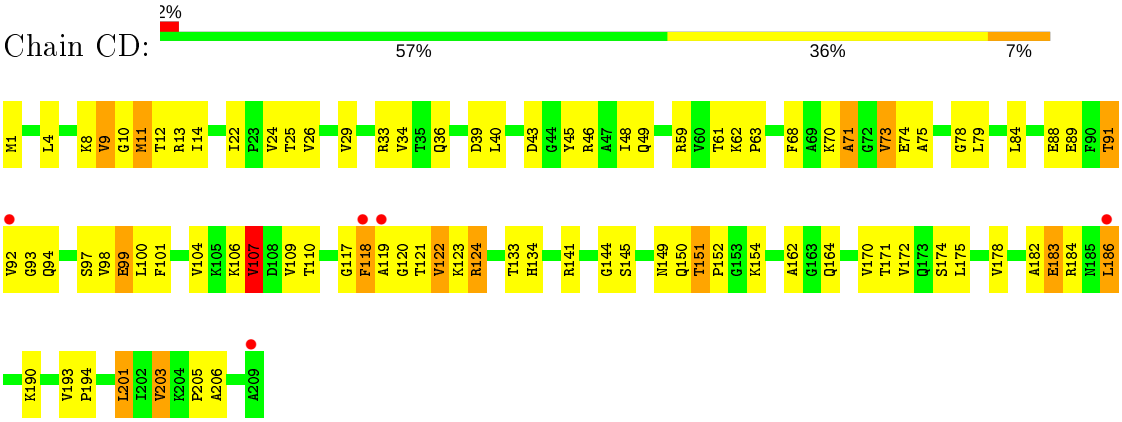


• Molecule 4: 50S ribosomal protein L3



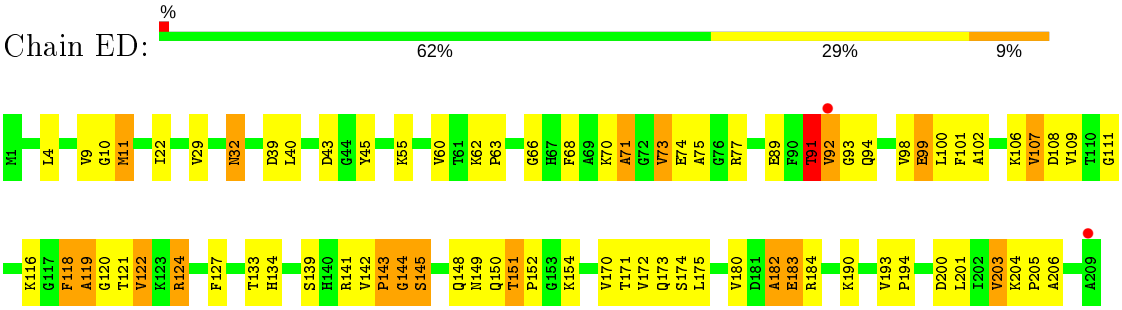
• Molecule 4: 50S ribosomal protein L3

Chain CD:



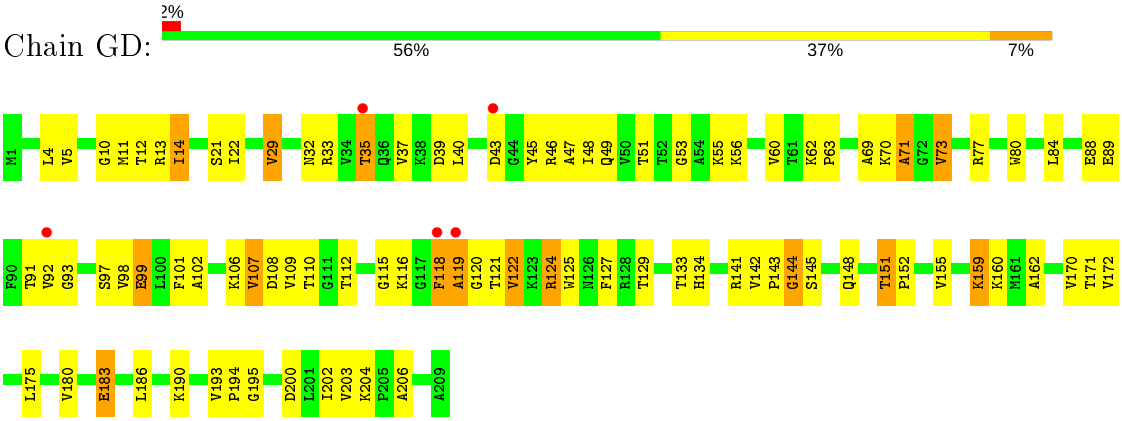
• Molecule 4: 50S ribosomal protein L3

Chain ED:



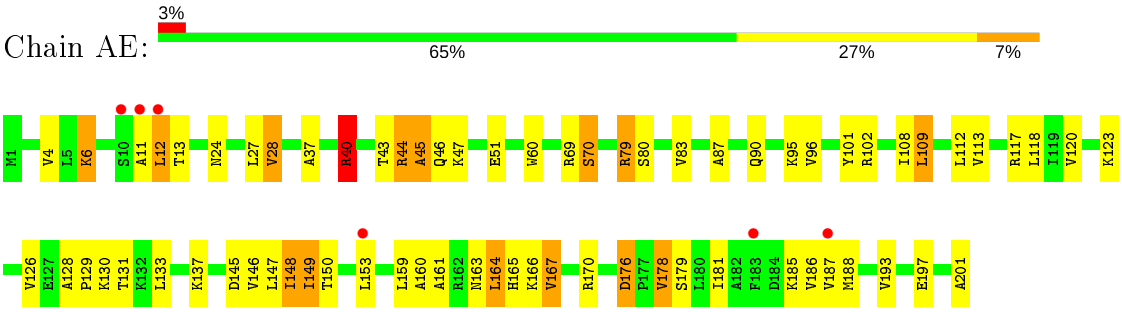
• Molecule 4: 50S ribosomal protein L3

Chain GD:



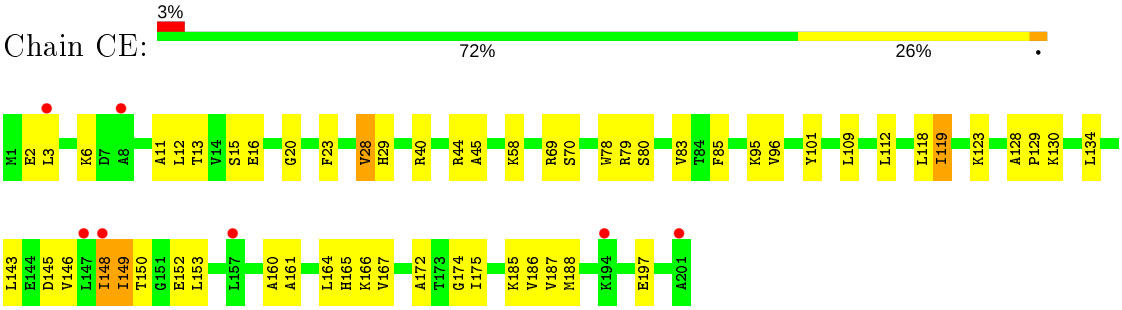
• Molecule 5: 50S ribosomal protein L4

Chain AE:



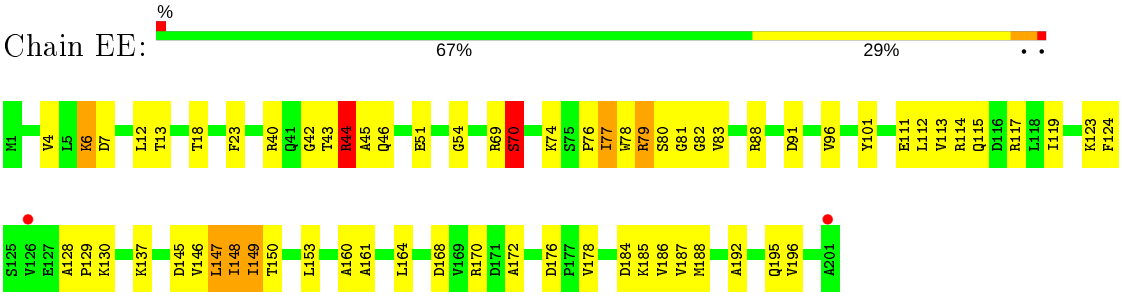
• Molecule 5: 50S ribosomal protein L4

Chain CE:



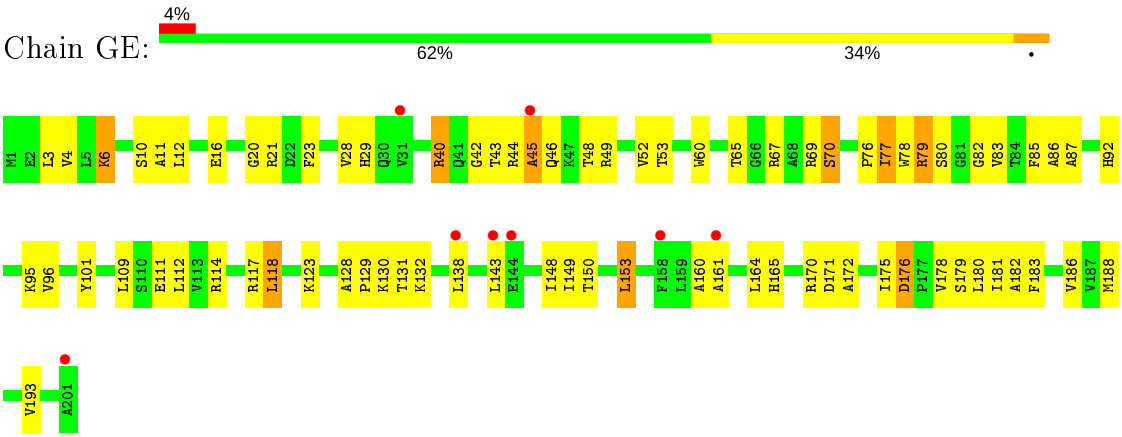
• Molecule 5: 50S ribosomal protein L4

Chain EE:



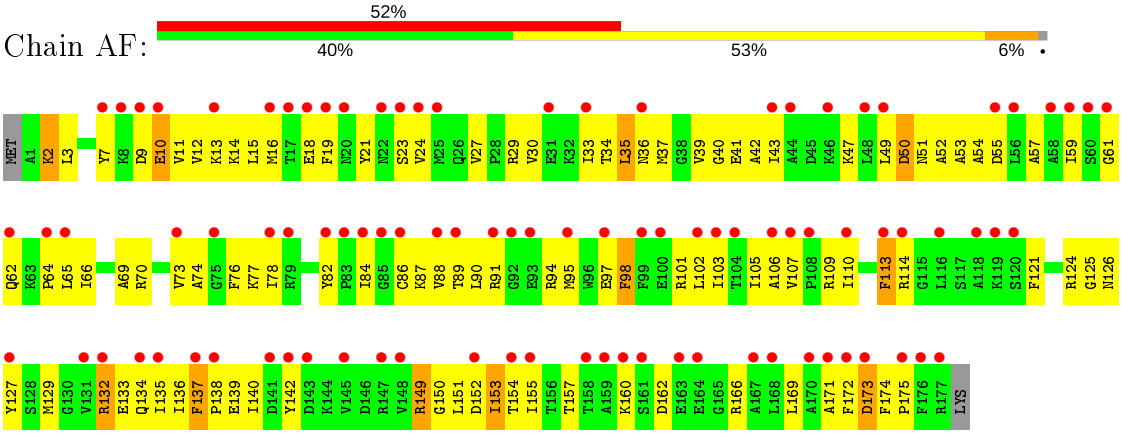
• Molecule 5: 50S ribosomal protein L4

Chain GE:



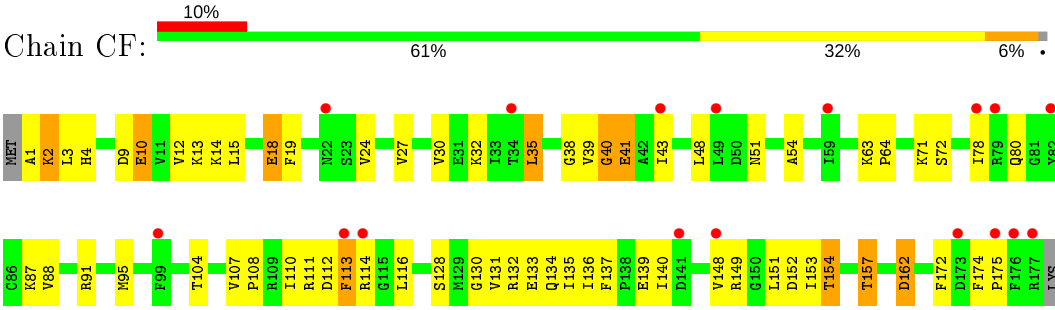
• Molecule 6: 50S ribosomal protein L5

Chain AF:



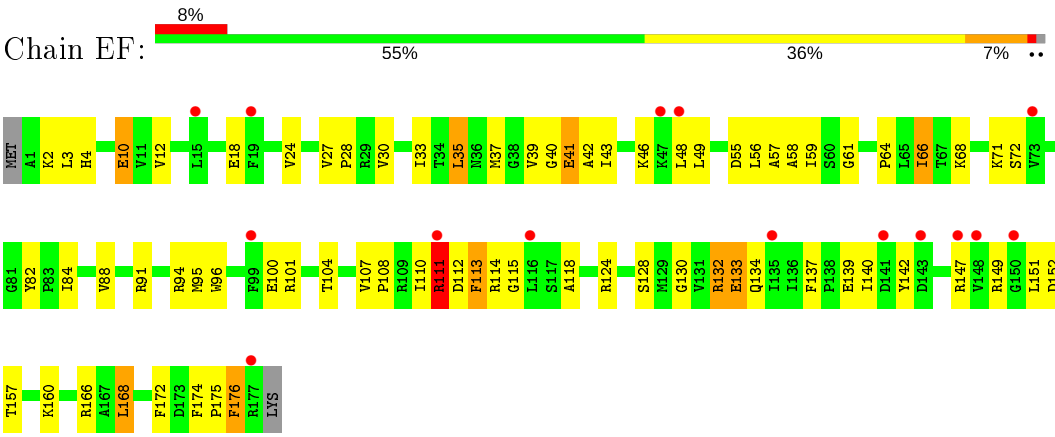
• Molecule 6: 50S ribosomal protein L5

Chain CF:



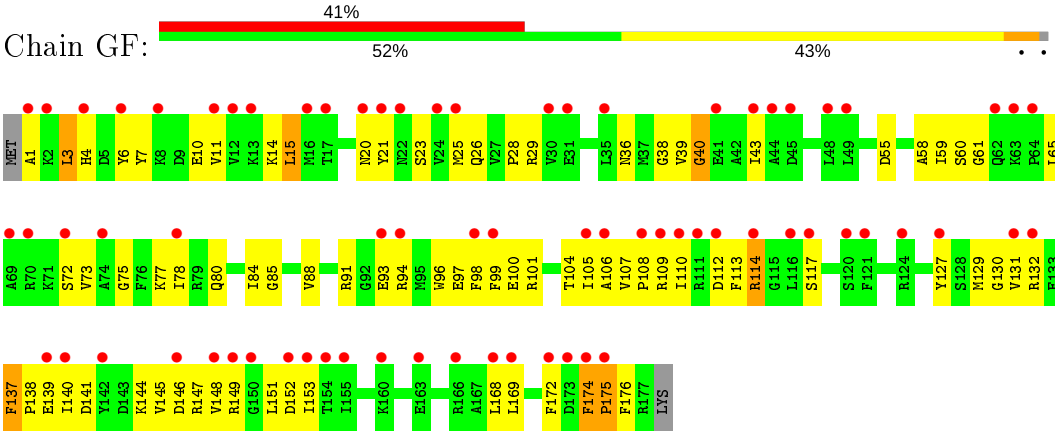
• Molecule 6: 50S ribosomal protein L5

Chain EF:



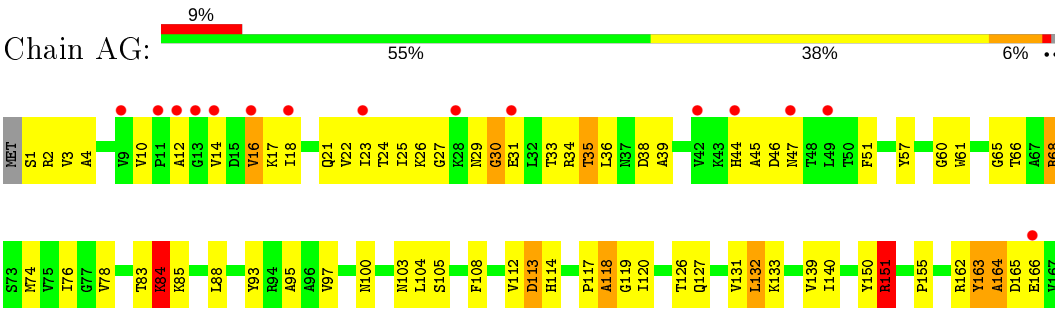
• Molecule 6: 50S ribosomal protein L5

Chain GF:



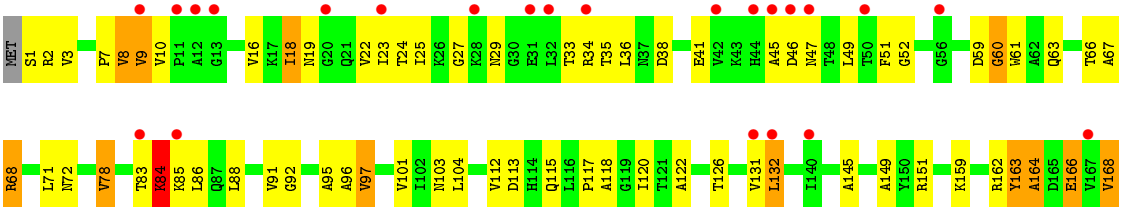
• Molecule 7: 50S ribosomal protein L6

Chain AG:



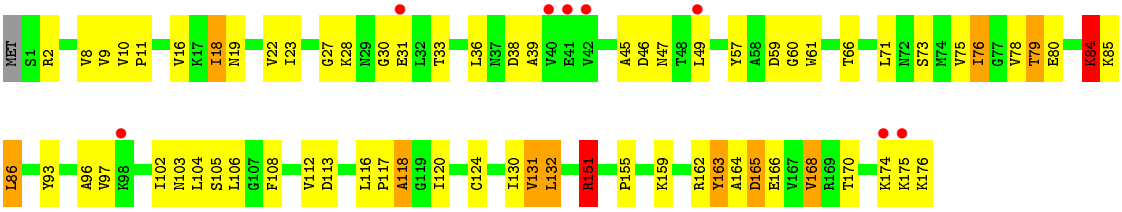
• Molecule 7: 50S ribosomal protein L6

Chain CG:



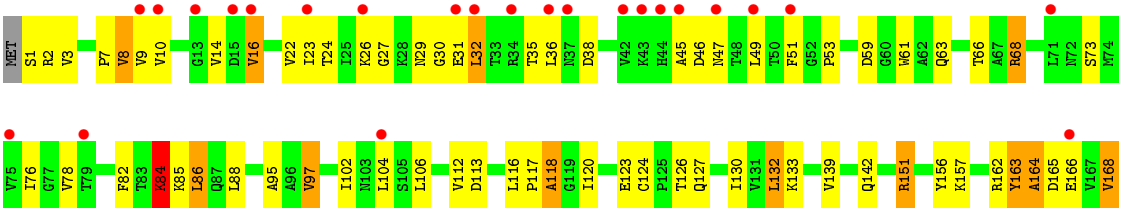
• Molecule 7: 50S ribosomal protein L6

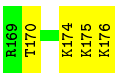
Chain EG:



• Molecule 7: 50S ribosomal protein L6

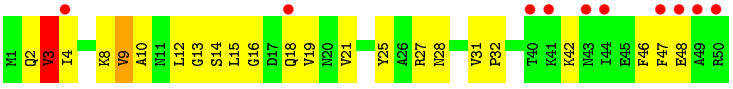
Chain GG:





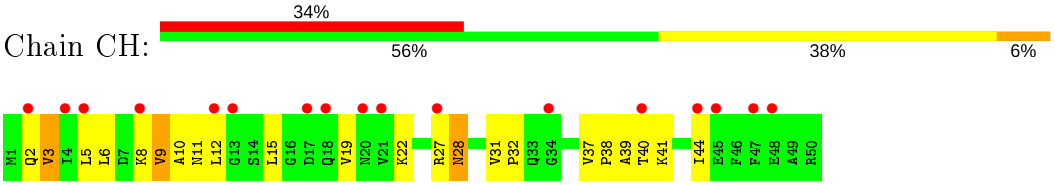
• Molecule 8: 50S ribosomal protein L9

Chain AH:



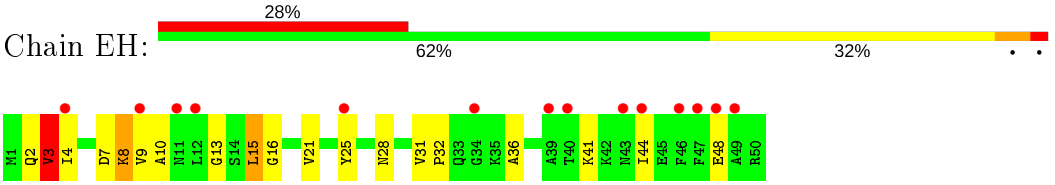
• Molecule 8: 50S ribosomal protein L9

Chain CH:



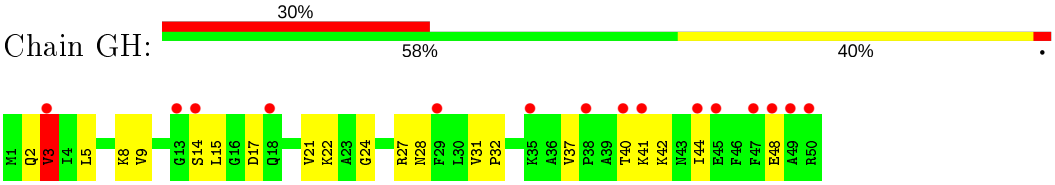
• Molecule 8: 50S ribosomal protein L9

Chain EH:



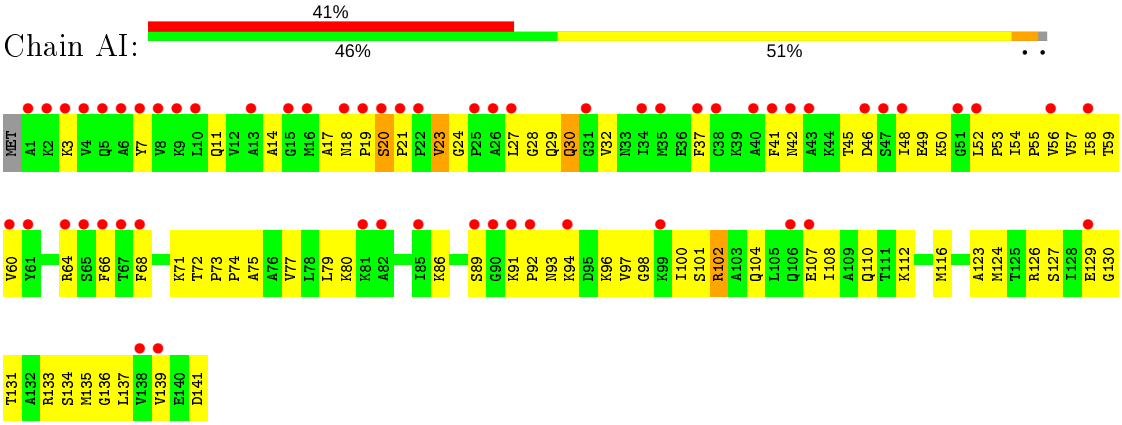
• Molecule 8: 50S ribosomal protein L9

Chain GH:



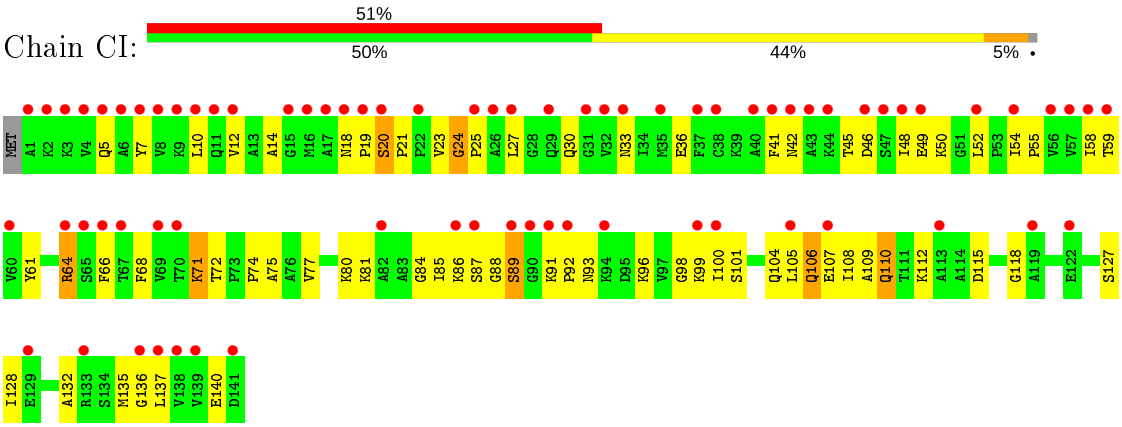
• Molecule 9: 50S ribosomal protein L11

Chain AI:



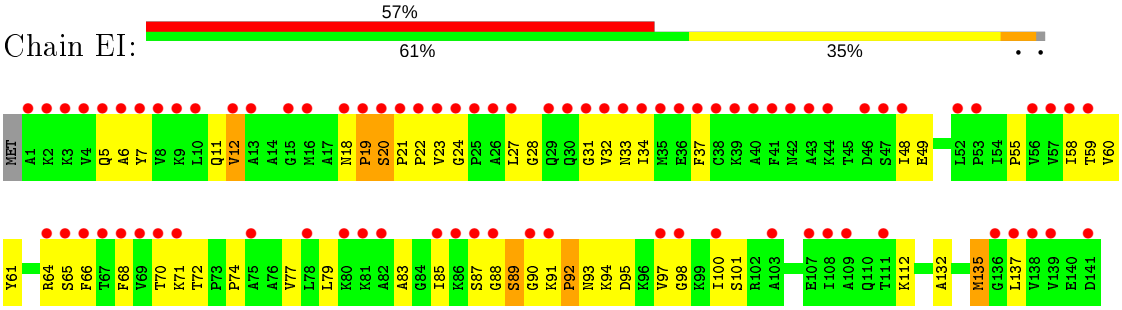
• Molecule 9: 50S ribosomal protein L11

Chain CI:



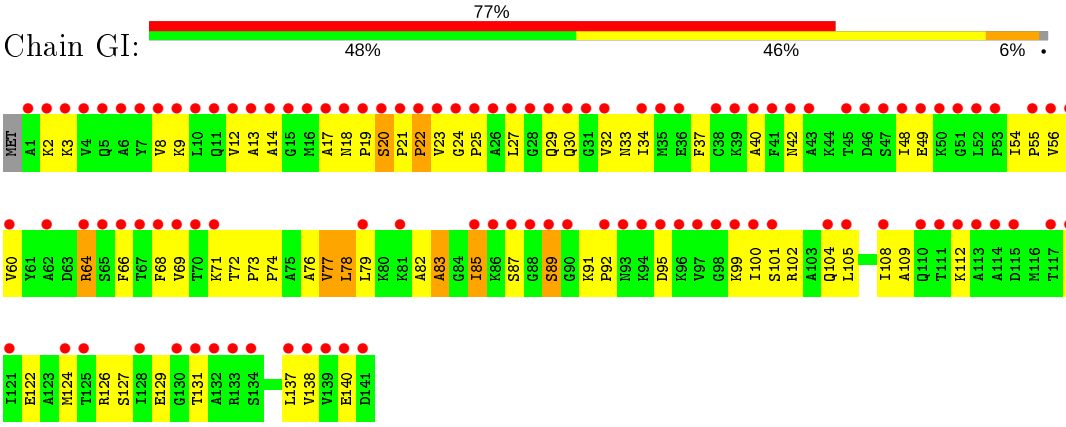
• Molecule 9: 50S ribosomal protein L11

Chain EI:



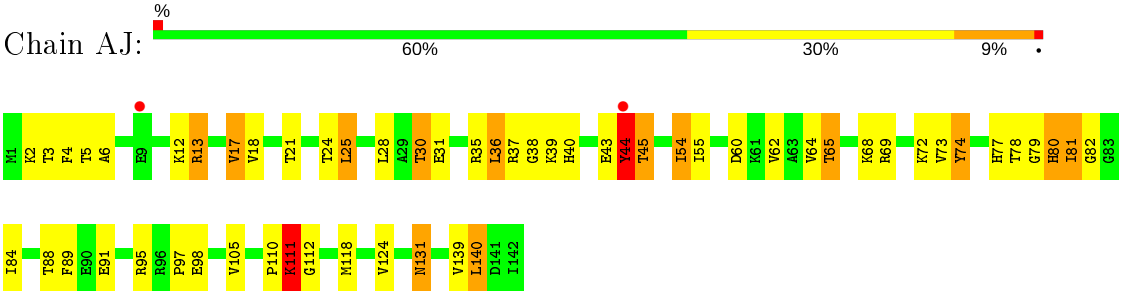
• Molecule 9: 50S ribosomal protein L11

Chain GI:



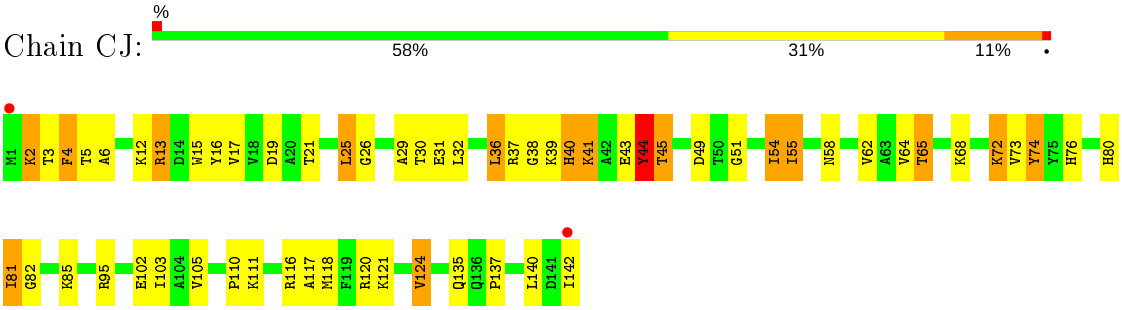
• Molecule 10: 50S ribosomal protein L13

Chain AJ:



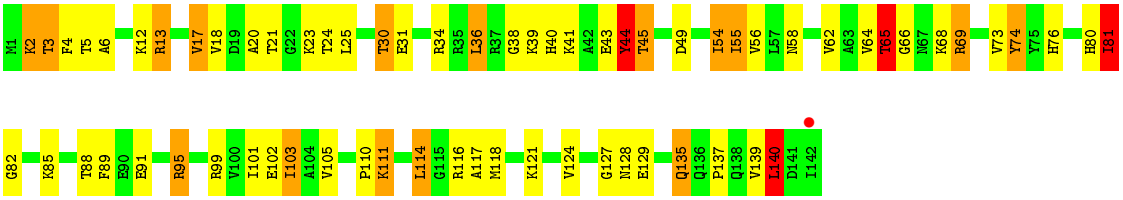
• Molecule 10: 50S ribosomal protein L13

Chain CJ:



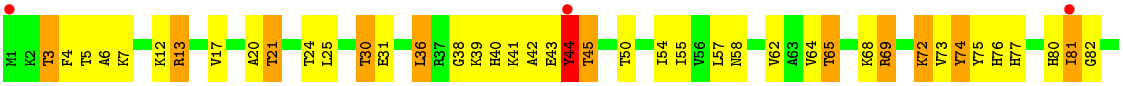
• Molecule 10: 50S ribosomal protein L13

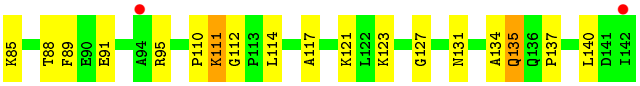
Chain EJ:



• Molecule 10: 50S ribosomal protein L13

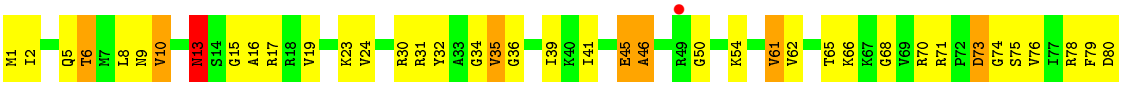
Chain GJ:





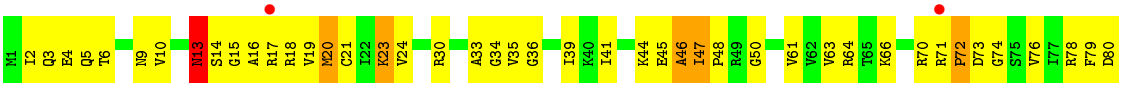
• Molecule 11: 50S ribosomal protein L14

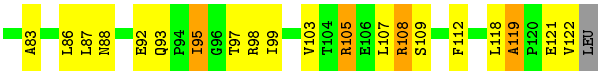
Chain AK:



• Molecule 11: 50S ribosomal protein L14

Chain CK:



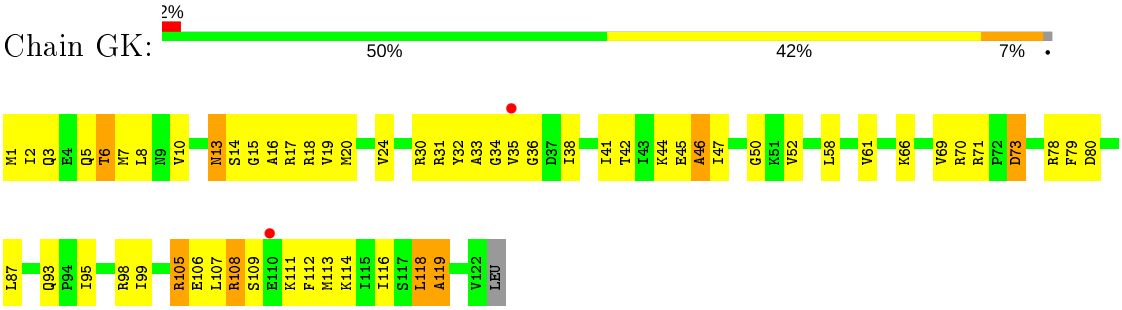


• Molecule 11: 50S ribosomal protein L14

Chain EK:

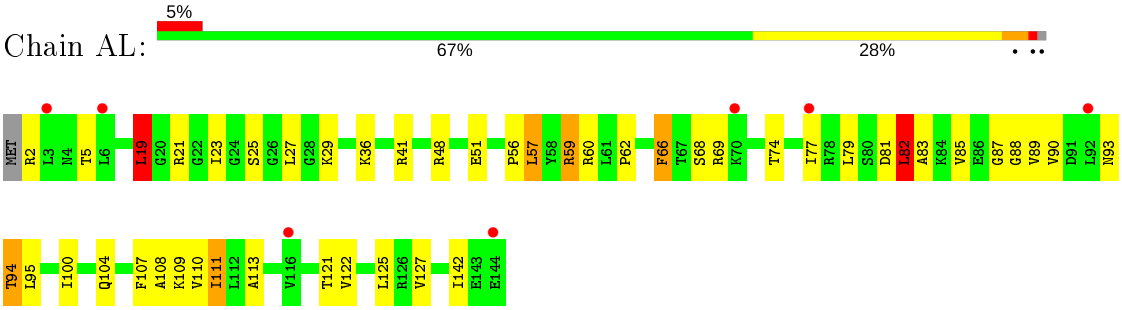
• Molecule 11: 50S ribosomal protein L14

Chain GK:



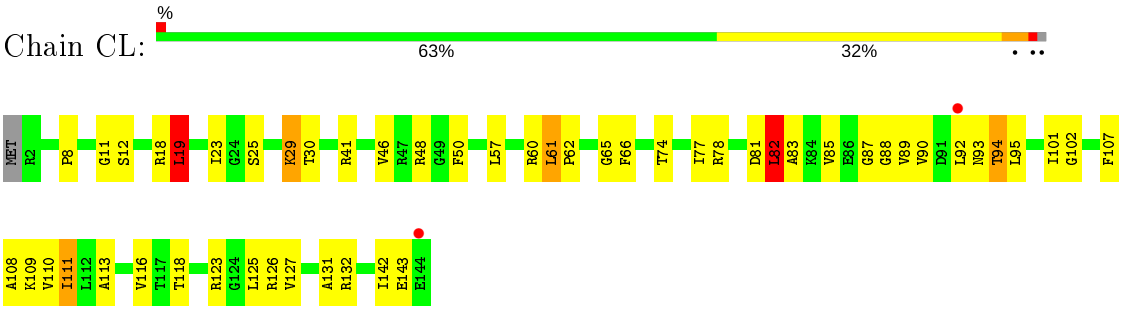
• Molecule 12: 50S ribosomal protein L15

Chain AL:



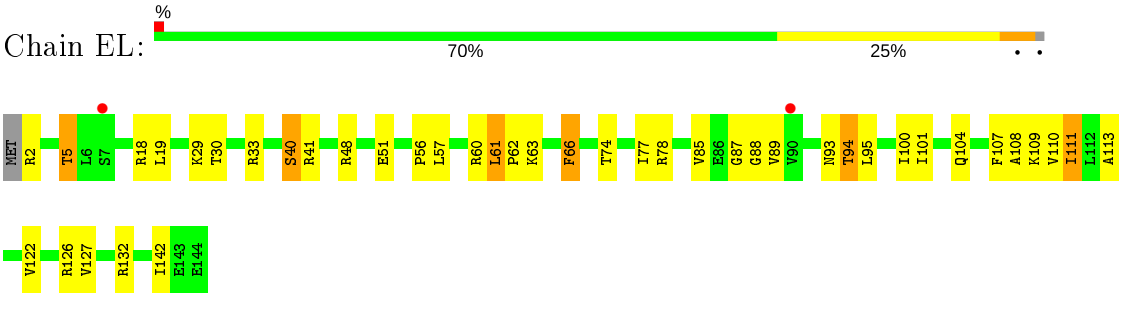
• Molecule 12: 50S ribosomal protein L15

Chain CL:



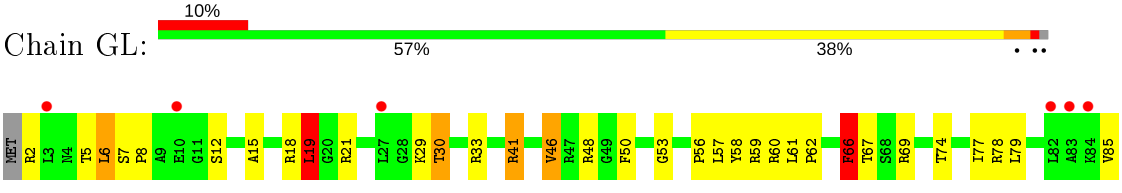
• Molecule 12: 50S ribosomal protein L15

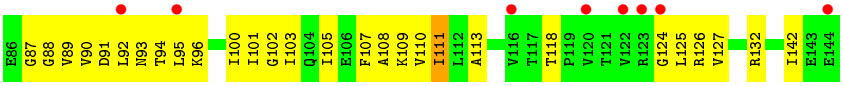
Chain EL:



• Molecule 12: 50S ribosomal protein L15

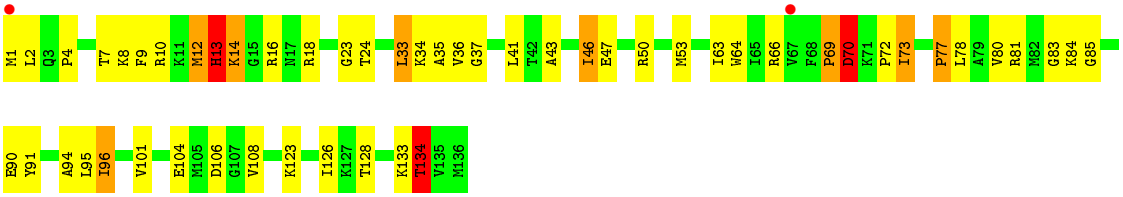
Chain GL:





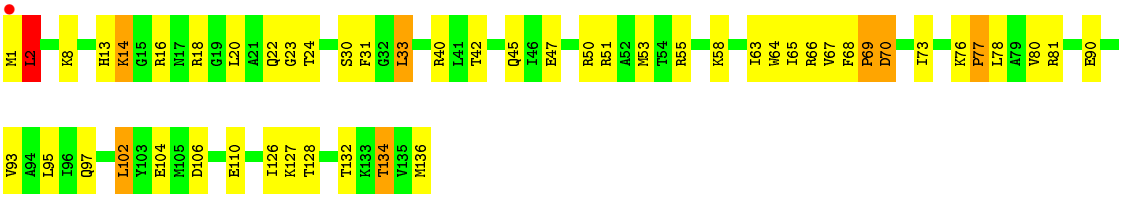
• Molecule 13: 50S ribosomal protein L16

Chain AM:



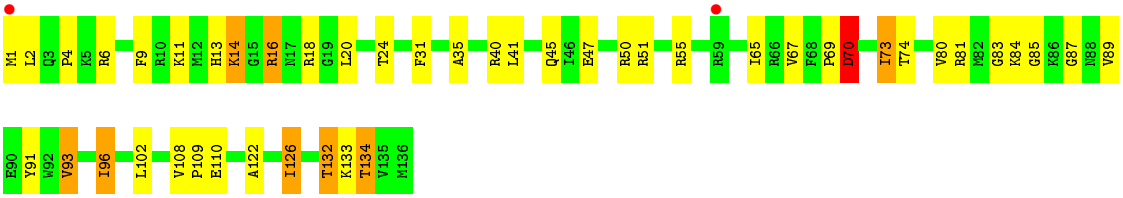
• Molecule 13: 50S ribosomal protein L16

Chain CM:



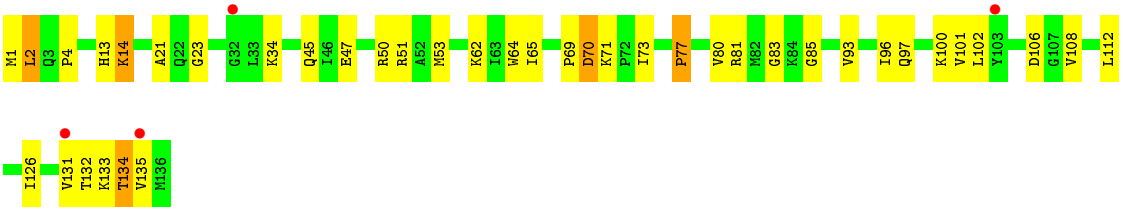
• Molecule 13: 50S ribosomal protein L16

Chain EM:



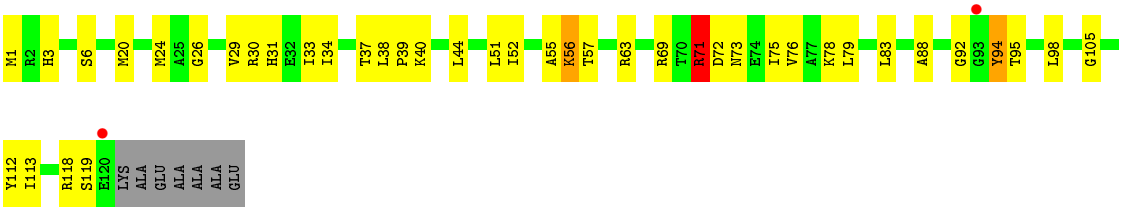
• Molecule 13: 50S ribosomal protein L16

Chain GM:



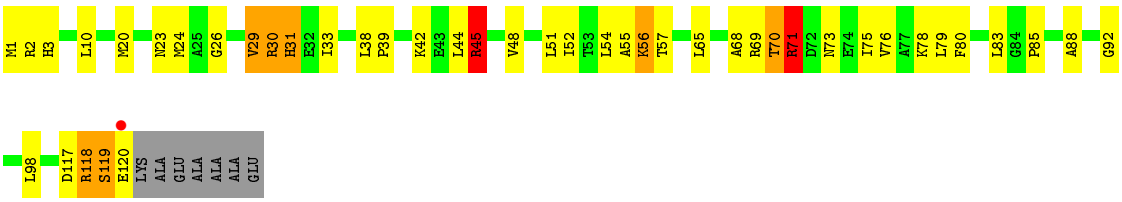
• Molecule 14: 50S ribosomal protein L17

Chain AN:



• Molecule 14: 50S ribosomal protein L17

Chain CN:

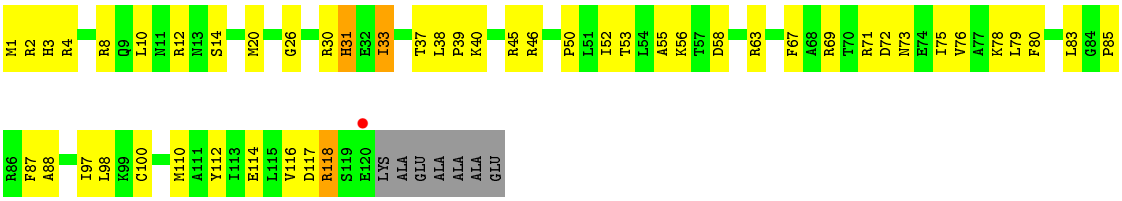


• Molecule 14: 50S ribosomal protein L17

Chain EN:

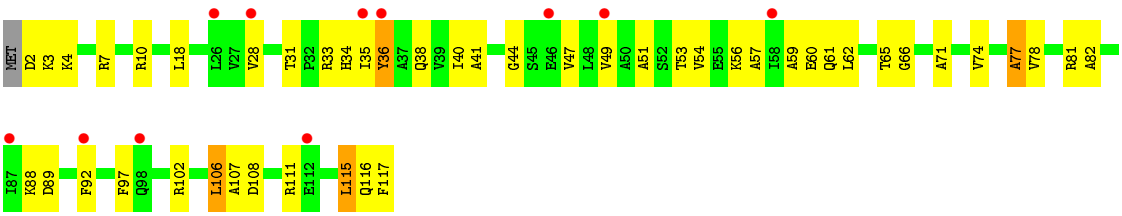
• Molecule 14: 50S ribosomal protein L17

Chain GN:



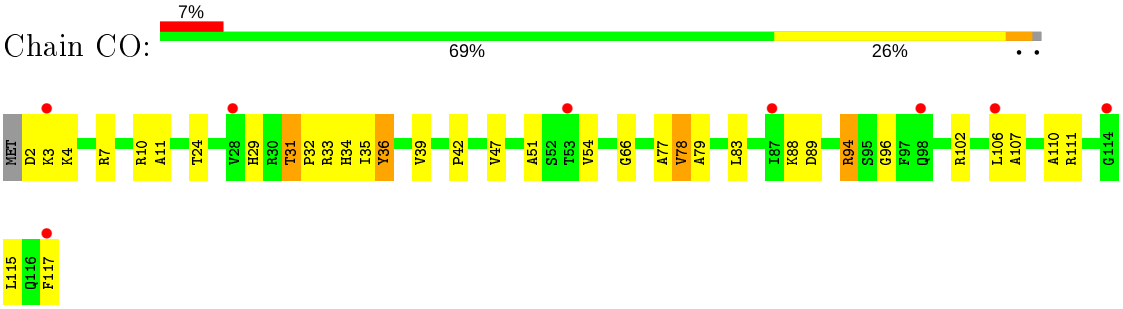
• Molecule 15: 50S ribosomal protein L18

Chain AO:



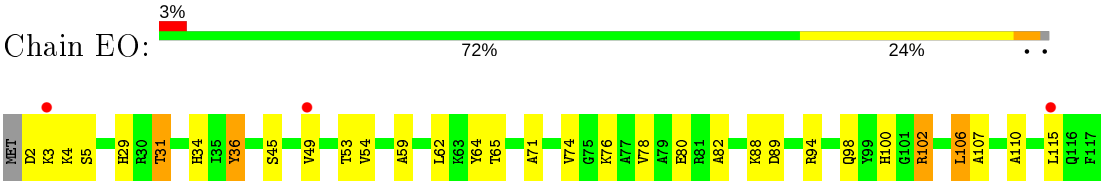
• Molecule 15: 50S ribosomal protein L18

Chain CO:



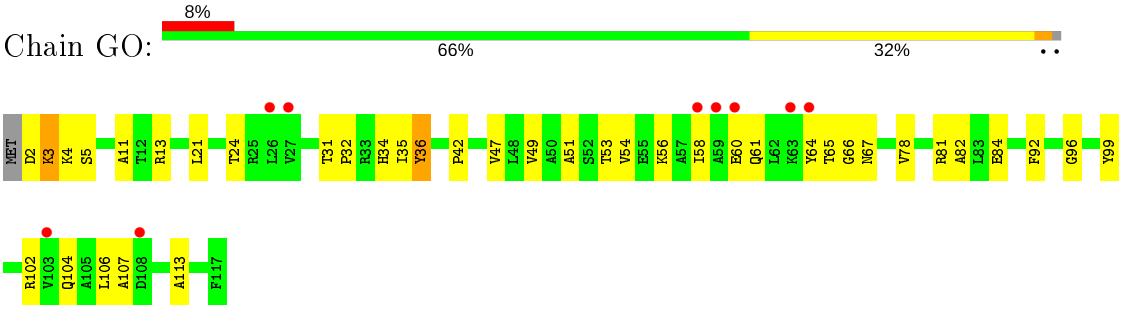
• Molecule 15: 50S ribosomal protein L18

Chain EO:



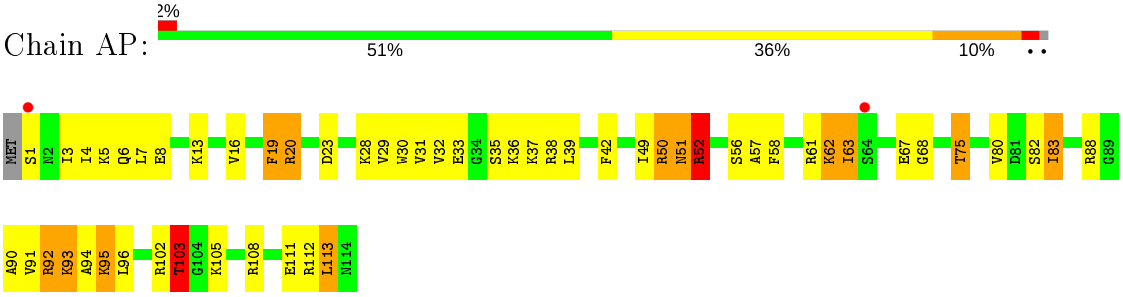
• Molecule 15: 50S ribosomal protein L18

Chain GO:



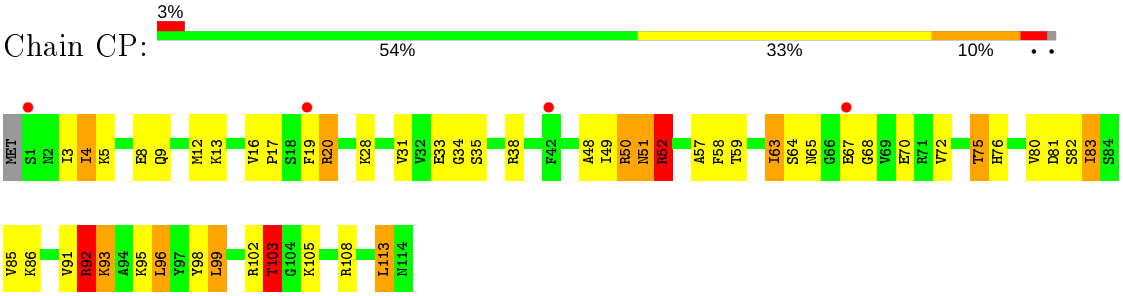
• Molecule 16: 50S ribosomal protein L19

Chain AP:



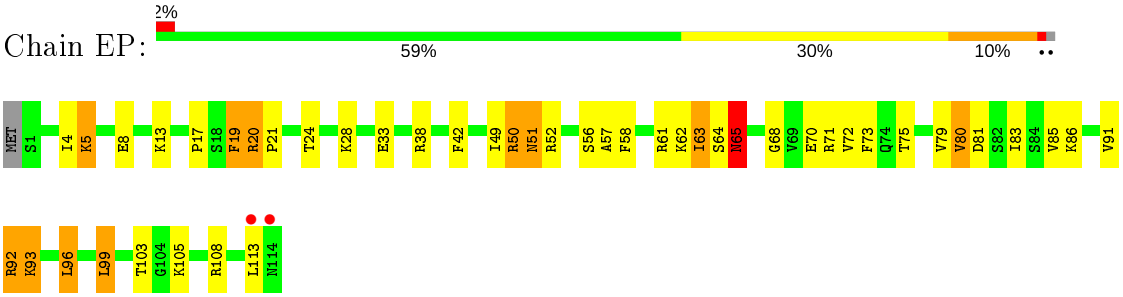
• Molecule 16: 50S ribosomal protein L19

Chain CP:



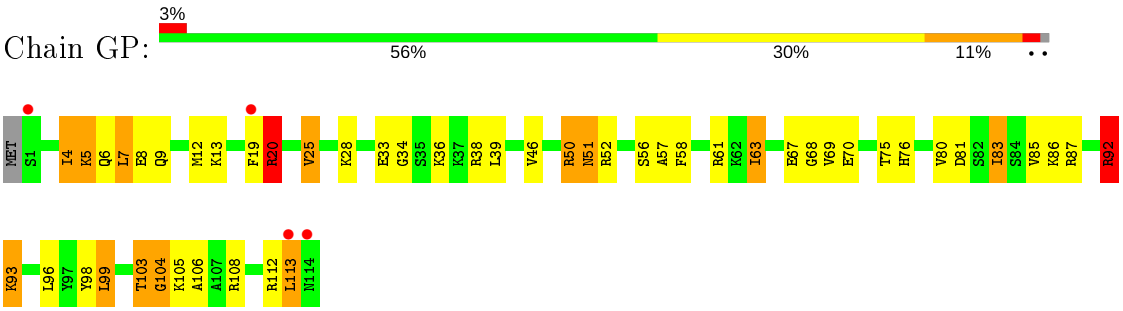
• Molecule 16: 50S ribosomal protein L19

Chain EP:



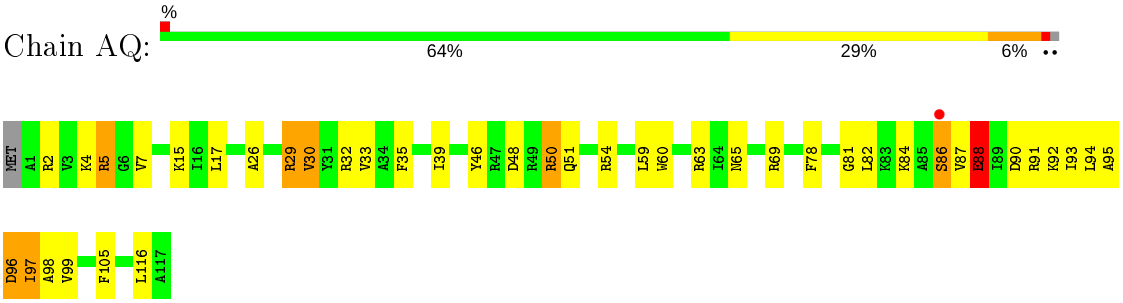
• Molecule 16: 50S ribosomal protein L19

Chain GP:



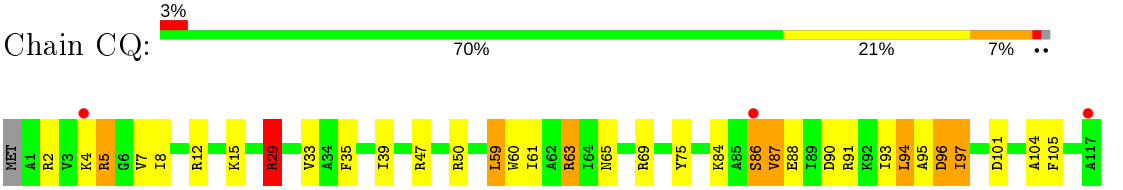
• Molecule 17: 50S ribosomal protein L20

Chain AQ:



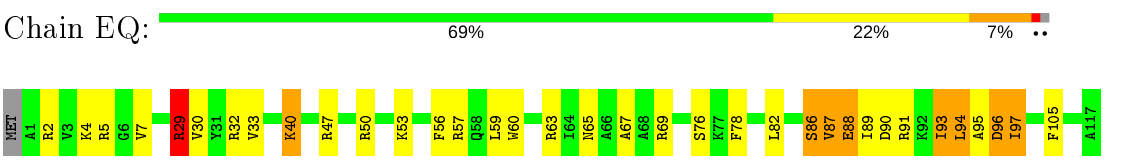
• Molecule 17: 50S ribosomal protein L20

Chain CQ:



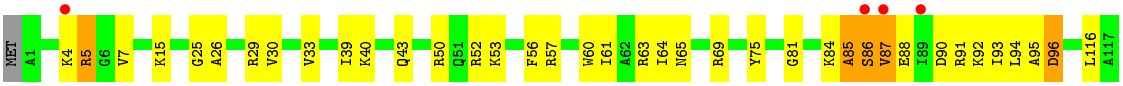
• Molecule 17: 50S ribosomal protein L20

Chain EQ:



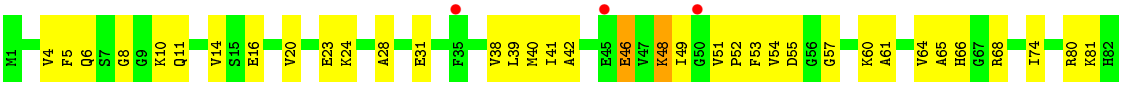
• Molecule 17: 50S ribosomal protein L20

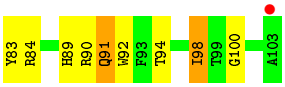
Chain GQ:



• Molecule 18: 50S ribosomal protein L21

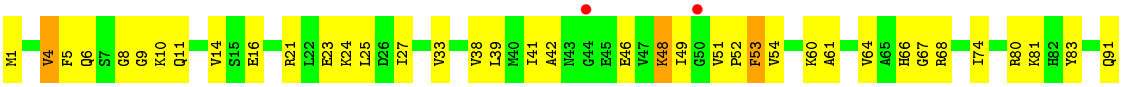
Chain AR:

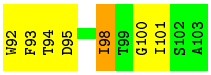




• Molecule 18: 50S ribosomal protein L21

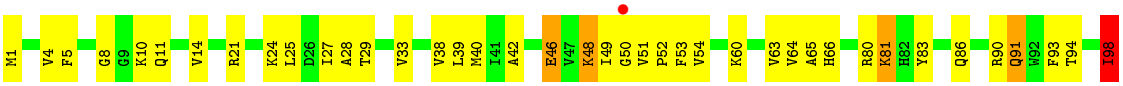
Chain CR:





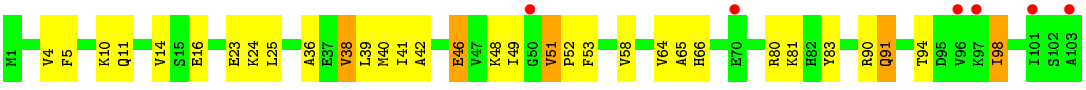
• Molecule 18: 50S ribosomal protein L21

Chain ER:



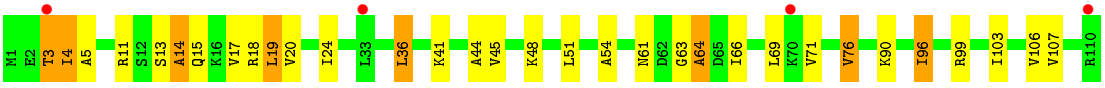
• Molecule 18: 50S ribosomal protein L21

Chain GR:



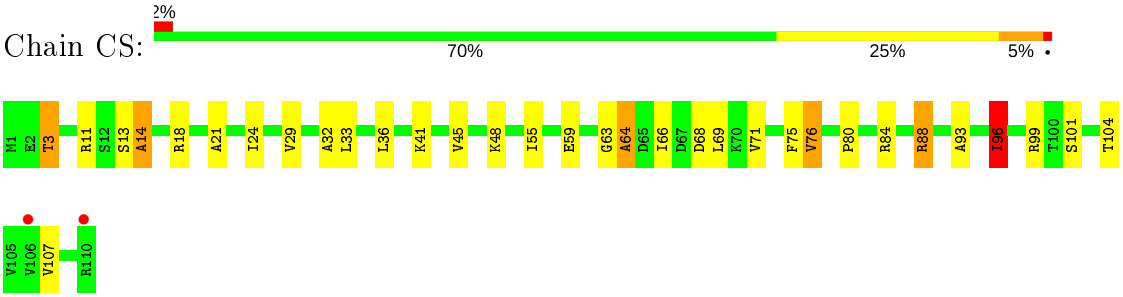
• Molecule 19: 50S ribosomal protein L22

Chain AS:



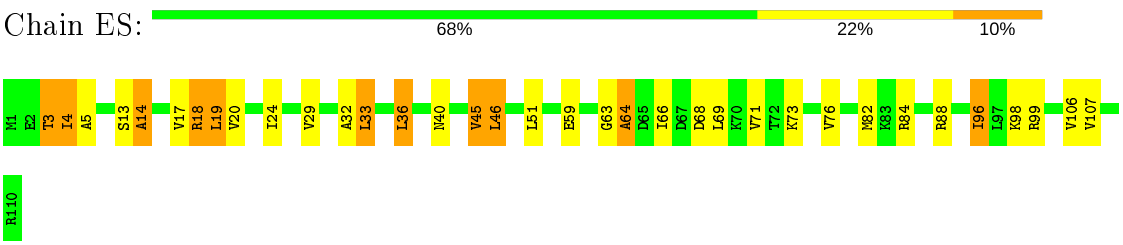
• Molecule 19: 50S ribosomal protein L22

Chain CS:



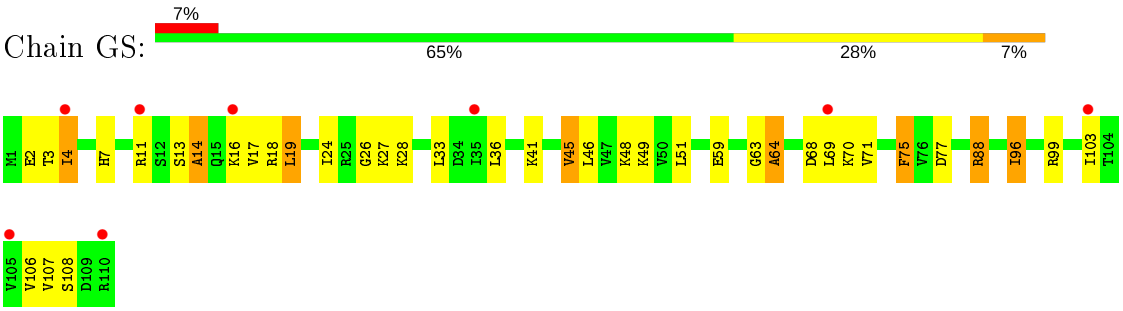
• Molecule 19: 50S ribosomal protein L22

Chain ES:



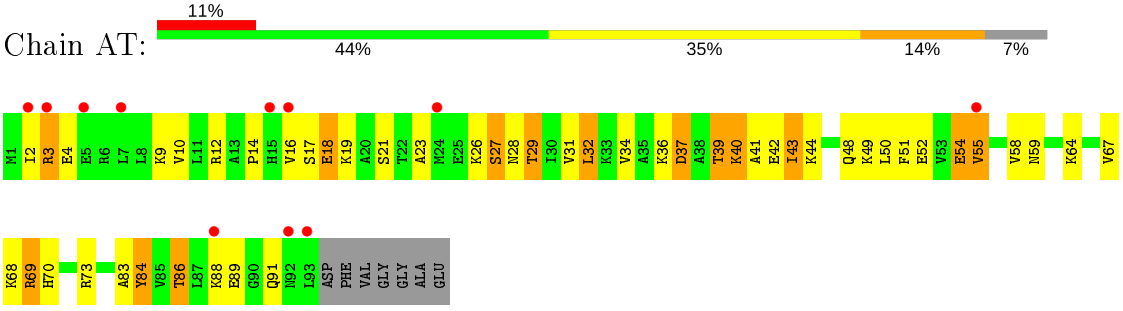
• Molecule 19: 50S ribosomal protein L22

Chain GS:



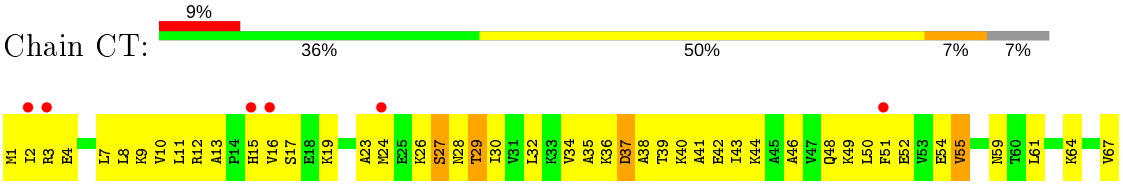
• Molecule 20: 50S ribosomal protein L23

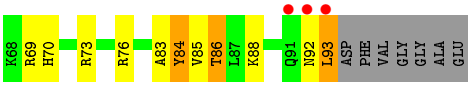
Chain AT:



• Molecule 20: 50S ribosomal protein L23

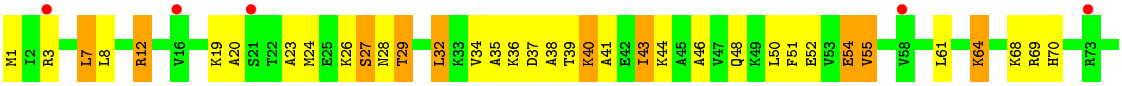
Chain CT:

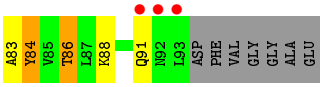




• Molecule 20: 50S ribosomal protein L23

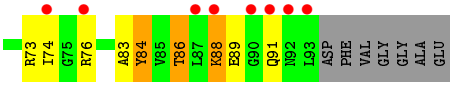
Chain ET:





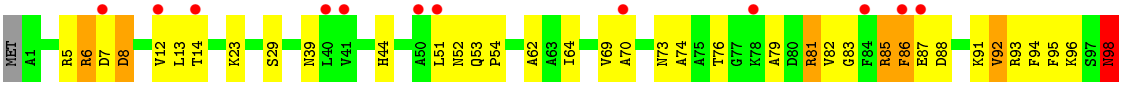
• Molecule 20: 50S ribosomal protein L23

Chain GT:



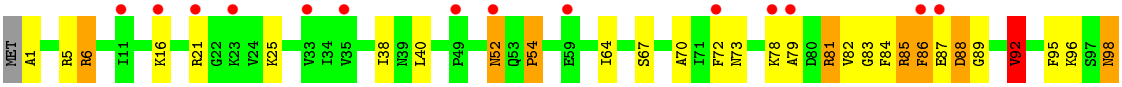
• Molecule 21: 50S ribosomal protein L24

Chain AU:



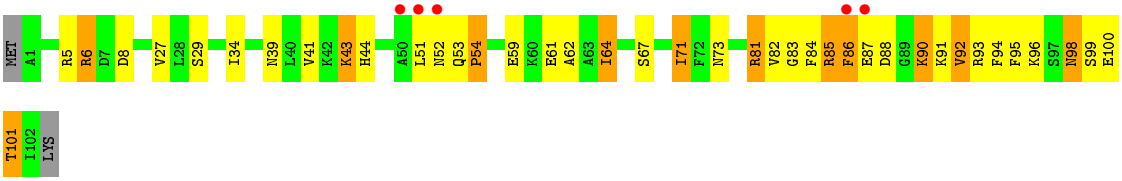
• Molecule 21: 50S ribosomal protein L24

Chain CU:

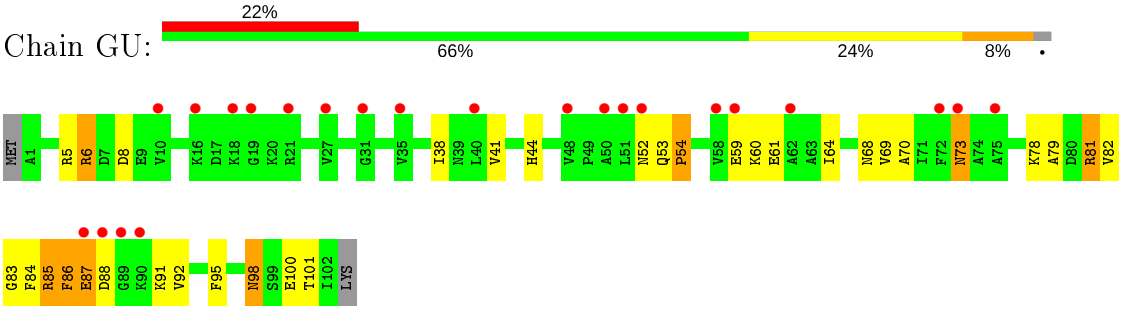


• Molecule 21: 50S ribosomal protein L24

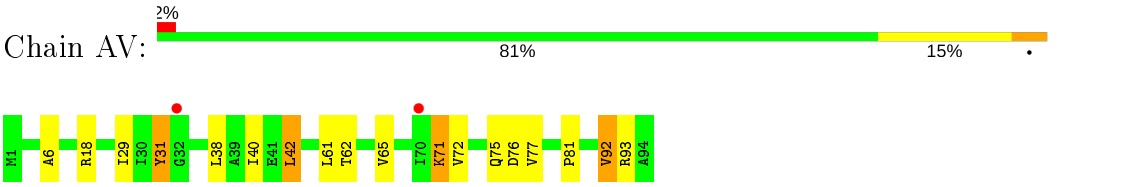
Chain EU:



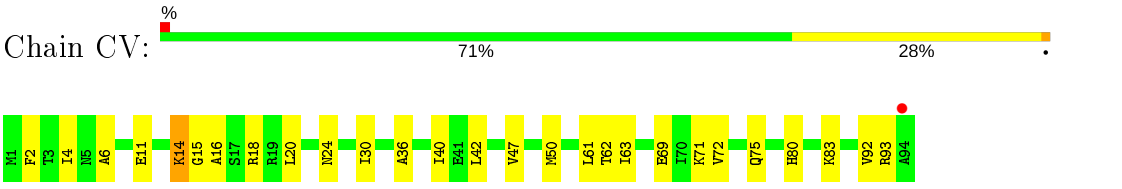
• Molecule 21: 50S ribosomal protein L24



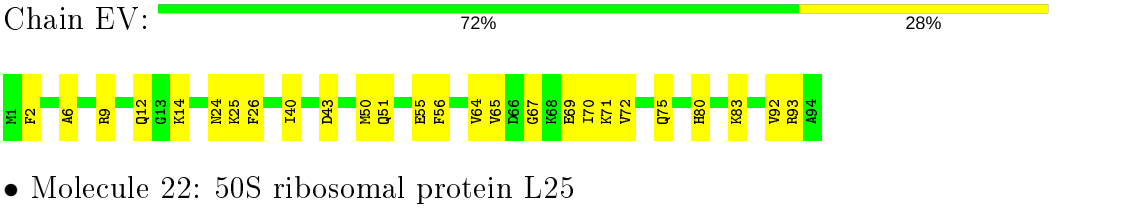
• Molecule 22: 50S ribosomal protein L25



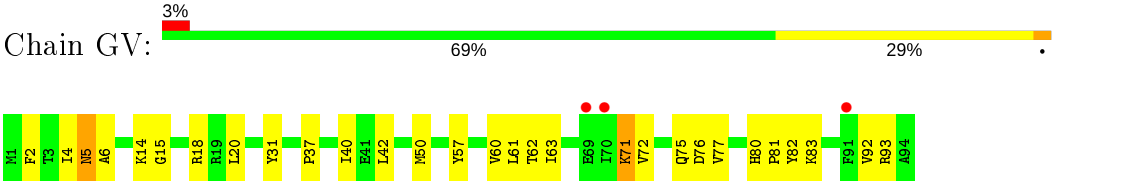
• Molecule 22: 50S ribosomal protein L25



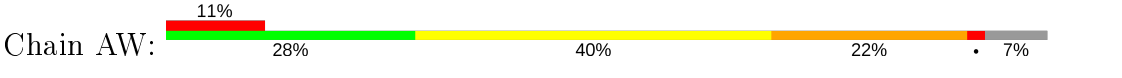
• Molecule 22: 50S ribosomal protein L25

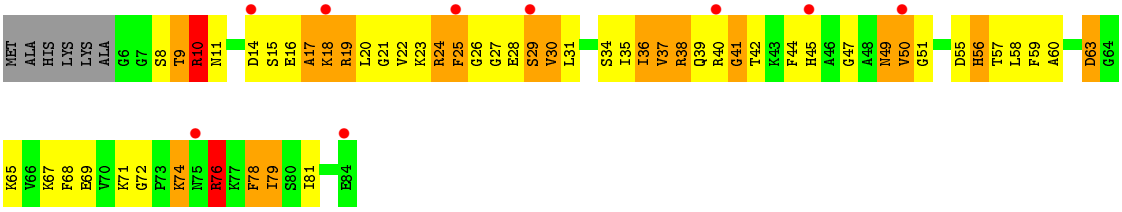


• Molecule 22: 50S ribosomal protein L25



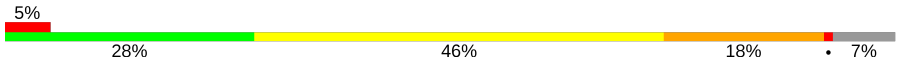
• Molecule 23: 50S ribosomal protein L27

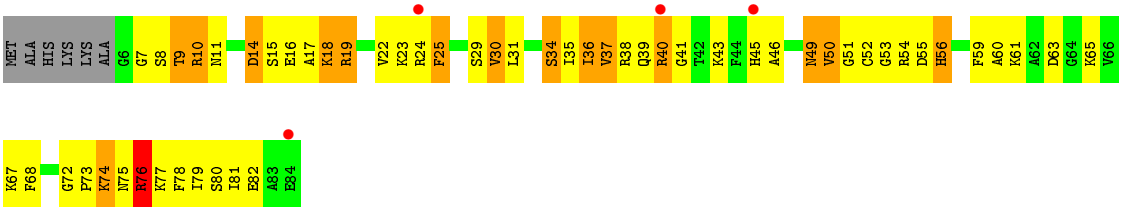




• Molecule 23: 50S ribosomal protein L27

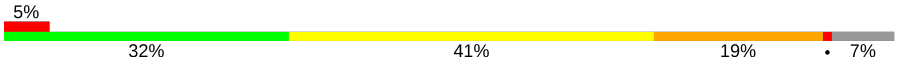
Chain CW:

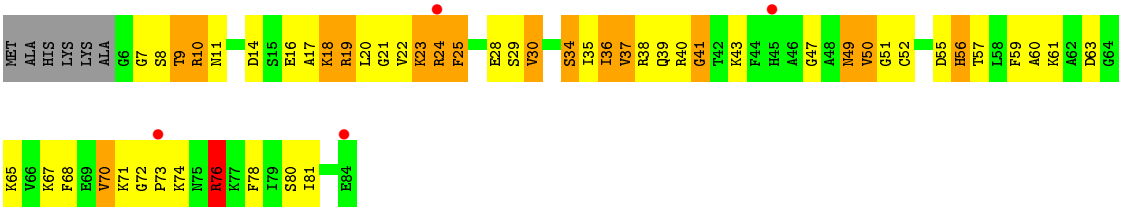




• Molecule 23: 50S ribosomal protein L27

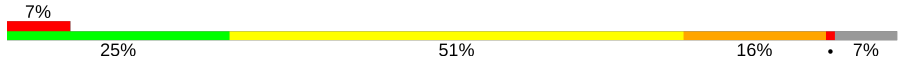
Chain EW:

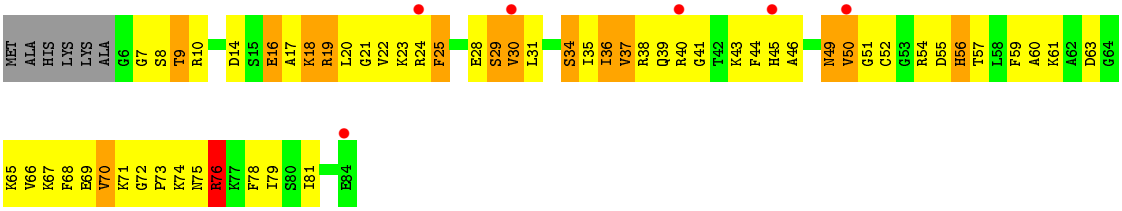




• Molecule 23: 50S ribosomal protein L27

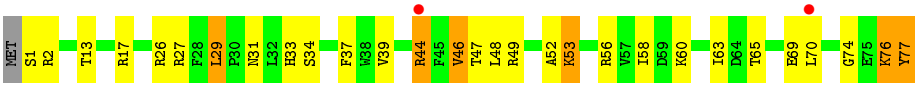
Chain GW:





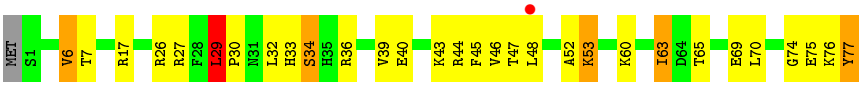
• Molecule 24: 50S ribosomal protein L28

Chain AX:



• Molecule 24: 50S ribosomal protein L28

Chain CX:

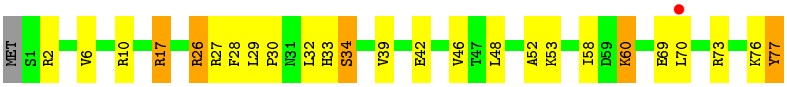


• Molecule 24: 50S ribosomal protein L28

Chain EX:

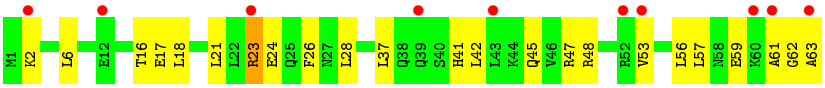
• Molecule 24: 50S ribosomal protein L28

Chain GX:



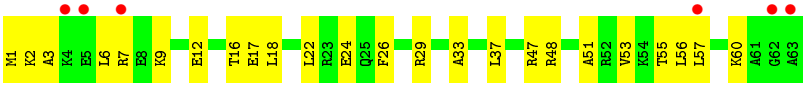
• Molecule 25: 50S ribosomal protein L29

Chain AY:



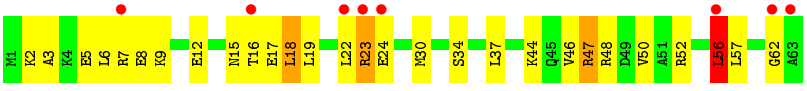
• Molecule 25: 50S ribosomal protein L29

Chain CY:



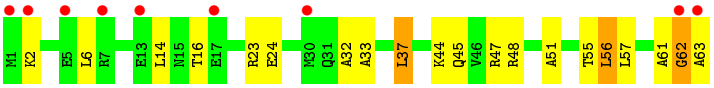
• Molecule 25: 50S ribosomal protein L29

Chain EY:



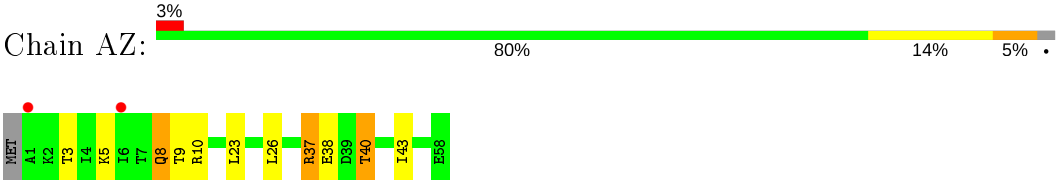
• Molecule 25: 50S ribosomal protein L29

Chain GY:



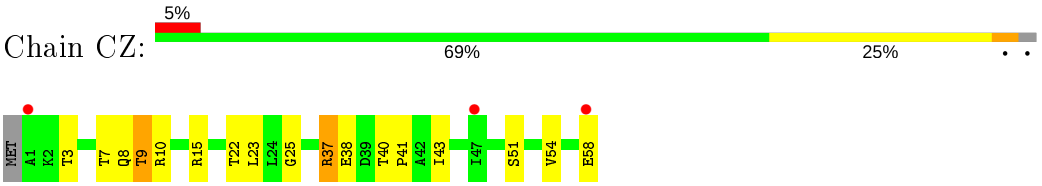
• Molecule 26: 50S ribosomal protein L30

Chain AZ:



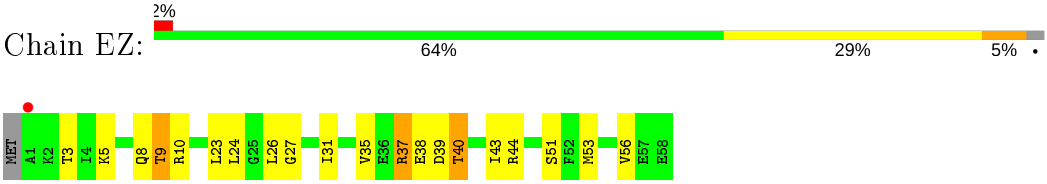
• Molecule 26: 50S ribosomal protein L30

Chain CZ:



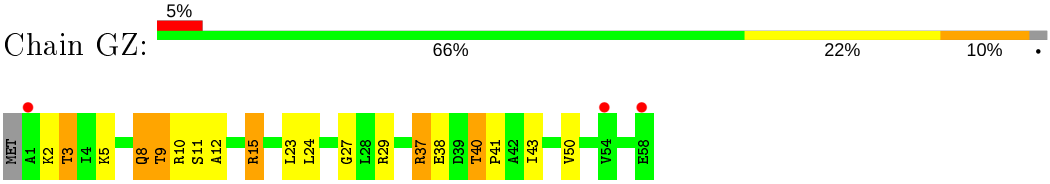
• Molecule 26: 50S ribosomal protein L30

Chain EZ:



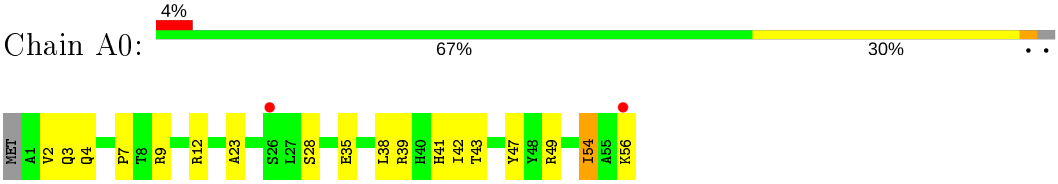
• Molecule 26: 50S ribosomal protein L30

Chain GZ:



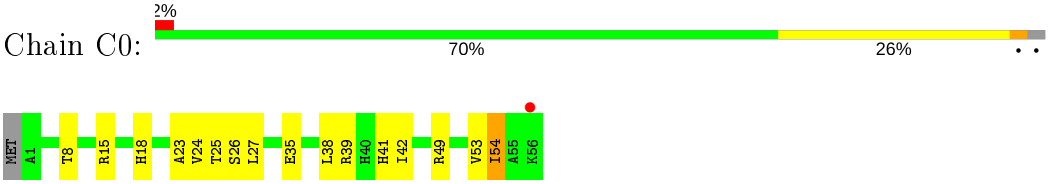
• Molecule 27: 50S ribosomal protein L32

Chain A0:



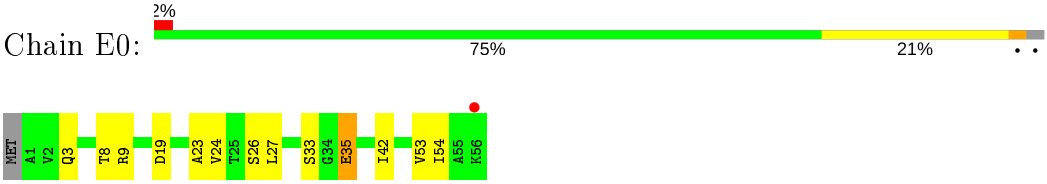
• Molecule 27: 50S ribosomal protein L32

Chain C0:



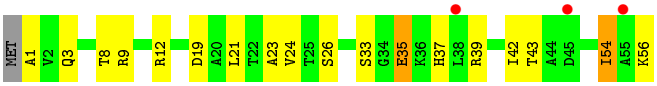
• Molecule 27: 50S ribosomal protein L32

Chain E0:



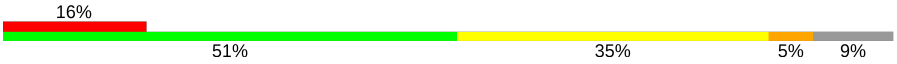
• Molecule 27: 50S ribosomal protein L32

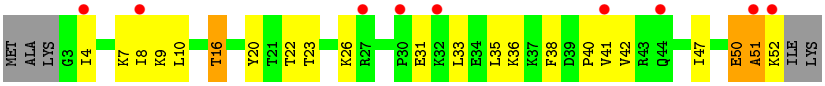
Chain G0:



• Molecule 28: 50S ribosomal protein L33

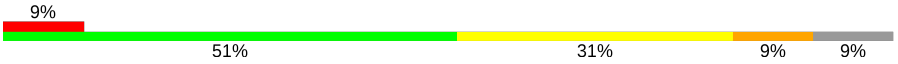
Chain A1:

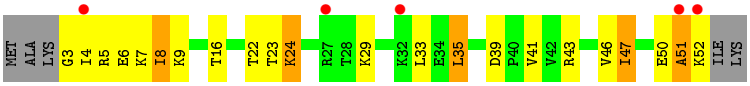




• Molecule 28: 50S ribosomal protein L33

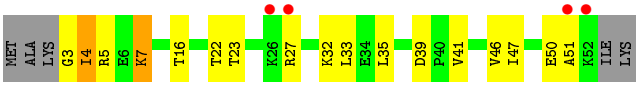
Chain C1:





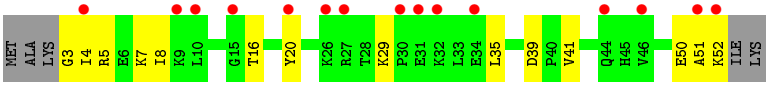
• Molecule 28: 50S ribosomal protein L33

Chain E1:



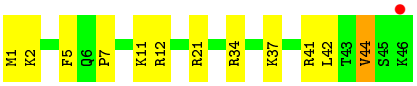
• Molecule 28: 50S ribosomal protein L33

Chain G1:



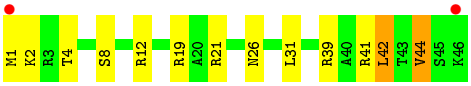
• Molecule 29: 50S ribosomal protein L34

Chain A2:



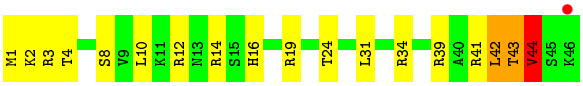
• Molecule 29: 50S ribosomal protein L34

Chain C2:



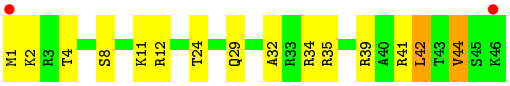
• Molecule 29: 50S ribosomal protein L34

Chain E2:



• Molecule 29: 50S ribosomal protein L34

Chain G2:

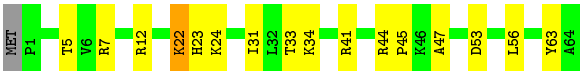


• Molecule 30: 50S ribosomal protein L35

Chain A3:

• Molecule 30: 50S ribosomal protein L35

Chain C3:

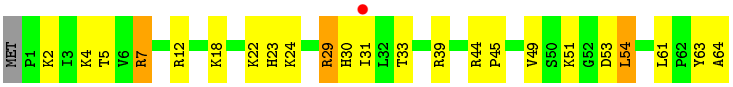


• Molecule 30: 50S ribosomal protein L35

Chain E3:

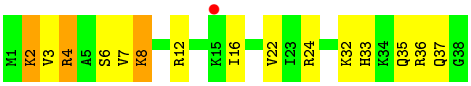
• Molecule 30: 50S ribosomal protein L35

Chain G3:



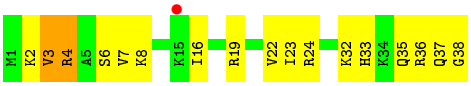
• Molecule 31: 50S ribosomal protein L36

Chain A4:



- Molecule 31: 50S ribosomal protein L36

Chain C4:

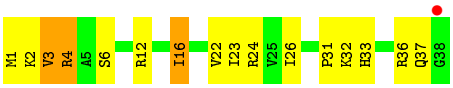


- Molecule 31: 50S ribosomal protein L36

Chain E4:

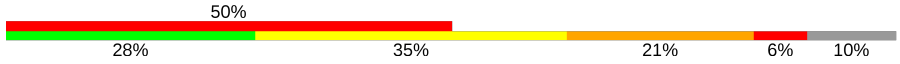
- Molecule 31: 50S ribosomal protein L36

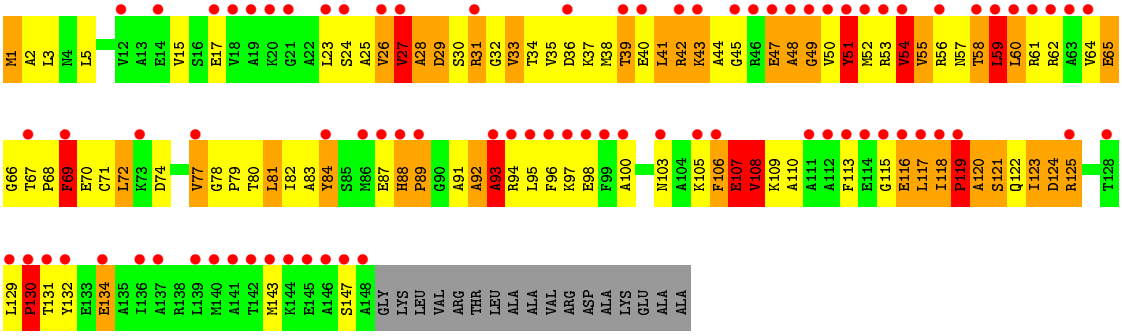
Chain G4:



- Molecule 32: 50S ribosomal protein L10

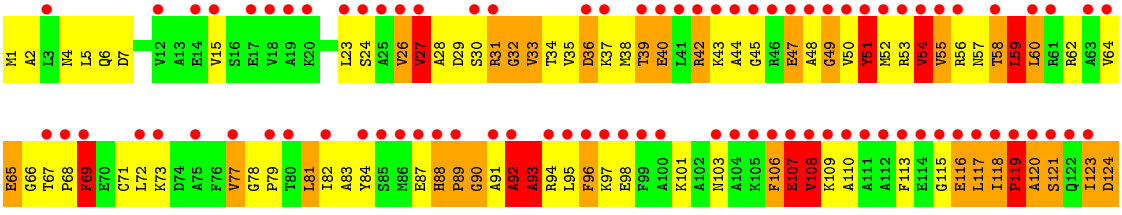
Chain A5:

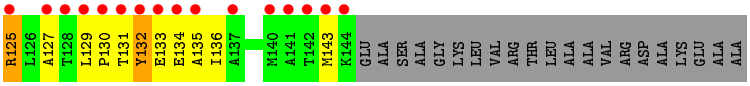




- Molecule 32: 50S ribosomal protein L10

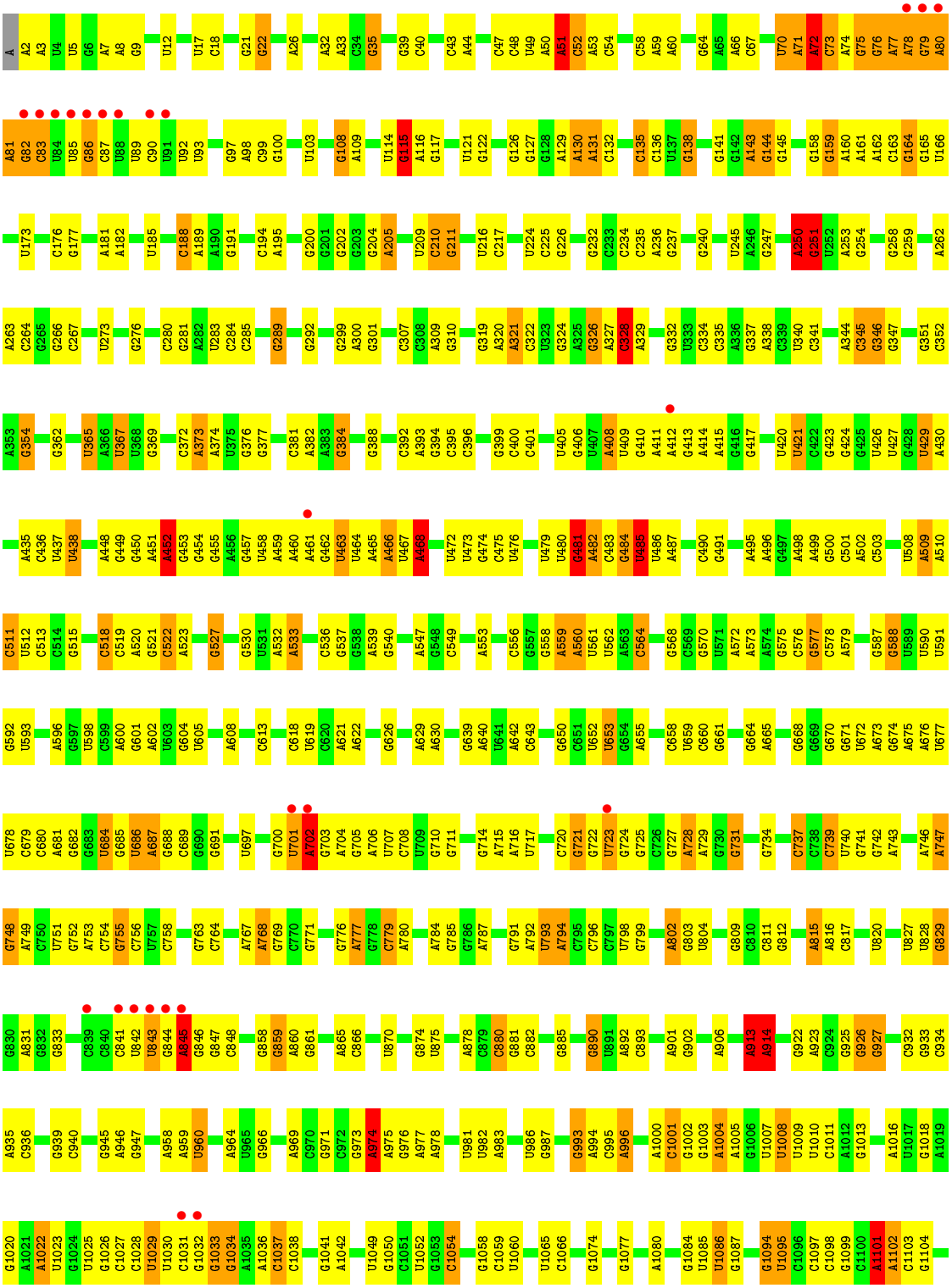
Chain E5:

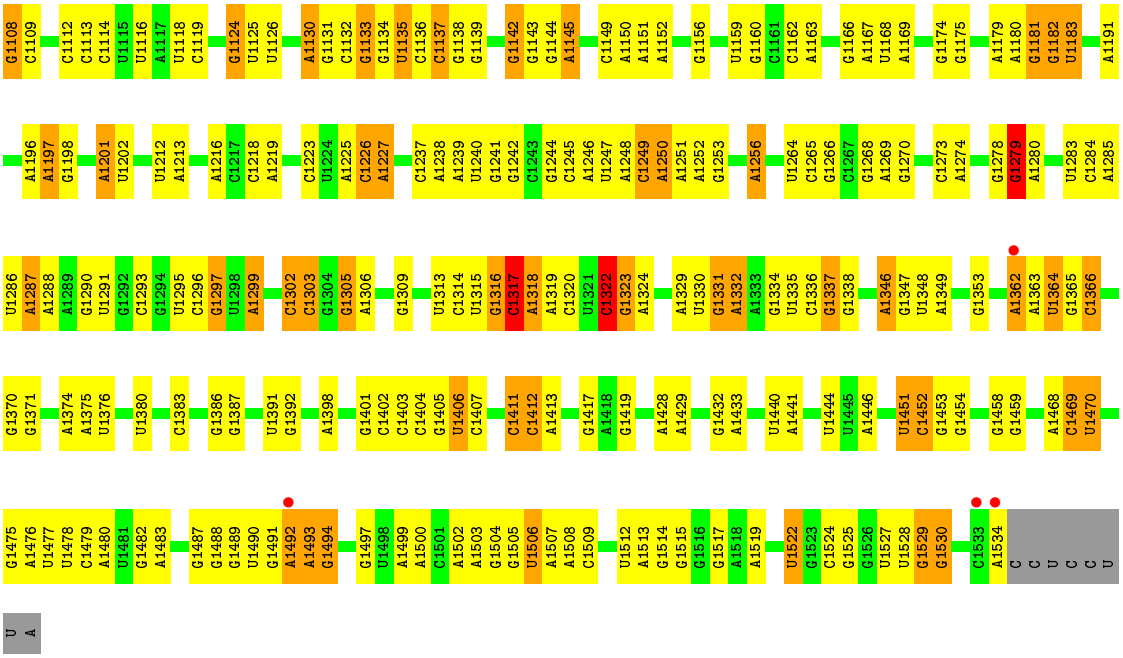




- Molecule 33: 16S rRNA

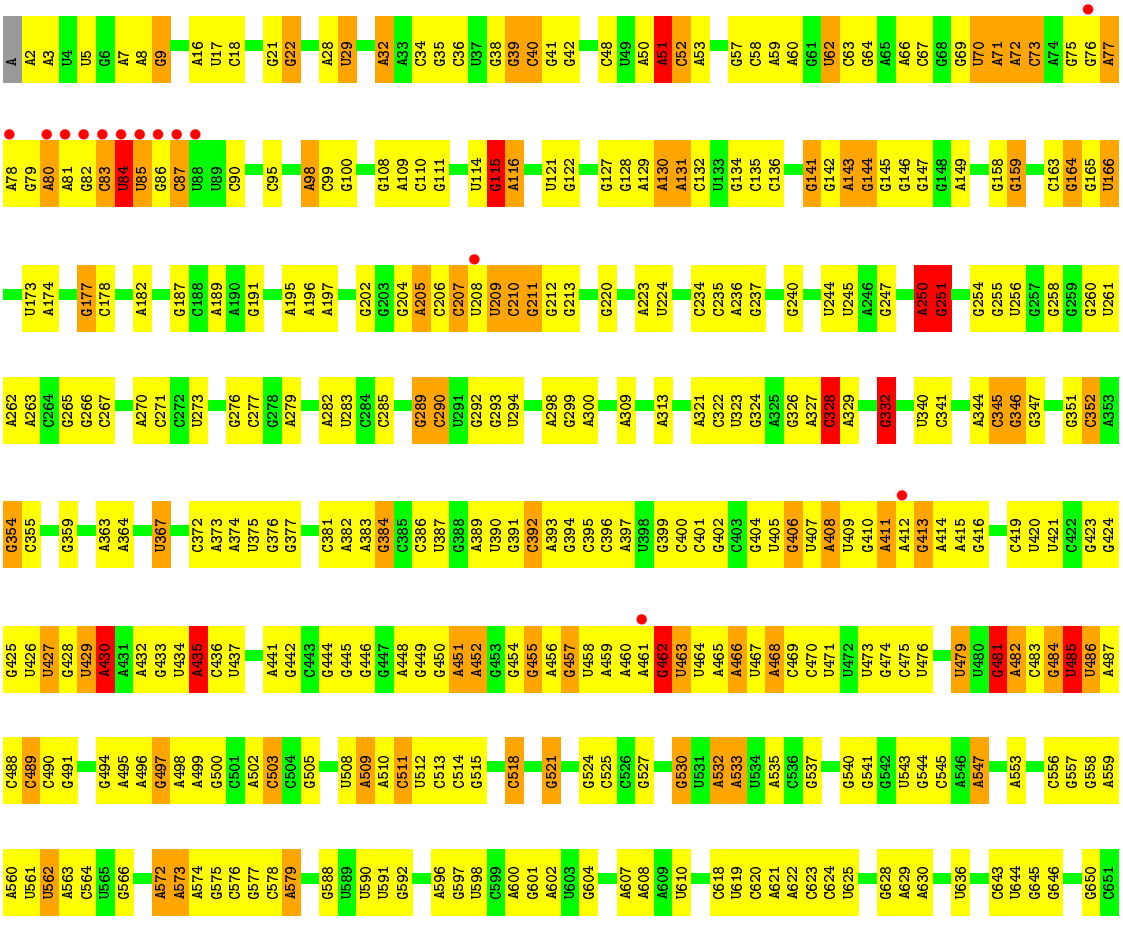
Chain BA:

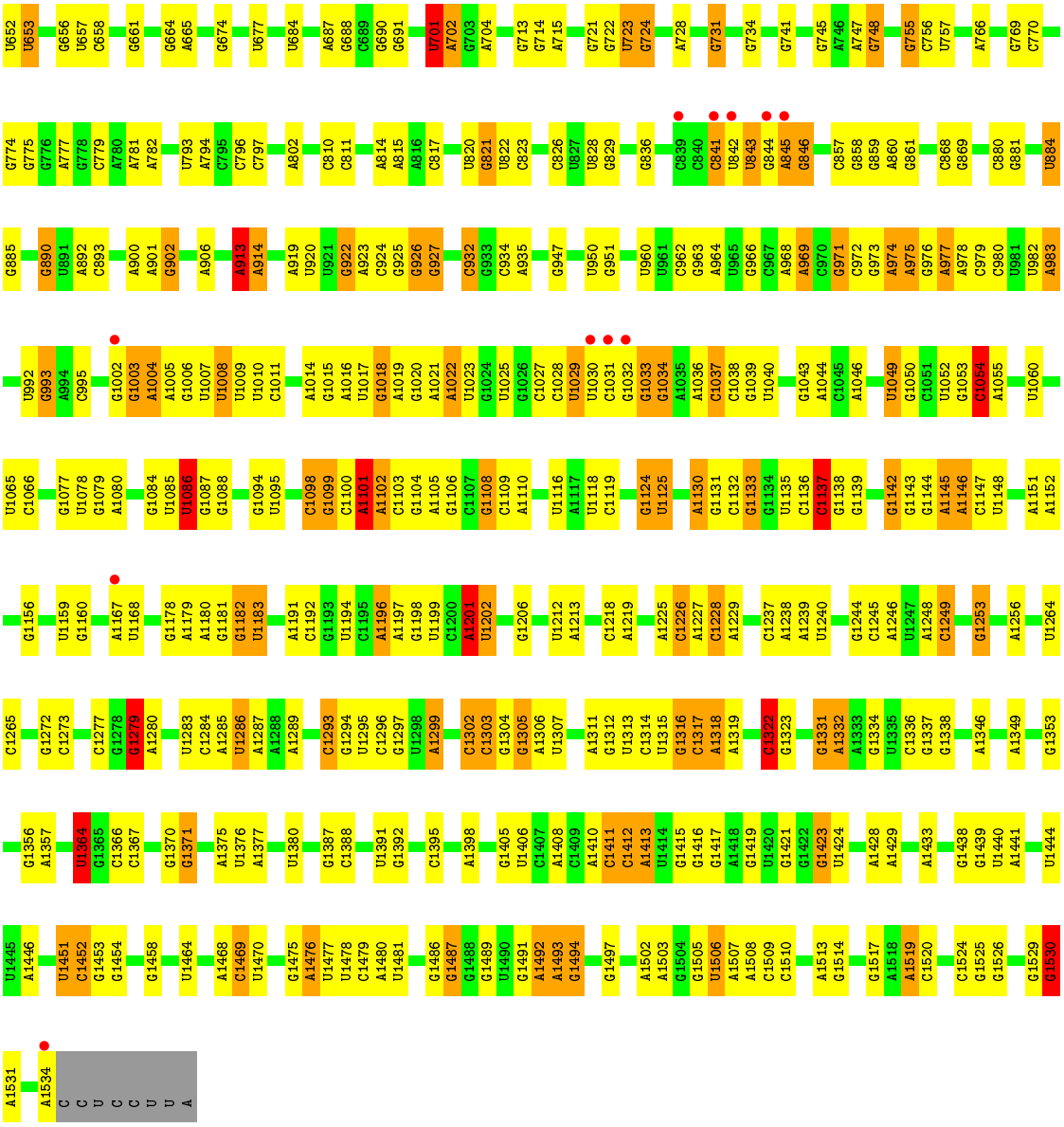




• Molecule 33: 16S rRNA

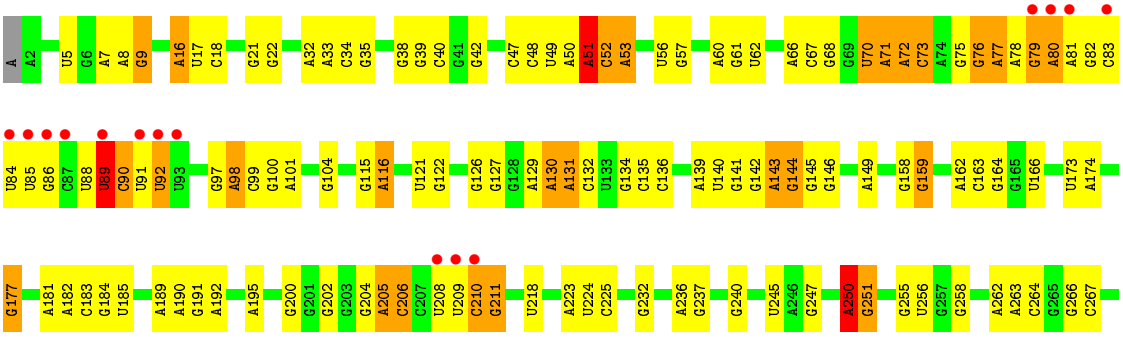
Chain DA:

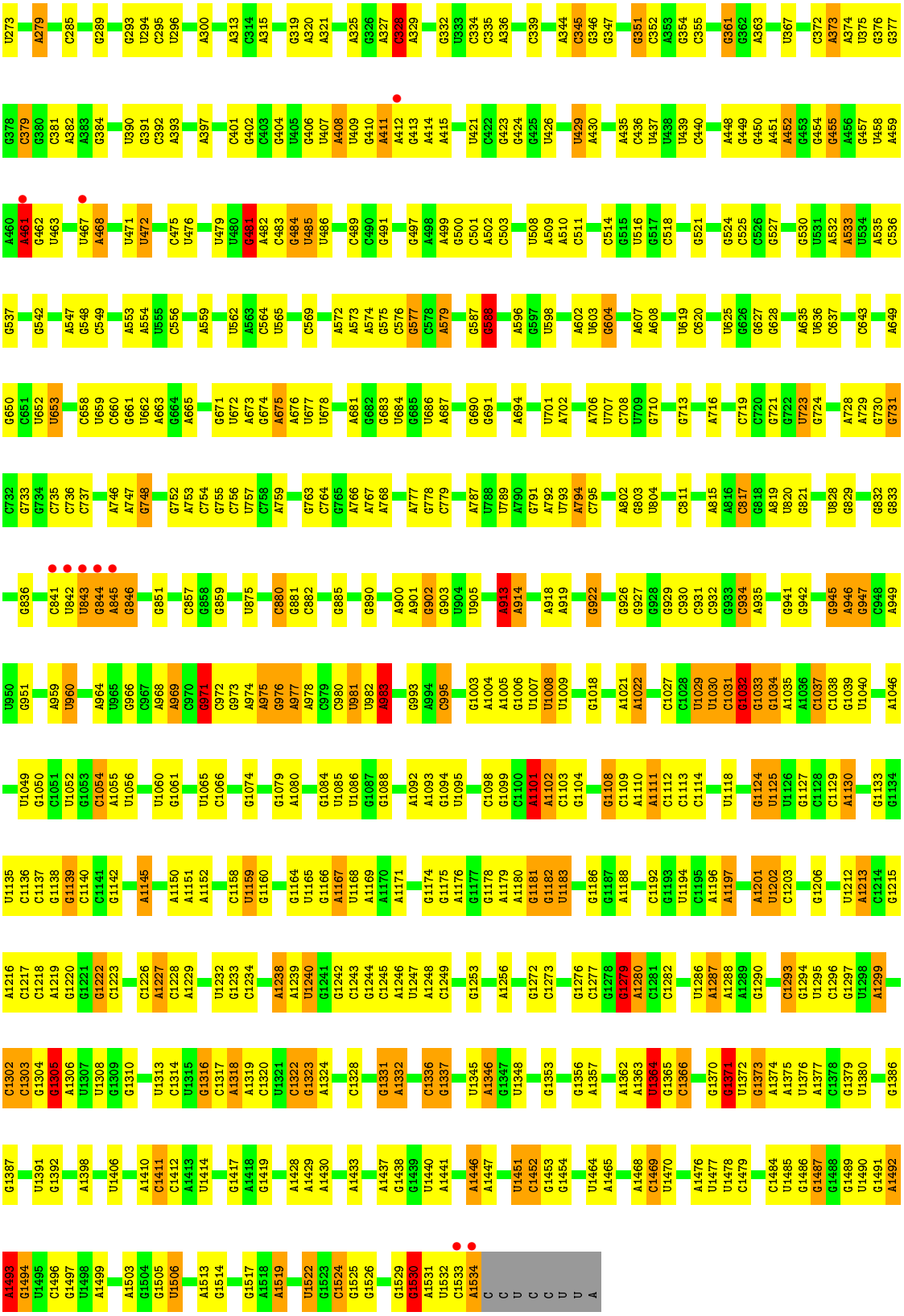




• Molecule 33: 16S rRNA

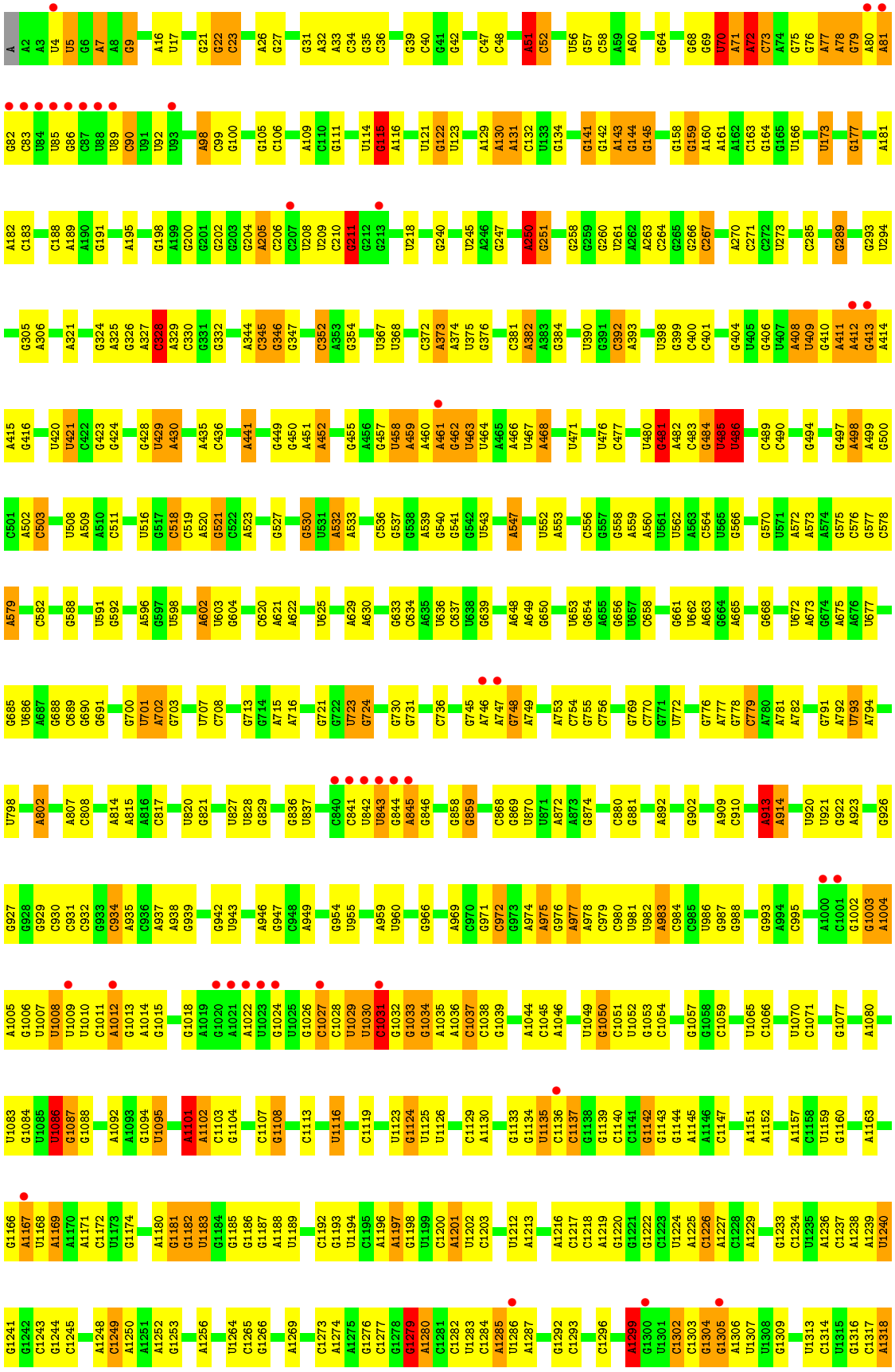
Chain FA:

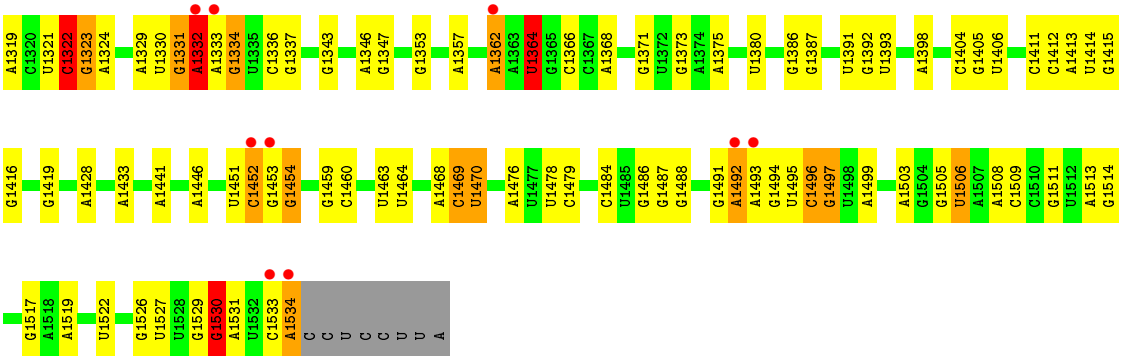




- Molecule 33: 16S rRNA

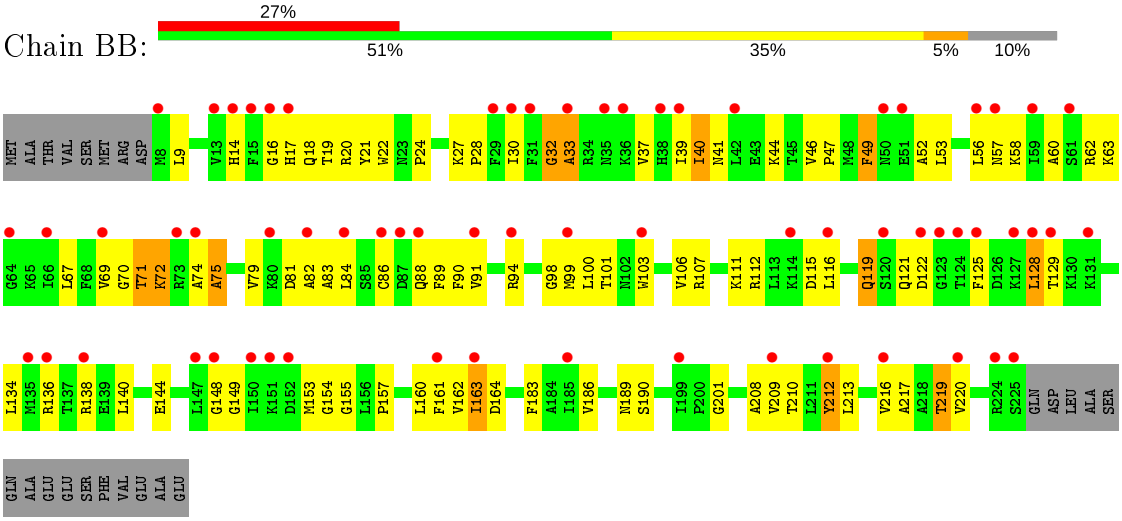
Chain HA:





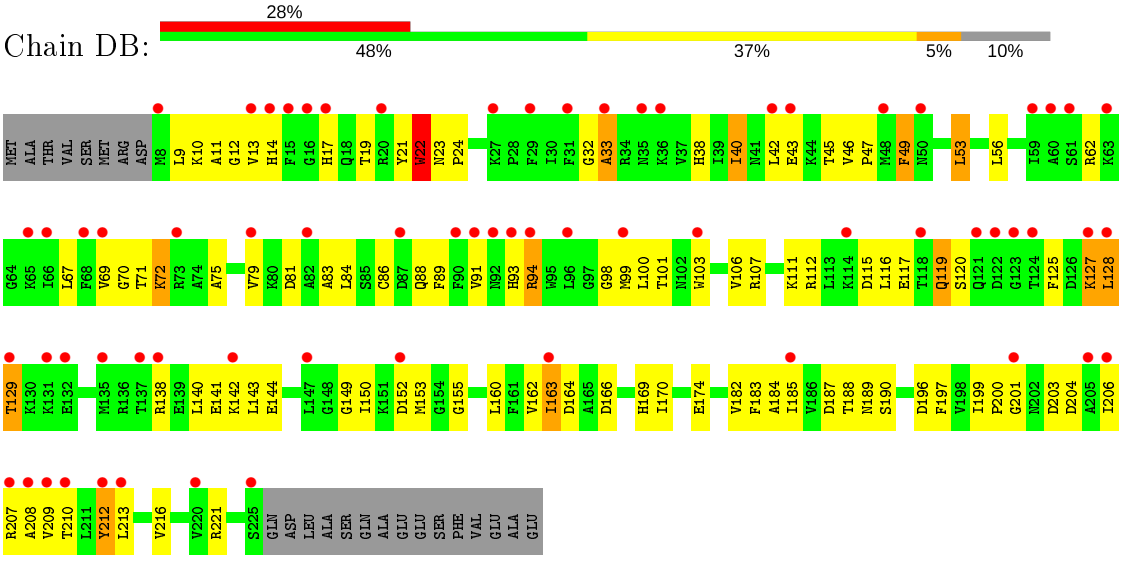
• Molecule 34: 30S ribosomal protein S2

Chain BB:



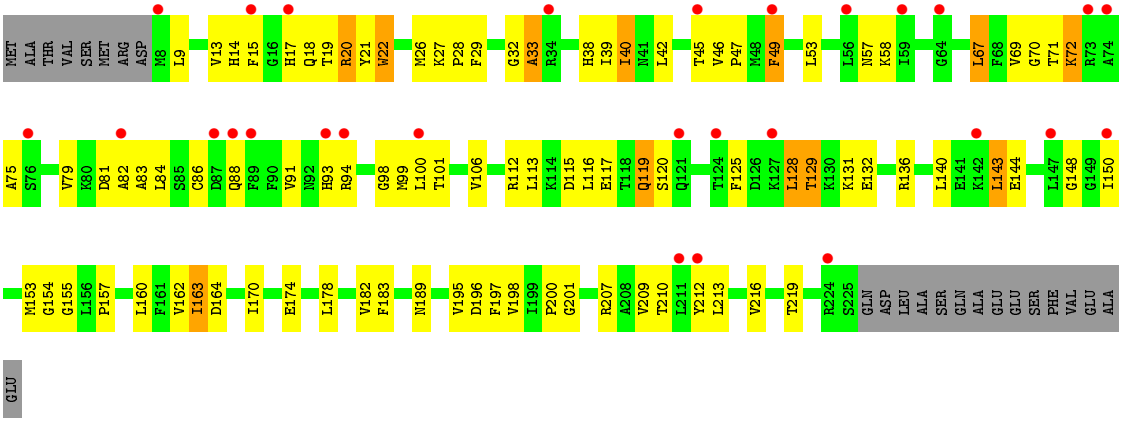
• Molecule 34: 30S ribosomal protein S2

Chain DB:



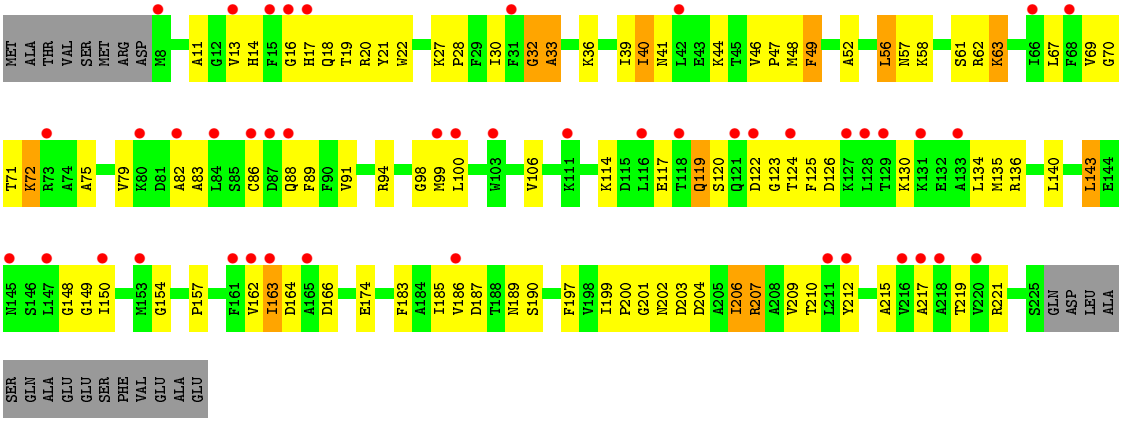
• Molecule 34: 30S ribosomal protein S2

Chain FB:



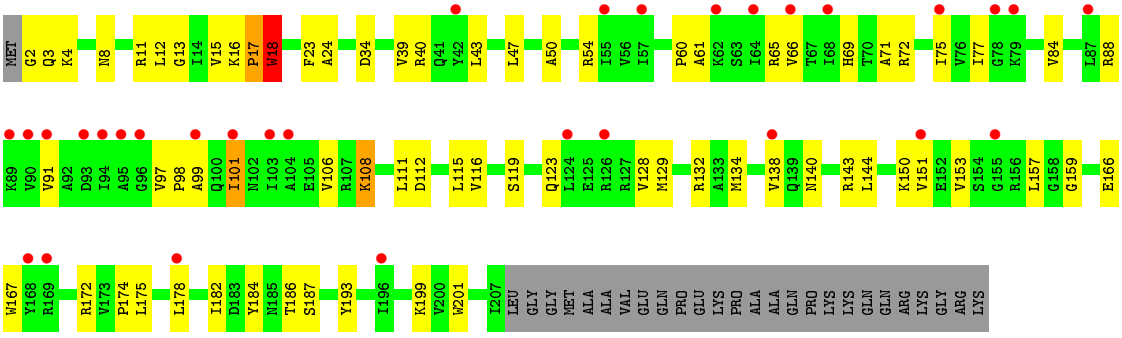
• Molecule 34: 30S ribosomal protein S2

Chain HB:



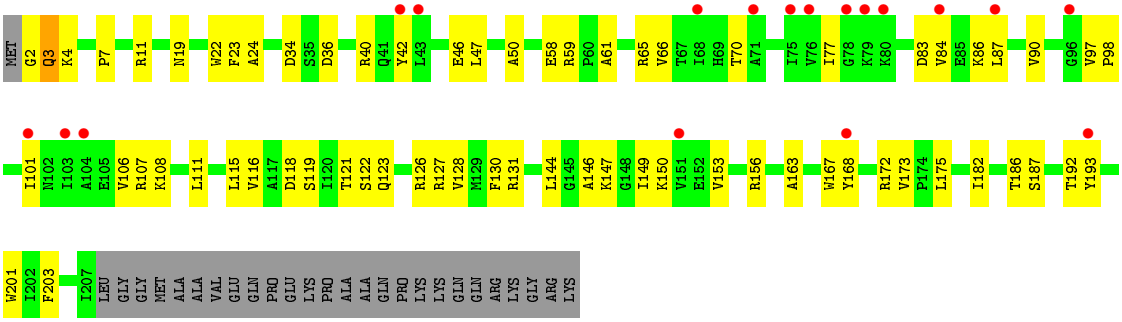
• Molecule 35: 30S ribosomal protein S3

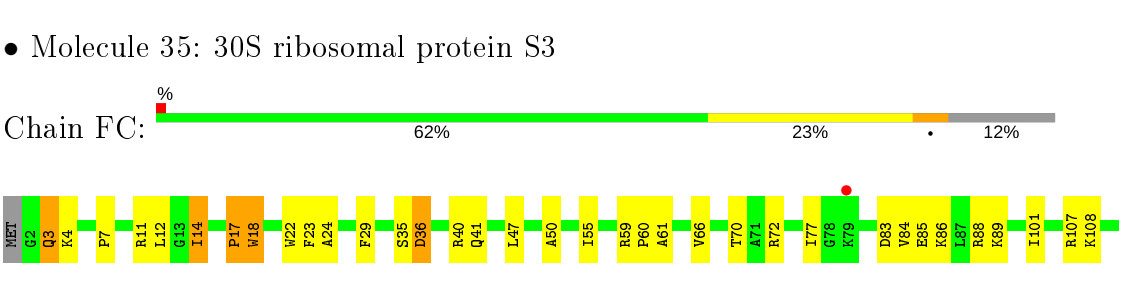
Chain BC:

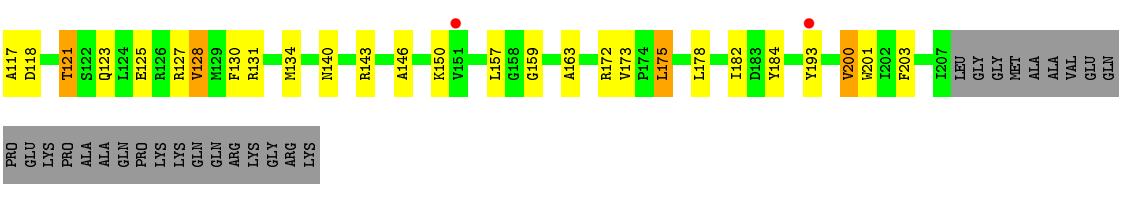


• Molecule 35: 30S ribosomal protein S3

Chain DC:





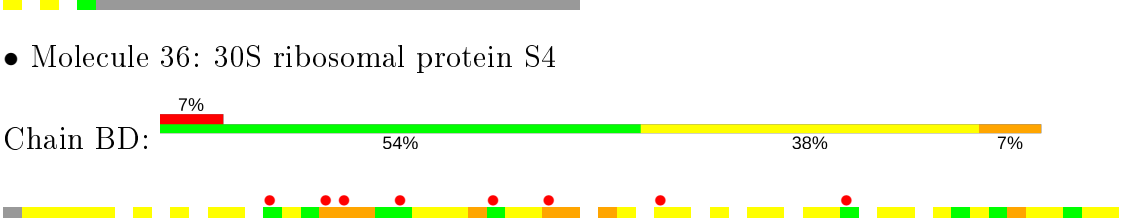


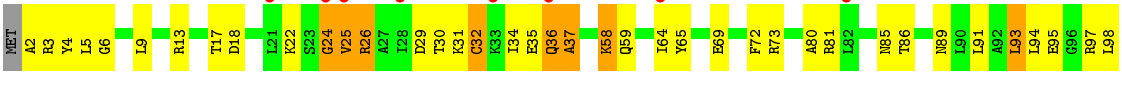
• Molecule 35: 30S ribosomal protein S3

Chain FC:

• Molecule 35: 30S ribosomal protein S3

Chain HC:



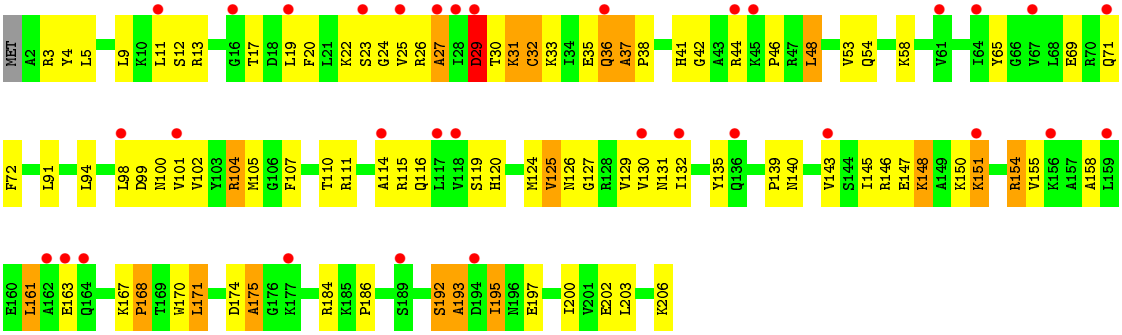


• Molecule 36: 30S ribosomal protein S4

Chain BD:

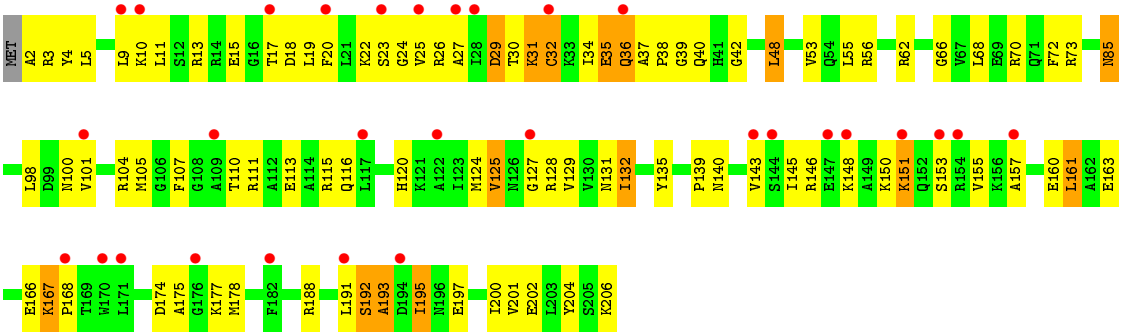
• Molecule 36: 30S ribosomal protein S4

Chain DD:



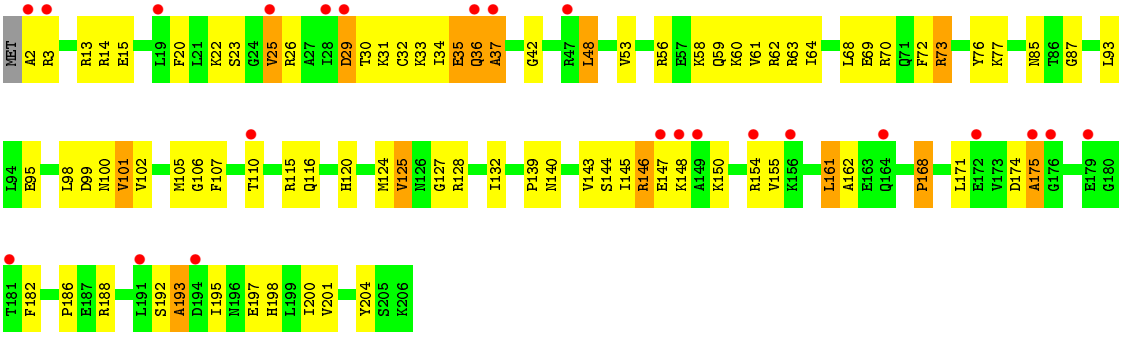
• Molecule 36: 30S ribosomal protein S4

Chain FD:



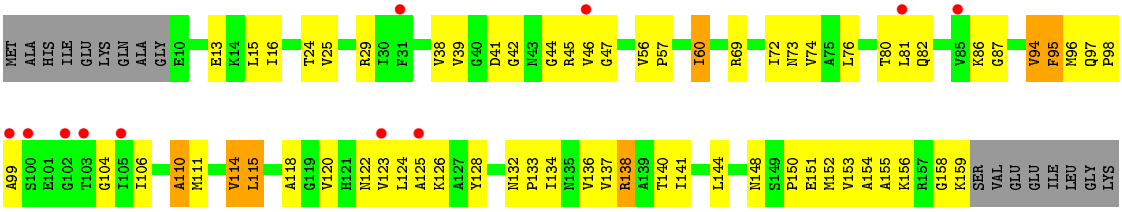
• Molecule 36: 30S ribosomal protein S4

Chain HD:



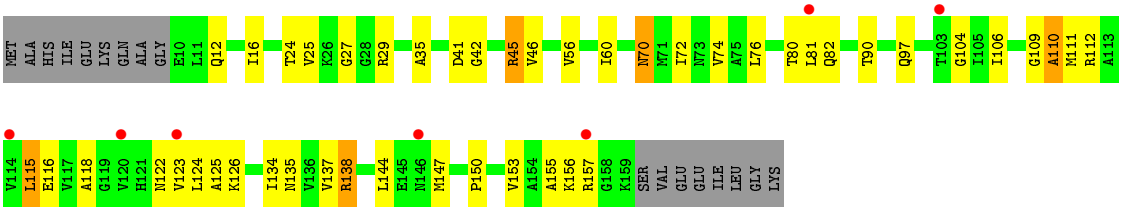
• Molecule 37: 30S ribosomal protein S5

Chain BE:



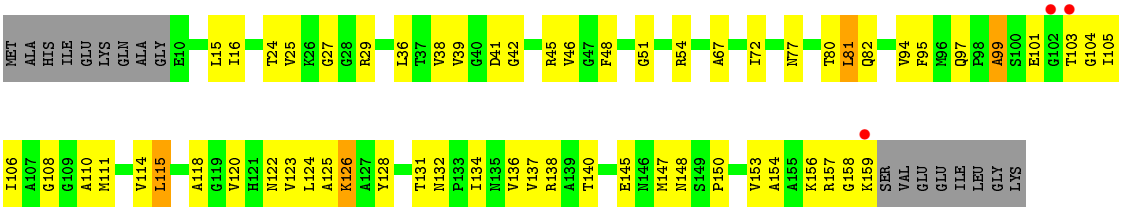
• Molecule 37: 30S ribosomal protein S5

Chain DE:



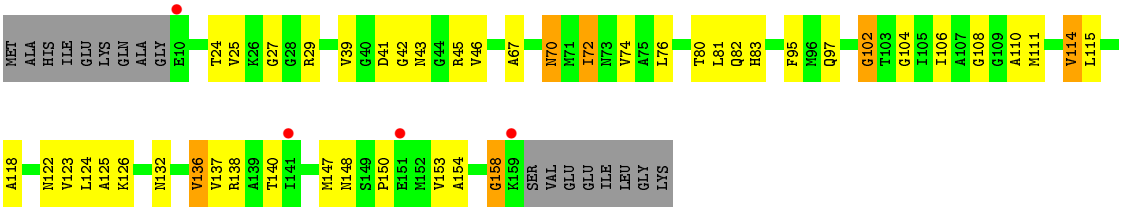
• Molecule 37: 30S ribosomal protein S5

Chain FE:



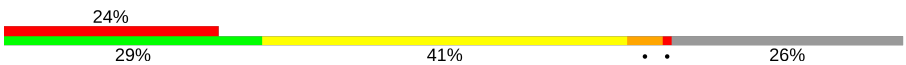
• Molecule 37: 30S ribosomal protein S5

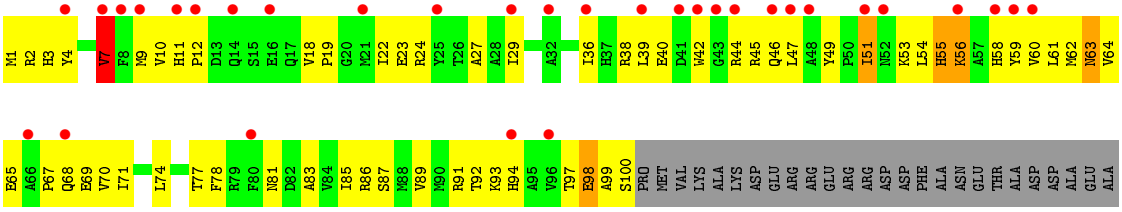
Chain HE:



• Molecule 38: 30S ribosomal protein S6

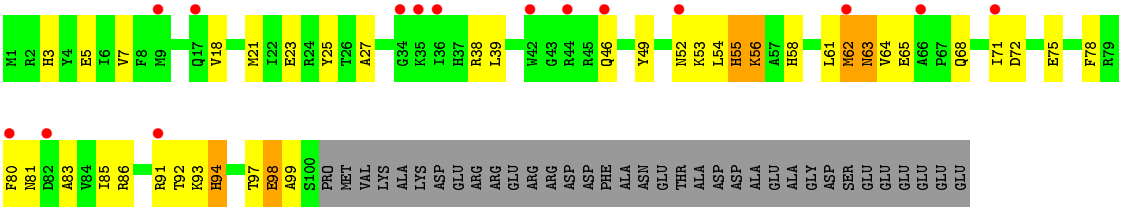
Chain BF:





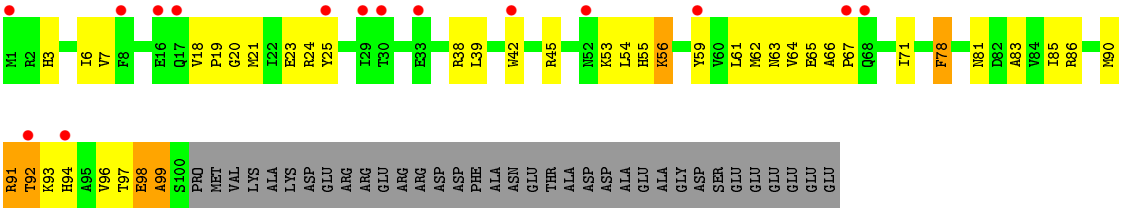
• Molecule 38: 30S ribosomal protein S6

Chain DF:



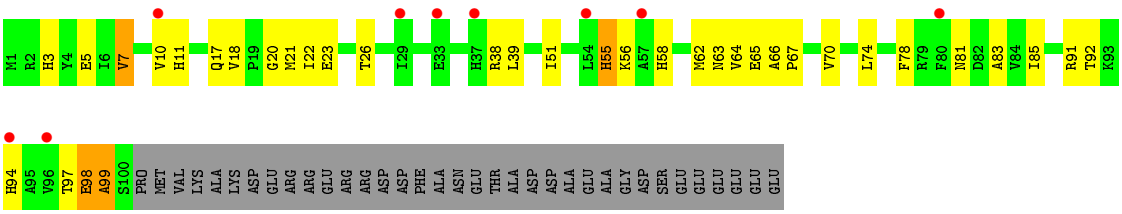
• Molecule 38: 30S ribosomal protein S6

Chain FF:



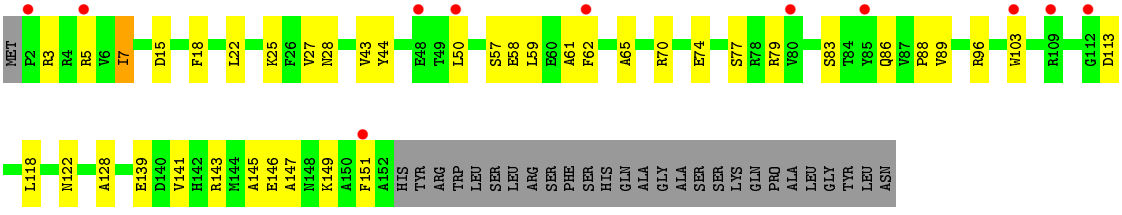
• Molecule 38: 30S ribosomal protein S6

Chain HF:



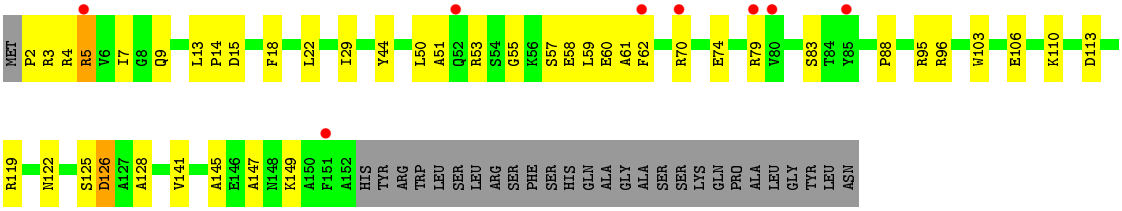
• Molecule 39: 30S ribosomal protein S7

Chain BG:



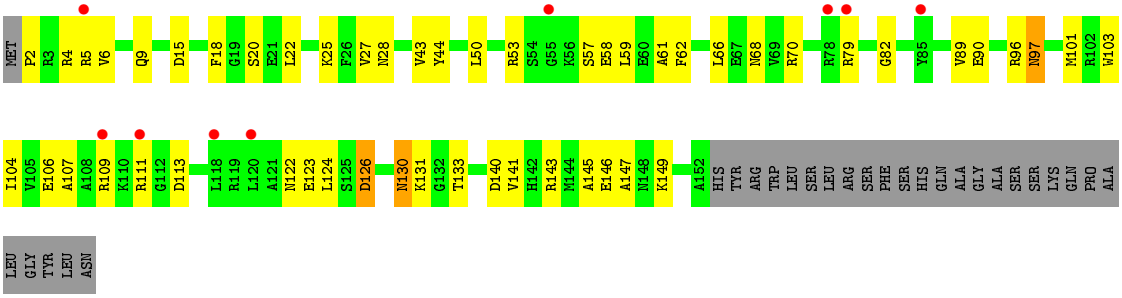
• Molecule 39: 30S ribosomal protein S7

Chain DG:



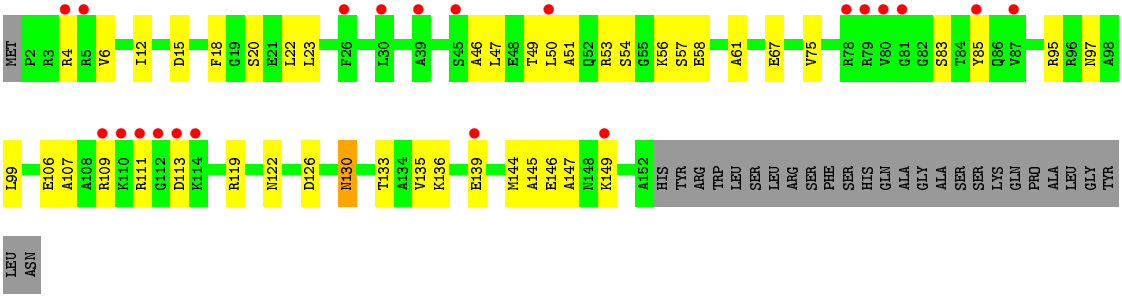
• Molecule 39: 30S ribosomal protein S7

Chain FG:



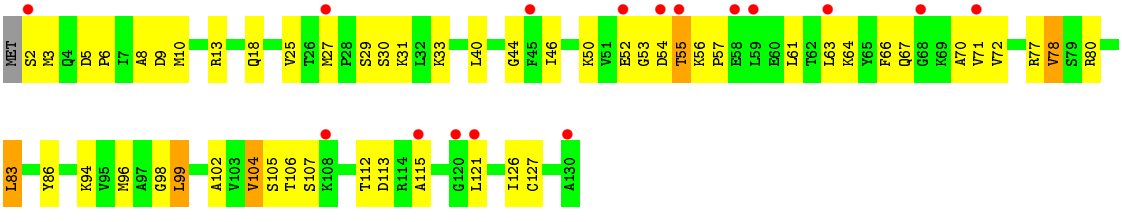
• Molecule 39: 30S ribosomal protein S7

Chain HG:



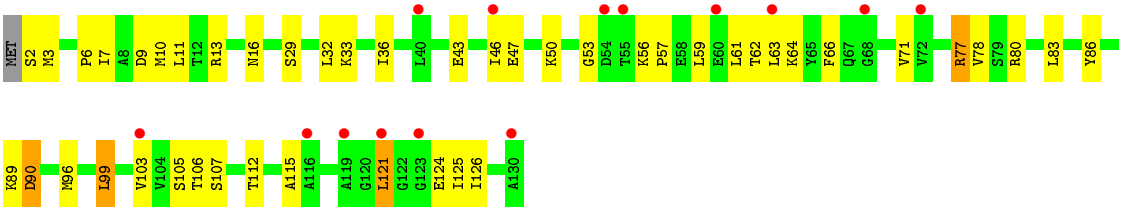
• Molecule 40: 30S ribosomal protein S8

Chain BH:



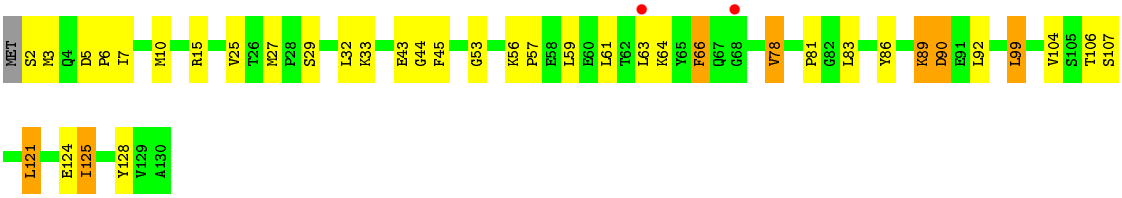
• Molecule 40: 30S ribosomal protein S8

Chain DH:



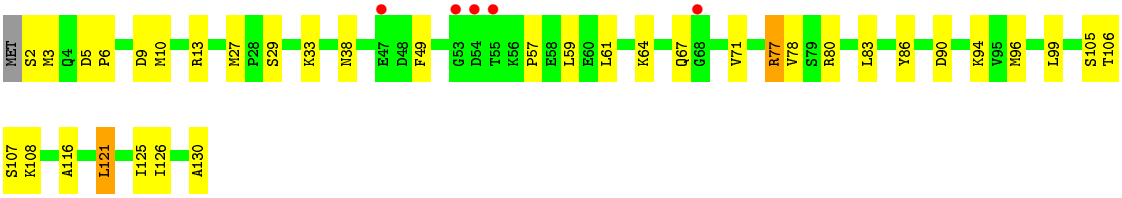
• Molecule 40: 30S ribosomal protein S8

Chain FH:



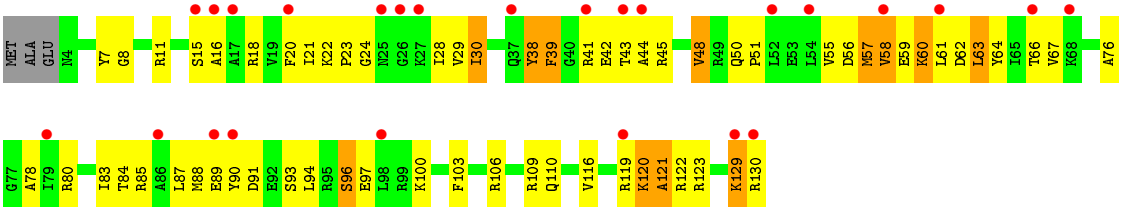
• Molecule 40: 30S ribosomal protein S8

Chain HH:



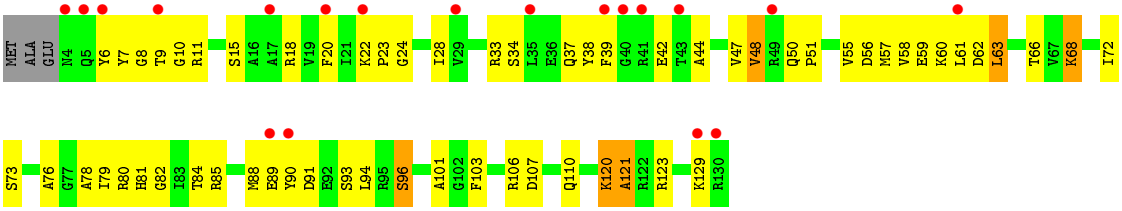
• Molecule 41: 30S ribosomal protein S9

Chain BI:



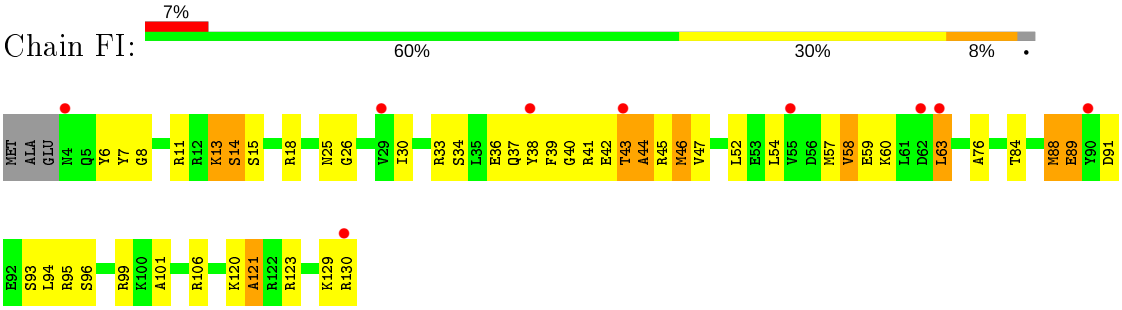
• Molecule 41: 30S ribosomal protein S9

Chain DI:



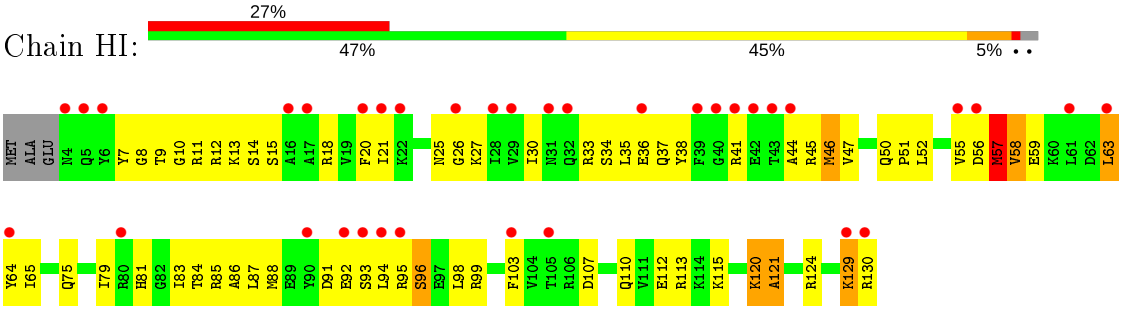
• Molecule 41: 30S ribosomal protein S9

Chain FI:



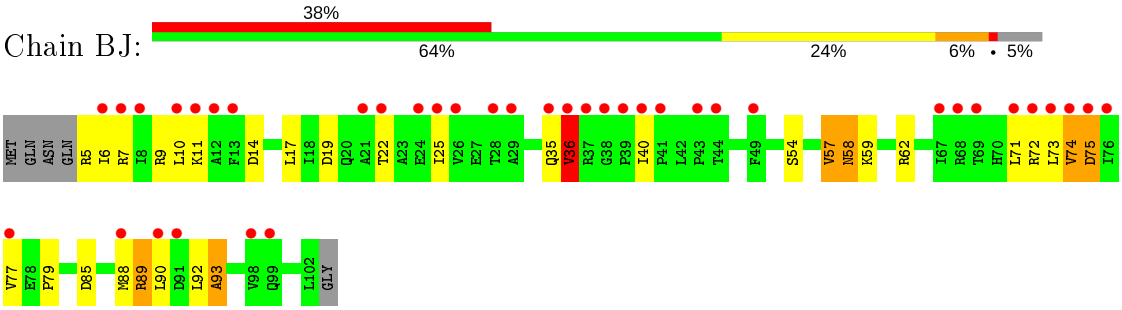
• Molecule 41: 30S ribosomal protein S9

Chain HI:



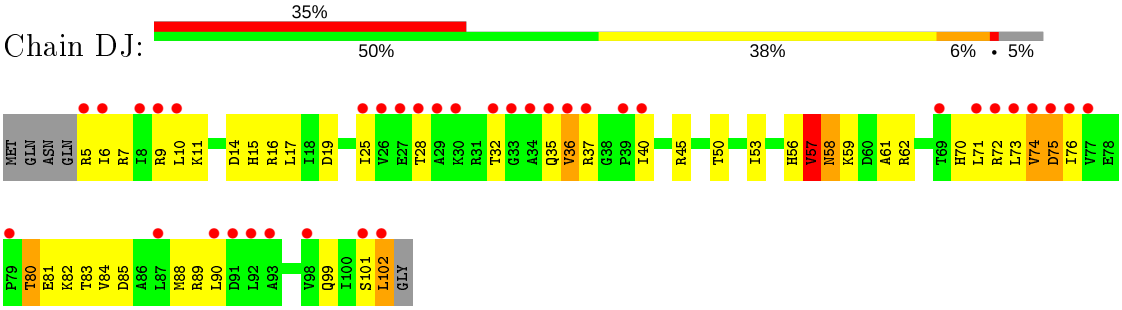
• Molecule 42: 30S ribosomal protein S10

Chain BJ:



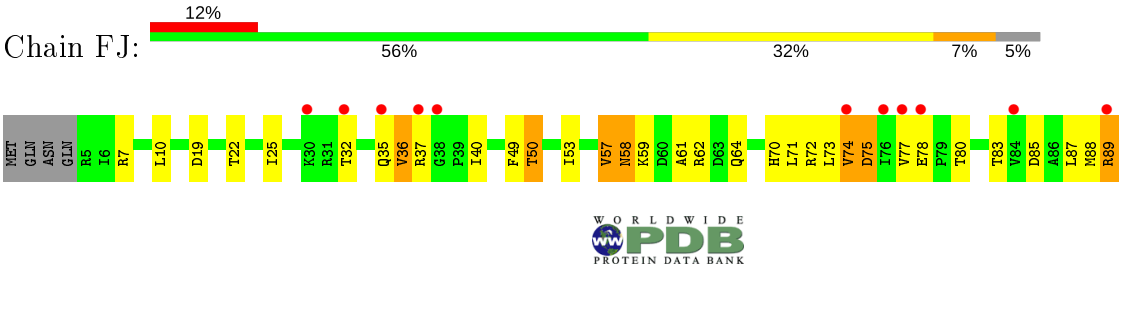
• Molecule 42: 30S ribosomal protein S10

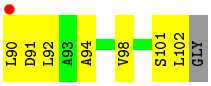
Chain DJ:



• Molecule 42: 30S ribosomal protein S10

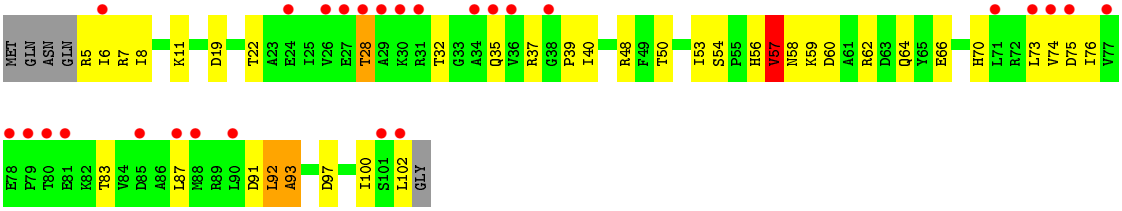
Chain FJ:





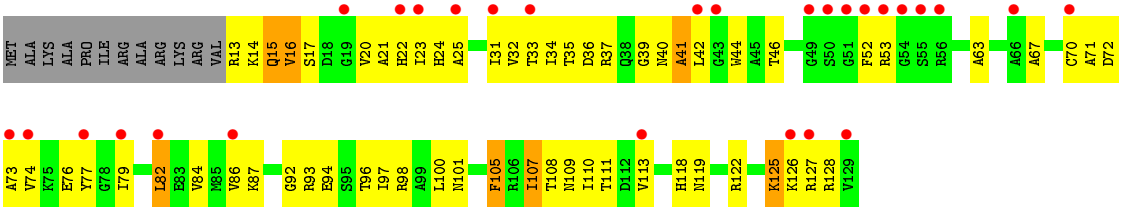
- Molecule 42: 30S ribosomal protein S10

Chain HJ:



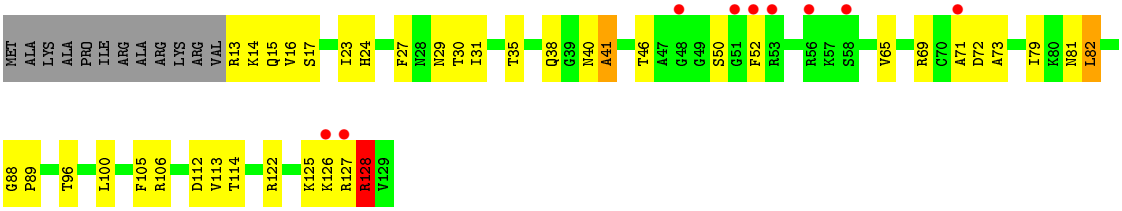
- Molecule 43: 30S ribosomal protein S11

Chain BK:



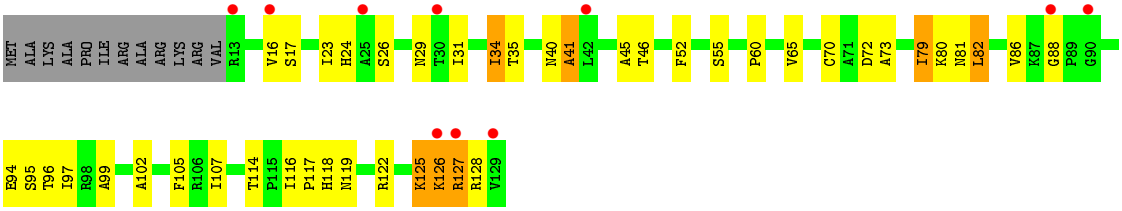
- Molecule 43: 30S ribosomal protein S11

Chain DK:



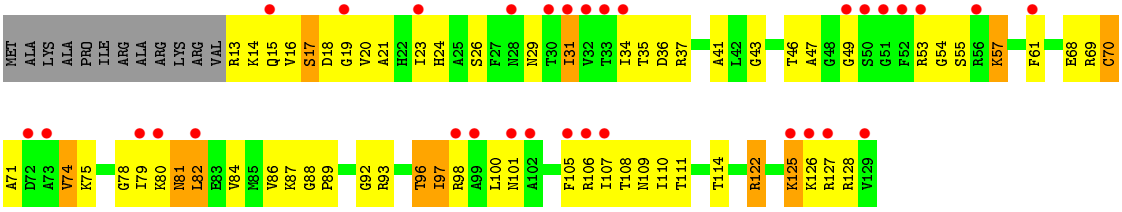
- Molecule 43: 30S ribosomal protein S11

Chain FK:



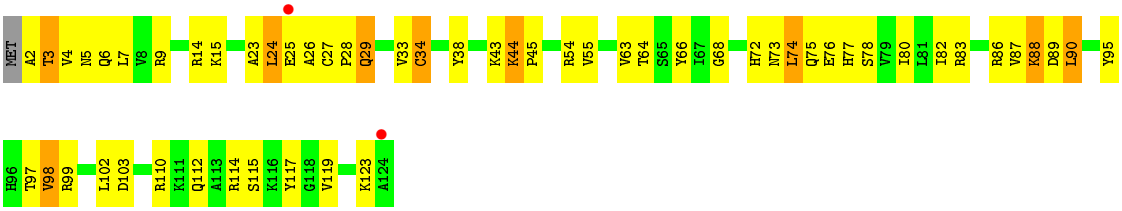
- Molecule 43: 30S ribosomal protein S11

Chain HK:



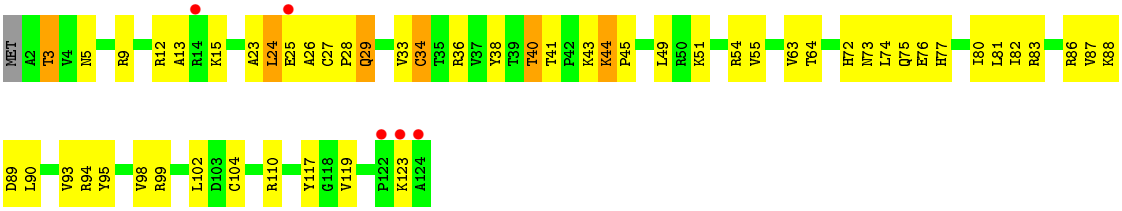
• Molecule 44: 30S ribosomal protein S12

Chain BL:



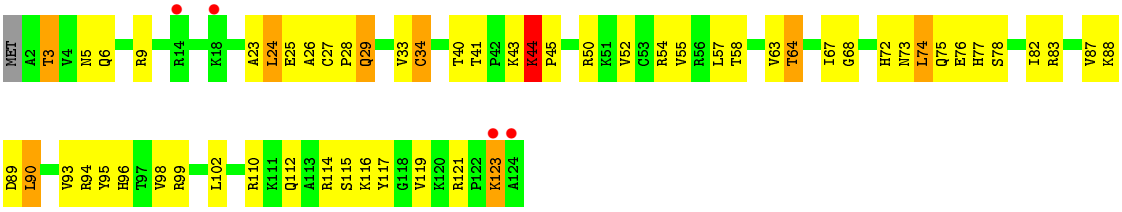
• Molecule 44: 30S ribosomal protein S12

Chain DL:



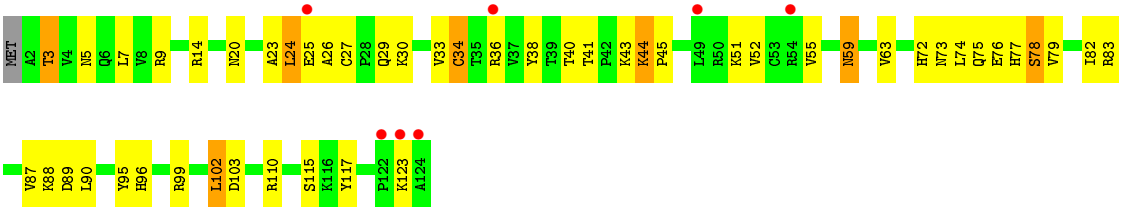
• Molecule 44: 30S ribosomal protein S12

Chain FL:



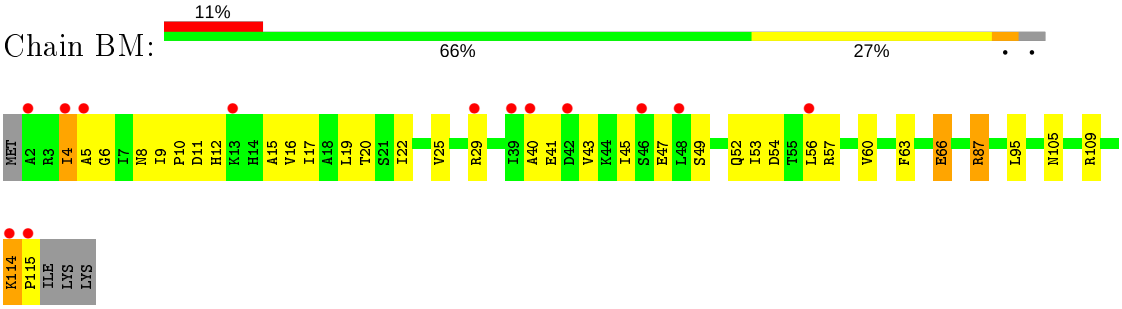
• Molecule 44: 30S ribosomal protein S12

Chain HL:



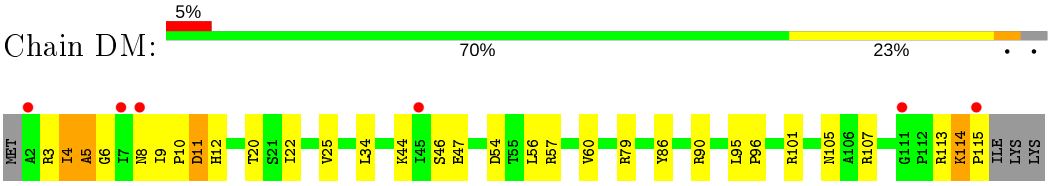
• Molecule 45: 30S ribosomal protein S13

Chain BM:



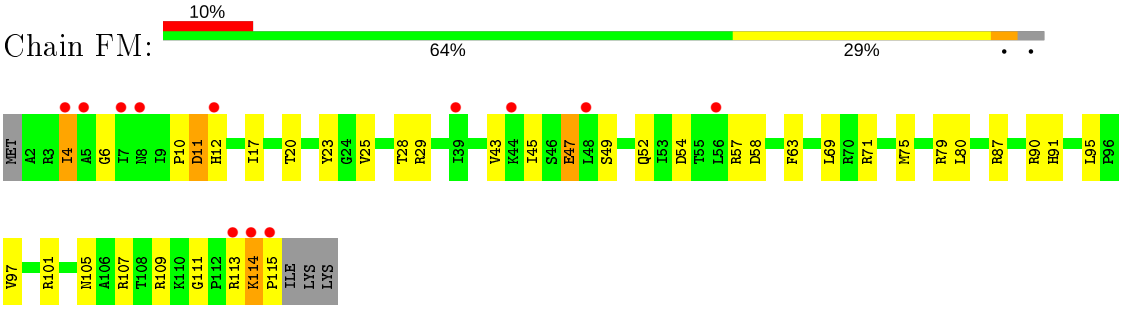
• Molecule 45: 30S ribosomal protein S13

Chain DM:



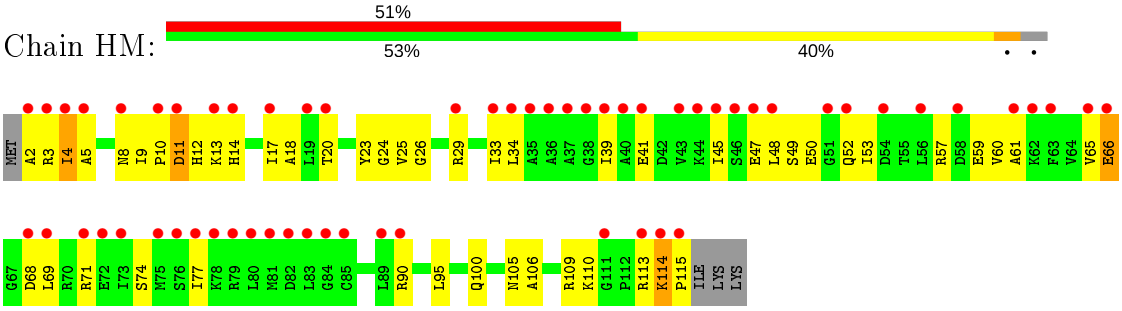
• Molecule 45: 30S ribosomal protein S13

Chain FM:



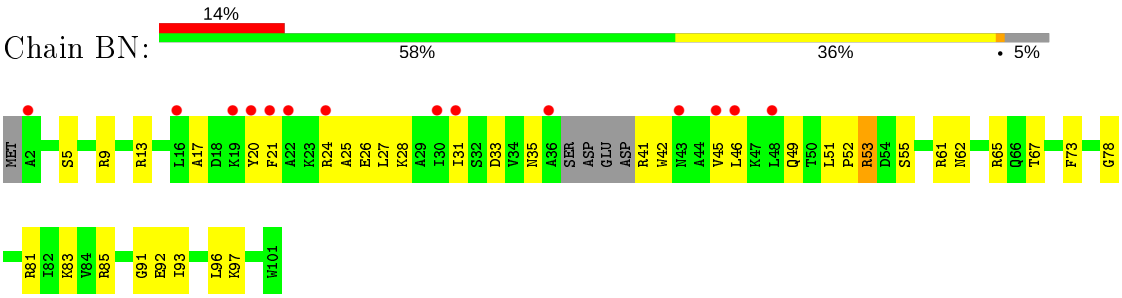
• Molecule 45: 30S ribosomal protein S13

Chain HM:



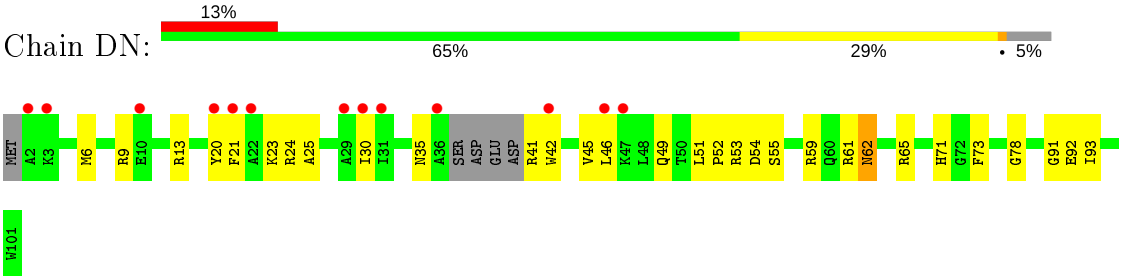
• Molecule 46: 30S ribosomal protein S14

Chain BN:



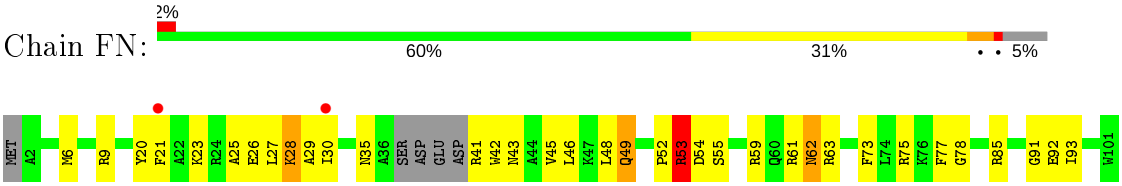
- Molecule 46: 30S ribosomal protein S14

Chain DN:



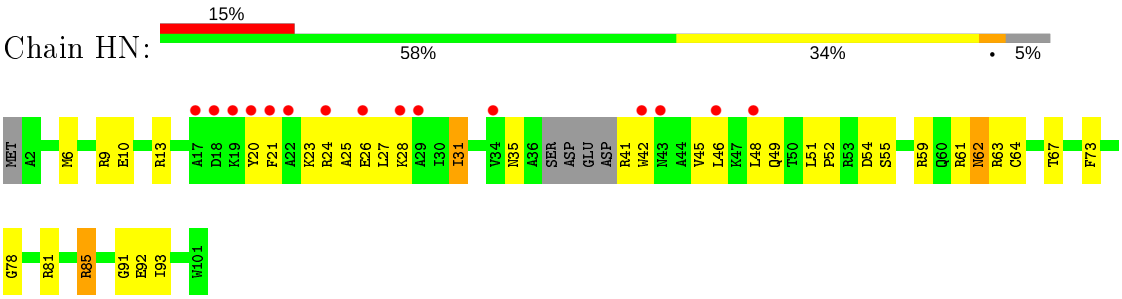
- Molecule 46: 30S ribosomal protein S14

Chain FN:



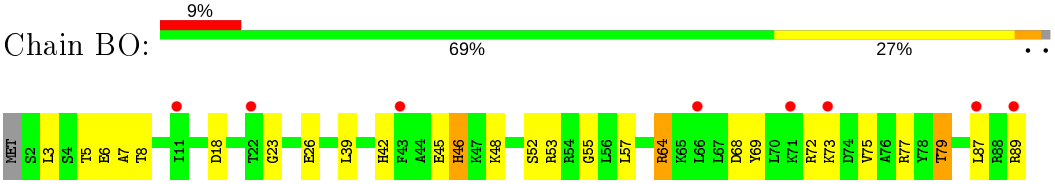
- Molecule 46: 30S ribosomal protein S14

Chain HN:



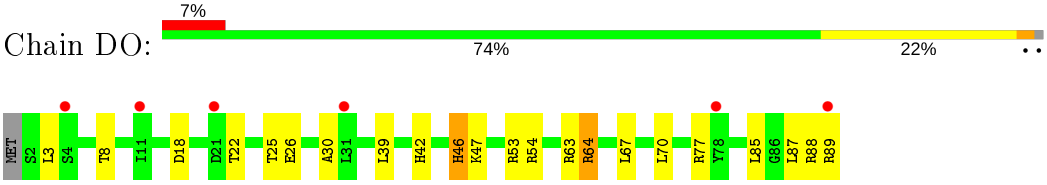
- Molecule 47: 30S ribosomal protein S15

Chain BO:



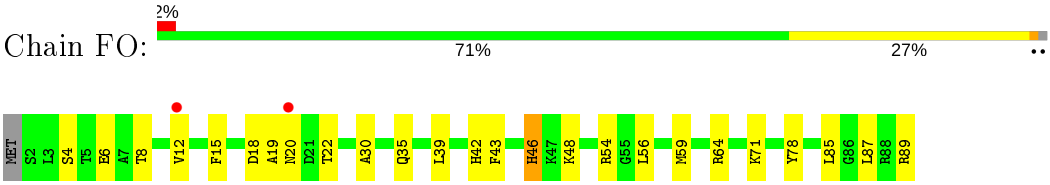
- Molecule 47: 30S ribosomal protein S15

Chain DO:



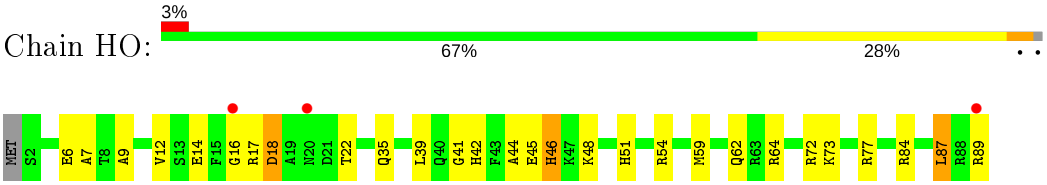
- Molecule 47: 30S ribosomal protein S15

Chain FO:



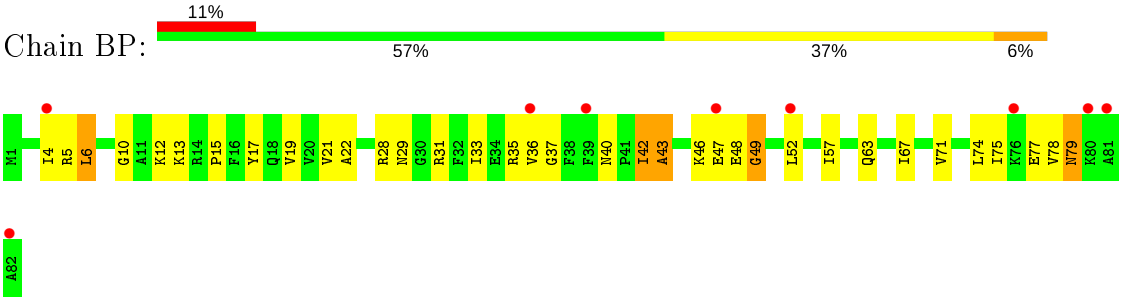
• Molecule 47: 30S ribosomal protein S15

Chain HO:



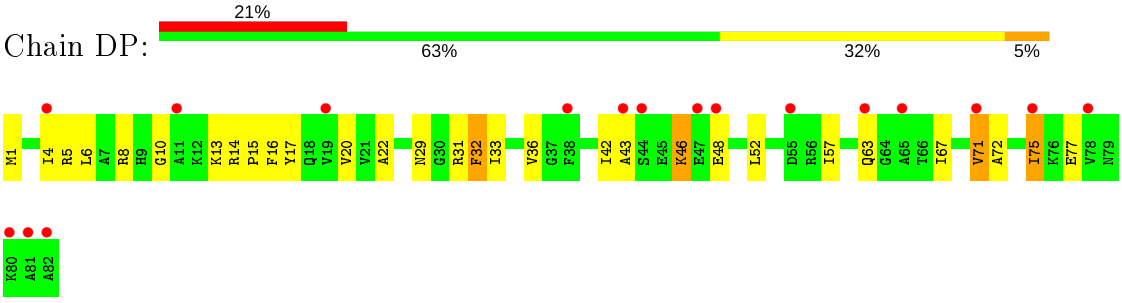
• Molecule 48: 30S ribosomal protein S16

Chain BP:



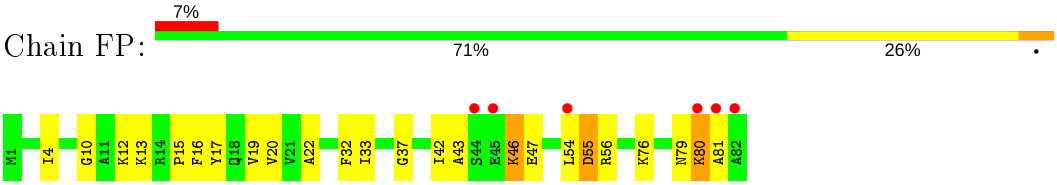
• Molecule 48: 30S ribosomal protein S16

Chain DP:



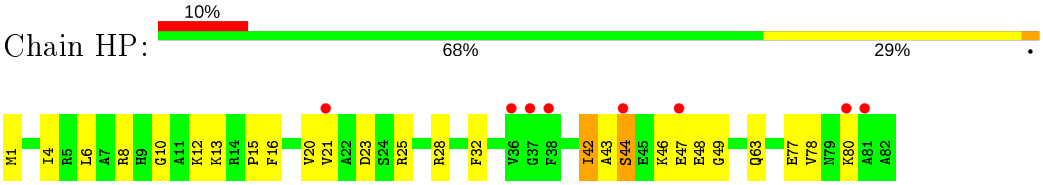
• Molecule 48: 30S ribosomal protein S16

Chain FP:



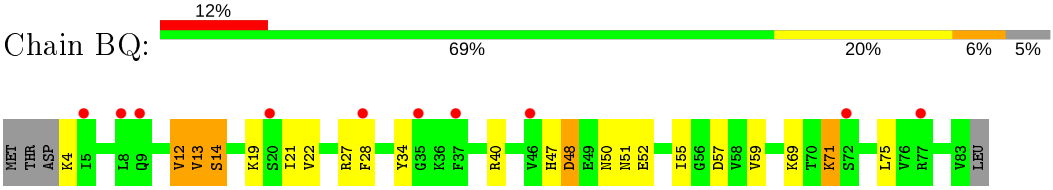
• Molecule 48: 30S ribosomal protein S16

Chain HP:



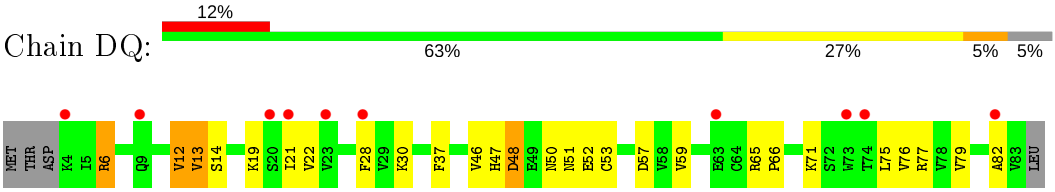
• Molecule 49: 30S ribosomal protein S17

Chain BQ:



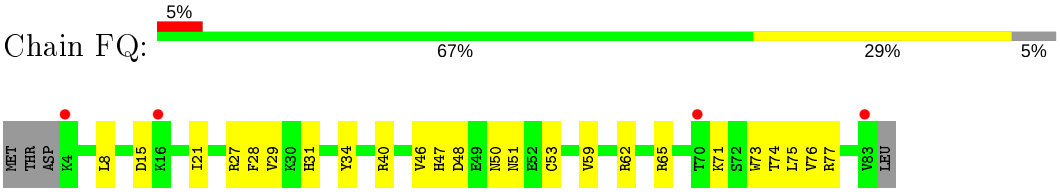
• Molecule 49: 30S ribosomal protein S17

Chain DQ:



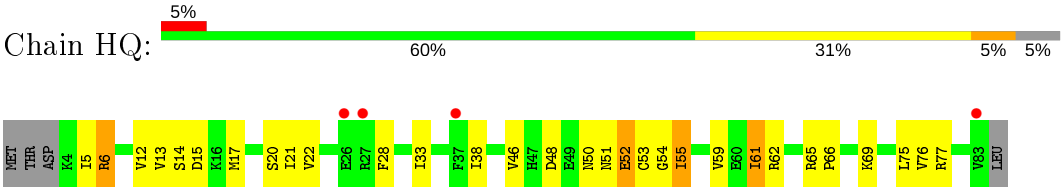
• Molecule 49: 30S ribosomal protein S17

Chain FQ:



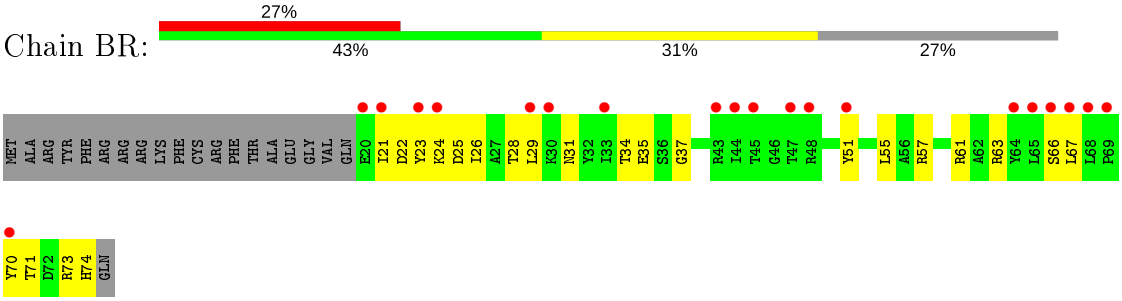
• Molecule 49: 30S ribosomal protein S17

Chain HQ:



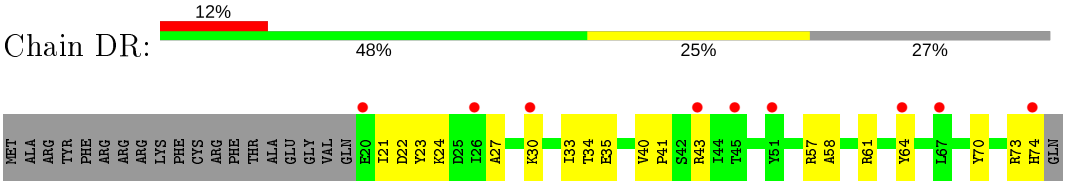
• Molecule 50: 30S ribosomal protein S18

Chain BR:



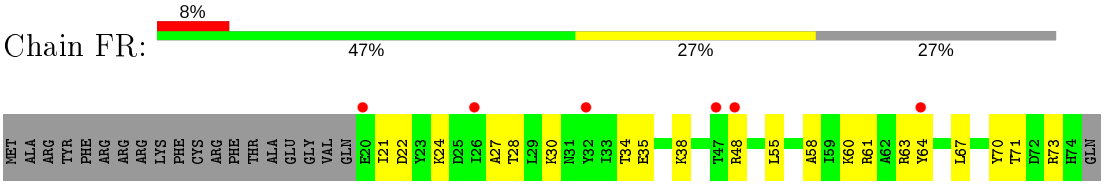
• Molecule 50: 30S ribosomal protein S18

Chain DR:



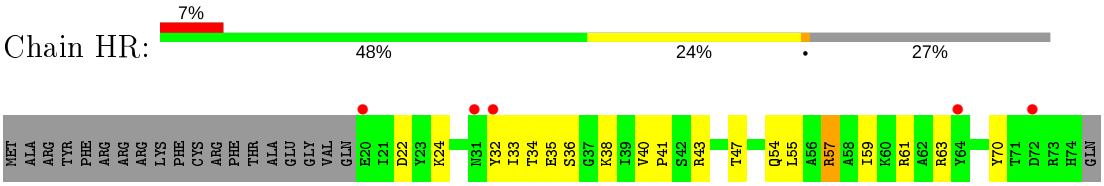
• Molecule 50: 30S ribosomal protein S18

Chain FR:



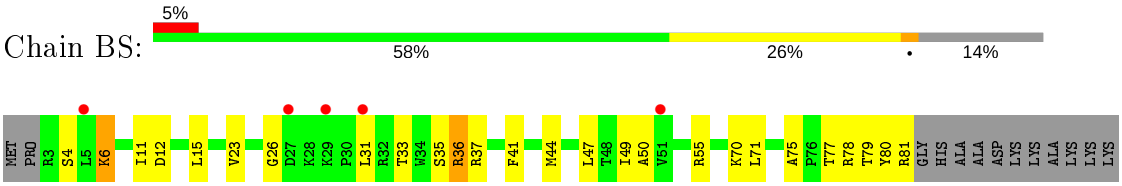
• Molecule 50: 30S ribosomal protein S18

Chain HR:



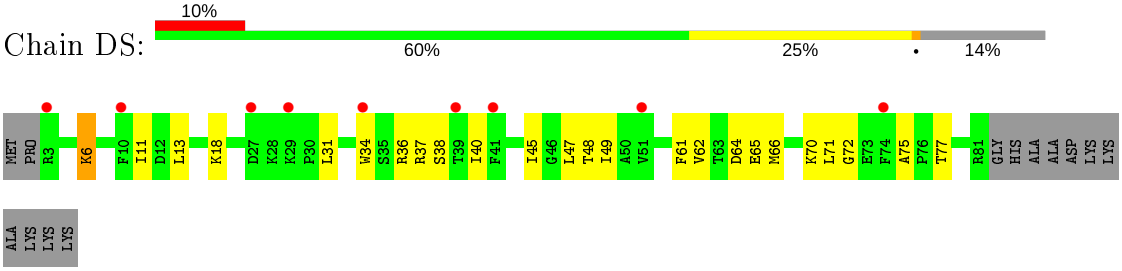
- Molecule 51: 30S ribosomal protein S19

Chain BS:



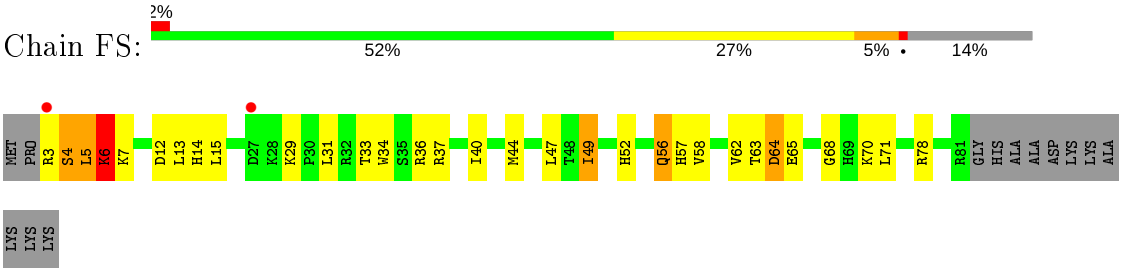
- Molecule 51: 30S ribosomal protein S19

Chain DS:



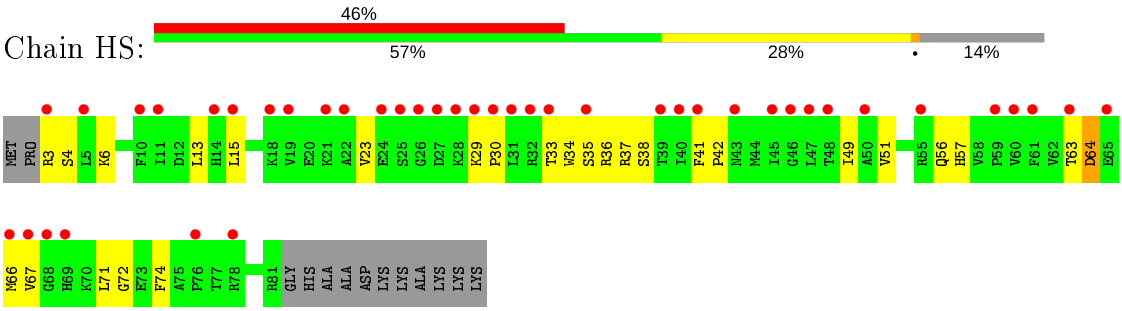
- Molecule 51: 30S ribosomal protein S19

Chain FS:



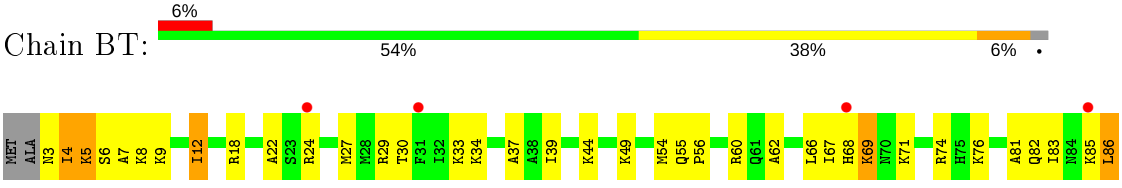
- Molecule 51: 30S ribosomal protein S19

Chain HS:



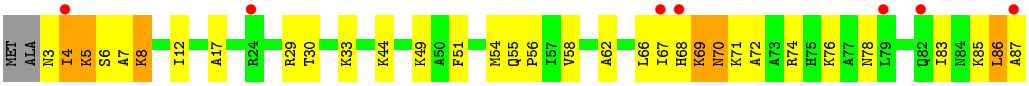
- Molecule 52: 30S ribosomal protein S20

Chain BT:



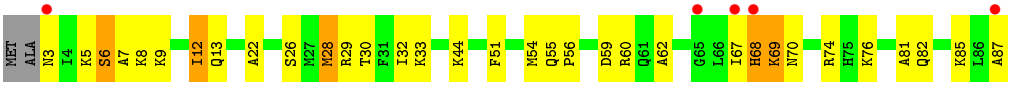
• Molecule 52: 30S ribosomal protein S20

Chain DT:



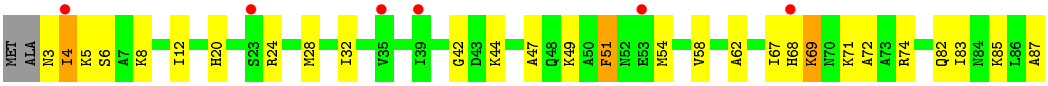
• Molecule 52: 30S ribosomal protein S20

Chain FT:



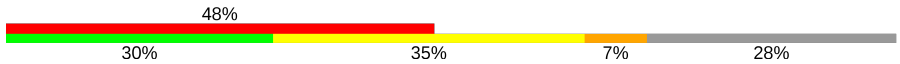
• Molecule 52: 30S ribosomal protein S20

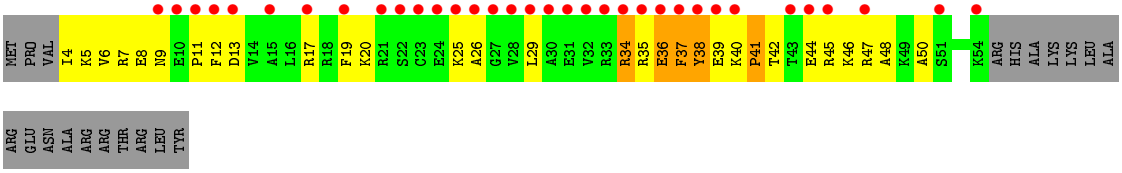
Chain HT:



• Molecule 53: 30S ribosomal protein S21

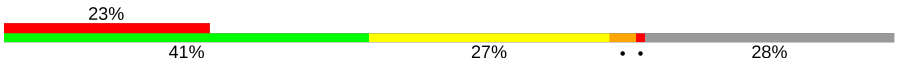
Chain BU:

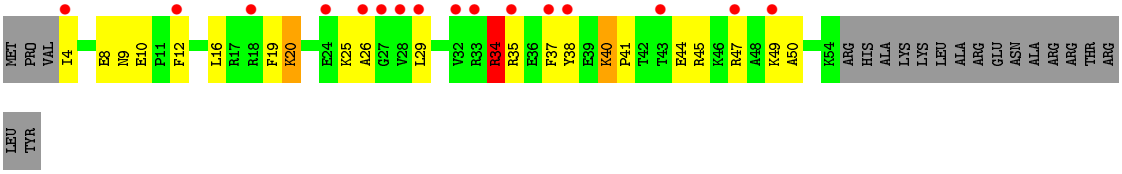




• Molecule 53: 30S ribosomal protein S21

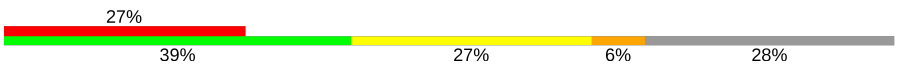
Chain DU:

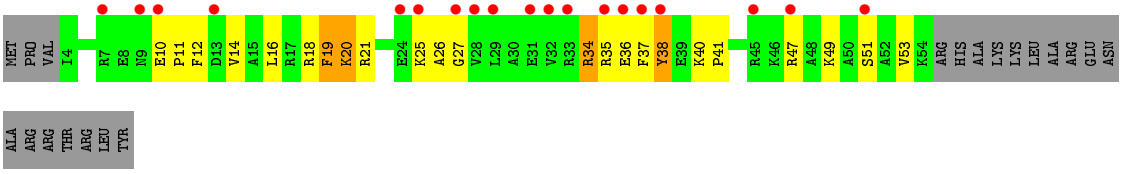




• Molecule 53: 30S ribosomal protein S21

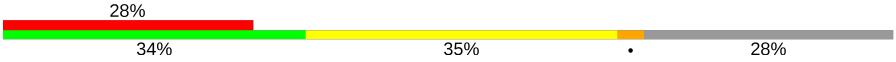
Chain FU:

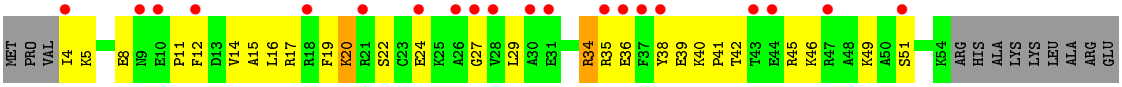




• Molecule 53: 30S ribosomal protein S21

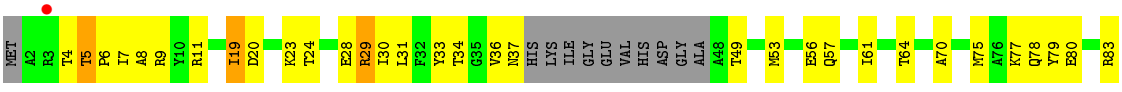
Chain HU:

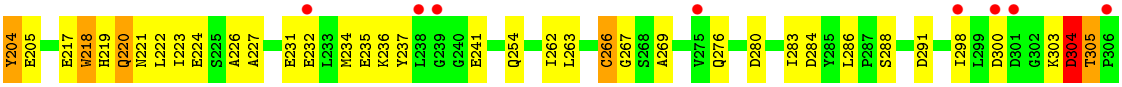


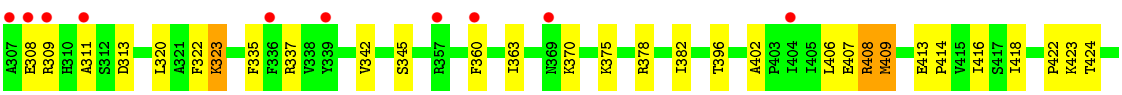


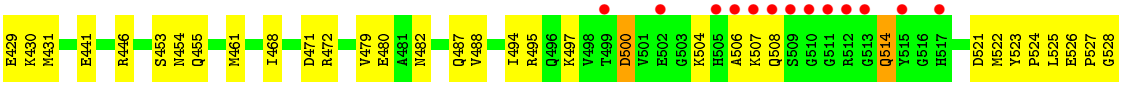
• Molecule 54: elongation factor G

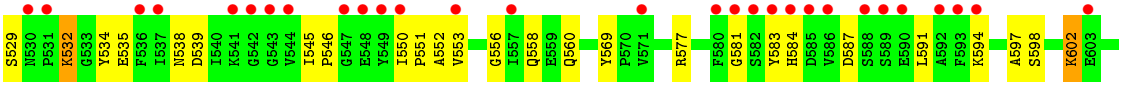
Chain BV:

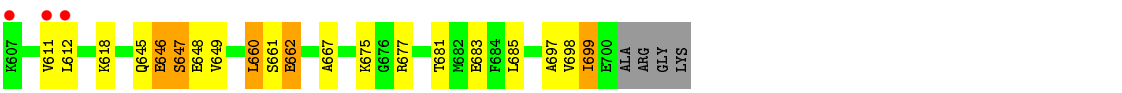






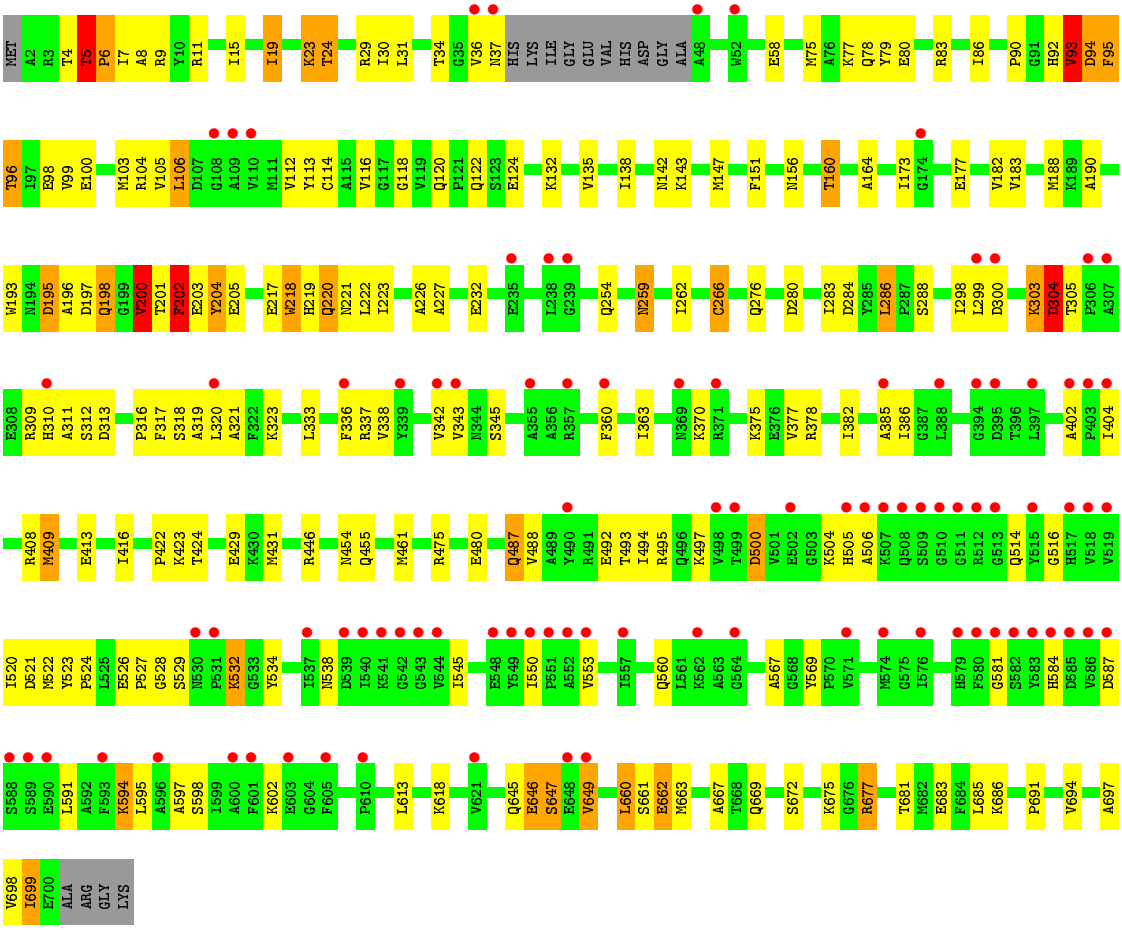






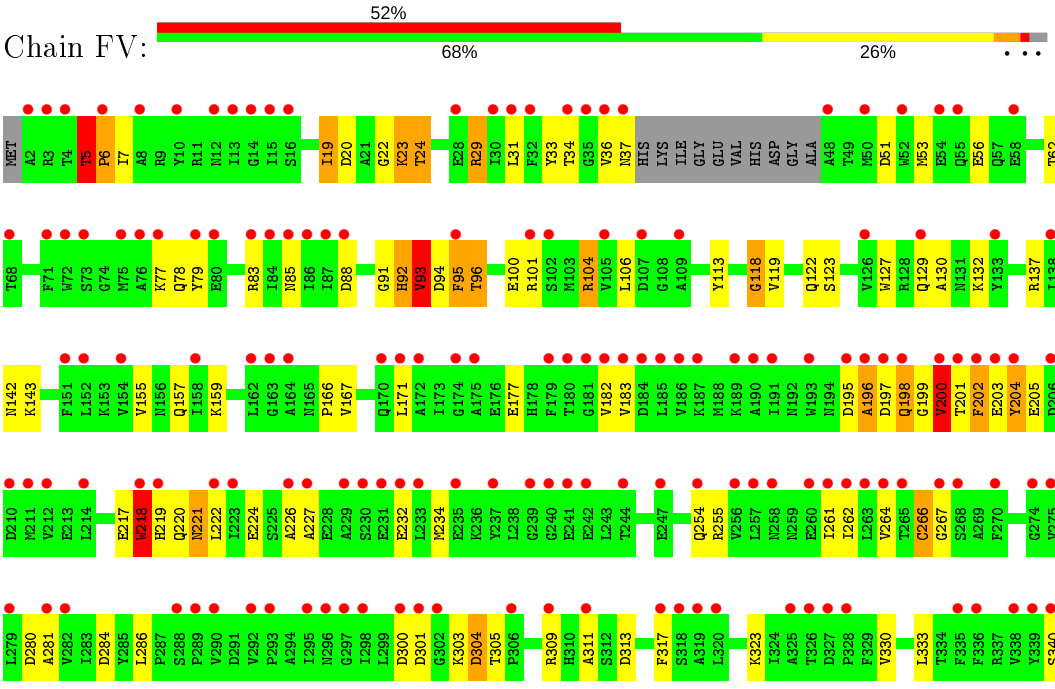
• Molecule 54: elongation factor G

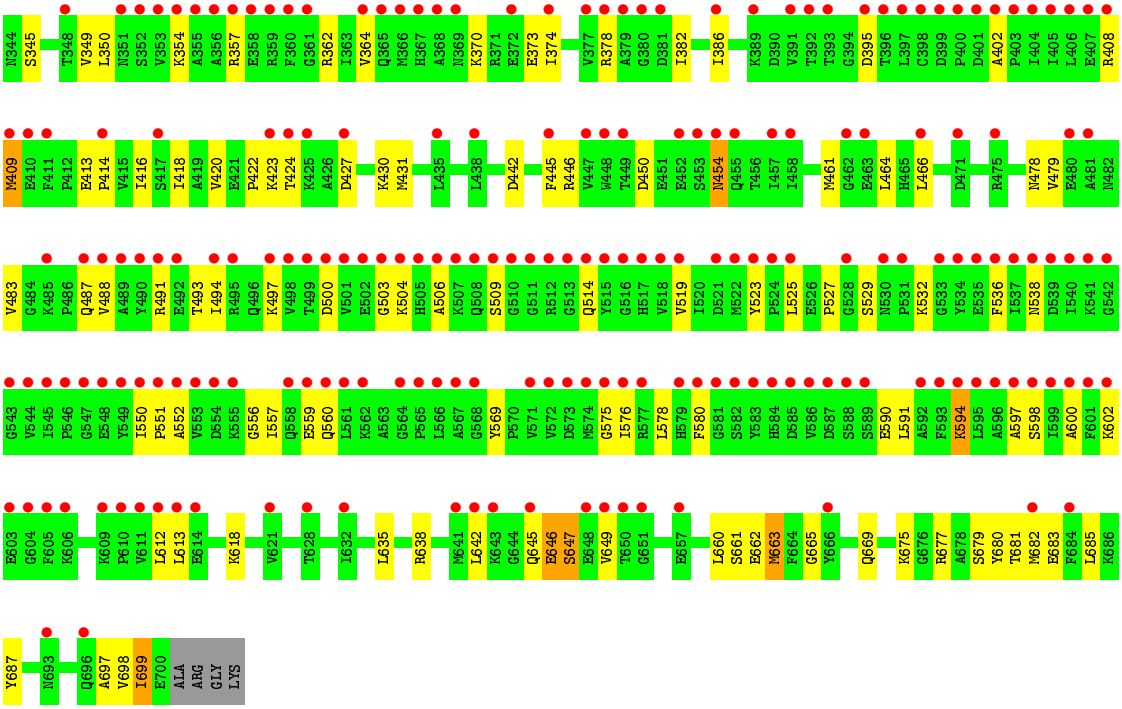
Chain DV:



• Molecule 54: elongation factor G

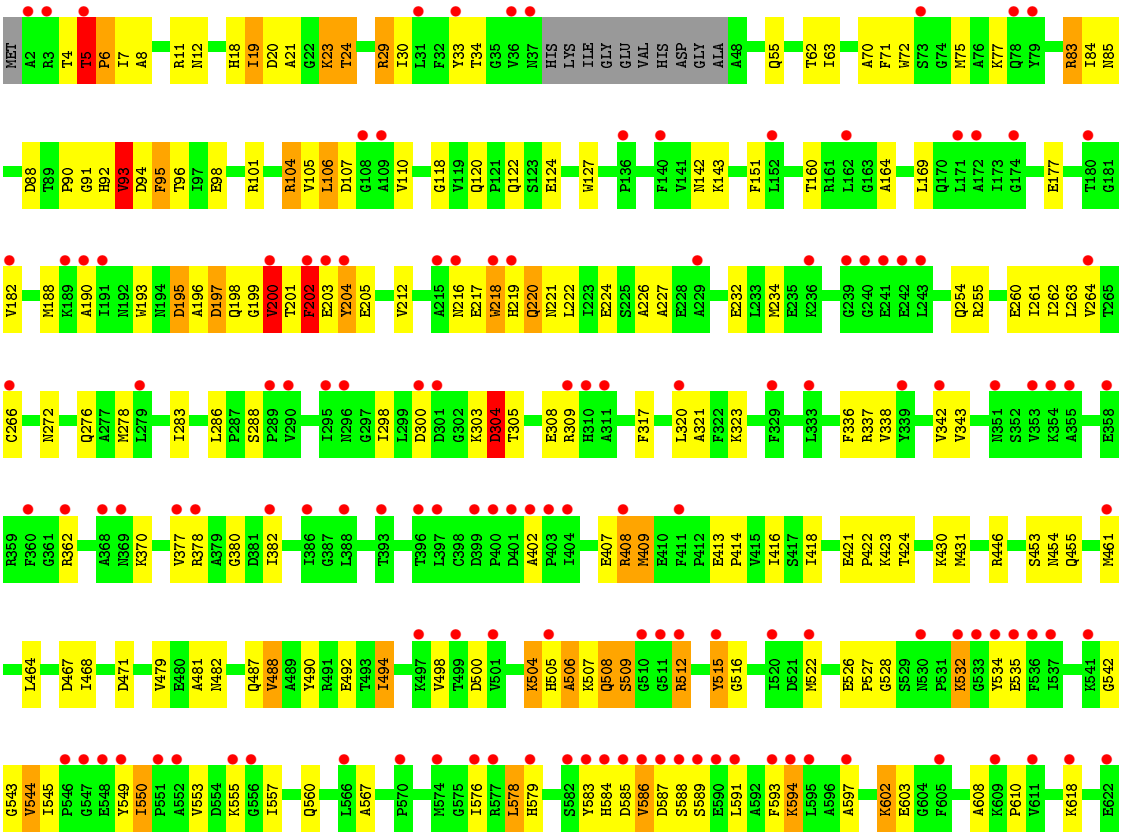
Chain FV:

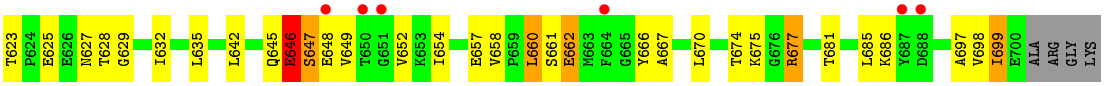




• Molecule 54: elongation factor G

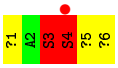
Chain HV:





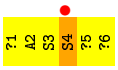
- Molecule 55: Viomycin

Chain BW:



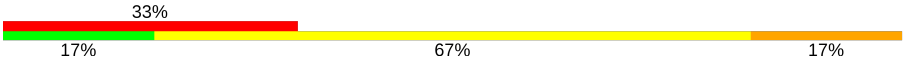
- Molecule 55: Viomycin

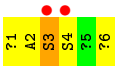
Chain DW:



- Molecule 55: Viomycin

Chain FW:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	361.14Å 360.51Å 429.73Å 90.00° 103.22° 90.00°	Depositor
Resolution (Å)	70.00 – 2.90 69.13 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (70.00-2.90) 77.4 (69.13-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.24 (at 2.81Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.215 , 0.267 0.217 , 0.268	Depositor DCC
R_{free} test set	3893 reflections (0.19%)	wwPDB-VP
Wilson B-factor (Å^2)	54.5	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 39.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	590573	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.58 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.8072e-03.*

[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: ZN, DPP, MG, KBE, GCP, UAL, 5OH

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	AA	0.74	9/68626 (0.0%)	1.28	446/107056 (0.4%)
1	CA	0.76	7/68626 (0.0%)	1.27	404/107056 (0.4%)
1	EA	0.90	29/68626 (0.0%)	1.41	729/107056 (0.7%)
1	GA	0.72	11/68626 (0.0%)	1.25	345/107056 (0.3%)
2	AB	0.67	0/2828	1.20	13/4410 (0.3%)
2	CB	0.61	0/2828	1.15	11/4410 (0.2%)
2	EB	0.75	1/2828 (0.0%)	1.38	18/4410 (0.4%)
2	GB	0.62	0/2828	1.09	2/4410 (0.0%)
3	AC	0.55	0/2121	0.83	3/2852 (0.1%)
3	CC	0.60	0/2121	0.81	0/2852
3	EC	0.62	0/2121	0.83	1/2852 (0.0%)
3	GC	0.59	0/2121	0.84	1/2852 (0.0%)
4	AD	0.60	0/1586	0.81	1/2134 (0.0%)
4	CD	0.55	0/1586	0.75	1/2134 (0.0%)
4	ED	0.63	0/1586	0.81	0/2134
4	GD	0.54	0/1586	0.78	1/2134 (0.0%)
5	AE	0.50	0/1571	0.76	1/2113 (0.0%)
5	CE	0.53	0/1571	0.71	0/2113
5	EE	0.59	0/1571	0.79	2/2113 (0.1%)
5	GE	0.49	0/1571	0.68	0/2113
6	AF	0.69	0/1434	0.89	0/1926
6	CF	0.52	0/1434	0.70	0/1926
6	EF	0.51	0/1434	0.73	0/1926
6	GF	0.58	0/1434	0.77	1/1926 (0.1%)
7	AG	0.54	0/1343	0.72	0/1816
7	CG	0.52	0/1343	0.73	0/1816
7	EG	0.53	0/1343	0.74	0/1816
7	GG	0.52	0/1343	0.72	0/1816
8	AH	0.54	0/389	0.71	0/523
8	CH	0.60	0/389	0.76	0/523
8	EH	0.57	0/389	0.73	0/523
8	GH	0.57	0/389	0.74	0/523

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
9	AI	0.58	0/1046	0.77	0/1410
9	CI	0.58	0/1046	0.74	0/1410
9	EI	0.61	0/1046	0.75	0/1410
9	GI	0.71	0/1046	0.84	0/1410
10	AJ	0.53	0/1152	0.77	0/1551
10	CJ	0.57	1/1152 (0.1%)	0.78	0/1551
10	EJ	0.70	1/1152 (0.1%)	0.82	1/1551 (0.1%)
10	GJ	0.55	1/1152 (0.1%)	0.71	0/1551
11	AK	0.62	0/947	0.79	0/1268
11	CK	0.63	0/947	0.78	0/1268
11	EK	0.59	0/947	0.83	0/1268
11	GK	0.55	0/947	0.80	0/1268
12	AL	0.53	0/1054	0.78	2/1403 (0.1%)
12	CL	0.53	0/1054	0.81	2/1403 (0.1%)
12	EL	0.61	0/1054	0.81	0/1403
12	GL	0.52	0/1054	0.78	0/1403
13	AM	0.61	1/1093 (0.1%)	0.81	1/1460 (0.1%)
13	CM	0.53	0/1093	0.75	0/1460
13	EM	0.62	0/1093	0.87	2/1460 (0.1%)
13	GM	0.52	0/1093	0.73	0/1460
14	AN	0.51	0/973	0.75	1/1301 (0.1%)
14	CN	0.46	0/973	0.77	4/1301 (0.3%)
14	EN	0.57	0/973	0.74	0/1301
14	GN	0.49	0/973	0.69	0/1301
15	AO	0.48	0/902	0.72	0/1209
15	CO	0.47	0/902	0.70	0/1209
15	EO	0.48	0/902	0.75	0/1209
15	GO	0.48	0/902	0.74	0/1209
16	AP	0.56	0/929	0.87	2/1242 (0.2%)
16	CP	0.56	0/929	0.85	2/1242 (0.2%)
16	EP	0.63	1/929 (0.1%)	0.89	1/1242 (0.1%)
16	GP	0.58	0/929	0.80	0/1242
17	AQ	0.56	0/960	0.75	1/1278 (0.1%)
17	CQ	0.60	0/960	0.78	1/1278 (0.1%)
17	EQ	0.70	0/960	0.88	2/1278 (0.2%)
17	GQ	0.53	0/960	0.74	0/1278
18	AR	0.59	0/829	0.75	0/1107
18	CR	0.59	0/829	0.75	0/1107
18	ER	0.68	2/829 (0.2%)	0.79	0/1107
18	GR	0.56	0/829	0.75	0/1107
19	AS	0.52	0/864	0.76	0/1156
19	CS	0.52	0/864	0.73	0/1156
19	ES	0.62	0/864	0.84	1/1156 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
19	GS	0.49	0/864	0.72	0/1156
20	AT	0.60	0/744	0.84	0/994
20	CT	0.56	0/744	0.89	0/994
20	ET	0.65	0/744	0.92	1/994 (0.1%)
20	GT	0.57	0/744	0.91	1/994 (0.1%)
21	AU	0.56	0/787	0.76	0/1051
21	CU	0.52	0/787	0.75	0/1051
21	EU	0.61	0/787	0.81	0/1051
21	GU	0.52	0/787	0.77	0/1051
22	AV	0.48	0/766	0.67	0/1025
22	CV	0.55	1/766 (0.1%)	0.67	0/1025
22	EV	0.57	0/766	0.72	0/1025
22	GV	0.47	0/766	0.65	0/1025
23	AW	0.63	0/603	0.93	1/797 (0.1%)
23	CW	0.70	0/603	0.94	1/797 (0.1%)
23	EW	0.78	0/603	0.97	1/797 (0.1%)
23	GW	0.66	0/603	0.92	0/797
24	AX	0.52	0/635	0.83	1/848 (0.1%)
24	CX	0.58	0/635	0.80	2/848 (0.2%)
24	EX	0.56	0/635	0.79	1/848 (0.1%)
24	GX	0.51	0/635	0.79	0/848
25	AY	0.47	0/510	0.75	0/677
25	CY	0.51	0/510	0.76	0/677
25	EY	0.54	0/510	0.85	1/677 (0.1%)
25	GY	0.55	0/510	0.79	1/677 (0.1%)
26	AZ	0.53	0/453	0.65	0/605
26	CZ	0.49	0/453	0.75	0/605
26	EZ	0.58	0/453	0.82	0/605
26	GZ	0.48	0/453	0.73	0/605
27	A0	0.50	0/450	0.77	0/599
27	C0	0.49	0/450	0.72	0/599
27	E0	0.68	1/450 (0.2%)	0.80	1/599 (0.2%)
27	G0	0.52	1/450 (0.2%)	0.69	0/599
28	A1	0.54	0/416	0.78	0/554
28	C1	0.51	0/416	0.76	0/554
28	E1	0.54	0/416	0.72	0/554
28	G1	0.54	0/416	0.73	0/554
29	A2	0.52	0/380	0.77	0/498
29	C2	0.56	0/380	0.73	0/498
29	E2	0.75	1/380 (0.3%)	0.84	1/498 (0.2%)
29	G2	0.59	0/380	0.75	0/498
30	A3	0.51	0/513	0.74	0/676
30	C3	0.54	0/513	0.68	0/676

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
30	E3	0.64	0/513	0.81	0/676
30	G3	0.50	0/513	0.70	0/676
31	A4	0.61	0/303	0.78	0/397
31	C4	0.60	0/303	0.81	0/397
31	E4	0.60	0/303	0.82	0/397
31	G4	0.53	0/303	0.77	0/397
32	A5	0.83	0/1131	1.34	28/1524 (1.8%)
32	E5	0.74	0/1106	1.34	26/1490 (1.7%)
33	BA	0.64	0/36834	1.15	99/57462 (0.2%)
33	DA	0.63	0/36834	1.13	95/57462 (0.2%)
33	FA	0.65	1/36834 (0.0%)	1.18	114/57462 (0.2%)
33	HA	0.64	0/36834	1.13	101/57462 (0.2%)
34	BB	0.53	0/1735	0.72	0/2338
34	DB	0.49	0/1735	0.70	0/2338
34	FB	0.54	0/1735	0.73	0/2338
34	HB	0.52	0/1735	0.72	0/2338
35	BC	0.47	0/1651	0.64	0/2225
35	DC	0.47	0/1651	0.61	0/2225
35	FC	0.50	0/1651	0.71	0/2225
35	HC	0.48	0/1651	0.67	0/2225
36	BD	0.52	0/1665	0.74	0/2227
36	DD	0.54	0/1665	0.76	0/2227
36	FD	0.49	0/1665	0.71	0/2227
36	HD	0.52	0/1665	0.73	0/2227
37	BE	0.56	1/1118 (0.1%)	0.77	0/1504
37	DE	0.50	0/1118	0.74	0/1504
37	FE	0.54	0/1118	0.78	0/1504
37	HE	0.52	0/1118	0.76	0/1504
38	BF	0.64	0/835	0.75	0/1128
38	DF	0.55	0/835	0.73	0/1128
38	FF	0.54	0/835	0.73	0/1128
38	HF	0.58	0/835	0.72	0/1128
39	BG	0.48	0/1195	0.66	0/1602
39	DG	0.47	0/1195	0.66	0/1602
39	FG	0.51	0/1195	0.70	0/1602
39	HG	0.51	0/1195	0.73	0/1602
40	BH	0.48	0/989	0.63	0/1326
40	DH	0.50	0/989	0.65	0/1326
40	FH	0.50	0/989	0.72	0/1326
40	HH	0.45	0/989	0.66	0/1326
41	BI	0.52	0/1034	0.77	0/1375
41	DI	0.49	0/1034	0.72	1/1375 (0.1%)
41	FI	0.52	0/1034	0.80	0/1375

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
41	HI	0.56	0/1034	0.76	1/1375 (0.1%)
42	BJ	0.53	0/796	0.73	1/1077 (0.1%)
42	DJ	0.55	0/796	0.75	0/1077
42	FJ	0.55	0/796	0.78	0/1077
42	HJ	0.54	0/796	0.77	0/1077
43	BK	0.59	0/893	0.81	0/1205
43	DK	0.51	0/893	0.80	1/1205 (0.1%)
43	FK	0.52	0/893	0.72	0/1205
43	HK	0.71	0/893	0.92	2/1205 (0.2%)
44	BL	0.55	0/969	0.78	0/1300
44	DL	0.54	0/969	0.79	0/1300
44	FL	0.51	0/969	0.75	1/1300 (0.1%)
44	HL	0.50	0/969	0.78	0/1300
45	BM	0.48	0/892	0.72	0/1193
45	DM	0.48	0/892	0.70	0/1193
45	FM	0.46	0/892	0.72	0/1193
45	HM	0.60	0/892	0.83	0/1193
46	BN	0.53	0/785	0.73	0/1043
46	DN	0.53	0/785	0.68	0/1043
46	FN	0.59	0/785	0.80	0/1043
46	HN	0.48	0/785	0.67	0/1043
47	BO	0.46	0/722	0.65	0/964
47	DO	0.47	0/722	0.64	0/964
47	FO	0.44	0/722	0.63	0/964
47	HO	0.50	0/722	0.68	0/964
48	BP	0.51	0/659	0.74	0/884
48	DP	0.52	0/659	0.72	0/884
48	FP	0.48	0/659	0.70	0/884
48	HP	0.51	0/659	0.67	0/884
49	BQ	0.51	0/657	0.73	0/881
49	DQ	0.50	0/657	0.74	0/881
49	FQ	0.49	0/657	0.66	0/881
49	HQ	0.51	0/657	0.75	0/881
50	BR	0.53	0/462	0.67	0/621
50	DR	0.50	0/462	0.71	0/621
50	FR	0.48	0/462	0.63	0/621
50	HR	0.53	0/462	0.77	1/621 (0.2%)
51	BS	0.47	0/652	0.78	0/877
51	DS	0.49	0/652	0.70	0/877
51	FS	0.48	0/652	0.72	0/877
51	HS	0.66	0/652	0.79	0/877
52	BT	0.50	0/671	0.65	0/888
52	DT	0.49	0/671	0.64	0/888

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
52	FT	0.48	0/671	0.68	0/888
52	HT	0.49	0/671	0.72	0/888
53	BU	0.67	0/430	0.75	0/570
53	DU	0.67	0/430	0.83	1/570 (0.2%)
53	FU	0.69	0/430	0.83	0/570
53	HU	0.78	0/430	0.82	0/570
54	BV	0.48	0/5418	0.68	1/7329 (0.0%)
54	DV	0.46	0/5418	0.66	1/7329 (0.0%)
54	FV	0.57	0/5418	0.68	1/7329 (0.0%)
54	HV	0.50	0/5418	0.70	1/7329 (0.0%)
55	BW	2.44	1/11 (9.1%)	1.38	0/13
55	DW	2.31	1/11 (9.1%)	1.57	0/13
55	FW	2.44	1/11 (9.1%)	2.53	1/13 (7.7%)
All	All	0.68	73/635346 (0.0%)	1.13	2493/946873 (0.3%)

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
3	CC	0	1
3	EC	0	1
3	GC	0	1
4	CD	0	2
4	ED	0	1
4	GD	0	1
32	A5	0	2
41	FI	0	1
44	BL	0	1
44	DL	0	1
44	FL	0	1
44	HL	0	1
54	BV	0	2
54	DV	0	2
54	FV	0	2
54	HV	0	3
All	All	0	23

The worst 5 of 73 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	EA	984	A	N9-C4	-10.08	1.31	1.37
1	EA	528	A	N9-C4	-9.15	1.32	1.37
37	BE	94	VAL	CB-CG2	9.12	1.72	1.52
13	AM	13	HIS	CG-CD2	8.66	1.50	1.35
10	EJ	44	TYR	CD1-CE1	-7.92	1.27	1.39

The worst 5 of 2493 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	EA	834	G	N1-C6-O6	16.23	129.64	119.90
1	EA	984	A	C2-N3-C4	-15.83	102.68	110.60
1	EA	974	G	C4-C5-N7	15.17	116.87	110.80
1	AA	2544	G	N1-C6-O6	14.98	128.89	119.90
1	AA	2053	G	N1-C6-O6	14.67	128.70	119.90

There are no chirality outliers.

5 of 23 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
32	A5	130	PRO	Peptide
32	A5	134	GLU	Peptide
44	BL	23	ALA	Peptide
54	BV	218	TRP	Peptide
54	BV	304	ASP	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	61274	0	30818	1057	0
1	CA	61274	0	30819	919	0
1	EA	61274	0	30819	835	0
1	GA	61274	0	30819	917	3
2	AB	2529	0	1281	36	0
2	CB	2529	0	1281	34	0
2	EB	2529	0	1281	35	0
2	GB	2529	0	1281	37	0
3	AC	2082	0	2157	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	CC	2082	0	2157	68	0
3	EC	2082	0	2157	65	0
3	GC	2082	0	2157	57	0
4	AD	1565	0	1616	78	0
4	CD	1565	0	1616	75	0
4	ED	1565	0	1616	72	0
4	GD	1565	0	1616	77	0
5	AE	1552	0	1619	63	0
5	CE	1552	0	1619	34	0
5	EE	1552	0	1619	42	0
5	GE	1552	0	1619	56	0
6	AF	1410	0	1447	133	0
6	CF	1410	0	1447	53	0
6	EF	1410	0	1447	60	0
6	GF	1410	0	1447	92	1
7	AG	1323	0	1374	65	0
7	CG	1323	0	1374	65	0
7	EG	1323	0	1374	48	0
7	GG	1323	0	1374	58	0
8	AH	384	0	405	12	0
8	CH	384	0	405	18	0
8	EH	384	0	405	15	0
8	GH	384	0	405	11	0
9	AI	1032	0	1088	70	0
9	CI	1032	0	1088	62	0
9	EI	1032	0	1088	48	0
9	GI	1032	0	1088	82	0
10	AJ	1129	0	1162	49	0
10	CJ	1129	0	1162	58	0
10	EJ	1129	0	1162	76	0
10	GJ	1129	0	1162	57	0
11	AK	938	0	1012	40	0
11	CK	938	0	1012	57	0
11	EK	938	0	1012	49	0
11	GK	938	0	1012	42	0
12	AL	1045	0	1117	51	0
12	CL	1045	0	1117	38	0
12	EL	1045	0	1117	35	0
12	GL	1045	0	1117	50	0
13	AM	1074	0	1157	29	0
13	CM	1074	0	1157	33	0
13	EM	1074	0	1157	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	GM	1074	0	1157	24	0
14	AN	960	0	1000	35	0
14	CN	960	0	1000	44	0
14	EN	960	0	1000	33	0
14	GN	960	0	1000	36	0
15	AO	892	0	923	41	0
15	CO	892	0	923	32	0
15	EO	892	0	923	21	0
15	GO	892	0	923	29	0
16	AP	917	0	965	63	0
16	CP	917	0	965	58	0
16	EP	917	0	965	52	0
16	GP	917	0	965	49	0
17	AQ	947	0	1022	53	0
17	CQ	947	0	1022	56	0
17	EQ	947	0	1022	58	0
17	GQ	947	0	1022	56	0
18	AR	816	0	839	41	0
18	CR	816	0	839	49	0
18	ER	816	0	839	46	0
18	GR	816	0	839	34	0
19	AS	857	0	922	21	0
19	CS	857	0	922	27	0
19	ES	857	0	922	26	0
19	GS	857	0	922	30	0
20	AT	738	0	807	51	0
20	CT	738	0	807	54	0
20	ET	738	0	807	34	0
20	GT	738	0	807	47	0
21	AU	779	0	834	31	0
21	CU	779	0	834	19	0
21	EU	779	0	834	28	0
21	GU	779	0	834	27	1
22	AV	753	0	780	10	0
22	CV	753	0	780	16	0
22	EV	753	0	780	16	0
22	GV	753	0	780	25	0
23	AW	596	0	610	83	0
23	CW	596	0	610	78	0
23	EW	596	0	610	100	0
23	GW	596	0	610	85	0
24	AX	625	0	655	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	CX	625	0	655	20	0
24	EX	625	0	655	26	0
24	GX	625	0	655	24	0
25	AY	509	0	543	12	0
25	CY	509	0	543	16	0
25	EY	509	0	543	17	0
25	GY	509	0	543	11	0
26	AZ	449	0	491	6	0
26	CZ	449	0	491	11	0
26	EZ	449	0	491	15	0
26	GZ	449	0	491	14	0
27	A0	444	0	461	20	0
27	C0	444	0	461	15	0
27	E0	444	0	461	6	0
27	G0	444	0	461	12	0
28	A1	409	0	440	18	0
28	C1	409	0	440	23	0
28	E1	409	0	440	14	0
28	G1	409	0	440	13	0
29	A2	377	0	418	12	0
29	C2	377	0	418	9	0
29	E2	377	0	418	15	0
29	G2	377	0	418	8	0
30	A3	504	0	574	20	0
30	C3	504	0	574	16	0
30	E3	504	0	574	14	0
30	G3	504	0	574	21	0
31	A4	302	0	340	14	0
31	C4	302	0	340	17	0
31	E4	302	0	340	14	0
31	G4	302	0	340	13	0
32	A5	1117	0	1155	135	0
32	E5	1092	0	1134	122	0
33	BA	32895	0	16553	571	0
33	DA	32895	0	16553	534	0
33	FA	32895	0	16553	435	3
33	HA	32895	0	16553	430	0
34	BB	1704	0	1732	67	0
34	DB	1704	0	1732	87	0
34	FB	1704	0	1732	79	0
34	HB	1704	0	1732	72	0
35	BC	1624	0	1696	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	DC	1624	0	1696	40	0
35	FC	1624	0	1696	38	0
35	HC	1624	0	1696	50	0
36	BD	1643	0	1707	80	0
36	DD	1643	0	1707	83	0
36	FD	1643	0	1707	73	0
36	HD	1643	0	1707	72	0
37	BE	1105	0	1148	61	0
37	DE	1105	0	1148	33	0
37	FE	1105	0	1148	50	0
37	HE	1105	0	1148	37	0
38	BF	817	0	808	51	0
38	DF	817	0	808	28	0
38	FF	817	0	808	28	0
38	HF	817	0	808	25	0
39	BG	1181	0	1238	25	0
39	DG	1181	0	1238	31	0
39	FG	1181	0	1238	35	0
39	HG	1181	0	1238	38	0
40	BH	979	0	1031	50	0
40	DH	979	0	1031	28	0
40	FH	979	0	1031	34	0
40	HH	979	0	1031	28	0
41	BI	1022	0	1070	58	0
41	DI	1022	0	1070	53	0
41	FI	1022	0	1070	44	0
41	HI	1022	0	1070	59	0
42	BJ	786	0	828	26	0
42	DJ	786	0	828	34	0
42	FJ	786	0	828	43	0
42	HJ	786	0	828	34	0
43	BK	877	0	887	75	0
43	DK	877	0	887	45	0
43	FK	877	0	887	38	0
43	HK	877	0	887	75	0
44	BL	955	0	1016	55	0
44	DL	955	0	1016	52	0
44	FL	955	0	1016	51	0
44	HL	955	0	1016	39	0
45	BM	883	0	941	26	0
45	DM	883	0	941	25	0
45	FM	883	0	941	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	HM	883	0	941	53	0
46	BN	774	0	824	32	0
46	DN	774	0	824	21	0
46	FN	774	0	824	30	0
46	HN	774	0	824	29	0
47	BO	714	0	734	18	0
47	DO	714	0	734	13	0
47	FO	714	0	734	17	0
47	HO	714	0	734	21	0
48	BP	649	0	666	29	0
48	DP	649	0	666	25	0
48	FP	649	0	666	18	0
48	HP	649	0	666	19	0
49	BQ	648	0	691	19	0
49	DQ	648	0	691	21	0
49	FQ	648	0	691	16	0
49	HQ	648	0	691	21	0
50	BR	455	0	478	19	0
50	DR	455	0	478	16	0
50	FR	455	0	478	16	0
50	HR	455	0	478	15	0
51	BS	637	0	665	23	0
51	DS	637	0	665	17	0
51	FS	637	0	665	30	0
51	HS	637	0	665	21	0
52	BT	665	0	714	30	0
52	DT	665	0	714	26	0
52	FT	665	0	714	30	0
52	HT	665	0	714	19	0
53	BU	425	0	449	40	0
53	DU	425	0	449	28	0
53	FU	425	0	449	24	0
53	HU	425	0	449	36	0
54	BV	5319	0	5228	105	0
54	DV	5319	0	5228	113	0
54	FV	5319	0	5229	111	0
54	HV	5319	0	5227	145	0
55	BW	48	0	41	7	0
55	DW	48	0	41	8	0
55	FW	48	0	39	9	0
56	A3	1	0	0	0	0
56	AA	130	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	AB	4	0	0	0	0
56	AC	3	0	0	0	0
56	AD	1	0	0	0	0
56	AE	1	0	0	0	0
56	AT	1	0	0	0	0
56	BA	40	0	0	0	0
56	BE	1	0	0	0	0
56	BL	1	0	0	0	0
56	BU	1	0	0	0	0
56	BV	1	0	0	0	0
56	C4	1	0	0	0	0
56	CA	134	0	0	0	0
56	CB	4	0	0	0	0
56	CD	1	0	0	0	0
56	CE	1	0	0	0	0
56	DA	42	0	0	0	0
56	DU	1	0	0	0	0
56	DV	1	0	0	0	0
56	EA	133	0	0	0	0
56	EB	4	0	0	0	0
56	EC	1	0	0	0	0
56	ED	2	0	0	0	0
56	EQ	1	0	0	0	0
56	FA	41	0	0	0	0
56	FE	1	0	0	0	0
56	FU	1	0	0	0	0
56	FV	1	0	0	0	0
56	GA	134	0	0	0	0
56	GB	4	0	0	0	0
56	GC	1	0	0	0	0
56	GL	1	0	0	0	0
56	GS	1	0	0	0	0
56	HA	40	0	0	0	0
56	HC	1	0	0	0	0
56	HE	1	0	0	0	0
56	HT	1	0	0	0	0
56	HV	1	0	0	0	0
57	A4	1	0	0	0	0
57	C4	1	0	0	0	0
57	E4	1	0	0	0	0
57	G4	1	0	0	0	0
58	BV	32	0	14	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	DV	32	0	14	1	0
58	FV	32	0	14	5	0
58	HV	32	0	14	1	0
59	A0	1	0	0	0	0
59	A3	1	0	0	0	0
59	A4	2	0	0	0	0
59	AA	608	0	0	111	0
59	AB	19	0	0	1	0
59	AC	10	0	0	0	0
59	AD	3	0	0	0	0
59	AE	1	0	0	0	0
59	AJ	1	0	0	1	0
59	AL	7	0	0	1	0
59	AN	4	0	0	0	0
59	AP	1	0	0	0	0
59	AQ	1	0	0	0	0
59	AS	1	0	0	0	0
59	AU	1	0	0	0	0
59	BA	197	0	0	36	0
59	BC	1	0	0	0	0
59	BD	1	0	0	0	0
59	BI	1	0	0	0	0
59	BK	1	0	0	0	0
59	BN	3	0	0	0	0
59	BT	2	0	0	0	0
59	BU	1	0	0	0	0
59	BV	1	0	0	1	0
59	C2	1	0	0	0	0
59	C3	1	0	0	0	0
59	C4	2	0	0	0	0
59	CA	604	0	0	104	0
59	CB	20	0	0	2	0
59	CC	11	0	0	4	0
59	CD	3	0	0	0	0
59	CE	1	0	0	0	0
59	CF	1	0	0	0	0
59	CJ	3	0	0	2	0
59	CL	6	0	0	1	0
59	CN	4	0	0	0	0
59	CS	1	0	0	0	0
59	CT	2	0	0	0	0
59	DA	193	0	0	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	DC	1	0	0	0	0
59	DE	2	0	0	0	0
59	DG	1	0	0	0	0
59	DK	1	0	0	0	0
59	DL	1	0	0	0	0
59	DN	6	0	0	0	0
59	DQ	1	0	0	0	0
59	DT	1	0	0	1	0
59	DU	1	0	0	0	0
59	DV	1	0	0	1	0
59	E0	2	0	0	0	0
59	E3	2	0	0	0	0
59	E4	1	0	0	0	0
59	EA	617	0	0	88	0
59	EB	20	0	0	1	0
59	EC	8	0	0	0	0
59	ED	1	0	0	0	0
59	EL	4	0	0	0	0
59	EN	2	0	0	0	0
59	ER	1	0	0	0	0
59	ET	1	0	0	0	0
59	EU	1	0	0	0	0
59	FA	198	0	0	21	0
59	FE	1	0	0	0	0
59	FK	1	0	0	0	0
59	FN	3	0	0	0	0
59	FQ	1	0	0	0	0
59	FT	4	0	0	1	0
59	FV	1	0	0	1	0
59	G2	2	0	0	0	0
59	G3	1	0	0	0	0
59	G4	1	0	0	0	0
59	GA	607	0	0	87	0
59	GB	19	0	0	1	0
59	GC	9	0	0	2	0
59	GD	4	0	0	0	0
59	GE	2	0	0	0	0
59	GL	4	0	0	1	0
59	GN	3	0	0	0	0
59	GQ	1	0	0	0	0
59	GR	2	0	0	0	0
59	GS	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	GT	1	0	0	0	0
59	GU	2	0	0	0	0
59	GV	1	0	0	1	0
59	HA	197	0	0	33	0
59	HD	1	0	0	0	0
59	HE	3	0	0	0	0
59	HN	5	0	0	0	0
59	HT	1	0	0	0	0
59	HU	1	0	0	0	0
59	HV	1	0	0	1	0
All	All	590573	0	402393	12569	4

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

The worst 5 of 12569 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:A5:117:LEU:CD2	32:A5:120:ALA:HA	1.56	1.35
32:A5:24:SER:CB	32:A5:116:GLU:HG2	1.59	1.32
32:A5:24:SER:O	32:A5:116:GLU:HB3	1.37	1.24
32:E5:117:LEU:CD2	32:E5:120:ALA:HA	1.70	1.20
32:E5:24:SER:CB	32:E5:116:GLU:HG2	1.75	1.16

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:FA:1029:U:O3'	1:GA:1508:A:N6[1_565]	2.13	0.07
33:FA:1029:U:OP2	1:GA:1509:A:N6[1_565]	2.16	0.04
33:FA:1029:U:O2'	1:GA:1508:A:N6[1_565]	2.16	0.04
6:GF:20:ASN:ND2	21:GU:52:ASN:OD1[2_556]	2.18	0.02

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AC	269/273 (98%)	220 (82%)	34 (13%)	15 (6%)	2	5
3	CC	269/273 (98%)	218 (81%)	35 (13%)	16 (6%)	1	5
3	EC	269/273 (98%)	219 (81%)	36 (13%)	14 (5%)	2	6
3	GC	269/273 (98%)	225 (84%)	30 (11%)	14 (5%)	2	6
4	AD	207/209 (99%)	161 (78%)	33 (16%)	13 (6%)	1	4
4	CD	207/209 (99%)	160 (77%)	33 (16%)	14 (7%)	1	3
4	ED	207/209 (99%)	155 (75%)	34 (16%)	18 (9%)	1	2
4	GD	207/209 (99%)	158 (76%)	34 (16%)	15 (7%)	1	3
5	AE	199/201 (99%)	163 (82%)	24 (12%)	12 (6%)	1	4
5	CE	199/201 (99%)	161 (81%)	26 (13%)	12 (6%)	1	4
5	EE	199/201 (99%)	162 (81%)	25 (13%)	12 (6%)	1	4
5	GE	199/201 (99%)	162 (81%)	25 (13%)	12 (6%)	1	4
6	AF	175/179 (98%)	128 (73%)	41 (23%)	6 (3%)	3	15
6	CF	175/179 (98%)	132 (75%)	37 (21%)	6 (3%)	3	15
6	EF	175/179 (98%)	139 (79%)	29 (17%)	7 (4%)	3	11
6	GF	175/179 (98%)	132 (75%)	40 (23%)	3 (2%)	9	31
7	AG	174/177 (98%)	124 (71%)	33 (19%)	17 (10%)	0	1
7	CG	174/177 (98%)	123 (71%)	37 (21%)	14 (8%)	1	2
7	EG	174/177 (98%)	120 (69%)	43 (25%)	11 (6%)	1	4
7	GG	174/177 (98%)	118 (68%)	41 (24%)	15 (9%)	1	2
8	AH	48/50 (96%)	24 (50%)	19 (40%)	5 (10%)	0	1
8	CH	48/50 (96%)	23 (48%)	19 (40%)	6 (12%)	0	0
8	EH	48/50 (96%)	24 (50%)	19 (40%)	5 (10%)	0	1
8	GH	48/50 (96%)	24 (50%)	21 (44%)	3 (6%)	1	4
9	AI	139/142 (98%)	87 (63%)	45 (32%)	7 (5%)	2	7
9	CI	139/142 (98%)	92 (66%)	37 (27%)	10 (7%)	1	3
9	EI	139/142 (98%)	90 (65%)	42 (30%)	7 (5%)	2	7
9	GI	139/142 (98%)	89 (64%)	38 (27%)	12 (9%)	1	2
10	AJ	140/142 (99%)	114 (81%)	18 (13%)	8 (6%)	1	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
10	CJ	140/142 (99%)	113 (81%)	19 (14%)	8 (6%)	1 5
10	EJ	140/142 (99%)	113 (81%)	19 (14%)	8 (6%)	1 5
10	GJ	140/142 (99%)	114 (81%)	17 (12%)	9 (6%)	1 4
11	AK	120/123 (98%)	93 (78%)	17 (14%)	10 (8%)	1 2
11	CK	120/123 (98%)	91 (76%)	21 (18%)	8 (7%)	1 3
11	EK	120/123 (98%)	92 (77%)	17 (14%)	11 (9%)	1 1
11	GK	120/123 (98%)	92 (77%)	19 (16%)	9 (8%)	1 2
12	AL	141/144 (98%)	107 (76%)	26 (18%)	8 (6%)	1 5
12	CL	141/144 (98%)	107 (76%)	27 (19%)	7 (5%)	2 7
12	EL	141/144 (98%)	108 (77%)	26 (18%)	7 (5%)	2 7
12	GL	141/144 (98%)	109 (77%)	25 (18%)	7 (5%)	2 7
13	AM	134/136 (98%)	105 (78%)	22 (16%)	7 (5%)	2 6
13	CM	134/136 (98%)	111 (83%)	16 (12%)	7 (5%)	2 6
13	EM	134/136 (98%)	110 (82%)	18 (13%)	6 (4%)	2 9
13	GM	134/136 (98%)	112 (84%)	16 (12%)	6 (4%)	2 9
14	AN	118/127 (93%)	101 (86%)	15 (13%)	2 (2%)	9 31
14	CN	118/127 (93%)	98 (83%)	17 (14%)	3 (2%)	5 21
14	EN	118/127 (93%)	101 (86%)	14 (12%)	3 (2%)	5 21
14	GN	118/127 (93%)	98 (83%)	19 (16%)	1 (1%)	19 51
15	AO	114/117 (97%)	99 (87%)	14 (12%)	1 (1%)	17 48
15	CO	114/117 (97%)	96 (84%)	17 (15%)	1 (1%)	17 48
15	EO	114/117 (97%)	96 (84%)	18 (16%)	0	100 100
15	GO	114/117 (97%)	97 (85%)	13 (11%)	4 (4%)	3 14
16	AP	112/115 (97%)	83 (74%)	22 (20%)	7 (6%)	1 4
16	CP	112/115 (97%)	81 (72%)	22 (20%)	9 (8%)	1 2
16	EP	112/115 (97%)	83 (74%)	22 (20%)	7 (6%)	1 4
16	GP	112/115 (97%)	79 (70%)	21 (19%)	12 (11%)	0 1
17	AQ	115/118 (98%)	101 (88%)	9 (8%)	5 (4%)	2 10
17	CQ	115/118 (98%)	102 (89%)	9 (8%)	4 (4%)	3 14
17	EQ	115/118 (98%)	102 (89%)	8 (7%)	5 (4%)	2 10
17	GQ	115/118 (98%)	103 (90%)	7 (6%)	5 (4%)	2 10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
18	AR	101/103 (98%)	83 (82%)	15 (15%)	3 (3%)	4 17
18	CR	101/103 (98%)	83 (82%)	15 (15%)	3 (3%)	4 17
18	ER	101/103 (98%)	83 (82%)	15 (15%)	3 (3%)	4 17
18	GR	101/103 (98%)	84 (83%)	13 (13%)	4 (4%)	3 11
19	AS	108/110 (98%)	93 (86%)	10 (9%)	5 (5%)	2 9
19	CS	108/110 (98%)	96 (89%)	8 (7%)	4 (4%)	3 13
19	ES	108/110 (98%)	91 (84%)	12 (11%)	5 (5%)	2 9
19	GS	108/110 (98%)	92 (85%)	11 (10%)	5 (5%)	2 9
20	AT	91/100 (91%)	59 (65%)	24 (26%)	8 (9%)	1 2
20	CT	91/100 (91%)	60 (66%)	23 (25%)	8 (9%)	1 2
20	ET	91/100 (91%)	59 (65%)	25 (28%)	7 (8%)	1 2
20	GT	91/100 (91%)	60 (66%)	22 (24%)	9 (10%)	0 1
21	AU	100/104 (96%)	73 (73%)	18 (18%)	9 (9%)	1 1
21	CU	100/104 (96%)	74 (74%)	16 (16%)	10 (10%)	0 1
21	EU	100/104 (96%)	74 (74%)	13 (13%)	13 (13%)	0 0
21	GU	100/104 (96%)	73 (73%)	18 (18%)	9 (9%)	1 1
22	AV	92/94 (98%)	82 (89%)	9 (10%)	1 (1%)	14 42
22	CV	92/94 (98%)	79 (86%)	12 (13%)	1 (1%)	14 42
22	EV	92/94 (98%)	82 (89%)	9 (10%)	1 (1%)	14 42
22	GV	92/94 (98%)	83 (90%)	8 (9%)	1 (1%)	14 42
23	AW	77/85 (91%)	41 (53%)	19 (25%)	17 (22%)	0 0
23	CW	77/85 (91%)	42 (54%)	21 (27%)	14 (18%)	0 0
23	EW	77/85 (91%)	42 (54%)	19 (25%)	16 (21%)	0 0
23	GW	77/85 (91%)	42 (54%)	21 (27%)	14 (18%)	0 0
24	AX	75/78 (96%)	65 (87%)	7 (9%)	3 (4%)	3 11
24	CX	75/78 (96%)	64 (85%)	8 (11%)	3 (4%)	3 11
24	EX	75/78 (96%)	64 (85%)	9 (12%)	2 (3%)	5 19
24	GX	75/78 (96%)	65 (87%)	9 (12%)	1 (1%)	12 37
25	AY	61/63 (97%)	40 (66%)	19 (31%)	2 (3%)	4 15
25	CY	61/63 (97%)	43 (70%)	17 (28%)	1 (2%)	9 32
25	EY	61/63 (97%)	38 (62%)	19 (31%)	4 (7%)	1 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
25	GY	61/63 (97%)	42 (69%)	17 (28%)	2 (3%)	4 15
26	AZ	56/59 (95%)	49 (88%)	5 (9%)	2 (4%)	3 14
26	CZ	56/59 (95%)	49 (88%)	5 (9%)	2 (4%)	3 14
26	EZ	56/59 (95%)	48 (86%)	6 (11%)	2 (4%)	3 14
26	GZ	56/59 (95%)	49 (88%)	5 (9%)	2 (4%)	3 14
27	A0	54/57 (95%)	45 (83%)	6 (11%)	3 (6%)	2 5
27	C0	54/57 (95%)	45 (83%)	6 (11%)	3 (6%)	2 5
27	E0	54/57 (95%)	45 (83%)	6 (11%)	3 (6%)	2 5
27	G0	54/57 (95%)	45 (83%)	6 (11%)	3 (6%)	2 5
28	A1	48/55 (87%)	40 (83%)	5 (10%)	3 (6%)	1 4
28	C1	48/55 (87%)	40 (83%)	6 (12%)	2 (4%)	3 10
28	E1	48/55 (87%)	42 (88%)	5 (10%)	1 (2%)	7 26
28	G1	48/55 (87%)	41 (85%)	5 (10%)	2 (4%)	3 10
29	A2	44/46 (96%)	39 (89%)	4 (9%)	1 (2%)	6 23
29	C2	44/46 (96%)	39 (89%)	4 (9%)	1 (2%)	6 23
29	E2	44/46 (96%)	39 (89%)	4 (9%)	1 (2%)	6 23
29	G2	44/46 (96%)	39 (89%)	4 (9%)	1 (2%)	6 23
30	A3	62/65 (95%)	56 (90%)	4 (6%)	2 (3%)	4 16
30	C3	62/65 (95%)	56 (90%)	4 (6%)	2 (3%)	4 16
30	E3	62/65 (95%)	55 (89%)	5 (8%)	2 (3%)	4 16
30	G3	62/65 (95%)	56 (90%)	4 (6%)	2 (3%)	4 16
31	A4	36/38 (95%)	31 (86%)	2 (6%)	3 (8%)	1 2
31	C4	36/38 (95%)	31 (86%)	3 (8%)	2 (6%)	2 5
31	E4	36/38 (95%)	31 (86%)	2 (6%)	3 (8%)	1 2
31	G4	36/38 (95%)	30 (83%)	4 (11%)	2 (6%)	2 5
32	A5	146/165 (88%)	80 (55%)	44 (30%)	22 (15%)	0 0
32	E5	142/165 (86%)	80 (56%)	39 (28%)	23 (16%)	0 0
34	BB	216/241 (90%)	147 (68%)	57 (26%)	12 (6%)	2 5
34	DB	216/241 (90%)	145 (67%)	59 (27%)	12 (6%)	2 5
34	FB	216/241 (90%)	146 (68%)	60 (28%)	10 (5%)	2 9
34	HB	216/241 (90%)	149 (69%)	55 (26%)	12 (6%)	2 5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
35	BC	204/233 (88%)	180 (88%)	16 (8%)	8 (4%)	3 12
35	DC	204/233 (88%)	177 (87%)	23 (11%)	4 (2%)	7 27
35	FC	204/233 (88%)	181 (89%)	17 (8%)	6 (3%)	4 18
35	HC	204/233 (88%)	183 (90%)	16 (8%)	5 (2%)	5 21
36	BD	203/206 (98%)	157 (77%)	34 (17%)	12 (6%)	1 5
36	DD	203/206 (98%)	157 (77%)	30 (15%)	16 (8%)	1 2
36	FD	203/206 (98%)	155 (76%)	34 (17%)	14 (7%)	1 3
36	HD	203/206 (98%)	159 (78%)	35 (17%)	9 (4%)	2 10
37	BE	148/167 (89%)	124 (84%)	19 (13%)	5 (3%)	3 15
37	DE	148/167 (89%)	125 (84%)	18 (12%)	5 (3%)	3 15
37	FE	148/167 (89%)	122 (82%)	22 (15%)	4 (3%)	5 19
37	HE	148/167 (89%)	122 (82%)	22 (15%)	4 (3%)	5 19
38	BF	98/135 (73%)	73 (74%)	20 (20%)	5 (5%)	2 7
38	DF	98/135 (73%)	71 (72%)	20 (20%)	7 (7%)	1 3
38	FF	98/135 (73%)	72 (74%)	16 (16%)	10 (10%)	0 1
38	HF	98/135 (73%)	75 (76%)	18 (18%)	5 (5%)	2 7
39	BG	149/179 (83%)	126 (85%)	23 (15%)	0	100 100
39	DG	149/179 (83%)	123 (83%)	25 (17%)	1 (1%)	22 54
39	FG	149/179 (83%)	126 (85%)	23 (15%)	0	100 100
39	HG	149/179 (83%)	122 (82%)	25 (17%)	2 (1%)	12 37
40	BH	127/130 (98%)	108 (85%)	18 (14%)	1 (1%)	19 51
40	DH	127/130 (98%)	110 (87%)	15 (12%)	2 (2%)	9 32
40	FH	127/130 (98%)	113 (89%)	12 (9%)	2 (2%)	9 32
40	HH	127/130 (98%)	111 (87%)	16 (13%)	0	100 100
41	BI	125/130 (96%)	96 (77%)	21 (17%)	8 (6%)	1 4
41	DI	125/130 (96%)	99 (79%)	19 (15%)	7 (6%)	2 5
41	FI	125/130 (96%)	97 (78%)	22 (18%)	6 (5%)	2 8
41	HI	125/130 (96%)	98 (78%)	21 (17%)	6 (5%)	2 8
42	BJ	96/103 (93%)	73 (76%)	16 (17%)	7 (7%)	1 3
42	DJ	96/103 (93%)	72 (75%)	18 (19%)	6 (6%)	1 4
42	FJ	96/103 (93%)	73 (76%)	17 (18%)	6 (6%)	1 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
42	HJ	96/103 (93%)	73 (76%)	19 (20%)	4 (4%)	3 10
43	BK	115/129 (89%)	92 (80%)	17 (15%)	6 (5%)	2 6
43	DK	115/129 (89%)	90 (78%)	23 (20%)	2 (2%)	9 31
43	FK	115/129 (89%)	92 (80%)	20 (17%)	3 (3%)	5 20
43	HK	115/129 (89%)	87 (76%)	24 (21%)	4 (4%)	3 14
44	BL	121/124 (98%)	95 (78%)	17 (14%)	9 (7%)	1 2
44	DL	121/124 (98%)	95 (78%)	18 (15%)	8 (7%)	1 3
44	FL	121/124 (98%)	96 (79%)	17 (14%)	8 (7%)	1 3
44	HL	121/124 (98%)	97 (80%)	15 (12%)	9 (7%)	1 2
45	BM	112/118 (95%)	98 (88%)	8 (7%)	6 (5%)	2 6
45	DM	112/118 (95%)	99 (88%)	7 (6%)	6 (5%)	2 6
45	FM	112/118 (95%)	98 (88%)	9 (8%)	5 (4%)	2 9
45	HM	112/118 (95%)	91 (81%)	14 (12%)	7 (6%)	1 4
46	BN	92/101 (91%)	71 (77%)	18 (20%)	3 (3%)	4 15
46	DN	92/101 (91%)	71 (77%)	19 (21%)	2 (2%)	6 24
46	FN	92/101 (91%)	69 (75%)	20 (22%)	3 (3%)	4 15
46	HN	92/101 (91%)	70 (76%)	20 (22%)	2 (2%)	6 24
47	BO	86/89 (97%)	72 (84%)	12 (14%)	2 (2%)	6 23
47	DO	86/89 (97%)	73 (85%)	11 (13%)	2 (2%)	6 23
47	FO	86/89 (97%)	72 (84%)	12 (14%)	2 (2%)	6 23
47	HO	86/89 (97%)	70 (81%)	14 (16%)	2 (2%)	6 23
48	BP	80/82 (98%)	60 (75%)	16 (20%)	4 (5%)	2 7
48	DP	80/82 (98%)	62 (78%)	16 (20%)	2 (2%)	5 21
48	FP	80/82 (98%)	65 (81%)	13 (16%)	2 (2%)	5 21
48	HP	80/82 (98%)	61 (76%)	15 (19%)	4 (5%)	2 7
49	BQ	78/84 (93%)	54 (69%)	19 (24%)	5 (6%)	1 4
49	DQ	78/84 (93%)	56 (72%)	16 (20%)	6 (8%)	1 2
49	FQ	78/84 (93%)	57 (73%)	18 (23%)	3 (4%)	3 13
49	HQ	78/84 (93%)	57 (73%)	16 (20%)	5 (6%)	1 4
50	BR	53/75 (71%)	41 (77%)	12 (23%)	0	100 100
50	DR	53/75 (71%)	43 (81%)	10 (19%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
50	FR	53/75 (71%)	40 (76%)	13 (24%)	0	100 100
50	HR	53/75 (71%)	43 (81%)	10 (19%)	0	100 100
51	BS	77/92 (84%)	69 (90%)	7 (9%)	1 (1%)	12 37
51	DS	77/92 (84%)	70 (91%)	6 (8%)	1 (1%)	12 37
51	FS	77/92 (84%)	67 (87%)	6 (8%)	4 (5%)	2 6
51	HS	77/92 (84%)	68 (88%)	9 (12%)	0	100 100
52	BT	83/87 (95%)	66 (80%)	15 (18%)	2 (2%)	6 22
52	DT	83/87 (95%)	69 (83%)	11 (13%)	3 (4%)	3 14
52	FT	83/87 (95%)	66 (80%)	15 (18%)	2 (2%)	6 22
52	HT	83/87 (95%)	68 (82%)	14 (17%)	1 (1%)	13 40
53	BU	49/71 (69%)	25 (51%)	20 (41%)	4 (8%)	1 2
53	DU	49/71 (69%)	27 (55%)	20 (41%)	2 (4%)	3 11
53	FU	49/71 (69%)	28 (57%)	19 (39%)	2 (4%)	3 11
53	HU	49/71 (69%)	24 (49%)	22 (45%)	3 (6%)	1 4
54	BV	685/704 (97%)	559 (82%)	90 (13%)	36 (5%)	2 6
54	DV	685/704 (97%)	558 (82%)	92 (13%)	35 (5%)	2 7
54	FV	685/704 (97%)	556 (81%)	91 (13%)	38 (6%)	2 5
54	HV	685/704 (97%)	556 (81%)	91 (13%)	38 (6%)	2 5
55	BW	2/6 (33%)	0	0	2 (100%)	0 0
55	DW	2/6 (33%)	1 (50%)	1 (50%)	0	100 100
55	FW	2/6 (33%)	2 (100%)	0	0	100 100
All	All	25122/26708 (94%)	19751 (79%)	4073 (16%)	1298 (5%)	2 6

5 of 1298 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AC	70	LYS
3	AC	104	LEU
3	AC	121	ALA
3	AC	140	VAL
3	AC	256	THR

5.3.2 Protein sidechains (i)

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
3	AC	216/218 (99%)	203 (94%)	13 (6%)	19 49
3	CC	216/218 (99%)	201 (93%)	15 (7%)	15 41
3	EC	216/218 (99%)	200 (93%)	16 (7%)	13 38
3	GC	216/218 (99%)	198 (92%)	18 (8%)	11 32
4	AD	164/164 (100%)	153 (93%)	11 (7%)	16 43
4	CD	164/164 (100%)	156 (95%)	8 (5%)	25 57
4	ED	164/164 (100%)	155 (94%)	9 (6%)	21 53
4	GD	164/164 (100%)	156 (95%)	8 (5%)	25 57
5	AE	165/165 (100%)	154 (93%)	11 (7%)	16 43
5	CE	165/165 (100%)	158 (96%)	7 (4%)	30 63
5	EE	165/165 (100%)	153 (93%)	12 (7%)	14 38
5	GE	165/165 (100%)	160 (97%)	5 (3%)	41 75
6	AF	148/150 (99%)	140 (95%)	8 (5%)	22 54
6	CF	148/150 (99%)	139 (94%)	9 (6%)	18 48
6	EF	148/150 (99%)	138 (93%)	10 (7%)	16 42
6	GF	148/150 (99%)	144 (97%)	4 (3%)	44 77
7	AG	137/138 (99%)	126 (92%)	11 (8%)	12 33
7	CG	137/138 (99%)	126 (92%)	11 (8%)	12 33
7	EG	137/138 (99%)	125 (91%)	12 (9%)	10 30
7	GG	137/138 (99%)	130 (95%)	7 (5%)	24 56
8	AH	40/40 (100%)	38 (95%)	2 (5%)	24 57
8	CH	40/40 (100%)	39 (98%)	1 (2%)	47 78
8	EH	40/40 (100%)	36 (90%)	4 (10%)	7 23
8	GH	40/40 (100%)	36 (90%)	4 (10%)	7 23
9	AI	109/110 (99%)	105 (96%)	4 (4%)	34 68
9	CI	109/110 (99%)	108 (99%)	1 (1%)	78 93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
9	EI	109/110 (99%)	108 (99%)	1 (1%)	78 93
9	GI	109/110 (99%)	108 (99%)	1 (1%)	78 93
10	AJ	116/116 (100%)	97 (84%)	19 (16%)	2 7
10	CJ	116/116 (100%)	102 (88%)	14 (12%)	5 15
10	EJ	116/116 (100%)	96 (83%)	20 (17%)	2 6
10	GJ	116/116 (100%)	103 (89%)	13 (11%)	6 18
11	AK	103/104 (99%)	93 (90%)	10 (10%)	8 25
11	CK	103/104 (99%)	94 (91%)	9 (9%)	10 30
11	EK	103/104 (99%)	95 (92%)	8 (8%)	12 34
11	GK	103/104 (99%)	96 (93%)	7 (7%)	16 42
12	AL	102/103 (99%)	96 (94%)	6 (6%)	19 49
12	CL	102/103 (99%)	96 (94%)	6 (6%)	19 49
12	EL	102/103 (99%)	97 (95%)	5 (5%)	25 57
12	GL	102/103 (99%)	94 (92%)	8 (8%)	12 34
13	AM	109/109 (100%)	94 (86%)	15 (14%)	3 10
13	CM	109/109 (100%)	96 (88%)	13 (12%)	5 15
13	EM	109/109 (100%)	100 (92%)	9 (8%)	11 32
13	GM	109/109 (100%)	102 (94%)	7 (6%)	17 45
14	AN	100/103 (97%)	94 (94%)	6 (6%)	19 49
14	CN	100/103 (97%)	93 (93%)	7 (7%)	15 41
14	EN	100/103 (97%)	98 (98%)	2 (2%)	55 82
14	GN	100/103 (97%)	96 (96%)	4 (4%)	31 65
15	AO	86/87 (99%)	81 (94%)	5 (6%)	20 50
15	CO	86/87 (99%)	80 (93%)	6 (7%)	15 41
15	EO	86/87 (99%)	79 (92%)	7 (8%)	11 33
15	GO	86/87 (99%)	83 (96%)	3 (4%)	36 70
16	AP	99/100 (99%)	85 (86%)	14 (14%)	3 10
16	CP	99/100 (99%)	88 (89%)	11 (11%)	6 19
16	EP	99/100 (99%)	91 (92%)	8 (8%)	11 33
16	GP	99/100 (99%)	88 (89%)	11 (11%)	6 19
17	AQ	89/90 (99%)	83 (93%)	6 (7%)	16 43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
17	CQ	89/90 (99%)	82 (92%)	7 (8%)	12 34
17	EQ	89/90 (99%)	80 (90%)	9 (10%)	7 23
17	GQ	89/90 (99%)	86 (97%)	3 (3%)	37 71
18	AR	84/84 (100%)	79 (94%)	5 (6%)	19 49
18	CR	84/84 (100%)	78 (93%)	6 (7%)	14 40
18	ER	84/84 (100%)	77 (92%)	7 (8%)	11 32
18	GR	84/84 (100%)	80 (95%)	4 (5%)	25 58
19	AS	93/93 (100%)	85 (91%)	8 (9%)	10 30
19	CS	93/93 (100%)	86 (92%)	7 (8%)	13 37
19	ES	93/93 (100%)	84 (90%)	9 (10%)	8 25
19	GS	93/93 (100%)	86 (92%)	7 (8%)	13 37
20	AT	80/84 (95%)	71 (89%)	9 (11%)	6 18
20	CT	80/84 (95%)	77 (96%)	3 (4%)	33 67
20	ET	80/84 (95%)	73 (91%)	7 (9%)	10 30
20	GT	80/84 (95%)	76 (95%)	4 (5%)	24 57
21	AU	83/85 (98%)	79 (95%)	4 (5%)	25 58
21	CU	83/85 (98%)	80 (96%)	3 (4%)	35 69
21	EU	83/85 (98%)	76 (92%)	7 (8%)	11 31
21	GU	83/85 (98%)	80 (96%)	3 (4%)	35 69
22	AV	78/78 (100%)	73 (94%)	5 (6%)	17 45
22	CV	78/78 (100%)	75 (96%)	3 (4%)	33 67
22	EV	78/78 (100%)	76 (97%)	2 (3%)	46 77
22	GV	78/78 (100%)	75 (96%)	3 (4%)	33 67
23	AW	59/63 (94%)	49 (83%)	10 (17%)	2 6
23	CW	59/63 (94%)	51 (86%)	8 (14%)	3 11
23	EW	59/63 (94%)	52 (88%)	7 (12%)	5 15
23	GW	59/63 (94%)	53 (90%)	6 (10%)	7 22
24	AX	67/68 (98%)	61 (91%)	6 (9%)	9 29
24	CX	67/68 (98%)	60 (90%)	7 (10%)	7 21
24	EX	67/68 (98%)	60 (90%)	7 (10%)	7 21
24	GX	67/68 (98%)	61 (91%)	6 (9%)	9 29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
25	AY	55/55 (100%)	49 (89%)	6 (11%)	6 19
25	CY	55/55 (100%)	53 (96%)	2 (4%)	35 69
25	EY	55/55 (100%)	49 (89%)	6 (11%)	6 19
25	GY	55/55 (100%)	51 (93%)	4 (7%)	14 38
26	AZ	48/49 (98%)	44 (92%)	4 (8%)	11 32
26	CZ	48/49 (98%)	43 (90%)	5 (10%)	7 21
26	EZ	48/49 (98%)	44 (92%)	4 (8%)	11 32
26	GZ	48/49 (98%)	43 (90%)	5 (10%)	7 21
27	A0	47/48 (98%)	47 (100%)	0	100 100
27	C0	47/48 (98%)	45 (96%)	2 (4%)	29 62
27	E0	47/48 (98%)	45 (96%)	2 (4%)	29 62
27	G0	47/48 (98%)	47 (100%)	0	100 100
28	A1	45/49 (92%)	42 (93%)	3 (7%)	16 43
28	C1	45/49 (92%)	41 (91%)	4 (9%)	9 29
28	E1	45/49 (92%)	43 (96%)	2 (4%)	28 61
28	G1	45/49 (92%)	44 (98%)	1 (2%)	52 81
29	A2	38/38 (100%)	37 (97%)	1 (3%)	46 77
29	C2	38/38 (100%)	35 (92%)	3 (8%)	12 34
29	E2	38/38 (100%)	33 (87%)	5 (13%)	4 12
29	G2	38/38 (100%)	34 (90%)	4 (10%)	7 21
30	A3	51/52 (98%)	49 (96%)	2 (4%)	32 66
30	C3	51/52 (98%)	50 (98%)	1 (2%)	55 82
30	E3	51/52 (98%)	47 (92%)	4 (8%)	12 34
30	G3	51/52 (98%)	47 (92%)	4 (8%)	12 34
31	A4	34/34 (100%)	32 (94%)	2 (6%)	19 49
31	C4	34/34 (100%)	32 (94%)	2 (6%)	19 49
31	E4	34/34 (100%)	32 (94%)	2 (6%)	19 49
31	G4	34/34 (100%)	31 (91%)	3 (9%)	10 30
32	A5	112/123 (91%)	95 (85%)	17 (15%)	3 8
32	E5	110/123 (89%)	96 (87%)	14 (13%)	4 13
34	BB	180/199 (90%)	171 (95%)	9 (5%)	24 57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
34	DB	180/199 (90%)	171 (95%)	9 (5%)	24 57
34	FB	180/199 (90%)	172 (96%)	8 (4%)	28 61
34	HB	180/199 (90%)	170 (94%)	10 (6%)	21 52
35	BC	170/190 (90%)	167 (98%)	3 (2%)	59 85
35	DC	170/190 (90%)	166 (98%)	4 (2%)	49 79
35	FC	170/190 (90%)	158 (93%)	12 (7%)	14 40
35	HC	170/190 (90%)	164 (96%)	6 (4%)	36 70
36	BD	172/173 (99%)	163 (95%)	9 (5%)	23 55
36	DD	172/173 (99%)	162 (94%)	10 (6%)	20 50
36	FD	172/173 (99%)	162 (94%)	10 (6%)	20 50
36	HD	172/173 (99%)	163 (95%)	9 (5%)	23 55
37	BE	113/126 (90%)	107 (95%)	6 (5%)	22 54
37	DE	113/126 (90%)	110 (97%)	3 (3%)	44 77
37	FE	113/126 (90%)	104 (92%)	9 (8%)	12 33
37	HE	113/126 (90%)	106 (94%)	7 (6%)	18 47
38	BF	87/116 (75%)	83 (95%)	4 (5%)	27 60
38	DF	87/116 (75%)	85 (98%)	2 (2%)	50 80
38	FF	87/116 (75%)	84 (97%)	3 (3%)	37 71
38	HF	87/116 (75%)	85 (98%)	2 (2%)	50 80
39	BG	124/147 (84%)	122 (98%)	2 (2%)	62 86
39	DG	124/147 (84%)	121 (98%)	3 (2%)	49 79
39	FG	124/147 (84%)	120 (97%)	4 (3%)	39 73
39	HG	124/147 (84%)	123 (99%)	1 (1%)	81 94
40	BH	104/105 (99%)	98 (94%)	6 (6%)	20 50
40	DH	104/105 (99%)	97 (93%)	7 (7%)	16 43
40	FH	104/105 (99%)	97 (93%)	7 (7%)	16 43
40	HH	104/105 (99%)	98 (94%)	6 (6%)	20 50
41	BI	105/107 (98%)	96 (91%)	9 (9%)	10 30
41	DI	105/107 (98%)	102 (97%)	3 (3%)	42 76
41	FI	105/107 (98%)	98 (93%)	7 (7%)	16 43
41	HI	105/107 (98%)	99 (94%)	6 (6%)	20 51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
42	BJ	86/90 (96%)	85 (99%)	1 (1%)	71 91
42	DJ	86/90 (96%)	80 (93%)	6 (7%)	15 41
42	FJ	86/90 (96%)	84 (98%)	2 (2%)	50 80
42	HJ	86/90 (96%)	83 (96%)	3 (4%)	36 70
43	BK	90/99 (91%)	87 (97%)	3 (3%)	38 72
43	DK	90/99 (91%)	88 (98%)	2 (2%)	52 81
43	FK	90/99 (91%)	85 (94%)	5 (6%)	21 52
43	HK	90/99 (91%)	82 (91%)	8 (9%)	9 29
44	BL	103/104 (99%)	100 (97%)	3 (3%)	42 76
44	DL	103/104 (99%)	101 (98%)	2 (2%)	57 84
44	FL	103/104 (99%)	97 (94%)	6 (6%)	20 50
44	HL	103/104 (99%)	94 (91%)	9 (9%)	10 30
45	BM	92/96 (96%)	89 (97%)	3 (3%)	38 72
45	DM	92/96 (96%)	92 (100%)	0	100 100
45	FM	92/96 (96%)	92 (100%)	0	100 100
45	HM	92/96 (96%)	92 (100%)	0	100 100
46	BN	79/84 (94%)	79 (100%)	0	100 100
46	DN	79/84 (94%)	78 (99%)	1 (1%)	69 90
46	FN	79/84 (94%)	75 (95%)	4 (5%)	24 56
46	HN	79/84 (94%)	77 (98%)	2 (2%)	47 78
47	BO	76/77 (99%)	72 (95%)	4 (5%)	22 54
47	DO	76/77 (99%)	74 (97%)	2 (3%)	46 77
47	FO	76/77 (99%)	74 (97%)	2 (3%)	46 77
47	HO	76/77 (99%)	74 (97%)	2 (3%)	46 77
48	BP	65/65 (100%)	63 (97%)	2 (3%)	40 74
48	DP	65/65 (100%)	60 (92%)	5 (8%)	13 35
48	FP	65/65 (100%)	64 (98%)	1 (2%)	65 87
48	HP	65/65 (100%)	63 (97%)	2 (3%)	40 74
49	BQ	74/78 (95%)	70 (95%)	4 (5%)	22 54
49	DQ	74/78 (95%)	72 (97%)	2 (3%)	44 77
49	FQ	74/78 (95%)	73 (99%)	1 (1%)	67 89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
49	HQ	74/78 (95%)	69 (93%)	5 (7%)	16 42
50	BR	48/65 (74%)	48 (100%)	0	100 100
50	DR	48/65 (74%)	48 (100%)	0	100 100
50	FR	48/65 (74%)	46 (96%)	2 (4%)	30 63
50	HR	48/65 (74%)	48 (100%)	0	100 100
51	BS	70/79 (89%)	69 (99%)	1 (1%)	67 89
51	DS	70/79 (89%)	67 (96%)	3 (4%)	29 62
51	FS	70/79 (89%)	64 (91%)	6 (9%)	10 30
51	HS	70/79 (89%)	67 (96%)	3 (4%)	29 62
52	BT	65/66 (98%)	60 (92%)	5 (8%)	13 35
52	DT	65/66 (98%)	58 (89%)	7 (11%)	6 20
52	FT	65/66 (98%)	60 (92%)	5 (8%)	13 35
52	HT	65/66 (98%)	60 (92%)	5 (8%)	13 35
53	BU	44/61 (72%)	42 (96%)	2 (4%)	27 61
53	DU	44/61 (72%)	41 (93%)	3 (7%)	16 42
53	FU	44/61 (72%)	41 (93%)	3 (7%)	16 42
53	HU	44/61 (72%)	42 (96%)	2 (4%)	27 61
54	BV	557/578 (96%)	503 (90%)	54 (10%)	8 25
54	DV	557/578 (96%)	508 (91%)	49 (9%)	10 30
54	FV	557/578 (96%)	508 (91%)	49 (9%)	10 30
54	HV	557/578 (96%)	507 (91%)	50 (9%)	9 29
55	BW	2/2 (100%)	1 (50%)	1 (50%)	0 0
55	DW	2/2 (100%)	1 (50%)	1 (50%)	0 0
55	FW	2/2 (100%)	2 (100%)	0	100 100
All	All	20824/21780 (96%)	19507 (94%)	1317 (6%)	18 46

5 of 1317 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
49	DQ	48	ASP
10	EJ	95	ARG
40	HH	94	LYS
54	DV	77	LYS
3	EC	176	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 87 such sidechains are listed below:

Mol	Chain	Res	Type
7	EG	115	GLN
34	FB	57	ASN
51	HS	52	HIS
9	EI	33	ASN
22	EV	80	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	2850/2904 (98%)	472 (16%)	48 (1%)
1	CA	2850/2904 (98%)	470 (16%)	50 (1%)
1	EA	2850/2904 (98%)	471 (16%)	45 (1%)
1	GA	2850/2904 (98%)	471 (16%)	51 (1%)
2	AB	117/120 (97%)	17 (14%)	0
2	CB	117/120 (97%)	18 (15%)	1 (0%)
2	EB	117/120 (97%)	17 (14%)	0
2	GB	117/120 (97%)	19 (16%)	0
33	BA	1532/1542 (99%)	272 (17%)	18 (1%)
33	DA	1532/1542 (99%)	269 (17%)	18 (1%)
33	FA	1532/1542 (99%)	265 (17%)	17 (1%)
33	HA	1532/1542 (99%)	273 (17%)	18 (1%)
All	All	17996/18264 (98%)	3034 (16%)	266 (1%)

5 of 3034 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	10	A
1	AA	12	U
1	AA	15	G
1	AA	34	U
1	AA	35	G

5 of 266 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
33	DA	250	A
1	EA	764	A
1	GA	2756	U
33	DA	499	A
1	EA	119	A

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

12 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	$\#\|Z\|>2$
55	5OH	FW	6	55	8,12,13	1.80	2 (25%)	3,16,18	1.42	0
55	DPP	BW	2	55	3,5,6	1.07	0	1,5,7	0.68	0
55	KBE	FW	1	55	8,8,9	0.97	0	7,8,10	1.91	1 (14%)
55	5OH	BW	6	55	8,12,13	1.51	1 (12%)	3,16,18	1.02	0
55	KBE	DW	1	55	8,8,9	0.91	0	7,8,10	1.12	1 (14%)
55	KBE	BW	1	55	8,8,9	0.90	0	7,8,10	1.07	1 (14%)
55	5OH	DW	6	55	8,12,13	1.68	2 (25%)	3,16,18	1.60	1 (33%)
55	UAL	FW	5	55	7,8,9	2.44	4 (57%)	5,9,11	3.73	3 (60%)
55	DPP	FW	2	55	3,5,6	0.81	0	1,5,7	0.00	0
55	UAL	DW	5	55	7,8,9	2.62	4 (57%)	5,9,11	4.77	2 (40%)
55	DPP	DW	2	55	3,5,6	0.79	0	1,5,7	0.27	0
55	UAL	BW	5	55	7,8,9	2.89	4 (57%)	5,9,11	5.14	2 (40%)

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
55	5OH	FW	6	55	-	0/2/18/20	0/1/1/1
55	DPP	BW	2	55	-	0/2/4/6	-
55	KBE	FW	1	55	-	2/7/7/8	-
55	5OH	BW	6	55	-	2/2/18/20	0/1/1/1
55	KBE	DW	1	55	-	5/7/7/8	-
55	KBE	BW	1	55	-	3/7/7/8	-
55	5OH	DW	6	55	-	1/2/18/20	0/1/1/1
55	UAL	FW	5	55	-	0/3/7/9	-
55	DPP	FW	2	55	-	0/2/4/6	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	UAL	DW	5	55	-	1/3/7/9	-
55	DPP	DW	2	55	-	0/2/4/6	-
55	UAL	BW	5	55	-	1/3/7/9	-

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	BW	5	UAL	CB-N1	4.26	1.46	1.35
55	BW	5	UAL	C-CA	4.23	1.51	1.45
55	DW	5	UAL	CB-N1	4.08	1.46	1.35
55	FW	5	UAL	CB-N1	3.85	1.45	1.35
55	DW	5	UAL	C1-N1	3.72	1.46	1.40

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	BW	5	UAL	O-C-CA	-8.90	114.08	125.39
55	DW	5	UAL	O-C-CA	-8.50	114.58	125.39
55	BW	5	UAL	CA-CB-N1	-6.87	112.65	125.60
55	FW	5	UAL	CA-CB-N1	-6.21	113.88	125.60
55	DW	5	UAL	CA-CB-N1	-6.01	114.27	125.60

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	FW	1	KBE	C-CA-CB-N
55	FW	1	KBE	C-CA-CB-CG
55	BW	6	5OH	C-CA-CB-CR
55	DW	1	KBE	N-CB-CG-CD
55	BW	1	KBE	O-C-CA-CB

There are no ring outliers.

10 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	FW	6	5OH	3	0
55	FW	1	KBE	1	0
55	BW	6	5OH	1	0
55	DW	1	KBE	1	0
55	BW	1	KBE	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	DW	6	5OH	3	0
55	FW	2	DPP	1	0
55	DW	5	UAL	2	0
55	DW	2	DPP	1	0
55	BW	5	UAL	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 748 ligands modelled in this entry, 744 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
58	GCP	HV	801	56	26,34,34	2.68	10 (38%)	31,54,54	1.61	5 (16%)
58	GCP	BV	801	56	26,34,34	2.83	10 (38%)	31,54,54	1.71	5 (16%)
58	GCP	DV	801	56	26,34,34	2.79	9 (34%)	31,54,54	1.47	4 (12%)
58	GCP	FV	801	56	26,34,34	2.50	8 (30%)	31,54,54	1.28	3 (9%)

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
58	GCP	HV	801	56	-	4/18/38/38	0/3/3/3
58	GCP	BV	801	56	-	4/18/38/38	0/3/3/3
58	GCP	DV	801	56	-	3/18/38/38	0/3/3/3
58	GCP	FV	801	56	-	5/18/38/38	0/3/3/3

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	FV	801	GCP	C4-N9	-10.32	1.34	1.47
58	BV	801	GCP	C5-C6	-8.24	1.38	1.52
58	DV	801	GCP	C5-C6	-8.06	1.39	1.52
58	BV	801	GCP	C4-N9	-7.94	1.37	1.47
58	DV	801	GCP	C4-N9	-7.77	1.37	1.47

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	HV	801	GCP	PA-O3A-PB	-4.54	118.16	132.56
58	HV	801	GCP	C4-C5-N7	4.48	108.40	102.46
58	BV	801	GCP	C4'-O4'-C1'	-4.21	100.17	109.47
58	BV	801	GCP	C4-C5-N7	4.17	107.99	102.46
58	DV	801	GCP	C4-C5-N7	4.01	107.77	102.46

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	DV	801	GCP	C2'-C1'-N9-C4
58	BV	801	GCP	PB-C3B-PG-O1G
58	BV	801	GCP	PB-C3B-PG-O2G
58	BV	801	GCP	PB-C3B-PG-O3G
58	BV	801	GCP	C2'-C1'-N9-C4

There are no ring outliers.

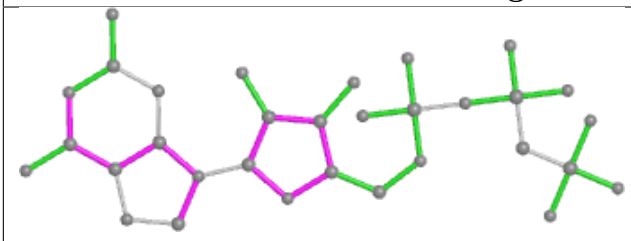
4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	HV	801	GCP	1	0
58	BV	801	GCP	2	0
58	DV	801	GCP	1	0
58	FV	801	GCP	5	0

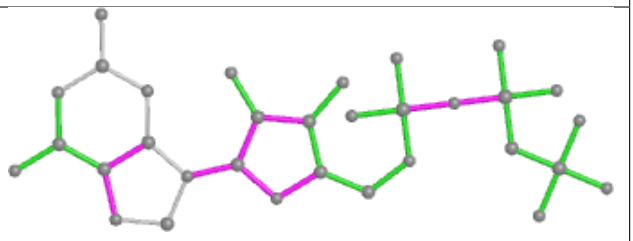
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

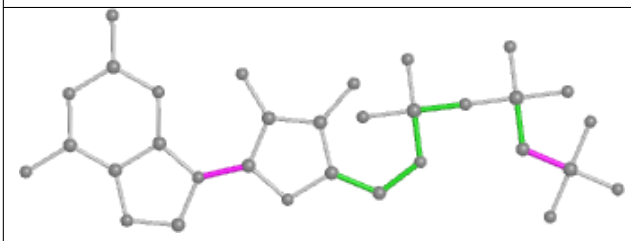
Ligand GCP HV 801



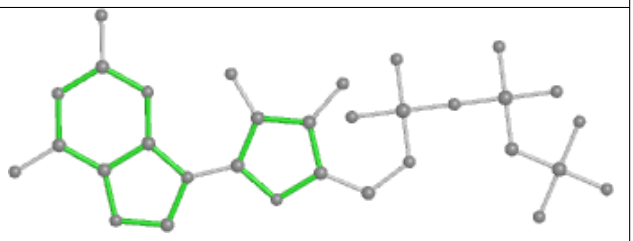
Bond lengths



Bond angles

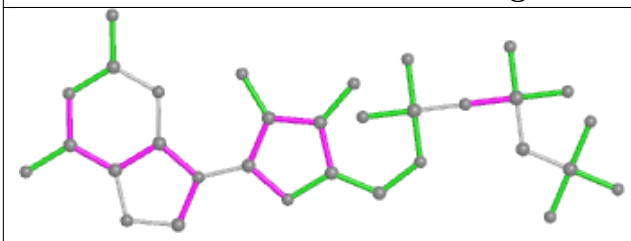


Torsions

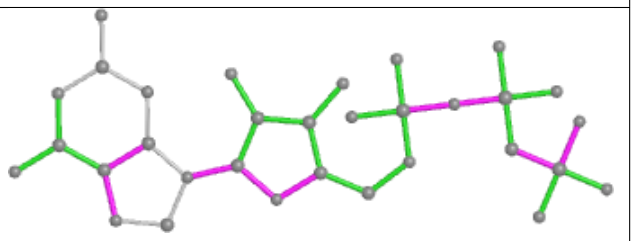


Rings

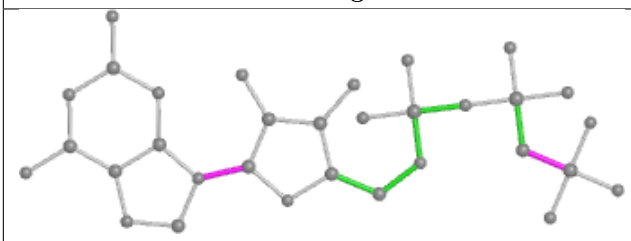
Ligand GCP BV 801



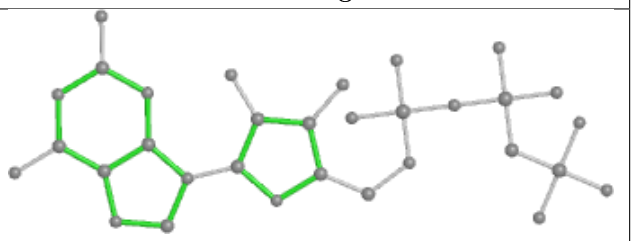
Bond lengths



Bond angles

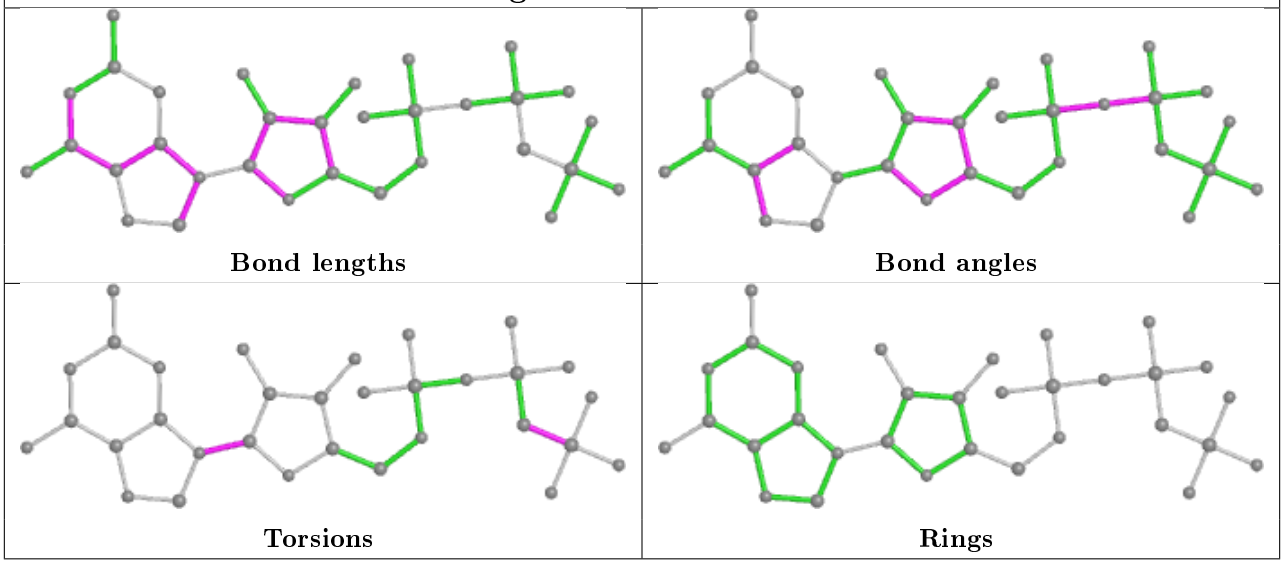


Torsions

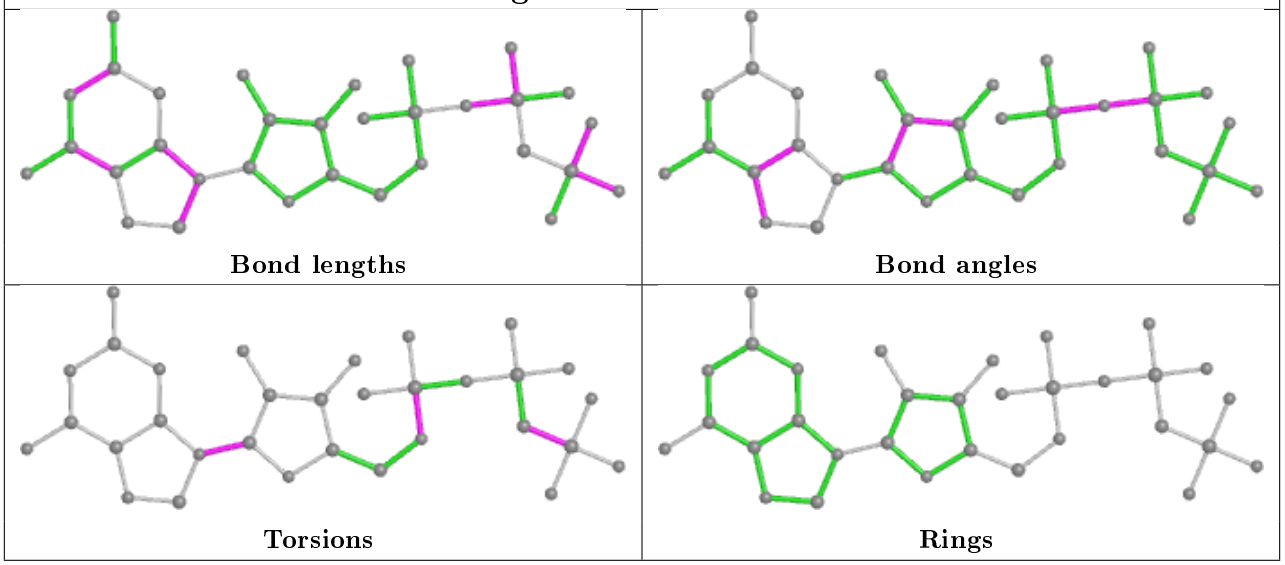


Rings

Ligand GCP DV 801



Ligand GCP FV 801



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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, 95^{th} 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	AA	2854/2904 (98%)	-0.24	60 (2%) 63 61	4, 28, 65, 87	0
1	CA	2854/2904 (98%)	-0.26	58 (2%) 65 63	3, 25, 63, 88	0
1	EA	2854/2904 (98%)	-0.25	45 (1%) 72 71	1, 14, 60, 92	0
1	GA	2854/2904 (98%)	-0.22	65 (2%) 60 58	5, 29, 68, 89	0
2	AB	118/120 (98%)	-0.49	0 100 100	18, 48, 62, 72	0
2	CB	118/120 (98%)	-0.61	0 100 100	18, 41, 54, 72	0
2	EB	118/120 (98%)	-0.52	0 100 100	3, 25, 45, 56	0
2	GB	118/120 (98%)	-0.52	1 (0%) 86 86	23, 44, 61, 78	0
3	AC	271/273 (99%)	-0.14	1 (0%) 92 93	5, 26, 40, 60	0
3	CC	271/273 (99%)	-0.23	0 100 100	2, 18, 34, 44	0
3	EC	271/273 (99%)	-0.30	0 100 100	1, 15, 32, 57	0
3	GC	271/273 (99%)	-0.28	0 100 100	3, 17, 30, 42	0
4	AD	209/209 (100%)	-0.09	2 (0%) 82 82	6, 27, 47, 60	0
4	CD	209/209 (100%)	-0.02	5 (2%) 59 56	3, 31, 52, 61	0
4	ED	209/209 (100%)	-0.18	2 (0%) 82 82	1, 20, 43, 56	0
4	GD	209/209 (100%)	0.08	5 (2%) 59 56	4, 36, 54, 62	0
5	AE	201/201 (100%)	0.17	6 (2%) 50 45	7, 33, 55, 63	0
5	CE	201/201 (100%)	0.13	7 (3%) 44 38	4, 33, 54, 60	0
5	EE	201/201 (100%)	-0.05	2 (0%) 82 82	2, 19, 45, 69	0
5	GE	201/201 (100%)	0.25	8 (3%) 38 33	7, 41, 56, 67	0
6	AF	177/179 (98%)	2.43	93 (52%) 0 0	45, 61, 71, 79	0
6	CF	177/179 (98%)	0.66	18 (10%) 6 5	32, 49, 63, 67	0
6	EF	177/179 (98%)	0.55	15 (8%) 10 8	19, 42, 61, 68	0
6	GF	177/179 (98%)	2.01	74 (41%) 0 0	36, 61, 72, 76	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
7	AG	176/177 (99%)	0.40	16 (9%) 9 6	20, 42, 60, 69	0
7	CG	176/177 (99%)	0.61	24 (13%) 3 2	23, 46, 61, 69	0
7	EG	176/177 (99%)	0.11	8 (4%) 33 29	19, 37, 55, 63	0
7	GG	176/177 (99%)	0.60	24 (13%) 3 2	32, 48, 63, 68	0
8	AH	50/50 (100%)	1.28	10 (20%) 1 0	28, 51, 67, 77	0
8	CH	50/50 (100%)	1.48	17 (34%) 0 0	39, 56, 68, 74	0
8	EH	50/50 (100%)	1.31	14 (28%) 0 0	24, 49, 69, 79	0
8	GH	50/50 (100%)	1.16	15 (30%) 0 0	26, 46, 64, 69	0
9	AI	141/142 (99%)	2.13	58 (41%) 0 0	44, 64, 75, 82	0
9	CI	141/142 (99%)	2.46	73 (51%) 0 0	49, 63, 73, 76	0
9	EI	141/142 (99%)	2.84	81 (57%) 0 0	48, 65, 77, 82	0
9	GI	141/142 (99%)	3.94	109 (77%) 0 0	49, 68, 77, 81	0
10	AJ	142/142 (100%)	-0.10	2 (1%) 75 75	12, 29, 41, 60	0
10	CJ	142/142 (100%)	-0.03	2 (1%) 75 75	13, 29, 42, 58	0
10	EJ	142/142 (100%)	-0.19	1 (0%) 87 87	3, 13, 30, 47	0
10	GJ	142/142 (100%)	0.05	5 (3%) 44 38	15, 32, 47, 61	0
11	AK	122/123 (99%)	-0.20	1 (0%) 86 86	5, 19, 34, 54	0
11	CK	122/123 (99%)	-0.14	2 (1%) 72 71	9, 22, 39, 56	0
11	EK	122/123 (99%)	-0.07	2 (1%) 72 71	4, 18, 37, 49	0
11	GK	122/123 (99%)	0.19	2 (1%) 72 71	13, 27, 42, 59	0
12	AL	143/144 (99%)	0.21	7 (4%) 29 26	10, 30, 48, 58	0
12	CL	143/144 (99%)	0.04	2 (1%) 75 75	3, 29, 47, 62	0
12	EL	143/144 (99%)	0.08	2 (1%) 75 75	1, 18, 39, 54	0
12	GL	143/144 (99%)	0.48	14 (9%) 7 5	10, 35, 53, 67	0
13	AM	136/136 (100%)	-0.07	2 (1%) 73 73	8, 19, 37, 55	0
13	CM	136/136 (100%)	-0.08	1 (0%) 87 87	8, 21, 38, 56	0
13	EM	136/136 (100%)	-0.21	2 (1%) 73 73	1, 11, 29, 60	0
13	GM	136/136 (100%)	0.18	4 (2%) 51 47	11, 28, 45, 58	0
14	AN	120/127 (94%)	0.08	2 (1%) 70 69	14, 29, 41, 62	0
14	CN	120/127 (94%)	0.00	1 (0%) 86 86	18, 31, 43, 62	0
14	EN	120/127 (94%)	-0.10	1 (0%) 86 86	6, 19, 32, 61	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
14	GN	120/127 (94%)	-0.00	1 (0%) 86 86	19, 31, 43, 72	0
15	AO	116/117 (99%)	0.60	11 (9%) 8 6	28, 47, 56, 62	0
15	CO	116/117 (99%)	0.40	8 (6%) 16 13	28, 42, 55, 61	0
15	EO	116/117 (99%)	0.09	3 (2%) 56 52	16, 30, 43, 55	0
15	GO	116/117 (99%)	0.49	9 (7%) 13 10	28, 40, 58, 63	0
16	AP	114/115 (99%)	0.08	2 (1%) 68 67	13, 31, 47, 62	0
16	CP	114/115 (99%)	0.06	4 (3%) 44 38	17, 35, 49, 62	0
16	EP	114/115 (99%)	-0.21	2 (1%) 68 67	6, 24, 43, 66	0
16	GP	114/115 (99%)	0.21	4 (3%) 44 38	14, 35, 50, 59	0
17	AQ	117/118 (99%)	0.01	1 (0%) 84 84	10, 26, 43, 56	0
17	CQ	117/118 (99%)	-0.05	3 (2%) 56 52	6, 24, 39, 60	0
17	EQ	117/118 (99%)	-0.18	0 100 100	2, 9, 25, 46	0
17	GQ	117/118 (99%)	0.15	4 (3%) 45 40	19, 29, 42, 56	0
18	AR	103/103 (100%)	0.17	4 (3%) 39 35	10, 37, 52, 60	0
18	CR	103/103 (100%)	0.06	2 (1%) 66 65	9, 34, 49, 63	0
18	ER	103/103 (100%)	-0.20	1 (0%) 82 82	2, 21, 41, 52	0
18	GR	103/103 (100%)	0.46	6 (5%) 23 19	13, 40, 53, 63	0
19	AS	110/110 (100%)	0.15	4 (3%) 42 37	13, 28, 45, 62	0
19	CS	110/110 (100%)	0.11	2 (1%) 68 67	7, 27, 45, 65	0
19	ES	110/110 (100%)	-0.10	0 100 100	2, 12, 36, 49	0
19	GS	110/110 (100%)	0.40	8 (7%) 15 11	12, 31, 50, 69	0
20	AT	93/100 (93%)	0.59	11 (11%) 4 3	18, 37, 58, 63	0
20	CT	93/100 (93%)	0.36	9 (9%) 7 6	14, 37, 57, 67	0
20	ET	93/100 (93%)	0.36	8 (8%) 10 8	6, 24, 53, 61	0
20	GT	93/100 (93%)	0.65	17 (18%) 1 0	19, 36, 57, 62	0
21	AU	102/104 (98%)	0.73	13 (12%) 3 2	24, 40, 56, 64	0
21	CU	102/104 (98%)	0.76	15 (14%) 2 1	24, 41, 61, 73	0
21	EU	102/104 (98%)	0.34	5 (4%) 29 26	13, 28, 51, 65	0
21	GU	102/104 (98%)	1.23	23 (22%) 0 0	32, 46, 63, 75	0
22	AV	94/94 (100%)	-0.12	2 (2%) 63 61	23, 38, 48, 57	0
22	CV	94/94 (100%)	0.00	1 (1%) 80 80	25, 39, 52, 67	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
22	EV	94/94 (100%)	-0.34	0 100 100	9, 22, 40, 45	0
22	GV	94/94 (100%)	0.20	3 (3%) 47 43	29, 42, 55, 60	0
23	AW	79/85 (92%)	0.54	9 (11%) 5 3	17, 35, 52, 61	0
23	CW	79/85 (92%)	0.41	4 (5%) 28 24	15, 29, 51, 65	0
23	EW	79/85 (92%)	0.38	4 (5%) 28 24	5, 17, 44, 50	0
23	GW	79/85 (92%)	0.52	6 (7%) 13 10	15, 33, 55, 63	0
24	AX	77/78 (98%)	0.34	2 (2%) 56 52	16, 31, 47, 57	0
24	CX	77/78 (98%)	0.08	1 (1%) 77 77	8, 22, 46, 49	0
24	EX	77/78 (98%)	0.01	0 100 100	4, 18, 40, 50	0
24	GX	77/78 (98%)	-0.01	1 (1%) 77 77	14, 25, 46, 56	0
25	AY	63/63 (100%)	0.95	10 (15%) 1 1	30, 47, 61, 65	0
25	CY	63/63 (100%)	0.63	6 (9%) 8 6	27, 44, 58, 67	0
25	EY	63/63 (100%)	0.75	8 (12%) 3 2	13, 33, 51, 70	0
25	GY	63/63 (100%)	1.11	9 (14%) 2 2	29, 45, 60, 68	0
26	AZ	58/59 (98%)	0.38	2 (3%) 45 40	15, 31, 55, 71	0
26	CZ	58/59 (98%)	0.25	3 (5%) 27 23	17, 30, 53, 65	0
26	EZ	58/59 (98%)	-0.14	1 (1%) 70 69	2, 10, 35, 59	0
26	GZ	58/59 (98%)	0.27	3 (5%) 27 23	20, 32, 51, 53	0
27	A0	56/57 (98%)	0.37	2 (3%) 42 37	11, 33, 54, 62	0
27	C0	56/57 (98%)	0.18	1 (1%) 68 67	8, 35, 50, 60	0
27	E0	56/57 (98%)	0.11	1 (1%) 68 67	3, 25, 48, 56	0
27	G0	56/57 (98%)	0.31	3 (5%) 25 22	15, 35, 58, 67	0
28	A1	50/55 (90%)	1.09	9 (18%) 1 1	27, 38, 51, 61	0
28	C1	50/55 (90%)	0.79	5 (10%) 7 5	21, 35, 48, 59	0
28	E1	50/55 (90%)	0.44	4 (8%) 12 9	11, 26, 44, 47	0
28	G1	50/55 (90%)	1.24	15 (30%) 0 0	25, 38, 55, 61	0
29	A2	46/46 (100%)	0.07	1 (2%) 62 59	9, 22, 34, 55	0
29	C2	46/46 (100%)	-0.04	2 (4%) 35 31	7, 14, 30, 54	0
29	E2	46/46 (100%)	-0.22	1 (2%) 62 59	2, 7, 15, 53	0
29	G2	46/46 (100%)	0.05	2 (4%) 35 31	8, 17, 28, 51	0
30	A3	64/65 (98%)	-0.00	0 100 100	12, 22, 37, 40	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
30	C3	64/65 (98%)	-0.03	0 100 100	10, 18, 27, 35	0
30	E3	64/65 (98%)	-0.13	0 100 100	2, 8, 14, 27	0
30	G3	64/65 (98%)	0.04	1 (1%) 72 71	13, 22, 37, 48	0
31	A4	38/38 (100%)	0.10	1 (2%) 56 52	13, 22, 36, 38	0
31	C4	38/38 (100%)	0.14	1 (2%) 56 52	14, 27, 39, 46	0
31	E4	38/38 (100%)	-0.14	0 100 100	5, 16, 35, 38	0
31	G4	38/38 (100%)	0.34	1 (2%) 56 52	22, 33, 44, 49	0
32	A5	148/165 (89%)	2.99	83 (56%) 0 0	36, 54, 65, 74	0
32	E5	144/165 (87%)	3.51	102 (70%) 0 0	35, 61, 72, 82	0
33	BA	1533/1542 (99%)	-0.26	29 (1%) 66 65	11, 42, 70, 91	0
33	DA	1533/1542 (99%)	-0.27	25 (1%) 72 71	12, 43, 69, 85	0
33	FA	1533/1542 (99%)	-0.27	25 (1%) 72 71	8, 33, 61, 85	0
33	HA	1533/1542 (99%)	-0.13	50 (3%) 46 41	15, 41, 72, 90	0
34	BB	218/241 (90%)	1.32	65 (29%) 0 0	41, 58, 69, 79	0
34	DB	218/241 (90%)	1.46	67 (30%) 0 0	40, 57, 69, 79	0
34	FB	218/241 (90%)	0.69	28 (12%) 3 2	26, 49, 63, 69	0
34	HB	218/241 (90%)	1.11	45 (20%) 1 0	33, 51, 67, 73	0
35	BC	206/233 (88%)	0.63	31 (15%) 2 1	30, 50, 60, 69	0
35	DC	206/233 (88%)	0.40	18 (8%) 10 7	35, 50, 60, 67	0
35	FC	206/233 (88%)	-0.08	3 (1%) 73 73	13, 30, 46, 58	0
35	HC	206/233 (88%)	0.32	11 (5%) 26 22	21, 40, 56, 66	0
36	BD	205/206 (99%)	0.40	15 (7%) 15 11	23, 39, 57, 64	0
36	DD	205/206 (99%)	0.89	33 (16%) 1 1	26, 47, 60, 65	0
36	FD	205/206 (99%)	0.70	30 (14%) 2 1	27, 44, 60, 73	0
36	HD	205/206 (99%)	0.59	23 (11%) 5 4	25, 47, 61, 79	0
37	BE	150/167 (89%)	0.23	11 (7%) 15 11	17, 48, 63, 76	0
37	DE	150/167 (89%)	0.16	7 (4%) 31 28	25, 45, 62, 71	0
37	FE	150/167 (89%)	-0.09	3 (2%) 65 63	18, 34, 50, 65	0
37	HE	150/167 (89%)	0.06	4 (2%) 54 50	21, 37, 54, 67	0
38	BF	100/135 (74%)	1.50	32 (32%) 0 0	50, 62, 70, 74	0
38	DF	100/135 (74%)	0.61	15 (15%) 2 1	32, 49, 62, 69	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
38	FF	100/135 (74%)	0.77	15 (15%) 2 1	32, 51, 63, 66	0
38	HF	100/135 (74%)	0.54	9 (9%) 9 7	31, 51, 64, 71	0
39	BG	151/179 (84%)	0.38	11 (7%) 15 11	28, 49, 60, 66	0
39	DG	151/179 (84%)	0.34	8 (5%) 26 22	32, 46, 58, 63	0
39	FG	151/179 (84%)	0.33	9 (5%) 21 18	23, 39, 55, 63	0
39	HG	151/179 (84%)	0.79	21 (13%) 2 2	32, 48, 62, 68	0
40	BH	129/130 (99%)	0.70	16 (12%) 4 3	40, 51, 62, 70	0
40	DH	129/130 (99%)	0.58	14 (10%) 5 4	28, 47, 59, 73	0
40	FH	129/130 (99%)	-0.04	2 (1%) 72 71	20, 32, 47, 66	0
40	HH	129/130 (99%)	0.27	5 (3%) 39 35	23, 35, 51, 69	0
41	BI	127/130 (97%)	1.01	25 (19%) 1 0	24, 52, 65, 70	0
41	DI	127/130 (97%)	0.97	19 (14%) 2 1	31, 52, 64, 74	0
41	FI	127/130 (97%)	0.39	9 (7%) 16 12	14, 43, 60, 69	0
41	HI	127/130 (97%)	1.29	35 (27%) 0 0	29, 55, 70, 75	0
42	BJ	98/103 (95%)	1.84	39 (39%) 0 0	30, 55, 68, 72	0
42	DJ	98/103 (95%)	1.73	36 (36%) 0 0	35, 57, 70, 74	0
42	FJ	98/103 (95%)	0.54	12 (12%) 4 3	14, 32, 59, 65	0
42	HJ	98/103 (95%)	1.27	27 (27%) 0 0	30, 51, 69, 78	0
43	BK	117/129 (90%)	1.36	28 (23%) 0 0	33, 56, 66, 80	0
43	DK	117/129 (90%)	0.16	9 (7%) 13 10	26, 41, 56, 60	0
43	FK	117/129 (90%)	0.44	10 (8%) 10 8	18, 42, 59, 64	0
43	HK	117/129 (90%)	1.41	32 (27%) 0 0	23, 50, 70, 74	0
44	BL	123/124 (99%)	-0.10	2 (1%) 72 71	15, 24, 43, 74	0
44	DL	123/124 (99%)	0.02	5 (4%) 37 32	20, 34, 48, 61	0
44	FL	123/124 (99%)	-0.08	4 (3%) 46 41	9, 28, 44, 67	0
44	HL	123/124 (99%)	0.19	7 (5%) 23 19	21, 37, 55, 63	0
45	BM	114/118 (96%)	0.64	13 (11%) 5 3	28, 49, 64, 74	0
45	DM	114/118 (96%)	0.45	6 (5%) 26 22	36, 50, 63, 67	0
45	FM	114/118 (96%)	0.52	12 (10%) 6 5	19, 45, 63, 68	0
45	HM	114/118 (96%)	2.55	60 (52%) 0 0	42, 63, 72, 75	0
46	BN	96/101 (95%)	0.60	14 (14%) 2 1	32, 46, 60, 65	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
46	DN	96/101 (95%)	0.58	13 (13%) 3 2	30, 49, 62, 65	0
46	FN	96/101 (95%)	0.01	2 (2%) 63 61	11, 24, 53, 60	0
46	HN	96/101 (95%)	0.59	15 (15%) 2 1	27, 47, 64, 70	0
47	BO	88/89 (98%)	0.59	8 (9%) 9 6	35, 50, 61, 64	0
47	DO	88/89 (98%)	0.46	6 (6%) 17 13	31, 45, 56, 61	0
47	FO	88/89 (98%)	0.37	2 (2%) 60 58	23, 37, 49, 56	0
47	HO	88/89 (98%)	0.19	3 (3%) 45 40	22, 39, 53, 70	0
48	BP	82/82 (100%)	0.65	9 (10%) 5 4	24, 35, 61, 68	0
48	DP	82/82 (100%)	1.16	17 (20%) 1 0	28, 43, 62, 79	0
48	FP	82/82 (100%)	0.24	6 (7%) 15 11	21, 34, 62, 77	0
48	HP	82/82 (100%)	0.47	8 (9%) 7 5	22, 39, 62, 71	0
49	BQ	80/84 (95%)	0.75	10 (12%) 3 3	30, 45, 55, 63	0
49	DQ	80/84 (95%)	0.79	10 (12%) 3 3	29, 44, 57, 68	0
49	FQ	80/84 (95%)	0.23	4 (5%) 28 25	22, 38, 54, 63	0
49	HQ	80/84 (95%)	0.34	4 (5%) 28 25	27, 41, 51, 57	0
50	BR	55/75 (73%)	1.74	20 (36%) 0 0	46, 55, 66, 69	0
50	DR	55/75 (73%)	0.76	9 (16%) 1 1	35, 44, 60, 66	0
50	FR	55/75 (73%)	0.43	6 (10%) 5 4	35, 44, 53, 61	0
50	HR	55/75 (73%)	0.47	5 (9%) 9 6	26, 40, 55, 64	0
51	BS	79/92 (85%)	0.32	5 (6%) 20 16	30, 44, 59, 64	0
51	DS	79/92 (85%)	0.67	9 (11%) 5 3	36, 49, 63, 67	0
51	FS	79/92 (85%)	-0.20	2 (2%) 57 55	22, 32, 52, 63	0
51	HS	79/92 (85%)	2.44	42 (53%) 0 0	43, 58, 70, 74	0
52	BT	85/87 (97%)	0.53	5 (5%) 22 18	25, 40, 50, 59	0
52	DT	85/87 (97%)	0.53	7 (8%) 11 9	30, 40, 55, 73	0
52	FT	85/87 (97%)	0.22	5 (5%) 22 18	24, 36, 50, 63	0
52	HT	85/87 (97%)	0.71	6 (7%) 16 12	23, 38, 53, 56	0
53	BU	51/71 (71%)	3.67	34 (66%) 0 0	53, 62, 71, 82	0
53	DU	51/71 (71%)	1.58	16 (31%) 0 0	40, 54, 69, 74	0
53	FU	51/71 (71%)	1.37	19 (37%) 0 0	40, 53, 65, 69	0
53	HU	51/71 (71%)	2.31	20 (39%) 0 0	40, 57, 67, 71	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
54	BV	689/704 (97%)	0.39	65 (9%) 8 6	18, 46, 66, 76	0
54	DV	689/704 (97%)	0.58	94 (13%) 3 2	27, 50, 68, 77	0
54	FV	689/704 (97%)	2.68	365 (52%) 0 0	33, 66, 76, 82	0
54	HV	689/704 (97%)	1.00	139 (20%) 1 0	32, 56, 70, 80	0
55	BW	2/6 (33%)	4.04	1 (50%) 0 0	41, 41, 41, 43	2 (100%)
55	DW	2/6 (33%)	3.38	1 (50%) 0 0	40, 40, 40, 44	2 (100%)
55	FW	2/6 (33%)	2.96	2 (100%) 0 0	41, 41, 41, 42	2 (100%)
All	All	43562/44972 (96%)	0.24	3539 (8%) 12 9	1, 37, 66, 92	6 (0%)

The worst 5 of 3539 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
48	DP	81	ALA	19.9
9	GI	8	VAL	16.8
32	A5	112	ALA	16.8
26	AZ	1	ALA	16.7
54	FV	588	SER	15.3

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	DPP	FW	2	6/7	0.48	0.88	37,42,43,43	6
55	5OH	FW	6	12/13	0.55	0.73	37,42,45,46	12
55	KBE	FW	1	9/10	0.62	0.49	28,36,40,42	9
55	UAL	FW	5	9/10	0.67	0.57	35,37,39,41	9
55	KBE	DW	1	9/10	0.68	0.37	32,33,40,41	9
55	KBE	BW	1	9/10	0.68	0.60	37,39,42,44	9
55	UAL	BW	5	9/10	0.69	0.62	32,40,42,42	9
55	5OH	BW	6	12/13	0.72	0.49	36,37,41,43	12
55	5OH	DW	6	12/13	0.74	0.44	33,41,43,48	12
55	UAL	DW	5	9/10	0.78	0.44	35,39,42,46	9
55	DPP	DW	2	6/7	0.84	0.43	32,34,37,44	6
55	DPP	BW	2	6/7	0.85	0.57	34,36,39,40	6

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
56	MG	AA	3068	1/1	0.79	0.17	59,59,59,59	0
56	MG	AA	3115	1/1	0.80	0.14	32,32,32,32	0
56	MG	EA	3133	1/1	0.82	0.13	32,32,32,32	0
56	MG	EQ	201	1/1	0.82	0.66	31,31,31,31	0
56	MG	FA	1636	1/1	0.82	0.63	38,38,38,38	0
56	MG	BA	1614	1/1	0.82	0.38	26,26,26,26	0
56	MG	GA	3069	1/1	0.82	0.07	63,63,63,63	0
56	MG	HA	1617	1/1	0.83	0.16	62,62,62,62	0
56	MG	HA	1613	1/1	0.83	0.47	41,41,41,41	0
56	MG	AA	3078	1/1	0.83	0.24	29,29,29,29	0
56	MG	BA	1609	1/1	0.84	0.11	38,38,38,38	0
56	MG	HE	201	1/1	0.84	0.21	39,39,39,39	0
56	MG	FA	1627	1/1	0.84	0.26	23,23,23,23	0
56	MG	HT	101	1/1	0.86	0.46	41,41,41,41	0
56	MG	EA	3087	1/1	0.86	0.59	30,30,30,30	0
58	GCP	FV	801	32/32	0.87	0.20	43,58,69,87	0
56	MG	CA	3011	1/1	0.87	0.40	23,23,23,23	0
56	MG	EA	3109	1/1	0.88	0.17	8,8,8,8	0
56	MG	FE	201	1/1	0.88	0.51	52,52,52,52	0
56	MG	CA	3092	1/1	0.88	0.17	30,30,30,30	0
56	MG	ED	301	1/1	0.88	0.22	7,7,7,7	0
56	MG	FA	1610	1/1	0.88	0.28	35,35,35,35	0
56	MG	BE	201	1/1	0.88	0.14	43,43,43,43	0
56	MG	EA	3130	1/1	0.89	0.21	29,29,29,29	0
56	MG	FU	101	1/1	0.89	0.14	24,24,24,24	0
56	MG	HC	401	1/1	0.89	0.32	49,49,49,49	0
56	MG	CA	3118	1/1	0.89	0.33	29,29,29,29	0
56	MG	CA	3122	1/1	0.89	0.17	7,7,7,7	0
56	MG	DA	1602	1/1	0.90	0.34	31,31,31,31	0
56	MG	GA	3059	1/1	0.90	0.48	44,44,44,44	0
56	MG	CA	3077	1/1	0.90	0.27	35,35,35,35	0
56	MG	BU	101	1/1	0.91	0.26	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3091	1/1	0.91	0.21	40,40,40,40	0
56	MG	BL	201	1/1	0.91	0.23	51,51,51,51	0
56	MG	GA	3073	1/1	0.91	0.47	20,20,20,20	0
56	MG	CA	3110	1/1	0.91	0.11	20,20,20,20	0
56	MG	GA	3057	1/1	0.92	0.11	22,22,22,22	0
56	MG	GA	3082	1/1	0.92	0.11	35,35,35,35	0
56	MG	HA	1637	1/1	0.92	0.10	47,47,47,47	0
56	MG	CA	3114	1/1	0.92	0.56	25,25,25,25	0
56	MG	BA	1637	1/1	0.92	0.29	29,29,29,29	0
56	MG	CA	3044	1/1	0.92	0.13	22,22,22,22	0
56	MG	EA	3069	1/1	0.93	0.41	4,4,4,4	0
56	MG	AA	3087	1/1	0.93	0.15	31,31,31,31	0
56	MG	GB	1201	1/1	0.93	0.09	38,38,38,38	0
56	MG	HA	1626	1/1	0.93	0.28	32,32,32,32	0
56	MG	EA	3010	1/1	0.93	0.16	11,11,11,11	0
56	MG	AA	3015	1/1	0.93	0.15	22,22,22,22	0
56	MG	CB	1204	1/1	0.93	0.06	16,16,16,16	0
56	MG	AA	3011	1/1	0.93	0.17	18,18,18,18	0
56	MG	EA	3057	1/1	0.93	0.11	15,15,15,15	0
56	MG	GA	3083	1/1	0.93	0.27	33,33,33,33	0
56	MG	AT	201	1/1	0.93	0.18	36,36,36,36	0
56	MG	BA	1640	1/1	0.93	0.14	33,33,33,33	0
56	MG	DA	1629	1/1	0.93	0.48	54,54,54,54	0
56	MG	AA	3090	1/1	0.94	0.10	23,23,23,23	0
56	MG	GA	3060	1/1	0.94	0.28	23,23,23,23	0
56	MG	CA	3120	1/1	0.94	0.15	3,3,3,3	0
56	MG	CA	3111	1/1	0.94	0.16	13,13,13,13	0
56	MG	HA	1601	1/1	0.94	0.16	38,38,38,38	0
56	MG	HA	1633	1/1	0.94	0.19	52,52,52,52	0
56	MG	FA	1602	1/1	0.94	0.10	23,23,23,23	0
56	MG	DA	1641	1/1	0.94	0.12	30,30,30,30	0
56	MG	GA	3087	1/1	0.94	0.19	19,19,19,19	0
56	MG	EB	1201	1/1	0.94	0.14	26,26,26,26	0
56	MG	GS	201	1/1	0.94	0.48	33,33,33,33	0
56	MG	C4	101	1/1	0.94	0.06	22,22,22,22	0
56	MG	GA	3131	1/1	0.94	0.13	41,41,41,41	0
56	MG	HA	1619	1/1	0.94	0.15	34,34,34,34	0
56	MG	AA	3007	1/1	0.94	0.18	44,44,44,44	0
56	MG	AC	303	1/1	0.94	1.02	34,34,34,34	0
56	MG	GA	3133	1/1	0.94	0.23	4,4,4,4	0
56	MG	FA	1601	1/1	0.94	0.14	28,28,28,28	0
56	MG	CA	3097	1/1	0.94	0.67	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	HA	1609	1/1	0.94	0.13	29,29,29,29	0
56	MG	GA	3055	1/1	0.94	0.12	12,12,12,12	0
56	MG	EA	3096	1/1	0.94	0.15	15,15,15,15	0
56	MG	EA	3127	1/1	0.94	0.15	0,0,0,0	0
56	MG	CE	301	1/1	0.94	0.25	16,16,16,16	0
56	MG	GA	3103	1/1	0.94	0.24	12,12,12,12	0
56	MG	AA	3005	1/1	0.94	0.16	23,23,23,23	0
56	MG	DA	1627	1/1	0.94	0.11	21,21,21,21	0
56	MG	GA	3077	1/1	0.95	0.10	33,33,33,33	0
56	MG	AA	3093	1/1	0.95	0.26	34,34,34,34	0
56	MG	GA	3023	1/1	0.95	0.17	7,7,7,7	0
56	MG	AA	3077	1/1	0.95	0.06	36,36,36,36	0
56	MG	BA	1624	1/1	0.95	0.12	28,28,28,28	0
56	MG	HA	1625	1/1	0.95	0.32	22,22,22,22	0
56	MG	GA	3108	1/1	0.95	0.15	16,16,16,16	0
56	MG	HA	1630	1/1	0.95	0.14	40,40,40,40	0
56	MG	HA	1634	1/1	0.95	0.13	24,24,24,24	0
56	MG	AB	1201	1/1	0.95	0.11	38,38,38,38	0
56	MG	EA	3016	1/1	0.95	0.12	6,6,6,6	0
56	MG	GA	3061	1/1	0.95	0.21	10,10,10,10	0
56	MG	EA	3068	1/1	0.95	0.12	35,35,35,35	0
56	MG	EA	3079	1/1	0.95	0.23	0,0,0,0	0
56	MG	DA	1610	1/1	0.95	0.04	48,48,48,48	0
56	MG	AB	1202	1/1	0.95	0.24	44,44,44,44	0
56	MG	DA	1614	1/1	0.95	0.12	44,44,44,44	0
56	MG	AC	301	1/1	0.95	0.35	10,10,10,10	0
56	MG	HA	1608	1/1	0.95	0.14	14,14,14,14	0
56	MG	HA	1610	1/1	0.95	0.27	13,13,13,13	0
56	MG	CA	3005	1/1	0.96	0.17	31,31,31,31	0
56	MG	GA	3037	1/1	0.96	0.19	19,19,19,19	0
56	MG	DA	1606	1/1	0.96	0.11	26,26,26,26	0
56	MG	EA	3088	1/1	0.96	0.16	6,6,6,6	0
56	MG	CA	3069	1/1	0.96	0.15	45,45,45,45	0
56	MG	AA	3069	1/1	0.96	0.17	6,6,6,6	0
56	MG	EA	3050	1/1	0.96	0.24	13,13,13,13	0
56	MG	GA	3001	1/1	0.96	0.17	32,32,32,32	0
56	MG	GA	3093	1/1	0.96	0.49	28,28,28,28	0
56	MG	EA	3025	1/1	0.96	0.21	0,0,0,0	0
56	MG	AA	3059	1/1	0.96	0.50	12,12,12,12	0
56	MG	FA	1604	1/1	0.96	0.07	33,33,33,33	0
56	MG	DA	1628	1/1	0.96	0.33	37,37,37,37	0
56	MG	HA	1604	1/1	0.96	0.17	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3083	1/1	0.96	0.12	22,22,22,22	0
56	MG	BA	1612	1/1	0.96	0.22	5,5,5,5	0
56	MG	CB	1201	1/1	0.96	0.12	41,41,41,41	0
56	MG	EA	3082	1/1	0.96	0.07	13,13,13,13	0
56	MG	EA	3011	1/1	0.96	0.86	17,17,17,17	0
56	MG	CA	3015	1/1	0.96	0.16	14,14,14,14	0
56	MG	GA	3018	1/1	0.96	0.26	36,36,36,36	0
56	MG	CA	3106	1/1	0.96	0.16	13,13,13,13	0
56	MG	GA	3075	1/1	0.96	0.15	7,7,7,7	0
56	MG	BA	1631	1/1	0.96	0.07	28,28,28,28	0
56	MG	DA	1639	1/1	0.96	0.10	40,40,40,40	0
56	MG	DA	1642	1/1	0.96	0.16	29,29,29,29	0
56	MG	CA	3016	1/1	0.96	0.21	8,8,8,8	0
56	MG	HA	1624	1/1	0.96	0.12	14,14,14,14	0
56	MG	GB	1202	1/1	0.96	0.16	36,36,36,36	0
56	MG	DU	101	1/1	0.96	0.27	36,36,36,36	0
58	GCP	DV	801	32/32	0.96	0.14	20,38,49,52	0
56	MG	GA	3113	1/1	0.96	0.10	26,26,26,26	0
56	MG	EA	3044	1/1	0.96	0.13	11,11,11,11	0
56	MG	EA	3059	1/1	0.96	0.14	1,1,1,1	0
56	MG	CA	3094	1/1	0.96	0.08	34,34,34,34	0
56	MG	CA	3087	1/1	0.96	0.06	29,29,29,29	0
56	MG	CA	3061	1/1	0.96	0.12	3,3,3,3	0
56	MG	AA	3006	1/1	0.96	0.09	38,38,38,38	0
56	MG	EA	3090	1/1	0.96	0.07	29,29,29,29	0
56	MG	GA	3094	1/1	0.96	0.56	22,22,22,22	0
56	MG	BA	1623	1/1	0.97	0.10	24,24,24,24	0
56	MG	AD	301	1/1	0.97	0.14	6,6,6,6	0
56	MG	GA	3006	1/1	0.97	0.12	25,25,25,25	0
56	MG	EA	3125	1/1	0.97	0.10	3,3,3,3	0
56	MG	FA	1617	1/1	0.97	0.12	9,9,9,9	0
56	MG	EA	3117	1/1	0.97	0.10	11,11,11,11	0
56	MG	AA	3088	1/1	0.97	0.13	14,14,14,14	0
56	MG	EA	3005	1/1	0.97	0.12	27,27,27,27	0
56	MG	BA	1604	1/1	0.97	0.12	20,20,20,20	0
56	MG	CA	3057	1/1	0.97	0.11	1,1,1,1	0
56	MG	GA	3111	1/1	0.97	0.17	11,11,11,11	0
56	MG	EA	3108	1/1	0.97	0.12	31,31,31,31	0
56	MG	DA	1625	1/1	0.97	0.09	23,23,23,23	0
56	MG	DA	1624	1/1	0.97	0.17	48,48,48,48	0
56	MG	AA	3002	1/1	0.97	0.10	20,20,20,20	0
56	MG	AA	3092	1/1	0.97	0.05	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3020	1/1	0.97	0.16	19,19,19,19	0
56	MG	FV	802	1/1	0.97	0.12	48,48,48,48	0
56	MG	HA	1629	1/1	0.97	0.10	17,17,17,17	0
56	MG	BA	1621	1/1	0.97	0.23	52,52,52,52	0
56	MG	FA	1628	1/1	0.97	0.18	19,19,19,19	0
56	MG	FA	1639	1/1	0.97	0.26	25,25,25,25	0
56	MG	EA	3029	1/1	0.97	0.18	0,0,0,0	0
56	MG	GB	1203	1/1	0.97	0.13	16,16,16,16	0
56	MG	HA	1621	1/1	0.97	0.28	29,29,29,29	0
56	MG	FA	1641	1/1	0.97	0.17	18,18,18,18	0
56	MG	BA	1634	1/1	0.97	0.14	14,14,14,14	0
56	MG	AA	3044	1/1	0.97	0.14	17,17,17,17	0
56	MG	DA	1622	1/1	0.97	0.08	37,37,37,37	0
56	MG	BA	1636	1/1	0.97	0.12	40,40,40,40	0
56	MG	DA	1636	1/1	0.97	0.29	41,41,41,41	0
56	MG	AC	302	1/1	0.97	0.23	19,19,19,19	0
56	MG	CA	3085	1/1	0.97	0.27	28,28,28,28	0
56	MG	AA	3098	1/1	0.97	0.23	5,5,5,5	0
58	GCP	BV	801	32/32	0.97	0.13	17,36,43,49	0
56	MG	EA	3113	1/1	0.97	0.18	0,0,0,0	0
56	MG	GA	3118	1/1	0.97	0.29	9,9,9,9	0
56	MG	EA	3056	1/1	0.97	0.08	2,2,2,2	0
56	MG	AA	3063	1/1	0.97	0.08	9,9,9,9	0
56	MG	HV	802	1/1	0.97	0.13	38,38,38,38	0
56	MG	FA	1618	1/1	0.97	0.10	28,28,28,28	0
56	MG	GA	3102	1/1	0.97	0.35	40,40,40,40	0
56	MG	DA	1604	1/1	0.97	0.08	23,23,23,23	0
56	MG	AA	3111	1/1	0.97	0.16	21,21,21,21	0
56	MG	AA	3089	1/1	0.97	0.06	26,26,26,26	0
56	MG	DA	1601	1/1	0.97	0.11	37,37,37,37	0
56	MG	FA	1630	1/1	0.97	0.09	16,16,16,16	0
56	MG	CA	3103	1/1	0.97	0.17	0,0,0,0	0
56	MG	GA	3040	1/1	0.97	0.21	16,16,16,16	0
56	MG	GA	3100	1/1	0.97	0.22	19,19,19,19	0
56	MG	AA	3100	1/1	0.97	0.12	6,6,6,6	0
56	MG	DA	1611	1/1	0.97	0.10	15,15,15,15	0
56	MG	EB	1202	1/1	0.97	0.08	19,19,19,19	0
56	MG	AA	3086	1/1	0.97	0.07	35,35,35,35	0
56	MG	DA	1626	1/1	0.97	0.08	24,24,24,24	0
56	MG	GA	3046	1/1	0.97	0.07	35,35,35,35	0
56	MG	EA	3024	1/1	0.97	0.19	0,0,0,0	0
56	MG	EA	3098	1/1	0.97	0.16	6,6,6,6	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	GA	3110	1/1	0.97	0.19	12,12,12,12	0
56	MG	BA	1613	1/1	0.97	0.13	38,38,38,38	0
56	MG	AA	3024	1/1	0.97	0.18	20,20,20,20	0
56	MG	BA	1635	1/1	0.97	0.23	29,29,29,29	0
56	MG	EA	3055	1/1	0.97	0.43	14,14,14,14	0
56	MG	EA	3060	1/1	0.97	0.28	3,3,3,3	0
56	MG	BA	1629	1/1	0.97	0.15	41,41,41,41	0
56	MG	EA	3102	1/1	0.97	0.21	0,0,0,0	0
56	MG	EA	3080	1/1	0.97	0.20	3,3,3,3	0
56	MG	GA	3091	1/1	0.97	0.14	11,11,11,11	0
56	MG	GA	3029	1/1	0.97	0.20	5,5,5,5	0
56	MG	DA	1618	1/1	0.97	0.09	33,33,33,33	0
56	MG	GA	3072	1/1	0.97	0.15	13,13,13,13	0
58	GCP	HV	801	32/32	0.97	0.11	24,48,54,56	0
56	MG	CA	3007	1/1	0.97	0.09	15,15,15,15	0
56	MG	CA	3045	1/1	0.97	0.14	21,21,21,21	0
56	MG	DA	1631	1/1	0.97	0.17	25,25,25,25	0
56	MG	EA	3071	1/1	0.97	0.13	2,2,2,2	0
56	MG	BA	1606	1/1	0.97	0.54	39,39,39,39	0
56	MG	GA	3088	1/1	0.98	0.17	8,8,8,8	0
56	MG	EA	3103	1/1	0.98	0.21	10,10,10,10	0
56	MG	GA	3068	1/1	0.98	0.27	15,15,15,15	0
56	MG	DA	1608	1/1	0.98	0.14	14,14,14,14	0
56	MG	AE	301	1/1	0.98	0.12	11,11,11,11	0
56	MG	BA	1601	1/1	0.98	0.17	33,33,33,33	0
56	MG	GA	3095	1/1	0.98	0.18	2,2,2,2	0
56	MG	EA	3058	1/1	0.98	0.13	6,6,6,6	0
56	MG	CA	3105	1/1	0.98	0.17	6,6,6,6	0
56	MG	AA	3127	1/1	0.98	0.13	16,16,16,16	0
56	MG	FA	1640	1/1	0.98	0.18	23,23,23,23	0
56	MG	GA	3030	1/1	0.98	0.24	11,11,11,11	0
56	MG	EA	3076	1/1	0.98	0.10	18,18,18,18	0
56	MG	GA	3010	1/1	0.98	0.26	15,15,15,15	0
56	MG	GA	3106	1/1	0.98	0.21	3,3,3,3	0
56	MG	BA	1622	1/1	0.98	0.21	32,32,32,32	0
56	MG	EA	3083	1/1	0.98	0.14	1,1,1,1	0
56	MG	GA	3035	1/1	0.98	0.13	15,15,15,15	0
56	MG	AA	3085	1/1	0.98	0.08	30,30,30,30	0
56	MG	GA	3066	1/1	0.98	0.17	4,4,4,4	0
56	MG	CA	3076	1/1	0.98	0.08	25,25,25,25	0
56	MG	GA	3025	1/1	0.98	0.17	18,18,18,18	0
56	MG	BA	1617	1/1	0.98	0.13	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	HA	1602	1/1	0.98	0.37	48,48,48,48	0
56	MG	CA	3024	1/1	0.98	0.19	2,2,2,2	0
56	MG	EA	3004	1/1	0.98	0.09	13,13,13,13	0
56	MG	EA	3075	1/1	0.98	0.13	10,10,10,10	0
56	MG	EA	3022	1/1	0.98	0.15	0,0,0,0	0
56	MG	AA	3026	1/1	0.98	0.07	10,10,10,10	0
56	MG	EA	3052	1/1	0.98	0.20	2,2,2,2	0
56	MG	AA	3096	1/1	0.98	0.15	33,33,33,33	0
56	MG	DA	1638	1/1	0.98	0.04	40,40,40,40	0
56	MG	CA	3093	1/1	0.98	0.12	25,25,25,25	0
56	MG	GA	3033	1/1	0.98	0.24	12,12,12,12	0
56	MG	BA	1619	1/1	0.98	0.18	28,28,28,28	0
56	MG	DA	1632	1/1	0.98	0.15	28,28,28,28	0
56	MG	FA	1611	1/1	0.98	0.23	0,0,0,0	0
56	MG	GA	3047	1/1	0.98	0.18	27,27,27,27	0
56	MG	EA	3122	1/1	0.98	0.19	0,0,0,0	0
56	MG	AA	3091	1/1	0.98	0.14	16,16,16,16	0
56	MG	EA	3078	1/1	0.98	0.18	3,3,3,3	0
56	MG	GA	3076	1/1	0.98	0.14	23,23,23,23	0
56	MG	AA	3099	1/1	0.98	0.14	15,15,15,15	0
56	MG	GL	201	1/1	0.98	0.19	7,7,7,7	0
56	MG	CA	3006	1/1	0.98	0.09	15,15,15,15	0
56	MG	EA	3054	1/1	0.98	0.13	5,5,5,5	0
56	MG	GA	3104	1/1	0.98	0.20	6,6,6,6	0
56	MG	GB	1204	1/1	0.98	0.07	21,21,21,21	0
56	MG	AA	3074	1/1	0.98	0.17	9,9,9,9	0
56	MG	GA	3031	1/1	0.98	0.14	4,4,4,4	0
56	MG	EB	1204	1/1	0.98	0.06	12,12,12,12	0
56	MG	AA	3112	1/1	0.98	0.11	7,7,7,7	0
56	MG	DA	1630	1/1	0.98	0.10	34,34,34,34	0
56	MG	GA	3009	1/1	0.98	0.16	20,20,20,20	0
56	MG	EA	3121	1/1	0.98	0.24	1,1,1,1	0
56	MG	AA	3125	1/1	0.98	0.17	23,23,23,23	0
56	MG	FA	1629	1/1	0.98	0.10	16,16,16,16	0
56	MG	HA	1618	1/1	0.98	0.08	19,19,19,19	0
56	MG	EA	3031	1/1	0.98	0.23	2,2,2,2	0
56	MG	GA	3058	1/1	0.98	0.14	17,17,17,17	0
56	MG	EA	3086	1/1	0.98	0.07	34,34,34,34	0
56	MG	GA	3122	1/1	0.98	0.19	14,14,14,14	0
56	MG	EA	3094	1/1	0.98	0.11	15,15,15,15	0
56	MG	CA	3055	1/1	0.98	0.13	20,20,20,20	0
56	MG	BA	1625	1/1	0.98	0.20	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	1621	1/1	0.98	0.19	22,22,22,22	0
56	MG	EA	3120	1/1	0.98	0.22	0,0,0,0	0
56	MG	GA	3044	1/1	0.98	0.20	23,23,23,23	0
56	MG	GA	3071	1/1	0.98	0.18	20,20,20,20	0
56	MG	AA	3054	1/1	0.98	0.12	11,11,11,11	0
56	MG	CA	3127	1/1	0.98	0.08	11,11,11,11	0
56	MG	AA	3057	1/1	0.98	0.09	18,18,18,18	0
56	MG	FA	1638	1/1	0.98	0.10	33,33,33,33	0
56	MG	FA	1606	1/1	0.98	0.13	13,13,13,13	0
56	MG	FA	1605	1/1	0.98	0.15	36,36,36,36	0
56	MG	EA	3077	1/1	0.98	0.11	14,14,14,14	0
56	MG	CA	3013	1/1	0.98	0.08	7,7,7,7	0
56	MG	AA	3064	1/1	0.98	0.13	20,20,20,20	0
56	MG	BA	1626	1/1	0.98	0.16	36,36,36,36	0
56	MG	BA	1603	1/1	0.98	0.06	21,21,21,21	0
56	MG	AA	3050	1/1	0.98	0.09	7,7,7,7	0
56	MG	GA	3011	1/1	0.98	0.10	46,46,46,46	0
56	MG	CA	3068	1/1	0.98	0.13	13,13,13,13	0
56	MG	AA	3025	1/1	0.98	0.17	8,8,8,8	0
56	MG	CA	3009	1/1	0.98	0.15	18,18,18,18	0
56	MG	AA	3076	1/1	0.98	0.09	21,21,21,21	0
56	MG	HA	1639	1/1	0.98	0.17	20,20,20,20	0
56	MG	GA	3079	1/1	0.98	0.12	18,18,18,18	0
56	MG	EA	3019	1/1	0.98	0.08	13,13,13,13	0
56	MG	GA	3078	1/1	0.98	0.24	40,40,40,40	0
56	MG	BA	1630	1/1	0.98	0.11	25,25,25,25	0
56	MG	GA	3017	1/1	0.98	0.09	24,24,24,24	0
56	MG	A3	101	1/1	0.98	0.10	13,13,13,13	0
56	MG	AA	3105	1/1	0.98	0.19	12,12,12,12	0
56	MG	AA	3124	1/1	0.98	0.17	9,9,9,9	0
56	MG	CA	3008	1/1	0.98	0.17	15,15,15,15	0
56	MG	HA	1615	1/1	0.98	0.27	38,38,38,38	0
56	MG	FA	1632	1/1	0.98	0.13	28,28,28,28	0
56	MG	BA	1616	1/1	0.98	0.22	35,35,35,35	0
56	MG	GA	3084	1/1	0.98	0.30	25,25,25,25	0
56	MG	AA	3060	1/1	0.98	0.46	25,25,25,25	0
56	MG	CA	3037	1/1	0.98	0.20	1,1,1,1	0
56	MG	EA	3129	1/1	0.98	0.22	0,0,0,0	0
56	MG	GA	3126	1/1	0.98	0.09	18,18,18,18	0
56	MG	CB	1202	1/1	0.98	0.12	55,55,55,55	0
56	MG	CA	3028	1/1	0.98	0.21	7,7,7,7	0
56	MG	GA	3014	1/1	0.98	0.28	8,8,8,8	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	1627	1/1	0.98	0.08	25,25,25,25	0
56	MG	HA	1611	1/1	0.98	0.23	20,20,20,20	0
56	MG	AA	3029	1/1	0.98	0.09	21,21,21,21	0
56	MG	DA	1620	1/1	0.98	0.08	22,22,22,22	0
56	MG	AA	3082	1/1	0.98	0.03	29,29,29,29	0
56	MG	EA	3034	1/1	0.98	0.21	0,0,0,0	0
56	MG	CA	3132	1/1	0.98	0.17	2,2,2,2	0
56	MG	AA	3080	1/1	0.98	0.18	7,7,7,7	0
56	MG	FA	1603	1/1	0.98	0.11	30,30,30,30	0
56	MG	GA	3114	1/1	0.98	0.17	10,10,10,10	0
56	MG	GA	3022	1/1	0.98	0.16	16,16,16,16	0
56	MG	CA	3003	1/1	0.98	0.13	12,12,12,12	0
56	MG	DA	1612	1/1	0.98	0.19	11,11,11,11	0
56	MG	AA	3061	1/1	0.98	0.14	6,6,6,6	0
56	MG	DA	1607	1/1	0.98	0.13	16,16,16,16	0
56	MG	GA	3045	1/1	0.98	0.17	7,7,7,7	0
56	MG	CA	3060	1/1	0.98	0.22	13,13,13,13	0
56	MG	AA	3075	1/1	0.98	0.09	15,15,15,15	0
56	MG	EA	3020	1/1	0.98	0.24	4,4,4,4	0
56	MG	GA	3036	1/1	0.98	0.14	35,35,35,35	0
56	MG	GA	3002	1/1	0.98	0.17	14,14,14,14	0
56	MG	EA	3006	1/1	0.98	0.12	19,19,19,19	0
56	MG	GA	3098	1/1	0.98	0.15	25,25,25,25	0
56	MG	DA	1615	1/1	0.98	0.15	24,24,24,24	0
56	MG	AA	3030	1/1	0.98	0.16	13,13,13,13	0
56	MG	BA	1618	1/1	0.98	0.13	3,3,3,3	0
56	MG	CA	3030	1/1	0.98	0.21	11,11,11,11	0
56	MG	CA	3073	1/1	0.98	0.24	5,5,5,5	0
56	MG	HA	1603	1/1	0.98	0.36	38,38,38,38	0
56	MG	HA	1638	1/1	0.98	0.09	26,26,26,26	0
56	MG	CA	3019	1/1	0.98	0.10	22,22,22,22	0
56	MG	FA	1633	1/1	0.98	0.11	28,28,28,28	0
56	MG	EA	3014	1/1	0.98	0.19	0,0,0,0	0
56	MG	HA	1636	1/1	0.98	0.05	21,21,21,21	0
56	MG	BA	1620	1/1	0.98	0.05	20,20,20,20	0
56	MG	EA	3053	1/1	0.98	0.18	1,1,1,1	0
56	MG	FA	1621	1/1	0.98	0.18	10,10,10,10	0
56	MG	AA	3116	1/1	0.98	0.18	3,3,3,3	0
56	MG	GA	3089	1/1	0.98	0.13	14,14,14,14	0
56	MG	GA	3120	1/1	0.98	0.21	5,5,5,5	0
56	MG	FA	1615	1/1	0.98	0.18	16,16,16,16	0
56	MG	EA	3003	1/1	0.98	0.14	6,6,6,6	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	GA	3026	1/1	0.98	0.16	6,6,6,6	0
56	MG	CA	3123	1/1	0.98	0.17	8,8,8,8	0
56	MG	GA	3064	1/1	0.98	0.12	9,9,9,9	0
56	MG	AB	1204	1/1	0.98	0.07	8,8,8,8	0
56	MG	GA	3004	1/1	0.98	0.42	19,19,19,19	0
56	MG	FA	1607	1/1	0.98	0.10	18,18,18,18	0
56	MG	EA	3101	1/1	0.99	0.13	26,26,26,26	0
56	MG	EA	3124	1/1	0.99	0.11	5,5,5,5	0
56	MG	EA	3039	1/1	0.99	0.19	0,0,0,0	0
56	MG	GA	3125	1/1	0.99	0.11	5,5,5,5	0
56	MG	AA	3102	1/1	0.99	0.24	0,0,0,0	0
56	MG	AA	3045	1/1	0.99	0.13	18,18,18,18	0
56	MG	BA	1638	1/1	0.99	0.14	31,31,31,31	0
56	MG	BA	1607	1/1	0.99	0.26	8,8,8,8	0
56	MG	DA	1633	1/1	0.99	0.04	45,45,45,45	0
56	MG	AA	3048	1/1	0.99	0.12	2,2,2,2	0
56	MG	CA	3064	1/1	0.99	0.10	1,1,1,1	0
56	MG	CA	3100	1/1	0.99	0.17	1,1,1,1	0
56	MG	CA	3051	1/1	0.99	0.29	7,7,7,7	0
56	MG	EA	3119	1/1	0.99	0.22	0,0,0,0	0
56	MG	CA	3039	1/1	0.99	0.22	6,6,6,6	0
56	MG	EA	3030	1/1	0.99	0.16	0,0,0,0	0
56	MG	GA	3038	1/1	0.99	0.16	11,11,11,11	0
56	MG	GA	3065	1/1	0.99	0.15	3,3,3,3	0
56	MG	GA	3024	1/1	0.99	0.15	8,8,8,8	0
56	MG	EA	3085	1/1	0.99	0.19	4,4,4,4	0
56	MG	EA	3111	1/1	0.99	0.19	2,2,2,2	0
56	MG	GA	3132	1/1	0.99	0.14	7,7,7,7	0
56	MG	FA	1620	1/1	0.99	0.15	6,6,6,6	0
56	MG	CA	3017	1/1	0.99	0.18	2,2,2,2	0
56	MG	CA	3066	1/1	0.99	0.17	2,2,2,2	0
56	MG	EA	3021	1/1	0.99	0.12	5,5,5,5	0
56	MG	EA	3046	1/1	0.99	0.15	9,9,9,9	0
56	MG	FA	1608	1/1	0.99	0.18	14,14,14,14	0
56	MG	GA	3063	1/1	0.99	0.27	3,3,3,3	0
56	MG	EA	3043	1/1	0.99	0.10	4,4,4,4	0
56	MG	EA	3045	1/1	0.99	0.13	1,1,1,1	0
56	MG	CA	3056	1/1	0.99	0.11	7,7,7,7	0
56	MG	BA	1632	1/1	0.99	0.10	40,40,40,40	0
56	MG	HA	1620	1/1	0.99	0.08	14,14,14,14	0
56	MG	DA	1609	1/1	0.99	0.16	16,16,16,16	0
56	MG	AB	1203	1/1	0.99	0.12	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	EA	3026	1/1	0.99	0.10	28,28,28,28	0
56	MG	CA	3121	1/1	0.99	0.21	3,3,3,3	0
56	MG	BA	1628	1/1	0.99	0.12	26,26,26,26	0
56	MG	CA	3010	1/1	0.99	0.25	10,10,10,10	0
56	MG	CA	3041	1/1	0.99	0.13	13,13,13,13	0
56	MG	ED	302	1/1	0.99	0.17	2,2,2,2	0
56	MG	CA	3036	1/1	0.99	0.08	19,19,19,19	0
56	MG	CA	3026	1/1	0.99	0.09	5,5,5,5	0
56	MG	CA	3070	1/1	0.99	0.15	4,4,4,4	0
56	MG	HA	1614	1/1	0.99	0.12	37,37,37,37	0
56	MG	AA	3114	1/1	0.99	0.09	1,1,1,1	0
57	ZN	C4	102	1/1	0.99	0.09	76,76,76,76	0
56	MG	GA	3129	1/1	0.99	0.22	19,19,19,19	0
56	MG	CA	3063	1/1	0.99	0.16	2,2,2,2	0
57	ZN	A4	101	1/1	0.99	0.09	63,63,63,63	0
56	MG	GA	3099	1/1	0.99	0.13	12,12,12,12	0
56	MG	CA	3023	1/1	0.99	0.17	5,5,5,5	0
56	MG	EA	3015	1/1	0.99	0.51	1,1,1,1	0
56	MG	AA	3123	1/1	0.99	0.17	14,14,14,14	0
56	MG	AA	3108	1/1	0.99	0.16	21,21,21,21	0
56	MG	CA	3025	1/1	0.99	0.10	7,7,7,7	0
56	MG	GA	3051	1/1	0.99	0.19	4,4,4,4	0
56	MG	AA	3008	1/1	0.99	0.12	15,15,15,15	0
56	MG	CA	3004	1/1	0.99	0.08	6,6,6,6	0
56	MG	EA	3064	1/1	0.99	0.19	0,0,0,0	0
56	MG	CA	3065	1/1	0.99	0.11	1,1,1,1	0
56	MG	AA	3109	1/1	0.99	0.21	6,6,6,6	0
56	MG	AA	3037	1/1	0.99	0.19	9,9,9,9	0
56	MG	GA	3116	1/1	0.99	0.14	3,3,3,3	0
56	MG	FA	1612	1/1	0.99	0.31	17,17,17,17	0
56	MG	AA	3003	1/1	0.99	0.10	26,26,26,26	0
56	MG	HA	1623	1/1	0.99	0.11	18,18,18,18	0
56	MG	AA	3010	1/1	0.99	0.23	13,13,13,13	0
56	MG	GA	3092	1/1	0.99	0.07	17,17,17,17	0
56	MG	EA	3041	1/1	0.99	0.10	2,2,2,2	0
56	MG	CA	3115	1/1	0.99	0.16	12,12,12,12	0
56	MG	CA	3002	1/1	0.99	0.14	17,17,17,17	0
56	MG	AA	3052	1/1	0.99	0.12	2,2,2,2	0
56	MG	AA	3129	1/1	0.99	0.11	20,20,20,20	0
56	MG	EA	3100	1/1	0.99	0.14	0,0,0,0	0
56	MG	CA	3078	1/1	0.99	0.10	25,25,25,25	0
56	MG	EA	3007	1/1	0.99	0.07	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	GA	3053	1/1	0.99	0.15	4,4,4,4	0
56	MG	DA	1623	1/1	0.99	0.07	12,12,12,12	0
56	MG	CA	3035	1/1	0.99	0.16	3,3,3,3	0
56	MG	BA	1633	1/1	0.99	0.10	35,35,35,35	0
56	MG	GA	3041	1/1	0.99	0.09	10,10,10,10	0
56	MG	CA	3071	1/1	0.99	0.14	2,2,2,2	0
56	MG	AA	3101	1/1	0.99	0.17	7,7,7,7	0
56	MG	GA	3134	1/1	0.99	0.05	16,16,16,16	0
57	ZN	E4	101	1/1	0.99	0.09	54,54,54,54	0
56	MG	AA	3118	1/1	0.99	0.11	11,11,11,11	0
56	MG	GA	3097	1/1	0.99	0.17	26,26,26,26	0
56	MG	CA	3034	1/1	0.99	0.19	18,18,18,18	0
56	MG	CA	3038	1/1	0.99	0.18	7,7,7,7	0
56	MG	GA	3112	1/1	0.99	0.10	15,15,15,15	0
56	MG	AA	3009	1/1	0.99	0.22	12,12,12,12	0
56	MG	AA	3106	1/1	0.99	0.18	9,9,9,9	0
56	MG	GC	301	1/1	0.99	0.18	4,4,4,4	0
56	MG	CA	3129	1/1	0.99	0.17	9,9,9,9	0
56	MG	GA	3070	1/1	0.99	0.23	13,13,13,13	0
56	MG	CA	3101	1/1	0.99	0.15	10,10,10,10	0
56	MG	GA	3123	1/1	0.99	0.20	11,11,11,11	0
56	MG	EA	3067	1/1	0.99	0.26	4,4,4,4	0
56	MG	DA	1635	1/1	0.99	0.08	38,38,38,38	0
56	MG	GA	3096	1/1	0.99	0.16	4,4,4,4	0
56	MG	CA	3133	1/1	0.99	0.12	13,13,13,13	0
56	MG	AA	3065	1/1	0.99	0.16	2,2,2,2	0
56	MG	CA	3081	1/1	0.99	0.15	10,10,10,10	0
56	MG	CA	3075	1/1	0.99	0.22	20,20,20,20	0
56	MG	CA	3048	1/1	0.99	0.09	13,13,13,13	0
56	MG	EA	3092	1/1	0.99	0.14	7,7,7,7	0
56	MG	EA	3017	1/1	0.99	0.16	3,3,3,3	0
56	MG	CA	3088	1/1	0.99	0.10	28,28,28,28	0
56	MG	CA	3112	1/1	0.99	0.14	4,4,4,4	0
56	MG	GA	3081	1/1	0.99	0.19	16,16,16,16	0
56	MG	CA	3059	1/1	0.99	0.17	3,3,3,3	0
56	MG	GA	3115	1/1	0.99	0.23	23,23,23,23	0
56	MG	AA	3084	1/1	0.99	0.20	12,12,12,12	0
56	MG	GA	3012	1/1	0.99	0.19	2,2,2,2	0
56	MG	AA	3081	1/1	0.99	0.14	16,16,16,16	0
56	MG	GA	3028	1/1	0.99	0.12	10,10,10,10	0
56	MG	EA	3063	1/1	0.99	0.13	1,1,1,1	0
56	MG	CA	3049	1/1	0.99	0.18	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3052	1/1	0.99	0.10	10,10,10,10	0
56	MG	CA	3128	1/1	0.99	0.16	6,6,6,6	0
56	MG	GA	3090	1/1	0.99	0.07	26,26,26,26	0
56	MG	CA	3014	1/1	0.99	0.12	9,9,9,9	0
56	MG	GA	3003	1/1	0.99	0.11	15,15,15,15	0
56	MG	AA	3117	1/1	0.99	0.25	7,7,7,7	0
56	MG	AA	3053	1/1	0.99	0.10	6,6,6,6	0
56	MG	EA	3118	1/1	0.99	0.19	1,1,1,1	0
56	MG	AA	3028	1/1	0.99	0.28	2,2,2,2	0
56	MG	GA	3107	1/1	0.99	0.12	27,27,27,27	0
56	MG	FA	1631	1/1	0.99	0.06	21,21,21,21	0
56	MG	BA	1611	1/1	0.99	0.13	15,15,15,15	0
56	MG	HA	1605	1/1	0.99	0.11	39,39,39,39	0
56	MG	EA	3081	1/1	0.99	0.15	3,3,3,3	0
57	ZN	G4	101	1/1	0.99	0.09	69,69,69,69	0
56	MG	AA	3042	1/1	0.99	0.17	11,11,11,11	0
56	MG	CA	3022	1/1	0.99	0.12	0,0,0,0	0
56	MG	FA	1622	1/1	0.99	0.10	15,15,15,15	0
56	MG	CA	3047	1/1	0.99	0.10	31,31,31,31	0
56	MG	FA	1637	1/1	0.99	0.10	34,34,34,34	0
56	MG	GA	3074	1/1	0.99	0.14	2,2,2,2	0
56	MG	CA	3084	1/1	0.99	0.21	4,4,4,4	0
56	MG	BA	1639	1/1	0.99	0.13	19,19,19,19	0
56	MG	EA	3036	1/1	0.99	0.14	1,1,1,1	0
56	MG	EA	3110	1/1	0.99	0.11	24,24,24,24	0
56	MG	GA	3128	1/1	0.99	0.09	20,20,20,20	0
56	MG	GA	3109	1/1	0.99	0.09	9,9,9,9	0
56	MG	GA	3086	1/1	0.99	0.04	26,26,26,26	0
56	MG	EA	3106	1/1	0.99	0.15	0,0,0,0	0
56	MG	CA	3131	1/1	0.99	0.10	0,0,0,0	0
56	MG	AA	3121	1/1	0.99	0.10	20,20,20,20	0
56	MG	AA	3004	1/1	0.99	0.07	34,34,34,34	0
56	MG	GA	3117	1/1	0.99	0.07	22,22,22,22	0
56	MG	AA	3034	1/1	0.99	0.11	14,14,14,14	0
56	MG	EA	3126	1/1	0.99	0.17	2,2,2,2	0
56	MG	GA	3052	1/1	0.99	0.18	8,8,8,8	0
56	MG	HA	1640	1/1	0.99	0.10	15,15,15,15	0
56	MG	GA	3121	1/1	0.99	0.14	4,4,4,4	0
56	MG	AA	3001	1/1	0.99	0.09	11,11,11,11	0
56	MG	DA	1634	1/1	0.99	0.13	33,33,33,33	0
56	MG	CA	3108	1/1	0.99	0.12	3,3,3,3	0
56	MG	HA	1606	1/1	0.99	0.16	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3012	1/1	0.99	0.12	3,3,3,3	0
56	MG	GA	3130	1/1	0.99	0.09	9,9,9,9	0
56	MG	GA	3005	1/1	0.99	0.13	15,15,15,15	0
56	MG	EA	3009	1/1	0.99	0.20	0,0,0,0	0
56	MG	CA	3074	1/1	0.99	0.05	19,19,19,19	0
56	MG	GA	3124	1/1	0.99	0.12	16,16,16,16	0
56	MG	CA	3102	1/1	0.99	0.07	32,32,32,32	0
56	MG	EA	3066	1/1	0.99	0.19	0,0,0,0	0
56	MG	CA	3125	1/1	0.99	0.14	9,9,9,9	0
56	MG	CA	3124	1/1	0.99	0.15	0,0,0,0	0
56	MG	BA	1615	1/1	0.99	0.20	22,22,22,22	0
56	MG	FA	1634	1/1	0.99	0.07	19,19,19,19	0
56	MG	CA	3021	1/1	0.99	0.10	10,10,10,10	0
56	MG	FA	1623	1/1	0.99	0.21	7,7,7,7	0
56	MG	GA	3067	1/1	0.99	0.19	16,16,16,16	0
56	MG	CA	3096	1/1	0.99	0.21	10,10,10,10	0
56	MG	CA	3134	1/1	0.99	0.18	23,23,23,23	0
56	MG	CA	3119	1/1	0.99	0.21	3,3,3,3	0
56	MG	EA	3001	1/1	0.99	0.11	9,9,9,9	0
56	MG	FA	1613	1/1	0.99	0.11	9,9,9,9	0
56	MG	AA	3018	1/1	0.99	0.18	12,12,12,12	0
56	MG	AA	3051	1/1	0.99	0.08	4,4,4,4	0
56	MG	EA	3042	1/1	0.99	0.18	2,2,2,2	0
56	MG	GA	3105	1/1	0.99	0.15	3,3,3,3	0
56	MG	EA	3123	1/1	0.99	0.29	2,2,2,2	0
56	MG	EA	3116	1/1	0.99	0.15	0,0,0,0	0
56	MG	HA	1607	1/1	0.99	0.21	11,11,11,11	0
56	MG	CA	3116	1/1	0.99	0.12	13,13,13,13	0
56	MG	EA	3023	1/1	0.99	0.17	2,2,2,2	0
56	MG	EA	3093	1/1	0.99	0.09	21,21,21,21	0
56	MG	DA	1616	1/1	0.99	0.27	26,26,26,26	0
56	MG	EA	3013	1/1	0.99	0.14	0,0,0,0	0
56	MG	CA	3043	1/1	0.99	0.11	5,5,5,5	0
56	MG	CA	3001	1/1	0.99	0.15	10,10,10,10	0
56	MG	AA	3027	1/1	0.99	0.15	8,8,8,8	0
56	MG	CD	301	1/1	0.99	0.17	3,3,3,3	0
56	MG	AA	3019	1/1	0.99	0.18	33,33,33,33	0
56	MG	DA	1605	1/1	0.99	0.12	28,28,28,28	0
56	MG	AA	3020	1/1	0.99	0.13	24,24,24,24	0
56	MG	GA	3034	1/1	0.99	0.19	16,16,16,16	0
56	MG	HA	1622	1/1	0.99	0.10	36,36,36,36	0
56	MG	EA	3047	1/1	0.99	0.09	6,6,6,6	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	EA	3062	1/1	0.99	0.17	0,0,0,0	0
56	MG	GA	3049	1/1	0.99	0.17	8,8,8,8	0
56	MG	GA	3008	1/1	0.99	0.20	12,12,12,12	0
56	MG	EA	3074	1/1	0.99	0.18	4,4,4,4	0
56	MG	GA	3050	1/1	0.99	0.15	9,9,9,9	0
56	MG	AA	3094	1/1	0.99	0.06	20,20,20,20	0
56	MG	AA	3067	1/1	0.99	0.09	29,29,29,29	0
56	MG	CA	3029	1/1	0.99	0.07	8,8,8,8	0
56	MG	CA	3117	1/1	0.99	0.08	7,7,7,7	0
56	MG	CA	3095	1/1	0.99	0.11	21,21,21,21	0
56	MG	EA	3032	1/1	0.99	0.16	0,0,0,0	0
56	MG	HA	1631	1/1	0.99	0.10	28,28,28,28	0
56	MG	GA	3013	1/1	0.99	0.21	1,1,1,1	0
56	MG	GA	3043	1/1	0.99	0.10	8,8,8,8	0
56	MG	CA	3082	1/1	0.99	0.12	15,15,15,15	0
56	MG	AA	3013	1/1	0.99	0.16	5,5,5,5	0
56	MG	CA	3042	1/1	0.99	0.11	8,8,8,8	0
56	MG	EB	1203	1/1	0.99	0.14	3,3,3,3	0
56	MG	AA	3047	1/1	0.99	0.10	30,30,30,30	0
56	MG	AA	3062	1/1	0.99	0.18	2,2,2,2	0
56	MG	AA	3122	1/1	0.99	0.16	2,2,2,2	0
56	MG	EA	3027	1/1	0.99	0.20	0,0,0,0	0
56	MG	DA	1617	1/1	0.99	0.13	45,45,45,45	0
56	MG	AA	3039	1/1	0.99	0.18	5,5,5,5	0
56	MG	BA	1608	1/1	0.99	0.10	22,22,22,22	0
56	MG	EC	301	1/1	0.99	0.14	1,1,1,1	0
56	MG	AA	3095	1/1	0.99	0.10	9,9,9,9	0
56	MG	AA	3058	1/1	0.99	0.19	9,9,9,9	0
56	MG	FA	1609	1/1	0.99	0.32	16,16,16,16	0
56	MG	EA	3128	1/1	0.99	0.15	4,4,4,4	0
56	MG	EA	3012	1/1	0.99	0.17	1,1,1,1	0
56	MG	CA	3033	1/1	0.99	0.18	9,9,9,9	0
56	MG	FA	1619	1/1	0.99	0.10	25,25,25,25	0
56	MG	CA	3027	1/1	0.99	0.10	2,2,2,2	0
56	MG	BA	1602	1/1	0.99	0.12	15,15,15,15	0
56	MG	AA	3072	1/1	0.99	0.16	7,7,7,7	0
56	MG	EA	3095	1/1	0.99	0.17	5,5,5,5	0
56	MG	EA	3105	1/1	0.99	0.14	4,4,4,4	0
56	MG	FA	1635	1/1	0.99	0.13	8,8,8,8	0
56	MG	AA	3130	1/1	0.99	0.15	27,27,27,27	0
56	MG	EA	3084	1/1	0.99	0.17	2,2,2,2	0
56	MG	EA	3072	1/1	0.99	0.15	8,8,8,8	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	GA	3016	1/1	0.99	0.15	9,9,9,9	0
56	MG	AA	3041	1/1	0.99	0.18	2,2,2,2	0
56	MG	CA	3104	1/1	0.99	0.14	4,4,4,4	0
56	MG	FA	1625	1/1	0.99	0.09	18,18,18,18	0
56	MG	CA	3086	1/1	0.99	0.19	20,20,20,20	0
56	MG	HA	1635	1/1	0.99	0.15	17,17,17,17	0
56	MG	CA	3054	1/1	0.99	0.17	6,6,6,6	0
56	MG	AA	3120	1/1	0.99	0.18	6,6,6,6	0
56	MG	EA	3038	1/1	0.99	0.11	2,2,2,2	0
56	MG	DV	802	1/1	0.99	0.11	34,34,34,34	0
56	MG	HA	1627	1/1	0.99	0.14	24,24,24,24	0
56	MG	EA	3035	1/1	0.99	0.17	0,0,0,0	0
56	MG	CA	3067	1/1	0.99	0.11	4,4,4,4	0
56	MG	EA	3028	1/1	0.99	0.18	1,1,1,1	0
56	MG	AA	3046	1/1	0.99	0.15	7,7,7,7	0
56	MG	CA	3089	1/1	0.99	0.15	2,2,2,2	0
56	MG	DA	1640	1/1	0.99	0.18	21,21,21,21	0
56	MG	CA	3109	1/1	0.99	0.12	26,26,26,26	0
56	MG	FA	1624	1/1	0.99	0.18	18,18,18,18	0
56	MG	EA	3065	1/1	0.99	0.11	0,0,0,0	0
56	MG	CA	3113	1/1	0.99	0.11	14,14,14,14	0
56	MG	DA	1603	1/1	0.99	0.12	22,22,22,22	0
56	MG	AA	3040	1/1	0.99	0.12	24,24,24,24	0
56	MG	EA	3008	1/1	0.99	0.18	1,1,1,1	0
56	MG	AA	3083	1/1	0.99	0.27	33,33,33,33	0
56	MG	AA	3126	1/1	0.99	0.10	3,3,3,3	0
56	MG	HA	1628	1/1	0.99	0.14	30,30,30,30	0
56	MG	CA	3079	1/1	0.99	0.22	12,12,12,12	0
56	MG	AA	3021	1/1	0.99	0.11	11,11,11,11	0
56	MG	EA	3132	1/1	0.99	0.23	6,6,6,6	0
56	MG	CA	3018	1/1	0.99	0.10	26,26,26,26	0
56	MG	GA	3015	1/1	0.99	0.11	18,18,18,18	0
56	MG	GA	3119	1/1	0.99	0.16	5,5,5,5	0
56	MG	CA	3031	1/1	0.99	0.14	11,11,11,11	0
56	MG	GA	3101	1/1	0.99	0.10	15,15,15,15	0
56	MG	GA	3054	1/1	0.99	0.14	1,1,1,1	0
56	MG	AA	3104	1/1	0.99	0.13	12,12,12,12	0
56	MG	CA	3062	1/1	0.99	0.13	5,5,5,5	0
56	MG	AA	3036	1/1	0.99	0.24	25,25,25,25	0
56	MG	AA	3103	1/1	0.99	0.17	10,10,10,10	0
56	MG	GA	3032	1/1	0.99	0.13	8,8,8,8	0
56	MG	CA	3050	1/1	0.99	0.11	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	AA	3049	1/1	0.99	0.15	3,3,3,3	0
56	MG	GA	3027	1/1	0.99	0.17	6,6,6,6	0
56	MG	GA	3062	1/1	0.99	0.13	18,18,18,18	0
56	MG	CA	3072	1/1	0.99	0.15	11,11,11,11	0
56	MG	EA	3048	1/1	0.99	0.13	11,11,11,11	0
56	MG	CA	3032	1/1	0.99	0.17	3,3,3,3	0
56	MG	CA	3090	1/1	0.99	0.13	20,20,20,20	0
56	MG	AA	3035	1/1	0.99	0.20	3,3,3,3	0
56	MG	HA	1612	1/1	0.99	0.19	8,8,8,8	0
56	MG	EA	3131	1/1	0.99	0.20	5,5,5,5	0
56	MG	EA	3049	1/1	0.99	0.23	8,8,8,8	0
56	MG	EA	3073	1/1	0.99	0.19	0,0,0,0	0
56	MG	GA	3019	1/1	0.99	0.10	5,5,5,5	0
56	MG	AA	3014	1/1	0.99	0.18	4,4,4,4	0
56	MG	HA	1632	1/1	0.99	0.21	25,25,25,25	0
56	MG	AA	3022	1/1	0.99	0.11	8,8,8,8	0
56	MG	BA	1610	1/1	0.99	0.07	19,19,19,19	0
56	MG	EA	3114	1/1	0.99	0.18	1,1,1,1	0
56	MG	DA	1619	1/1	0.99	0.12	33,33,33,33	0
56	MG	EA	3061	1/1	0.99	0.22	0,0,0,0	0
56	MG	FA	1626	1/1	0.99	0.16	15,15,15,15	0
56	MG	GA	3007	1/1	0.99	0.07	28,28,28,28	0
56	MG	AA	3107	1/1	0.99	0.19	18,18,18,18	0
56	MG	AA	3110	1/1	0.99	0.21	4,4,4,4	0
56	MG	CA	3098	1/1	0.99	0.21	10,10,10,10	0
56	MG	FA	1616	1/1	0.99	0.19	16,16,16,16	0
56	MG	CA	3080	1/1	0.99	0.16	8,8,8,8	0
56	MG	AA	3056	1/1	0.99	0.13	24,24,24,24	0
56	MG	AA	3073	1/1	0.99	0.16	8,8,8,8	0
56	MG	AA	3038	1/1	0.99	0.11	6,6,6,6	0
56	MG	CA	3040	1/1	0.99	0.19	12,12,12,12	0
56	MG	GA	3020	1/1	0.99	0.21	3,3,3,3	0
56	MG	GA	3080	1/1	0.99	0.26	5,5,5,5	0
56	MG	DA	1637	1/1	0.99	0.11	23,23,23,23	0
56	MG	EA	3099	1/1	0.99	0.28	2,2,2,2	0
56	MG	GA	3127	1/1	0.99	0.12	1,1,1,1	0
56	MG	CA	3046	1/1	0.99	0.16	17,17,17,17	0
56	MG	HA	1616	1/1	0.99	0.16	33,33,33,33	0
56	MG	FA	1614	1/1	1.00	0.13	5,5,5,5	0
56	MG	GA	3085	1/1	1.00	0.15	16,16,16,16	0
56	MG	CA	3107	1/1	1.00	0.20	6,6,6,6	0
56	MG	AA	3031	1/1	1.00	0.17	8,8,8,8	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	AA	3033	1/1	1.00	0.17	8,8,8,8	0
56	MG	AA	3055	1/1	1.00	0.17	18,18,18,18	0
56	MG	CB	1203	1/1	1.00	0.11	6,6,6,6	0
56	MG	EA	3089	1/1	1.00	0.10	5,5,5,5	0
56	MG	EA	3051	1/1	1.00	0.15	0,0,0,0	0
56	MG	EA	3107	1/1	1.00	0.20	0,0,0,0	0
56	MG	EA	3091	1/1	1.00	0.14	11,11,11,11	0
56	MG	AA	3016	1/1	1.00	0.12	10,10,10,10	0
56	MG	AA	3066	1/1	1.00	0.17	6,6,6,6	0
56	MG	EA	3104	1/1	1.00	0.16	1,1,1,1	0
56	MG	DA	1613	1/1	1.00	0.10	12,12,12,12	0
56	MG	EA	3115	1/1	1.00	0.13	2,2,2,2	0
56	MG	GA	3056	1/1	1.00	0.12	4,4,4,4	0
56	MG	CA	3099	1/1	1.00	0.14	17,17,17,17	0
56	MG	EA	3097	1/1	1.00	0.19	2,2,2,2	0
56	MG	GA	3039	1/1	1.00	0.17	15,15,15,15	0
56	MG	AA	3032	1/1	1.00	0.16	14,14,14,14	0
56	MG	EA	3037	1/1	1.00	0.13	2,2,2,2	0
56	MG	AA	3128	1/1	1.00	0.14	2,2,2,2	0
56	MG	EA	3018	1/1	1.00	0.14	8,8,8,8	0
56	MG	GA	3048	1/1	1.00	0.19	6,6,6,6	0
56	MG	AA	3113	1/1	1.00	0.11	8,8,8,8	0
56	MG	BA	1605	1/1	1.00	0.12	21,21,21,21	0
56	MG	CA	3053	1/1	1.00	0.12	5,5,5,5	0
56	MG	AA	3070	1/1	1.00	0.13	11,11,11,11	0
56	MG	CA	3130	1/1	1.00	0.17	1,1,1,1	0
56	MG	EA	3040	1/1	1.00	0.18	1,1,1,1	0
56	MG	AA	3119	1/1	1.00	0.15	13,13,13,13	0
56	MG	AA	3043	1/1	1.00	0.13	21,21,21,21	0
56	MG	AA	3012	1/1	1.00	0.20	7,7,7,7	0
56	MG	CA	3126	1/1	1.00	0.14	7,7,7,7	0
56	MG	EA	3070	1/1	1.00	0.14	3,3,3,3	0
56	MG	AA	3097	1/1	1.00	0.18	8,8,8,8	0
56	MG	EA	3002	1/1	1.00	0.17	4,4,4,4	0
56	MG	CA	3058	1/1	1.00	0.13	5,5,5,5	0
56	MG	AA	3071	1/1	1.00	0.13	3,3,3,3	0
56	MG	AA	3023	1/1	1.00	0.17	3,3,3,3	0
56	MG	GA	3021	1/1	1.00	0.12	9,9,9,9	0
56	MG	EA	3112	1/1	1.00	0.15	5,5,5,5	0
56	MG	AA	3017	1/1	1.00	0.20	1,1,1,1	0
56	MG	GA	3042	1/1	1.00	0.14	24,24,24,24	0
56	MG	BV	802	1/1	1.00	0.17	27,27,27,27	0

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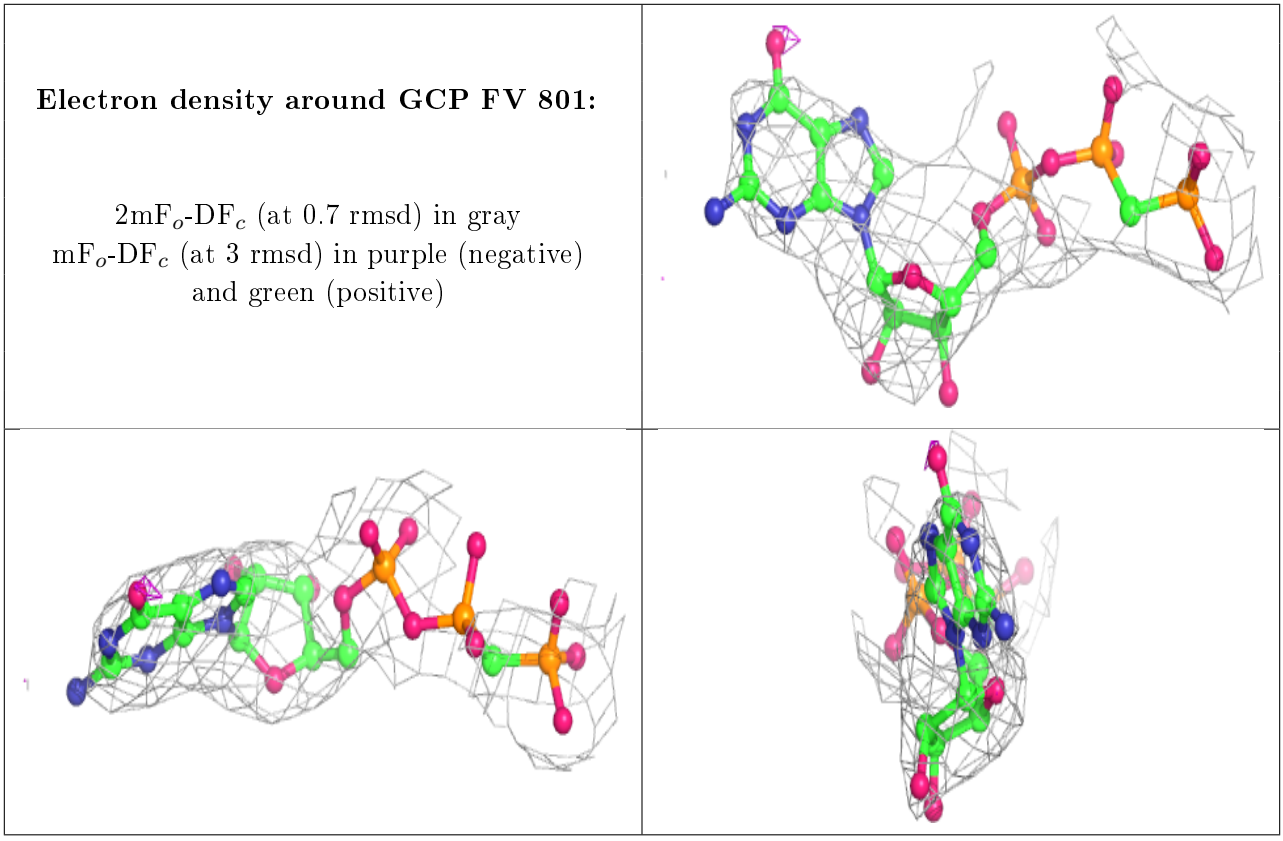
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	EA	3033	1/1	1.00	0.17	1,1,1,1	0
56	MG	AA	3079	1/1	1.00	0.16	11,11,11,11	0

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.

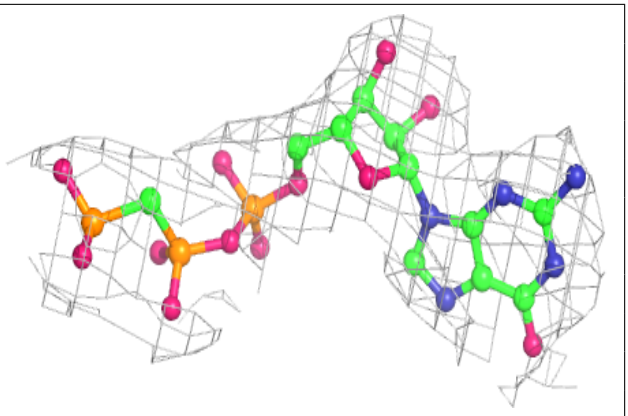
Electron density around GCP FV 801:

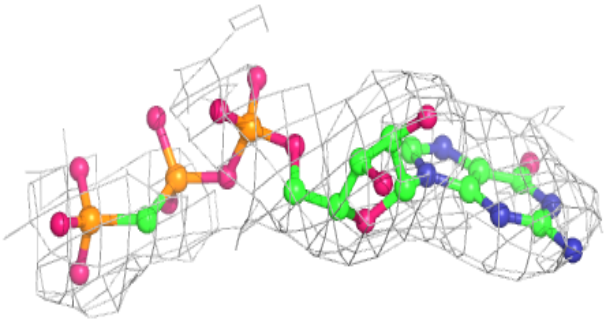
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

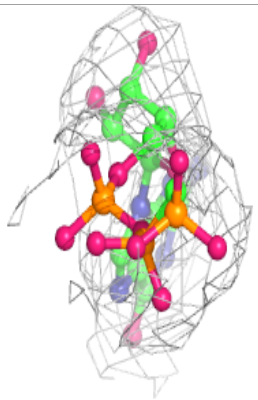


Electron density around GCP DV 801:

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

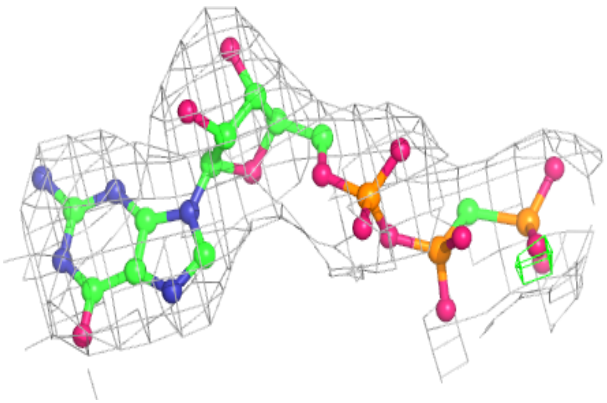


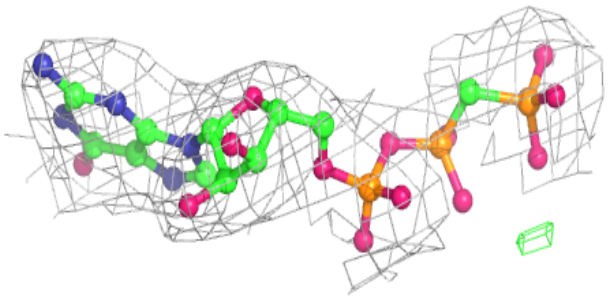


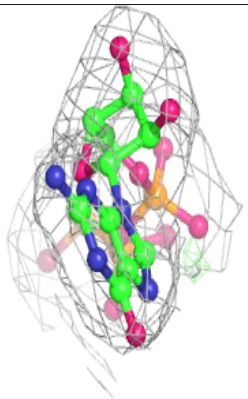


Electron density around GCP BV 801:

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

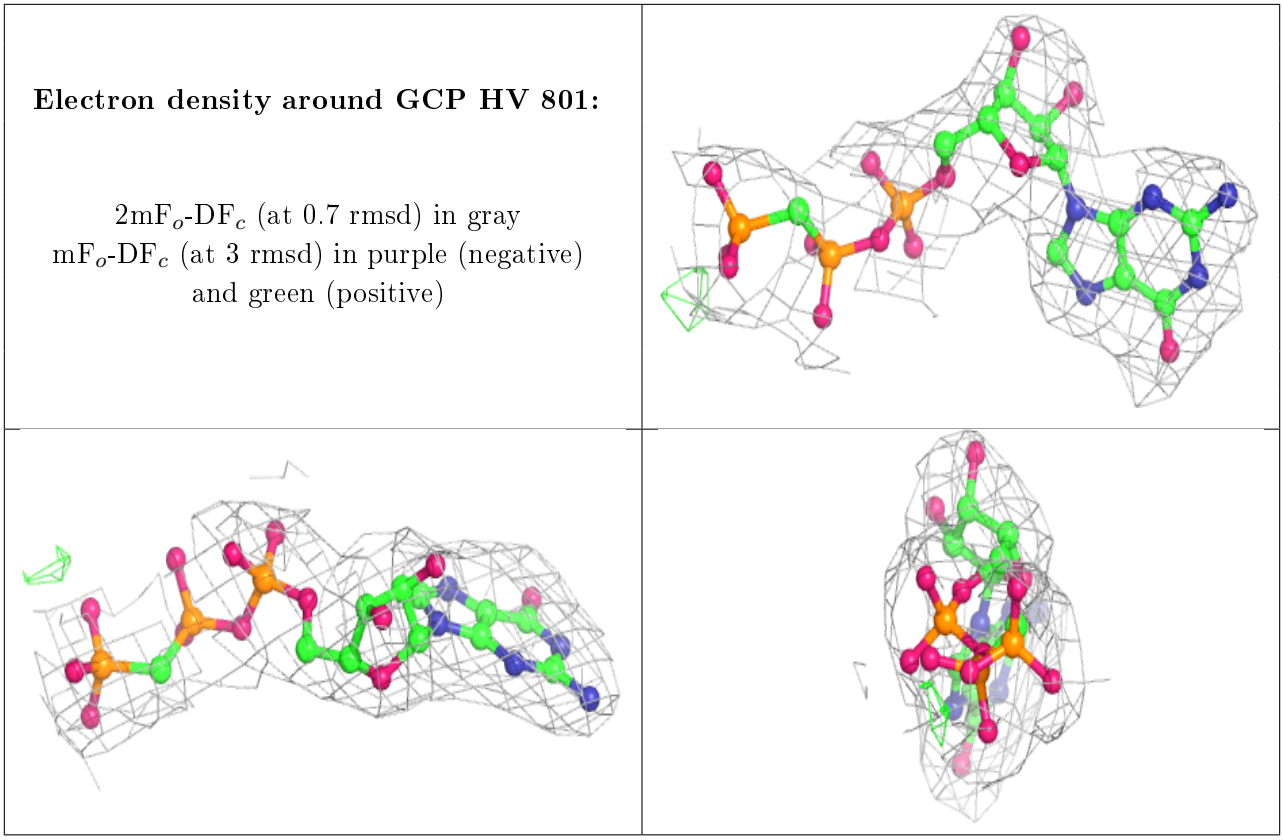






Electron density around GCP HV 801:

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



6.5 Other polymers (i)

There are no such residues in this entry.