



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 22, 2024 – 06:19 PM EDT

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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.37.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

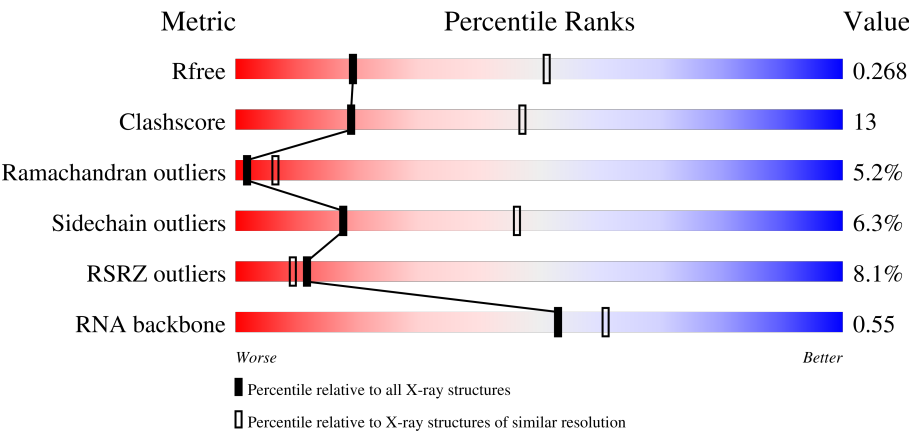
# 1 Overall quality at a glance i

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 <sub>free</sub>	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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	2904	<div><div>2%</div><div><div></div><div></div><div></div><div></div></div><div>47%38%12%..</div></div>
1	CA	2904	<div><div>2%</div><div><div></div><div></div><div></div><div></div></div><div>52%33%11%..</div></div>
1	EA	2904	<div><div>2%</div><div><div></div><div></div><div></div><div></div></div><div>50%34%12%..</div></div>
1	GA	2904	<div><div>2%</div><div><div></div><div></div><div></div><div></div></div><div>53%32%11%..</div></div>

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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	

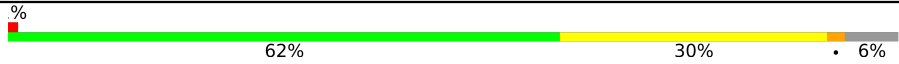

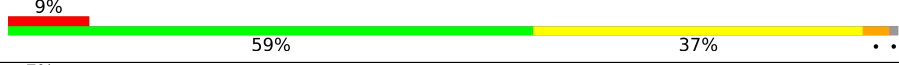

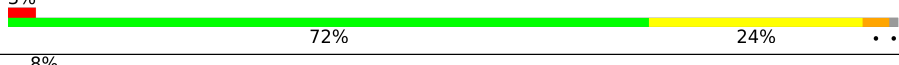
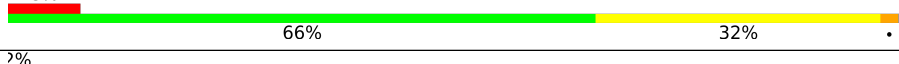
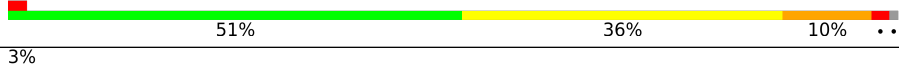

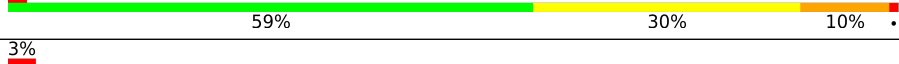


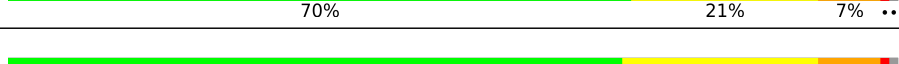
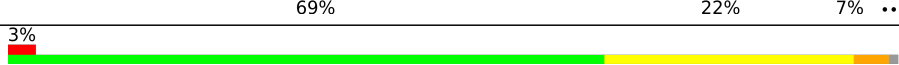
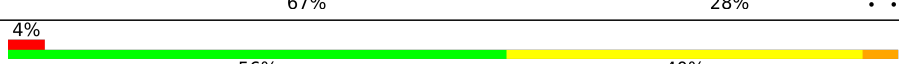

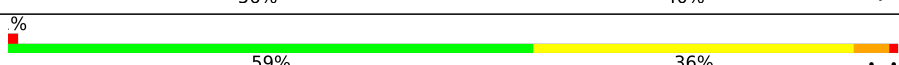
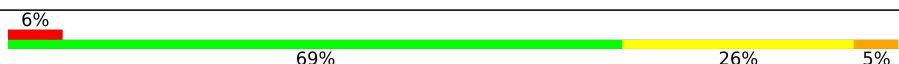
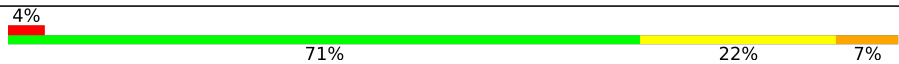
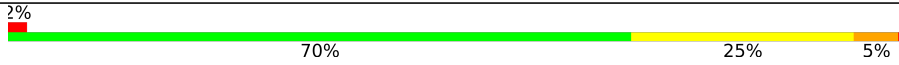


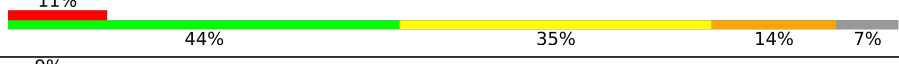



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Mol	Chain	Length	Quality of chain
8	CH	50	
8	EH	50	
8	GH	50	
9	AI	142	
9	CI	142	
9	EI	142	
9	GI	142	
10	AJ	142	
10	CJ	142	
10	EJ	142	
10	GJ	142	
11	AK	123	
11	CK	123	
11	EK	123	
11	GK	123	
12	AL	144	
12	CL	144	
12	EL	144	
12	GL	144	
13	AM	136	
13	CM	136	
13	EM	136	
13	GM	136	
14	AN	127	
14	CN	127	

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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	
16	AP	115	
16	CP	115	
16	EP	115	
16	GP	115	
17	AQ	118	
17	CQ	118	
17	EQ	118	
17	GQ	118	
18	AR	103	
18	CR	103	
18	ER	103	
18	GR	103	
19	AS	110	
19	CS	110	
19	ES	110	
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	
25	AY	63	
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
27	A0	57	
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	
34	BB	241	
34	DB	241	
34	FB	241	
34	HB	241	
35	BC	233	
35	DC	233	
35	FC	233	
35	HC	233	
36	BD	206	
36	DD	206	
36	FD	206	
36	HD	206	
37	BE	167	
37	DE	167	
37	FE	167	
37	HE	167	
38	BF	135	
38	DF	135	
38	FF	135	
38	HF	135	
39	BG	179	
39	DG	179	
39	FG	179	
39	HG	179	

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Mol	Chain	Length	Quality of chain
40	BH	130	
40	DH	130	
40	FH	130	
40	HH	130	
41	BI	130	
41	DI	130	
41	FI	130	
41	HI	130	
42	BJ	103	
42	DJ	103	
42	FJ	103	
42	HJ	103	
43	BK	129	
43	DK	129	
43	FK	129	
43	HK	129	
44	BL	124	
44	DL	124	
44	FL	124	
44	HL	124	
45	BM	118	
45	DM	118	
45	FM	118	
45	HM	118	
46	BN	101	

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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	
52	HT	87	
53	BU	71	
53	DU	71	
53	FU	71	
53	HU	71	
54	BV	704	
54	DV	704	
54	FV	704	
54	HV	704	
55	BW	6	
55	DW	6	
55	FW	6	

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	AA	130	Total	Mg	0	0
			130	130		
56	AB	4	Total	Mg	0	0
			4	4		
56	AC	3	Total	Mg	0	0
			3	3		
56	AD	1	Total	Mg	0	0
			1	1		
56	AE	1	Total	Mg	0	0
			1	1		
56	AT	1	Total	Mg	0	0
			1	1		
56	A3	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	BA	40	Total 40	Mg 40	0	0
56	BE	1	Total 1	Mg 1	0	0
56	BL	1	Total 1	Mg 1	0	0
56	BU	1	Total 1	Mg 1	0	0
56	BV	1	Total 1	Mg 1	0	0
56	CA	134	Total 134	Mg 134	0	0
56	CB	4	Total 4	Mg 4	0	0
56	CD	1	Total 1	Mg 1	0	0
56	CE	1	Total 1	Mg 1	0	0
56	C4	1	Total 1	Mg 1	0	0
56	DA	42	Total 42	Mg 42	0	0
56	DU	1	Total 1	Mg 1	0	0
56	DV	1	Total 1	Mg 1	0	0
56	EA	133	Total 133	Mg 133	0	0
56	EB	4	Total 4	Mg 4	0	0
56	EC	1	Total 1	Mg 1	0	0
56	ED	2	Total 2	Mg 2	0	0
56	EQ	1	Total 1	Mg 1	0	0
56	FA	41	Total 41	Mg 41	0	0
56	FE	1	Total 1	Mg 1	0	0
56	FU	1	Total 1	Mg 1	0	0

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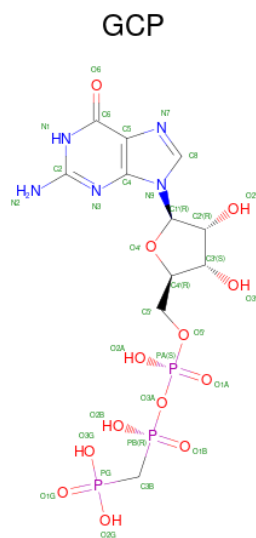
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	FV	1	Total 1	Mg 1	0	0
56	GA	134	Total 134	Mg 134	0	0
56	GB	4	Total 4	Mg 4	0	0
56	GC	1	Total 1	Mg 1	0	0
56	GL	1	Total 1	Mg 1	0	0
56	GS	1	Total 1	Mg 1	0	0
56	HA	40	Total 40	Mg 40	0	0
56	HC	1	Total 1	Mg 1	0	0
56	HE	1	Total 1	Mg 1	0	0
56	HT	1	Total 1	Mg 1	0	0
56	HV	1	Total 1	Mg 1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	A4	1	Total 1	Zn 1	0	0
57	C4	1	Total 1	Zn 1	0	0
57	E4	1	Total 1	Zn 1	0	0
57	G4	1	Total 1	Zn 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 32	C 11	N 5	O 13	P 3	0	0
58	DV	1	Total 32	C 11	N 5	O 13	P 3	0	0
58	FV	1	Total 32	C 11	N 5	O 13	P 3	0	0
58	HV	1	Total 32	C 11	N 5	O 13	P 3	0	0

- Molecule 59 is water.

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

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

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

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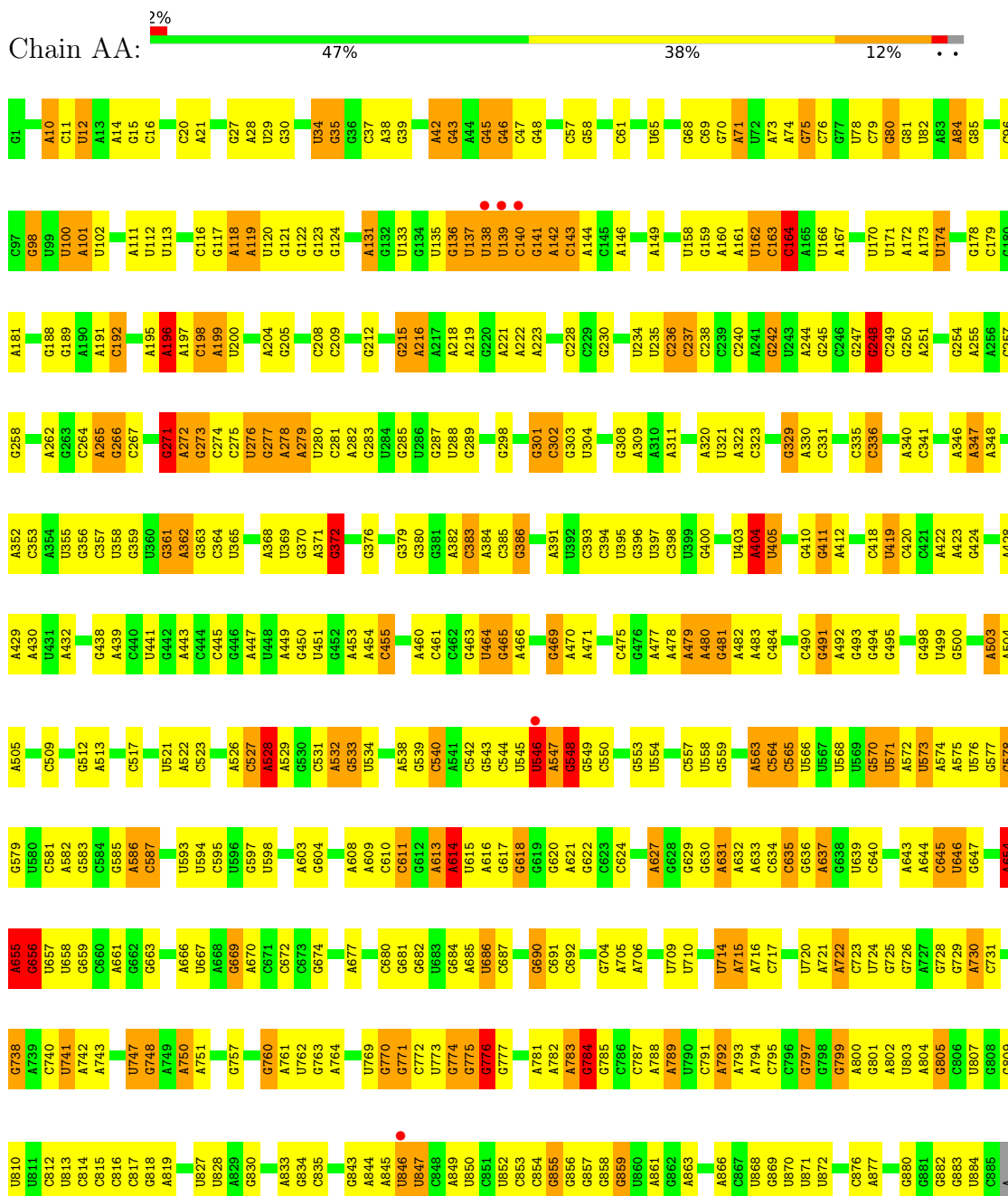
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	GD	4	Total 4	O 4	0	0
59	GE	2	Total 2	O 2	0	0
59	GL	4	Total 4	O 4	0	0
59	GN	3	Total 3	O 3	0	0
59	GQ	1	Total 1	O 1	0	0
59	GR	2	Total 2	O 2	0	0
59	GS	1	Total 1	O 1	0	0
59	GT	1	Total 1	O 1	0	0
59	GU	2	Total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

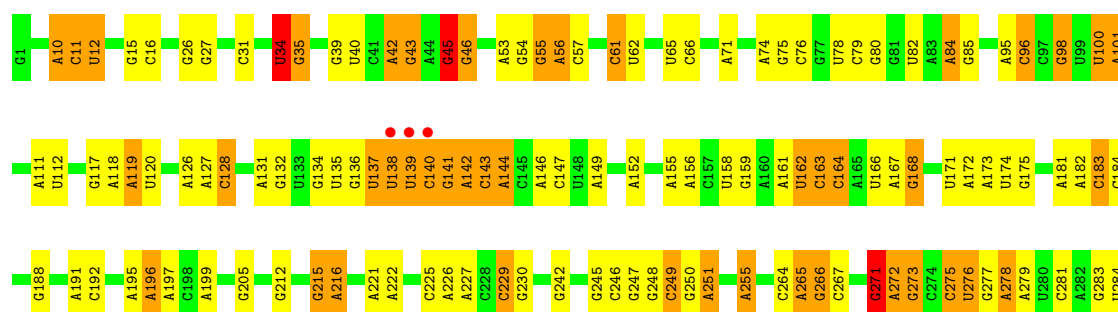
### 3 Residue-property plots

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

• Molecule 1: 23S rRNA

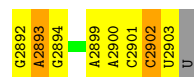


A2020	A1913	G1799	G1723	G1643	G1543	A1469	A1387	G1297	G1223	G1136	U1060	A981
C2021	C1914	C1800	G1724	G1644	A1543	A1470	G1388	C1298	G1227	G1137	U1061	C982
U2022	U1915	A1801	U1725	G1645	A1544	A1476	U1390	G1299	G1227	G1138	U1062	A983
C2023	A1916	A1802	C1726	G1646	A1548	U1474	U1394	A1301	U1231	G1139	G1063	A984
G2024	C1924	A1805	C1727	U1647	A1549	G1475	U1395	A1302	U1232	U1141	U1064	C985
G2025	U1926	C1806	U1728	U1648	A1551	G1476	A1395	C1305	G1233	A1142	U1065	A892
U2026	A1927	G1807	U1729	U1649	A1552	U1477	U1396	C1306	G1234	C1146	U1066	C893
G2027	G1928	A1808	C1730	A1650	C1555	G1478	U1397	A1307	U1235	C1147	A1067	A896
A2030	G1929	G1809	C1731	A1651	C1556	G1479	U1398	A1308	G1236	C1150	A1068	C897
G2031	G1930	G1811	C1732	A1652	C1557	G1480	C1399	G1309	G1237	C1151	A1070	C898
G2032	G1931	U1812	G1733	A1653	C1558	U1481	U1400	C1315	A1237	A1151	G1071	A910
A2033	G1932	G1813	G1734	G1654	C1559	U1482	G1401	U1316	G1238	C1161	A1072	A911
G1935	A1936	G1814	A1735	A1655	G1567	G1483	U1402	U1317	G1239	C1162	A1073	A912
A1937	A1937	G1815	U1736	A1656	G1568	U1484	U1403	U1318	U1240	A1165	G1074	G914
A1938	A1938	C1816	G1737	C1656	G1569	U1485	C1404	U1319	A1244	C1166	G1075	G915
U1939	U1939	G1817	U1738	U1657	A1569	U1487	U1405	C1319	G1245	C1167	A1076	G916
C2043	C2043	U1818	G1740	C1658	C1574	U1488	U1406	A1322	A1246	A1168	U1077	G917
C2047	C2047	A1819	C1741	A1665	U1578	G1493	G1410	A1327	A1247	C1170	U1078	A917
U1943	U1943	U1820	U1742	G1666	U1579	A1494	U1411	A1328	G1248	C1171	A1079	A918
G1945	G1945	G1821	G1743	G1667	C1581	A1495	U1412	U1329	U1249	C1172	A1080	U919
C2050	C2050	G1822	A1744	A1668	G1582	A1496	U1413	U1329	G1250	C1173	U1081	A920
A2051	A2051	G1823	A1745	A1669	A1583	G1500	G1416	C1330	C1251	C1174	U1082	C921
A2052	A2052	G1824	U1746	C1670	A1584	G1501	C1417	G1331	G1252	U1173	U1083	G922
G2053	G2053	G1825	C1747	U1671	C1585	A1504	G1418	G1332	A1253	A1175	A1084	G923
A2054	A2054	A1826	C1748	A1672	C1586	A1505	G1419	G1333	A1254	C1176	A1085	C1013
C2055	C2055	C1827	G1749	G1673	A1587	A1506	U1420	A1336	U1255	U1177	A1086	A1014
G2056	G2056	G1828	G1750	G1674	C1588	A1507	A1421	U1337	G1256	C1178	G1087	G1017
C2057	C2057	C1829	A1751	C1675	A1589	A1508	G1422	G1338	C1257	C1179	A1088	U931
A2058	A2058	G1830	A1752	A1676	C1590	A1509	G1423	G1339	U1258	C1180	U1089	U932
G2059	G2059	C1831	G1753	A1677	C1591	G1510	G1424	U1340	G1259	U1181	A1090	A933
A2060	A2060	U1832	G1754	U1678	C1592	G1511	G1425	U1341	A1260	G1182	A1091	U934
G2061	G2061	G1833	A1755	A1679	C1593	C1512	G1426	A1427	G1261	C1183	G1092	C935
A2062	A2062	C1834	U1756	C1680	C1594	U1513	G1427	C1428	C1262	U1184	U1093	U936
G1972	G1972	G1835	C1760	C1681	C1595	G1514	C1429	G1342	A1262	G1185	U1094	A941
C2065	C2065	A1847	C1761	G1686	G1601	A1515	G1430	U1344	U1263	C1186	U1097	G1025
G2066	G2066	A1848	G1762	G1687	U1602	G1516	A1431	U1345	A1264	G1026	A1098	A945
C2067	C2067	C1849	C1763	A1690	A1603	C1517	A1432	G1350	A1265	A1027	A1099	C946
U2068	U2068	A1853	U1764	C1691	C1604	G1518	A1433	C1351	G1266	C1187	G1100	U958
G2069	G2069	G1854	G1765	C1692	C1605	G1519	U1434	U1352	U1267	U1188	A1111	A959
A2070	A2070	A1857	C1771	U1693	C1606	U1520	G1435	G1369	A1268	A1189	G1112	A960
C2071	C2071	G1858	A1772	U1694	C1607	G1521	G1436	U1370	A1269	C1190	U1113	C961
G2072	G2072	U1865	A1773	C1695	A1608	U1522	U1437	G1360	G1270	G1193	C1114	G962
U2076	U2076	A1866	U1774	G1696	A1609	U1523	U1438	G1361	G1271	G1202	G1122	U963
C2077	C2077	C1867	U1775	A1705	A1610	G1524	G1441	A1365	A1272	C1203	A1122	C964
U2081	U2081	G1869	U1776	C1706	G1613	A1525	U1442	G1366	U1273	C1196	G1125	G1051
A2082	A2082	A1871	U1781	G1710	C1614	C1526	U1443	U1369	A1276	G1197	A1126	C1052
G2087	G2087	A1872	U1782	A1711	A1616	G1527	G1444	G1370	A1277	U1198	G1130	C1053
C2093	C2093	G1875	A1783	U1712	G1619	U1529	U1445	G1371	G1279	C1204	U1131	A972
A2094	A2094	C1876	A1784	A1713	C1622	C1530	G1446	G1372	G1280	A1205	G1132	A973
U2097	U2097	G1878	U1785	U1714	G1623	A1532	U1447	G1373	G1281	C1206	U1133	G974
G2098	G2098	C1879	A1786	U1715	C1624	C1533	G1448	U1374	A1285	C1207	A1134	A975
U2099	U2099	A1879	C1790	U1716	U1625	U1534	G1449	G1375	A1286	G1215	G1135	G1055
A2015	A2015	G1884	A1791	A1717	C1626	A1535	U1450	A1383	A1287	G1216	U1136	G1056
U2016	U2016	C1885	G1718	G1718	A1627	C1536	U1451	A1384	G1288	U1219	A1137	U1057
G2100	G2100	G1906	G1719	G1719	C1628	G1537	U1452	A1385	C1291	G1220	A1138	G1058
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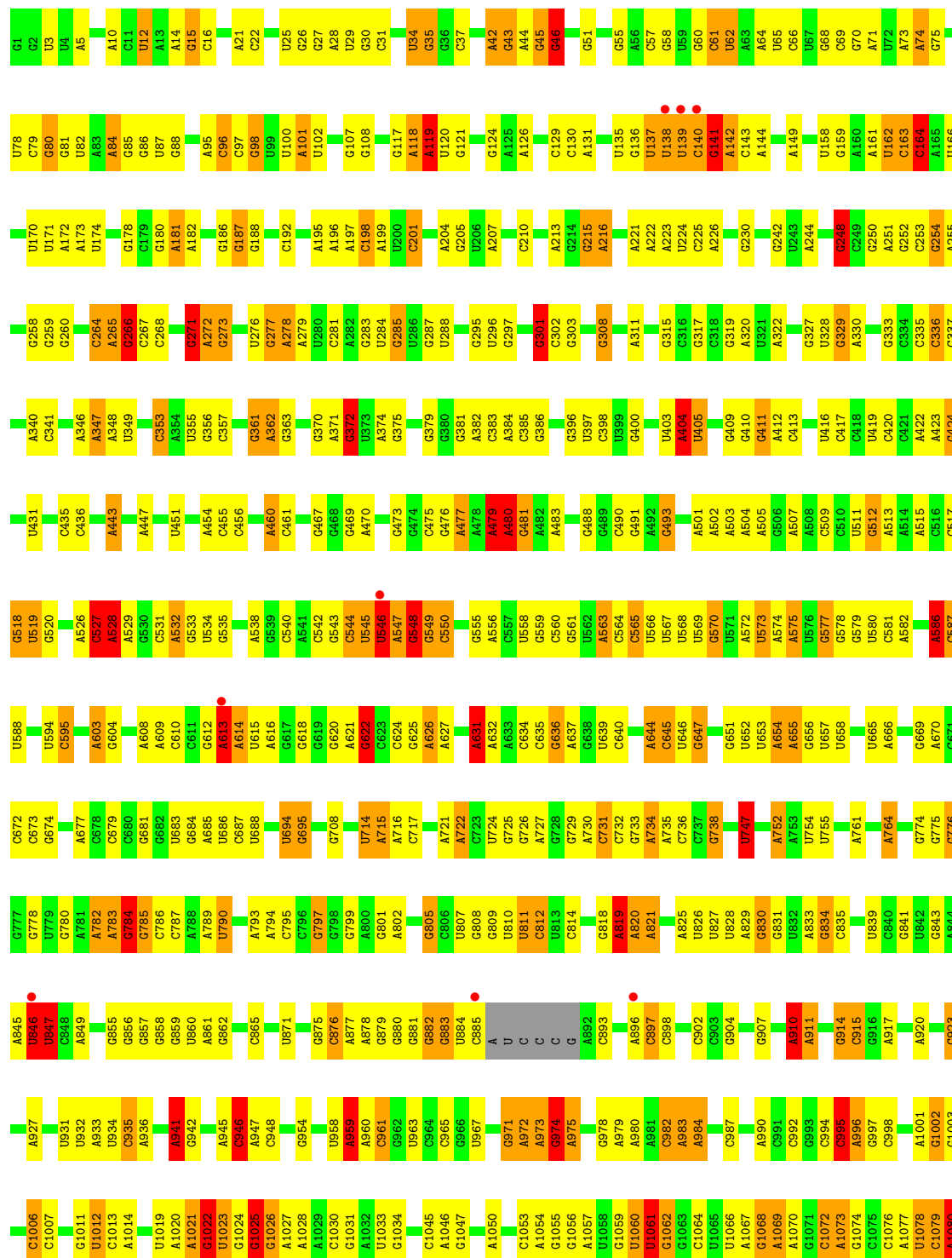


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A1522	A1427	A1336	A1254	C1161	A1077	A996	C912	U828	G738	C645	U567	C486	C385	G287
G1523	G1428	G1337	G1255	C1162	C1079	U999	U913	A829	A739	U646	U568	G489	G386	U288
A1524	G1435	G1341	G1256	C1163	A1080	A1000	G914	G830	C740	G647	U569	G490	U387	U296
C1525	G1436	G1342	C1257	A1165	U1081	A1001	C915	G831	U744	G648	G570	G491	G388	G297
G1527	A1437	A1343	A1262	C1166	U1082	A1002	U919	U832	G745	C650	A572	A492	G298	G299
C1533	U1438	G1344	G1263	G1167	U1083	A1003	C922	G833	G746	U653	A574	G493	A300	A299
U1534	A1439	U1345	A1264	A1168	A1084	A1004	U922	G834	U747	U654	A575	G494	G301	G302
A1535	U1440	C1349	A1265	C1170	A1085	C1005	G923	G843	G748	A653	A576	G495	A400	A401
C1536	G1441	G1350	G1266	G1171	U1086	C1006	U929	A844	U752	A655	U577	G496	A402	A309
G1537	U1442	U1352	U1267	U1174	A1088	C1007	G930	A845	A753	G656	G578	A503	A403	A310
C1541	G1443	A1353	A1268	A1175	A1089	A1008	U931	U847	U754	U657	U579	A504	U405	A311
U1549	U1444	A1354	A1269	A1176	A1090	A1009	U932	U848	U755	G658	U580	A505	A406	A312
C1550	G1445	G1355	G1270	C1177	U1091	A1010	U933	U849	G760	G659	U581	G506	U407	A313
A1556	C1447	U1358	G1271	G1178	U1092	G1011	A936	C853	G761	A661	A582	A508	G411	G315
A1569	G1448	G1359	U1272	C1179	U1093	U1012	C937	C854	A761	U666	U583	A509	A412	C316
A1570	G1452	A1360	U1273	G1180	U1094	C1013	U941	C855	C765	A667	A586	C509	C413	C323
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G1581	U1455	G1368	G1279	G1183	C1100	G1022	A941	G858	G771	A670	U589	A514	U416	A330
C1582	A1456	U1372	G1280	U1184	U1101	U1023	A945	G859	G772	C671	A590	C517	U417	G333
A1583	U1457	A1373	G1281	C1185	C1102	G1024	C946	U860	G773	C672	A591	C523	A422	C336
U1584	G1458	A1378	A1282	G1186	U1105	G1025	C947	A861	G774	A672	U592	C527	A423	C337
C1585	U1474	A1379	G1283	U1187	G1106	G1026	C948	G862	G775	C673	A603	A529	G424	G338
A1593	G1475	U1379	U1284	C1188	U1107	A1027	U955	G863	G776	U683	A604	A532	U431	A345
C1592	A1476	G1380	G1292	A1205	U1108	G1030	U956	G864	G777	A677	G608	A538	G442	A346
U1594	U1477	G1381	C1293	G1206	G1109	U1031	C957	C875	G778	A678	A609	G539	G445	A347
C1595	G1478	A1383	U1294	C1207	G1110	A1032	C958	C876	G779	U684	U612	A541	U431	A348
U1602	U1482	A1384	G1295	G1215	U1111	U1033	U959	A877	C786	A685	G613	C542	G442	A349
A1603	G1483	A1385	U1296	C1216	U1112	C1045	C961	G874	C787	A686	U614	C543	C445	U352
C1604	U1484	C1386	G1299	U1219	G1124	A1046	C962	C875	C788	U688	A615	C544	G450	C352
G1605	U1485	A1387	U1300	G1220	G1125	G1047	C963	C876	G789	A689	U616	U545	G455	C353
C1607	U1486	U1388	A1301	C1221	A1126	A1048	U964	A878	C789	C692	A617	C546	U355	G356
A1608	U1487	A1392	C1305	G1222	U1130	C1049	C964	G879	C791	U704	G618	U547	A460	C357
U1609	G1488	U1393	U1306	U1223	G1131	C1053	G971	G880	A792	U714	G619	A548	G465	G361
A1610	U1489	A1394	C1306	A1226	U1132	A1054	A972	G881	C793	A715	U620	G549	G468	A362
G1613	G1490	U1396	G1310	G1232	C1135	G1055	A975	G882	C794	A716	G621	C550	U365	U365
A1614	U1491	A1397	U1311	U1233	G1136	A1057	A979	G883	A795	A717	U622	G553	G470	G370
C1615	U1492	U1398	U1312	C1234	G1137	U1058	A980	U884	A796	G717	G623	U554	G473	A371
A1616	U1493	G1401	U1313	G1235	G1138	G1059	A981	C	C796	C723	A631	C557	G474	G372
G1617	U1494	U1400	U1314	G1236	U1139	U1060	A982	C	G797	U722	G634	U558	C475	U373
A1618	U1495	U1405	U1315	A1237	C1140	U1061	A983	A892	A802	G725	C635	G559	A478	A374
C1619	G1496	U1406	A1322	G1238	U1141	G1062	A984	G	A803	U724	G636	C560	A479	A480
U1621	U1497	G1407	U1323	U1239	A1142	G1063	C985	A892	G805	G726	U637	A563	A480	A481
G1620	U1498	U1408	G1324	U1240	A1143	A1069	A988	A893	C812	A727	C637	C560	A481	A482
A1621	U1499	A1416	U1325	A1244	A1144	A1070	A989	C897	C813	G728	C638	C561	A482	A483
C1622	U1500	U1419	A1327	A1245	C1152	G1071	G989	C898	C814	G729	C639	C562	A483	A484
A1623	G1501	A1420	U1328	G1246	C1153	A1072	A990	A899	C815	A730	C640	C563	A484	A485
C1624	U1502	U1421	U1329	U1247	A1156	G1073	A991	A900	C816	A731	C641	C564	A485	A486
A1625	U1503	G1422	U1330	U1248		G1074	C992	A901	A819	C731	C642	C565	A486	A487



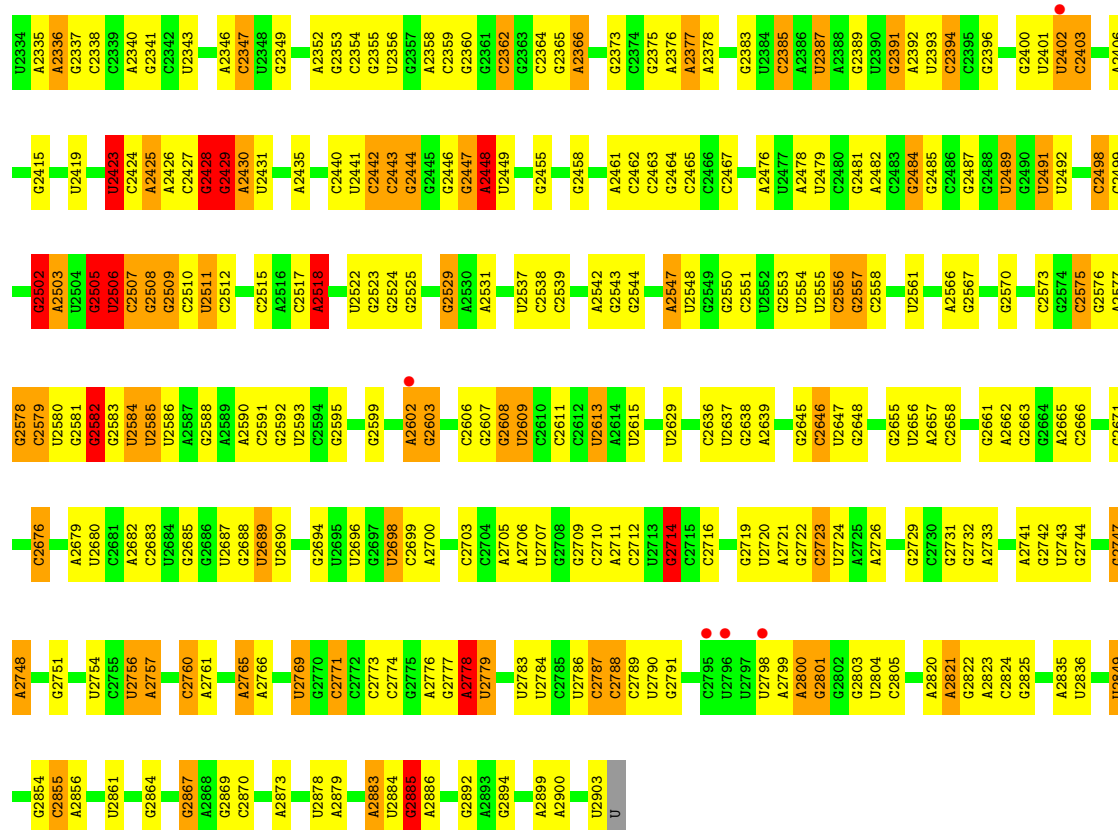


• Molecule 1: 23S rRNA

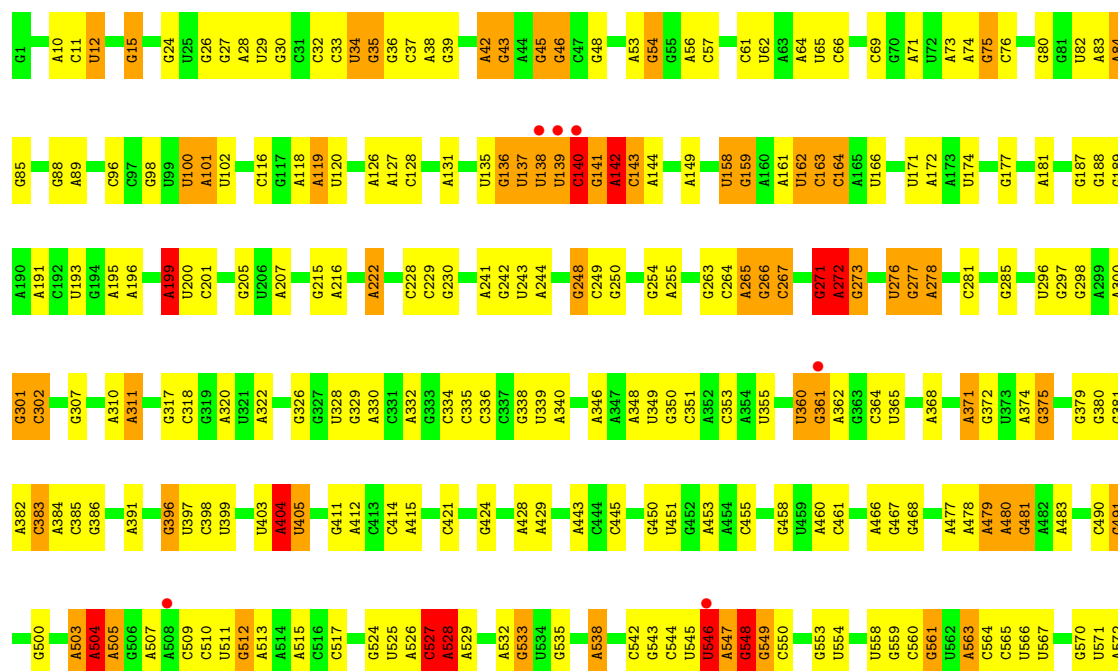








• Molecule 1: 23S rRNA



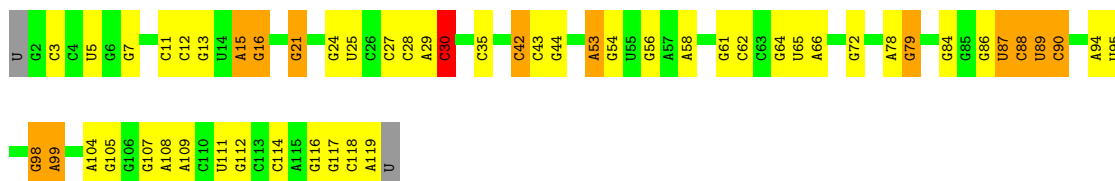
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U1797	G1797	U1714	G1475	C1297	G1226	G1131	A1054	U963	G864	U766	G651	A574
U1798	C1477	G1715	U1476	C1297	A1226	A1133	G1055	G966	C865	C772	U652	U576
G1799	G1478	C1799	G1478	G1300	U1231	C1134	G1056	U967	A866	G775	A654	G577
A1801	C1605	U1720	G1482	A1301	G1232	C1135	A1057	C968	G875	G776	A655	G578
A1802	C1606	G1721	U1396	C1305	G1233	G1136	U1058	G969	C876	G776	G656	G579
A1803	C1607	G1722	U1397	C1306	G1234	G1137	U1059	U970	A877	A782	U657	U580
A1804	C1608	G1723	U1486	A1307	G1235	G1138	U1060	G971	C878	A783	U658	C581
A1805	C1609	G1724	U1487	A1307	G1236	G1139	U1061	A972	A878	A784	G659	A586
A1805	A1610	U1725	U1405	U1405	G1236	C1140	G1062	A973	G879	G784	G659	C587
A1805	C1611	C1493	U1406	U1406	G1237	U1141	G1063	G974	G880	G785	G663	U588
A1808	C1727	C1727	U1503	G1311	G1238	A1142	C1064		G881			
A1811	C1614	G1728	A1504	U1312	G1239		U1065	A979	G882	A789	A666	U594
U1812	C1615	U1729	A1504	U1313		G1149	U1066	A980	G883		A666	C595
G1813	A1616	C1730	U1412	U1313	A1244	C1150	A1067	A981	U884	A792	G669	U596
G1814	C1617	G1731	A1413	G1317		A1151	G1068	C982	C885	A793	C672	U597
A1815	A1618	C1732		G1317	A1247	G1154	A1069	A984	A	A794	C672	U598
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A1829	U1647		U1532	A1337	U1258	G1169	A1080	G1002	C897	U807	A716	G617
C1830	U1648		C1533	A1337	G1259	C1170	U1081	G1003	C898	G808	C717	G618
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G1763			A1439	U1352	G1266	U1176	A1089	C1013			C736	A626
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G1770	G1659		G1441	A1354	A1268	C1178	G1091	U1019		U828	G738	G630
A1773	A1664		U1442	G1355	U1269	U1179	C1092	A1020	U929	A829	A739	A631
C1774	A1665		U1443	G1356	G1270	U1180	C1093	A1021	G830	G836	C740	A632
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U1778	A1669		G1448	C1362	A1272	G1182	A1095	U1023	U932	U832	A742	C634
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G1857	G1568		C1451	A1365	G1278	A1189	A1098	G1026			G748	A637
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A1784	C1577		U1457	A1378	U1283	G1198	G1106	G1031	C944	U846	U754	U641
A1785	U1578		G1459	U1379	U1284	U1201	G1110	A1032	A945	U847		
C1788	U1578		G1459	G1380	A1285	U1202	G1111	U1033	C946			A644
A1789	G1581		G1464	G1381	U1285	U1203	G1112	G1034	A947	C854	G760	C645
G1790	C1582		G1464	G1382	G1288	U1204	G1113	U1035	C948	G855	A761	U646
A1791	U1583		G1471	A1383	C1289	A1205	G1126	C1045	A959	G856	U762	G647
A1872	U1584		C1472	A1384	G1290	G1206	G1126	A1046	A960	G857	G763	G648
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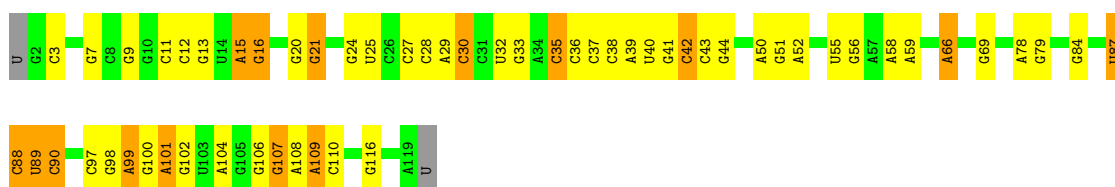
• Molecule 2: 5S rRNA

Chain CB: 54% 33% 10% ..



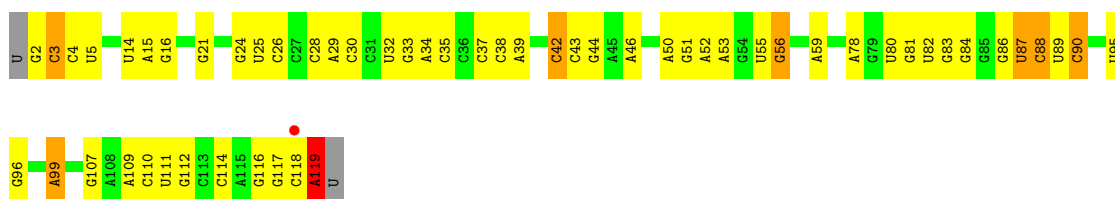
• Molecule 2: 5S rRNA

Chain EB: 51% 35% 12% .



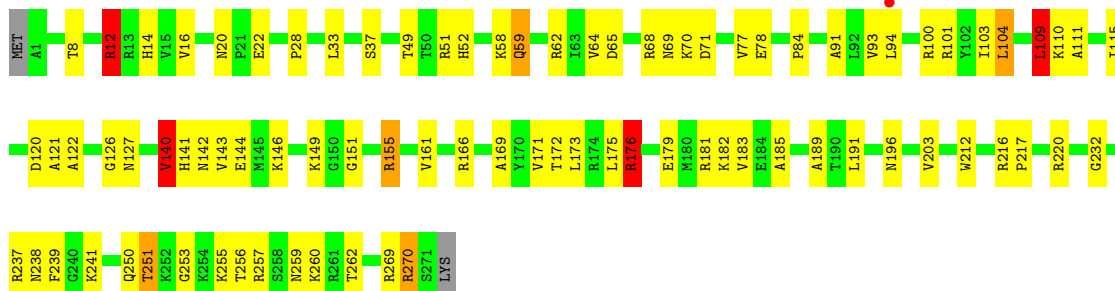
• Molecule 2: 5S rRNA

Chain GB: % 52% 40% 6% ..



• Molecule 3: 50S ribosomal protein L2

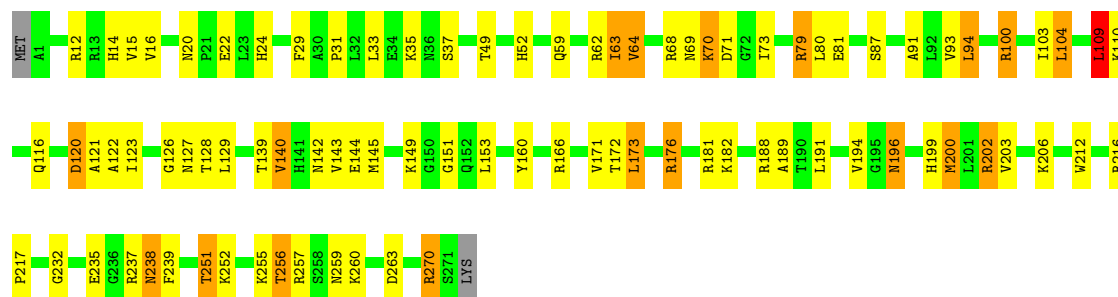
Chain AC: 68% 28% ...



• Molecule 3: 50S ribosomal protein L2

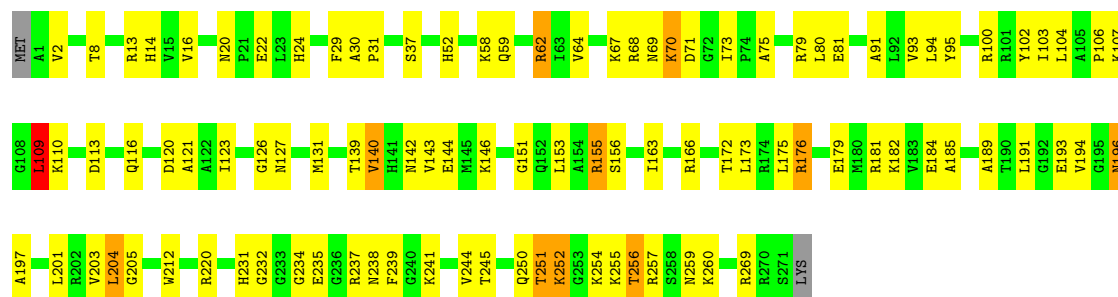
Chain CC: 67% 25% 7% .





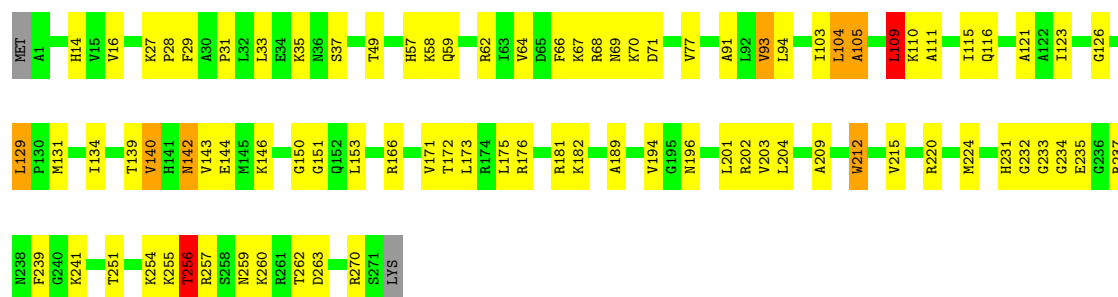
• Molecule 3: 50S ribosomal protein L2

Chain EC: 63% 33%



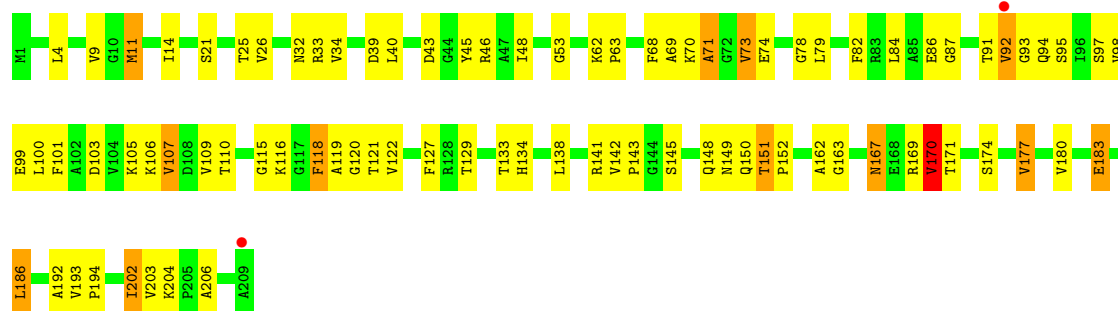
• Molecule 3: 50S ribosomal protein L2

Chain GC: 68% 28%

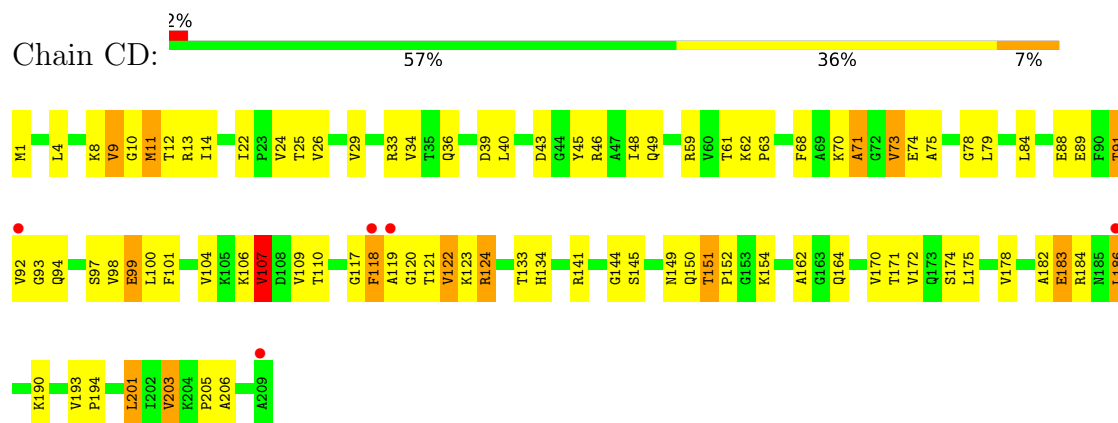


• Molecule 4: 50S ribosomal protein L3

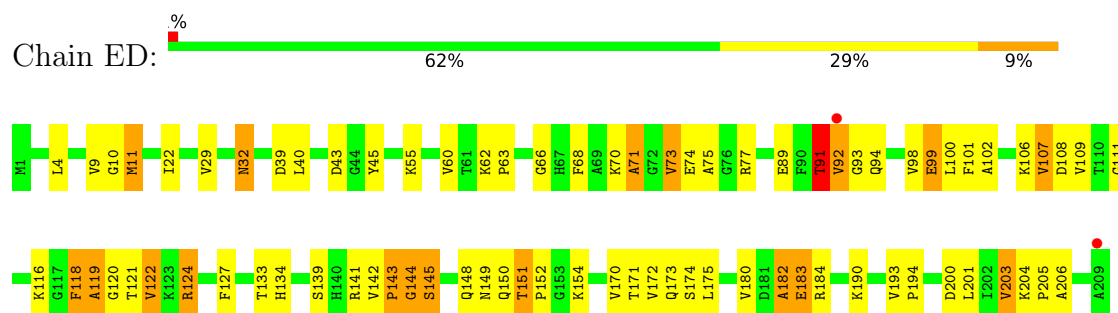
Chain AD: 59% 35% 6%



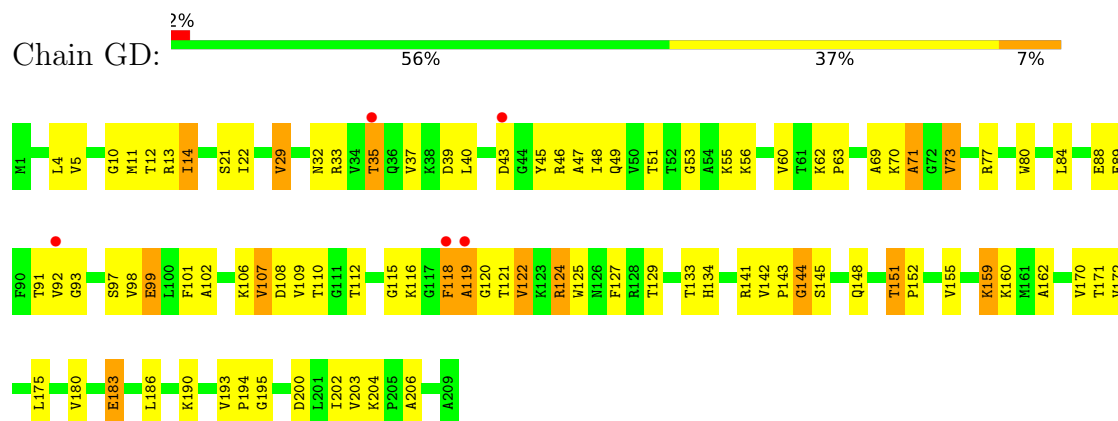
• Molecule 4: 50S ribosomal protein L3



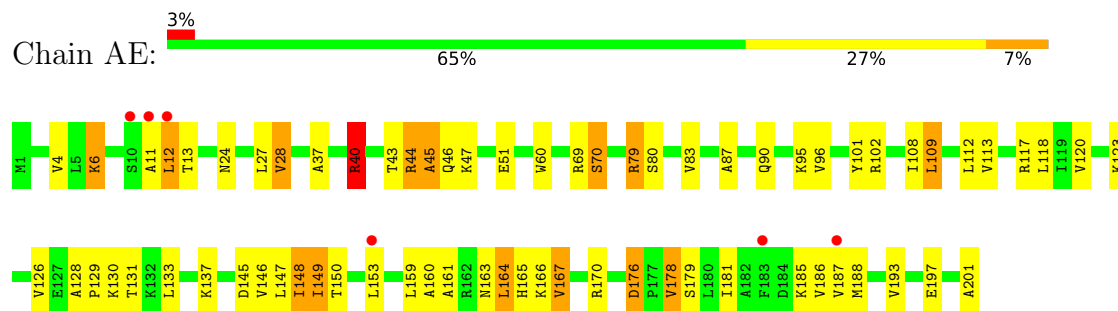
• Molecule 4: 50S ribosomal protein L3



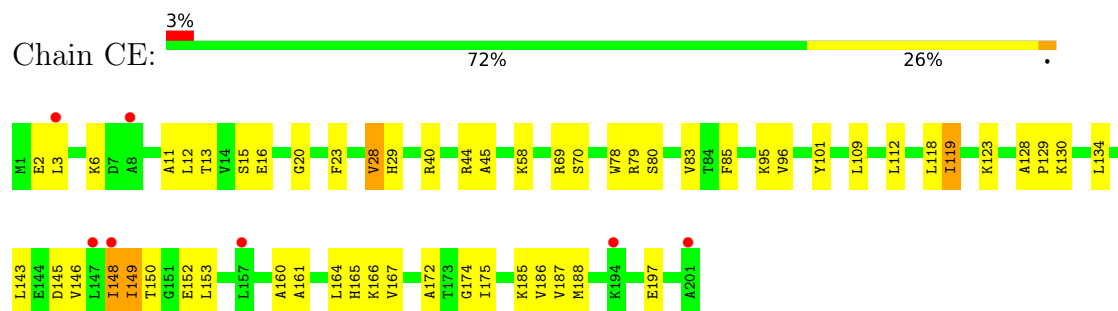
• Molecule 4: 50S ribosomal protein L3



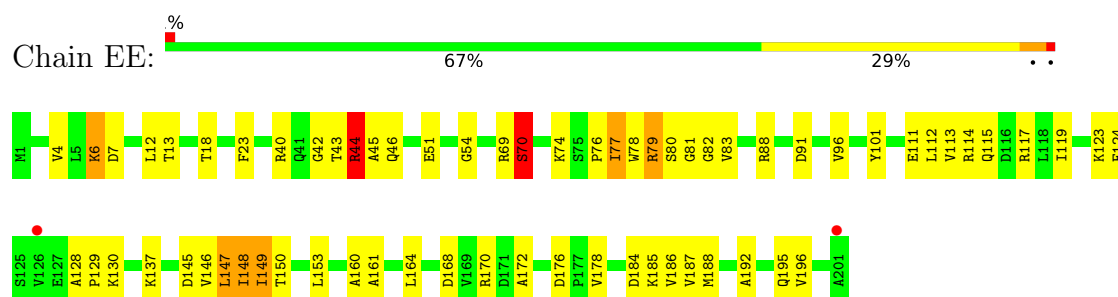
• Molecule 5: 50S ribosomal protein L4



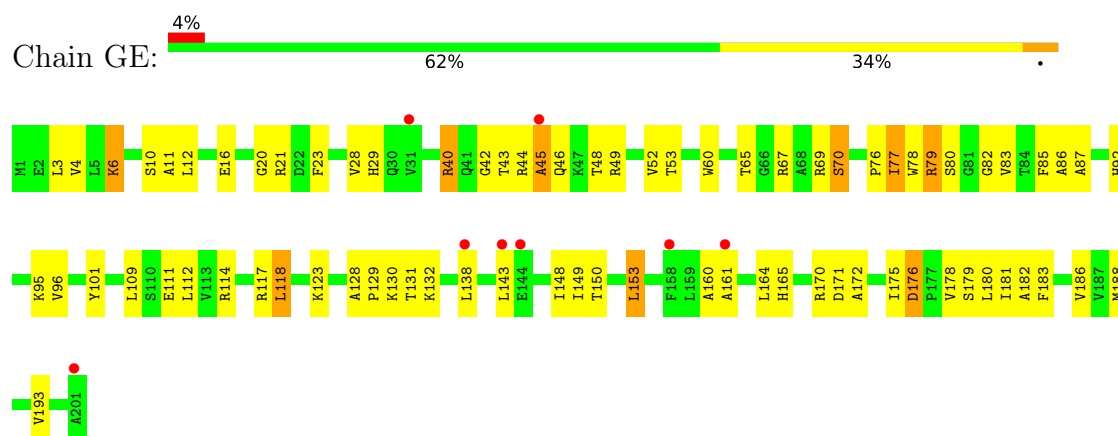
- Molecule 5: 50S ribosomal protein L4



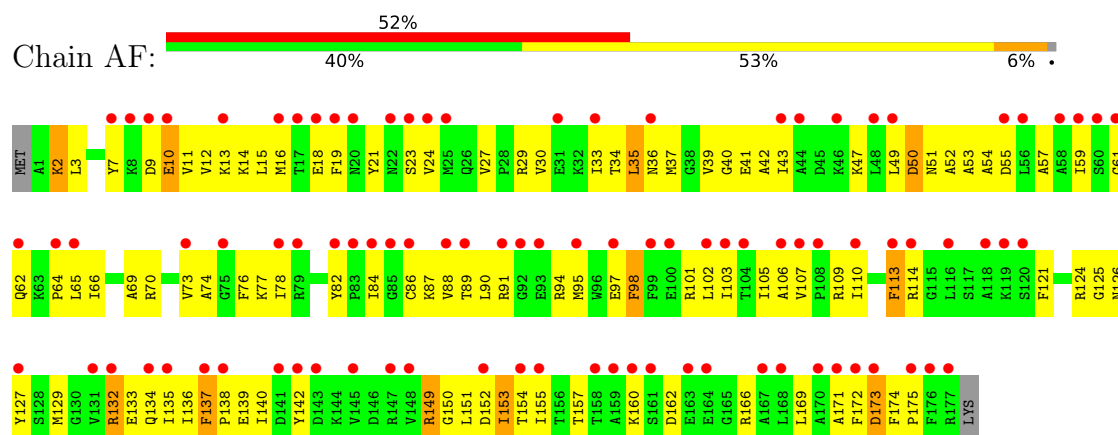
- Molecule 5: 50S ribosomal protein L4



- Molecule 5: 50S ribosomal protein L4

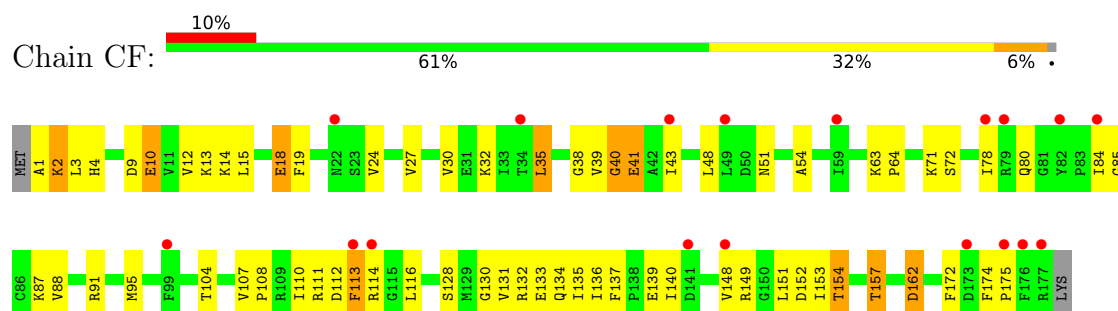


- Molecule 6: 50S ribosomal protein L5

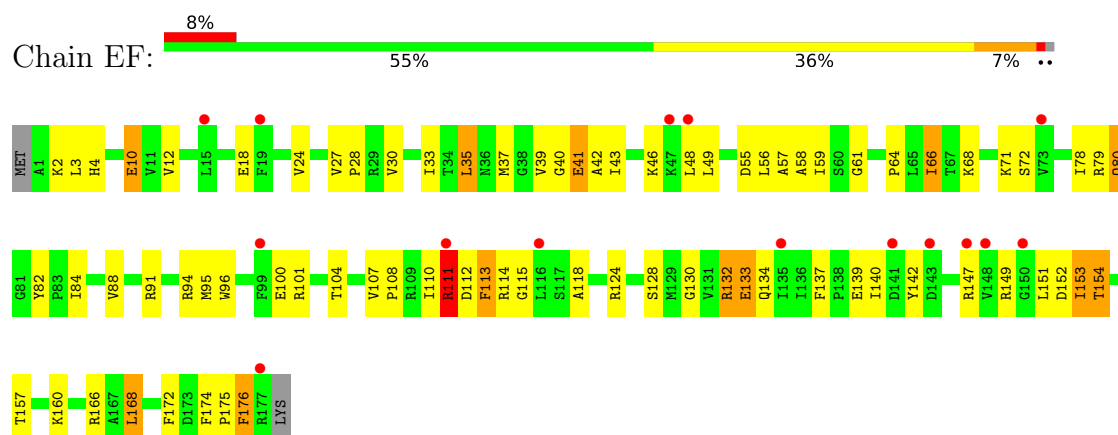




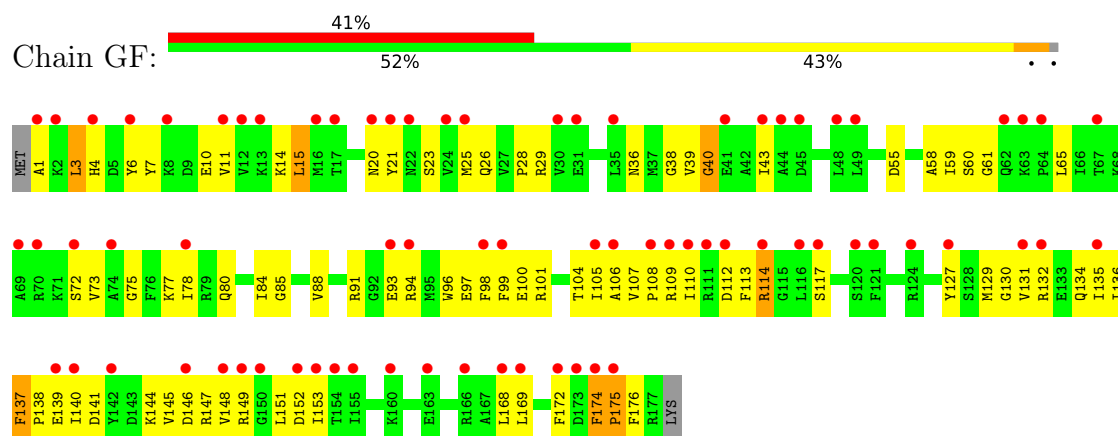
- Molecule 6: 50S ribosomal protein L5



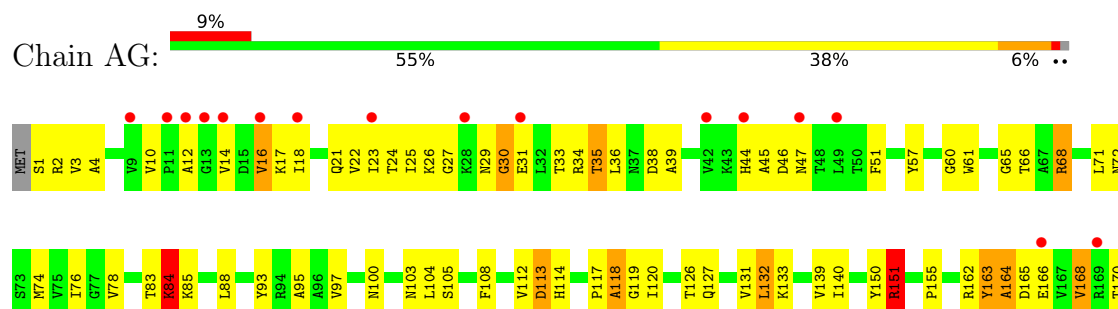
- Molecule 6: 50S ribosomal protein L5



- Molecule 6: 50S ribosomal protein L5



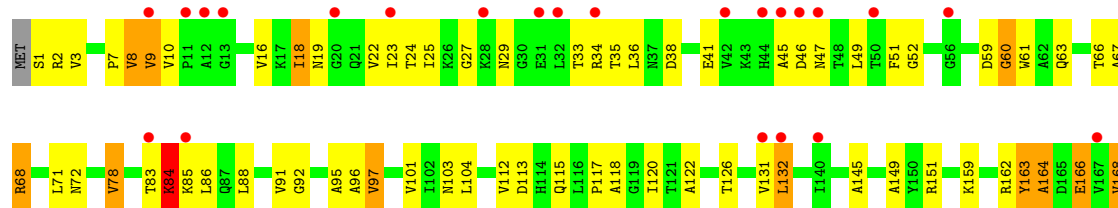
- Molecule 7: 50S ribosomal protein L6





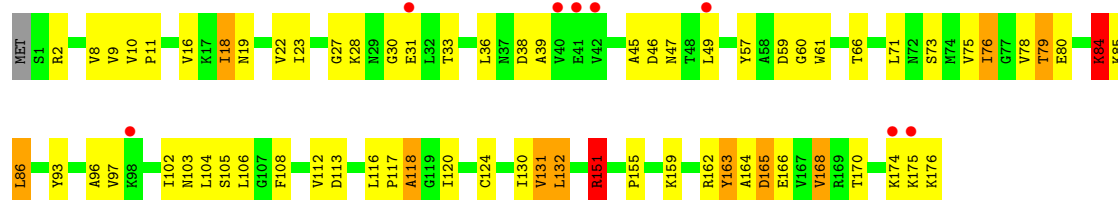
• Molecule 7: 50S ribosomal protein L6

Chain CG: 14% 58% 33% 7% ..



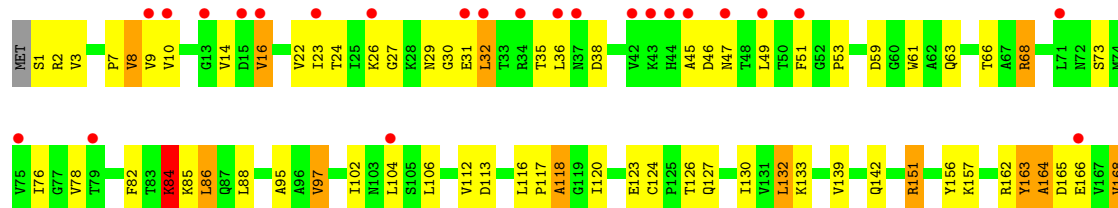
• Molecule 7: 50S ribosomal protein L6

Chain EG: 5% 60% 32% 6% ..



• Molecule 7: 50S ribosomal protein L6

Chain GG: 14% 58% 34% 7% ..

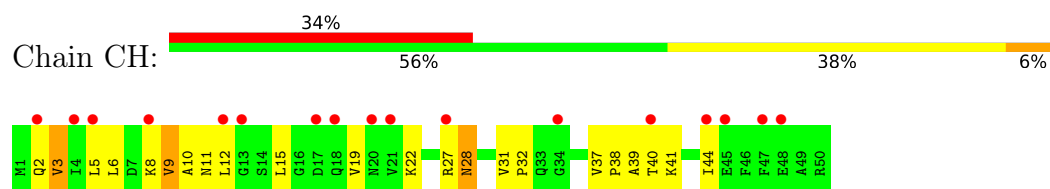


• Molecule 8: 50S ribosomal protein L9

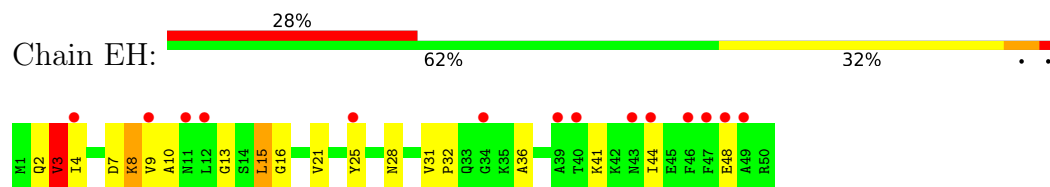
Chain AH: 20% 54% 42% ..



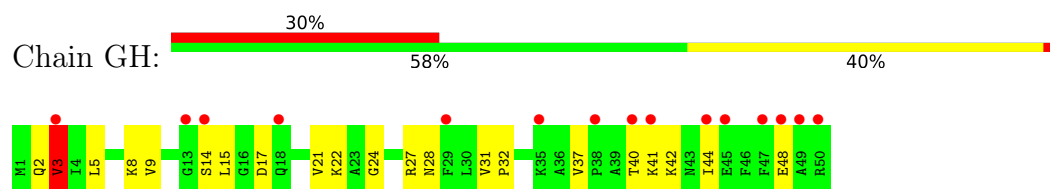
- Molecule 8: 50S ribosomal protein L9



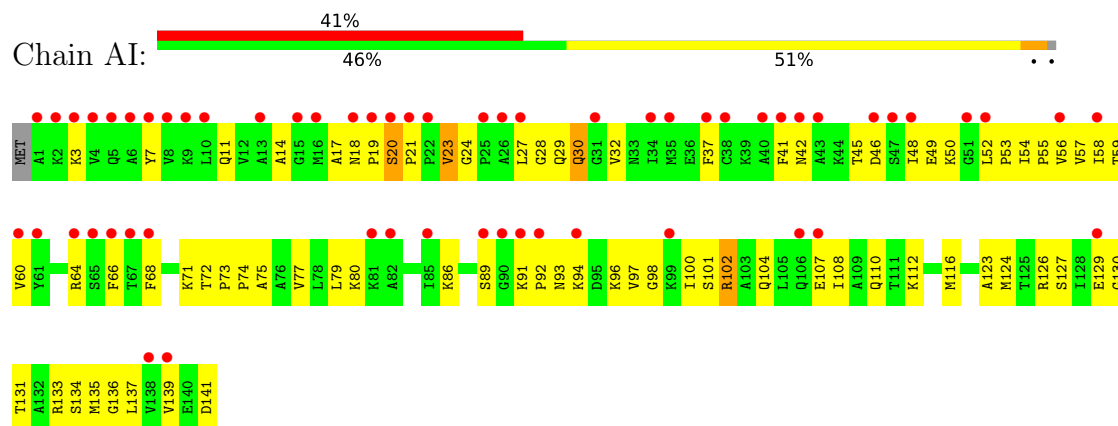
- Molecule 8: 50S ribosomal protein L9



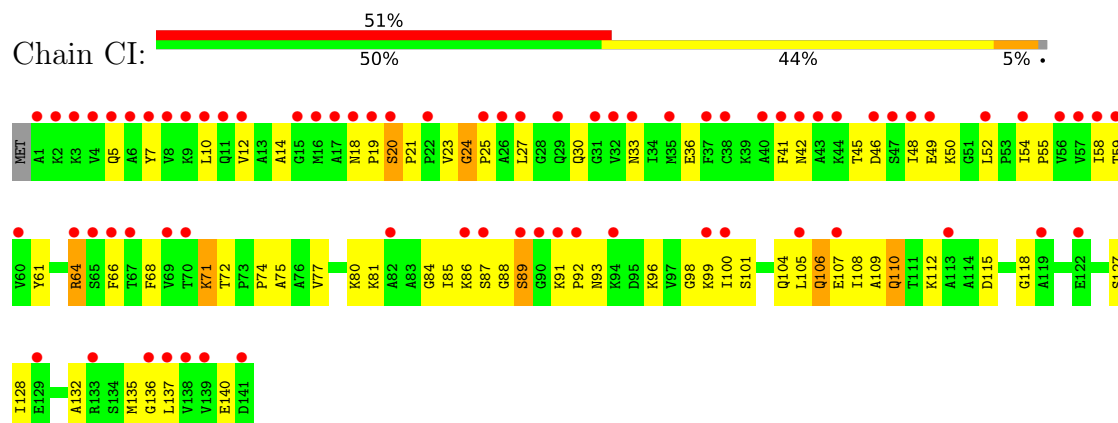
- Molecule 8: 50S ribosomal protein L9



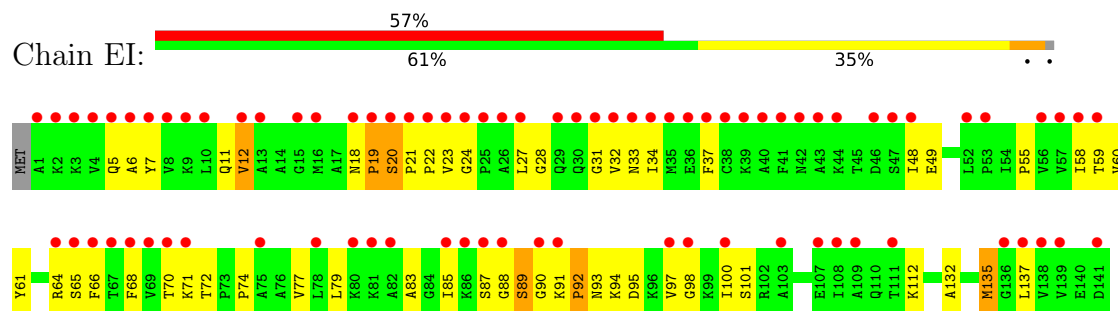
- Molecule 9: 50S ribosomal protein L11



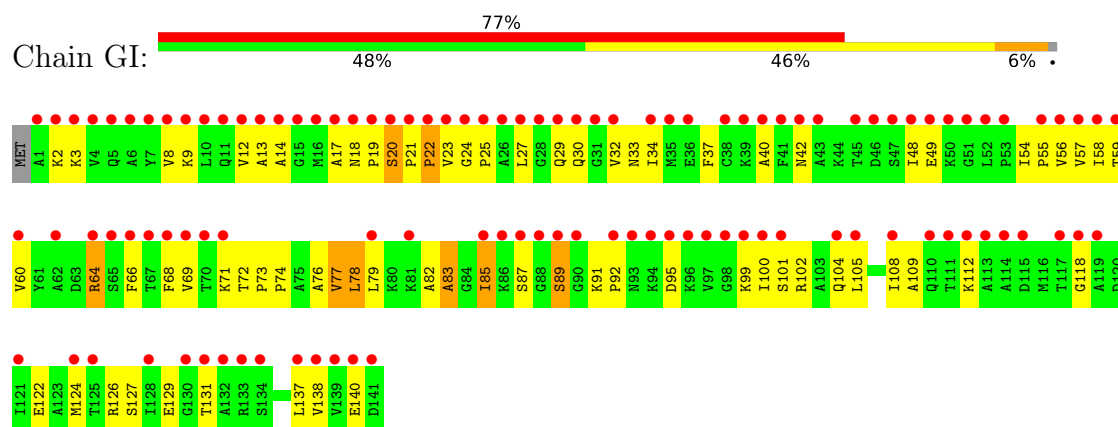
- Molecule 9: 50S ribosomal protein L11



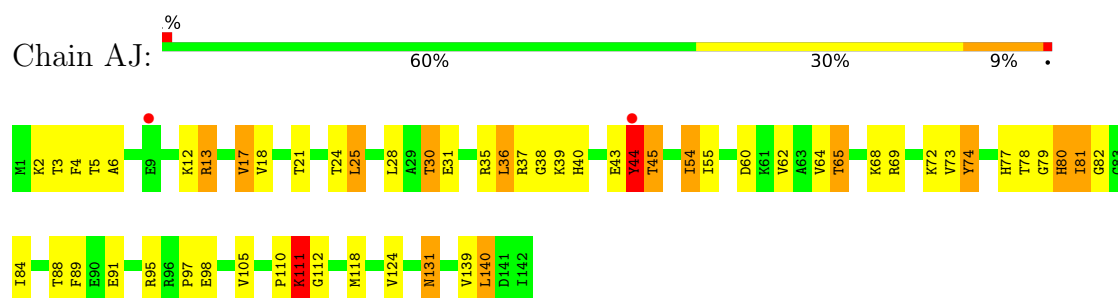
- Molecule 9: 50S ribosomal protein L11



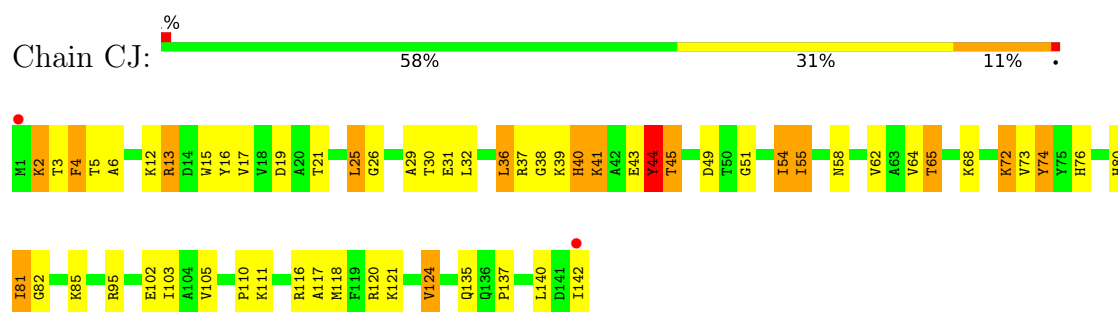
- Molecule 9: 50S ribosomal protein L11



- Molecule 10: 50S ribosomal protein L13

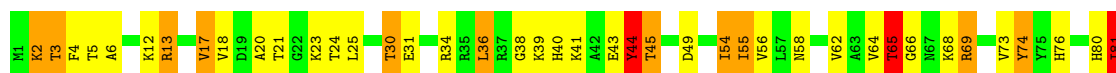


- Molecule 10: 50S ribosomal protein L13

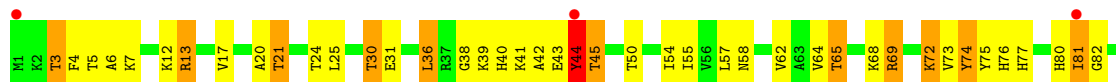


- Molecule 10: 50S ribosomal protein L13

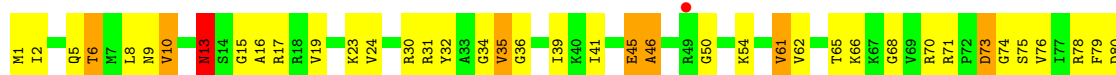




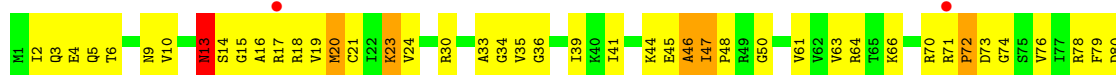
• Molecule 10: 50S ribosomal protein L13



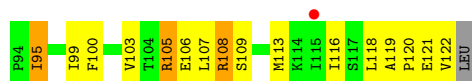
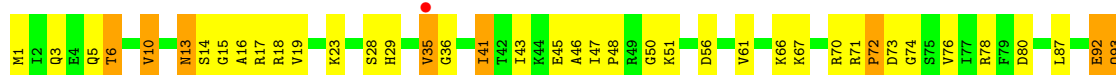
• Molecule 11: 50S ribosomal protein L14



• Molecule 11: 50S ribosomal protein L14

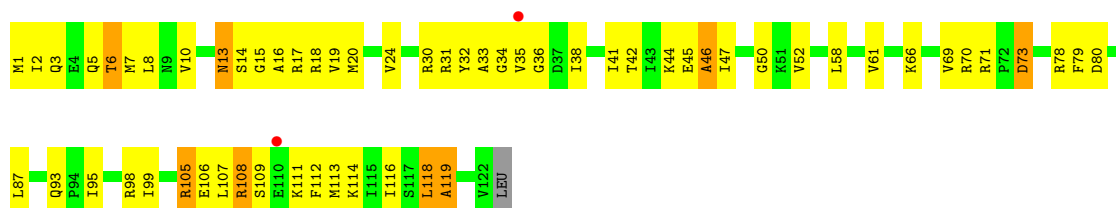


• Molecule 11: 50S ribosomal protein L14



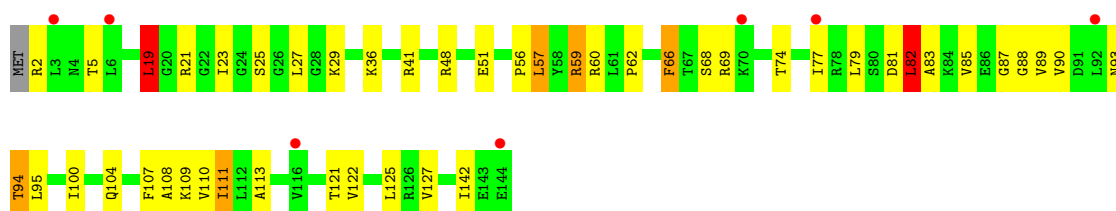
- Molecule 11: 50S ribosomal protein L14

Chain GK: 



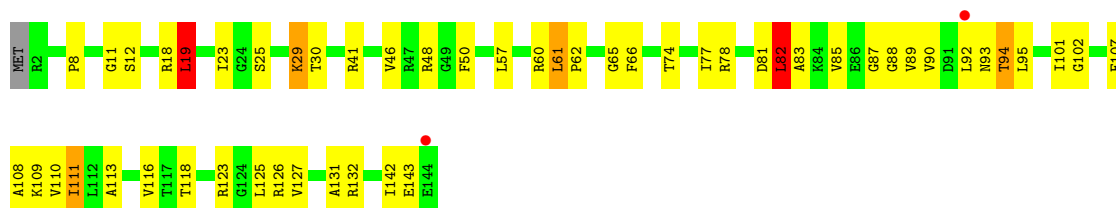
- Molecule 12: 50S ribosomal protein L15

Chain AL: 




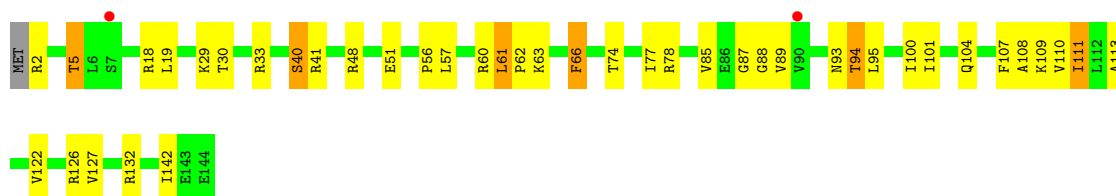
- Molecule 12: 50S ribosomal protein L15

Chain CL: 



- Molecule 12: 50S ribosomal protein L15

Chain EL: 



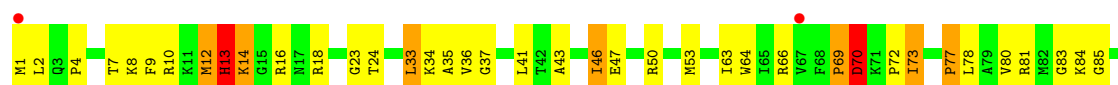
- Molecule 12: 50S ribosomal protein L15

Chain GL: 





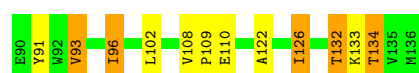
• Molecule 13: 50S ribosomal protein L16



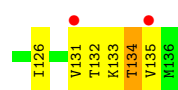
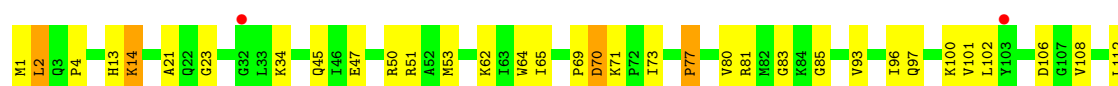
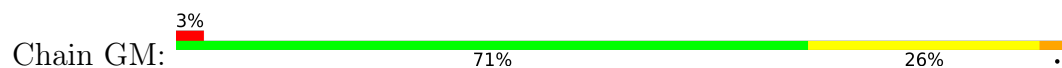
• Molecule 13: 50S ribosomal protein L16



• Molecule 13: 50S ribosomal protein L16

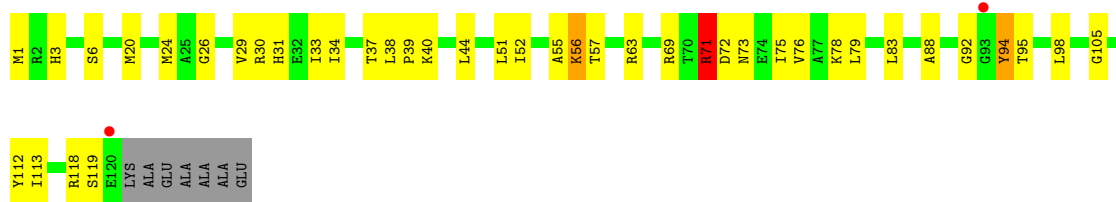


• Molecule 13: 50S ribosomal protein L16

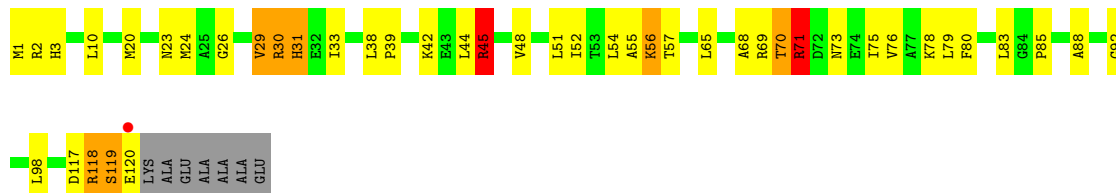


• Molecule 14: 50S ribosomal protein L17

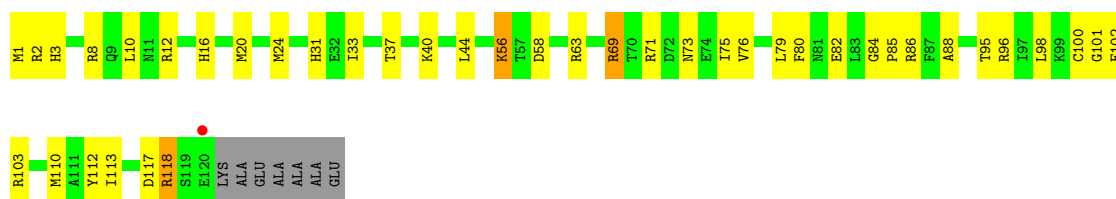




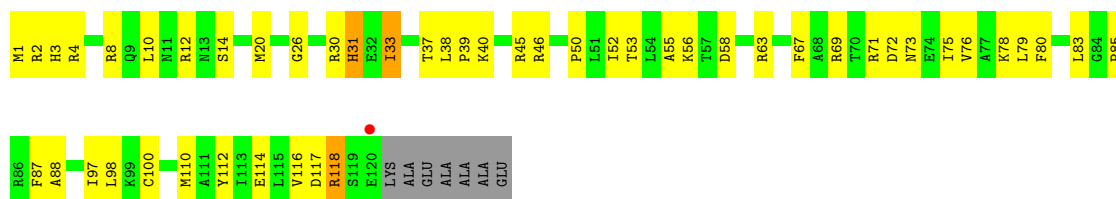
• Molecule 14: 50S ribosomal protein L17



• Molecule 14: 50S ribosomal protein L17



• Molecule 14: 50S ribosomal protein L17

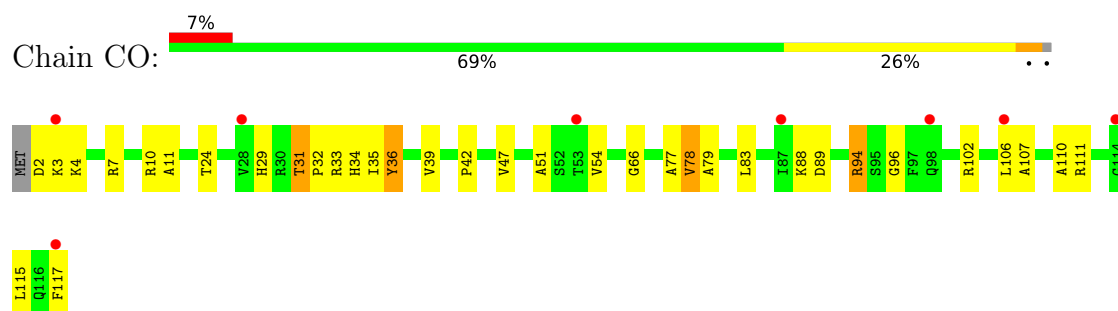


• Molecule 15: 50S ribosomal protein L18

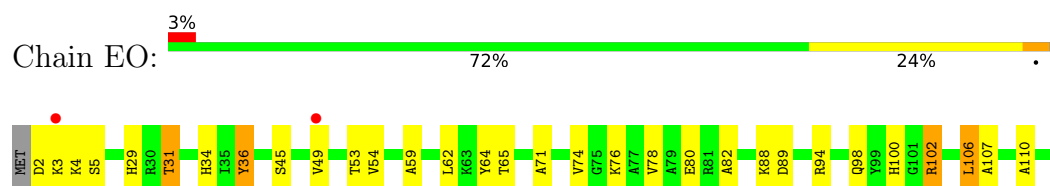




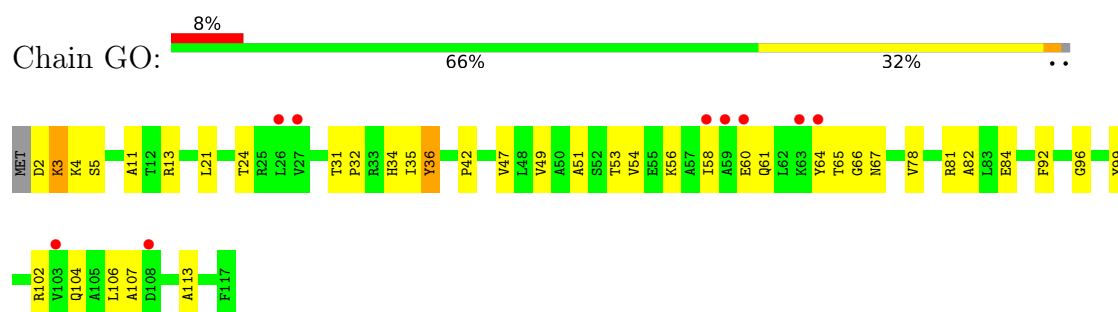
## • Molecule 15: 50S ribosomal protein L18



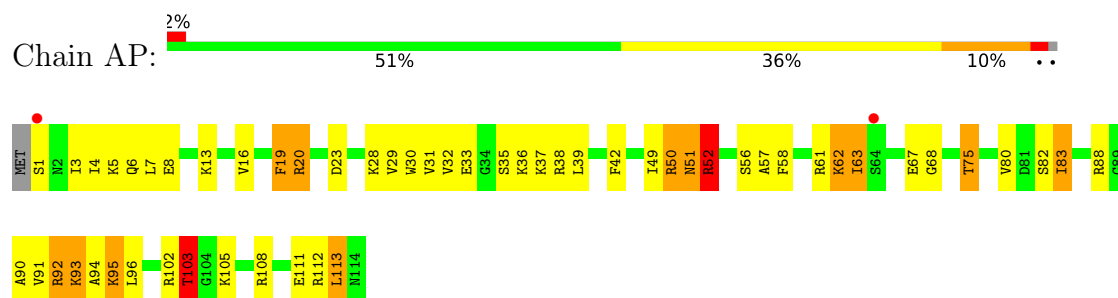
## • Molecule 15: 50S ribosomal protein L18



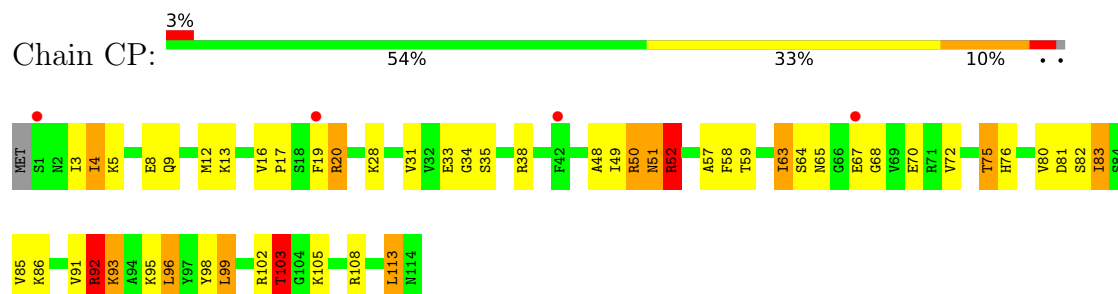
## • Molecule 15: 50S ribosomal protein L18



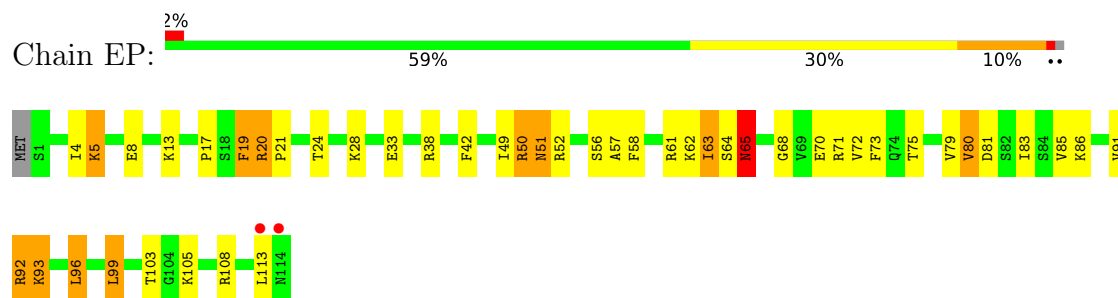
## • Molecule 16: 50S ribosomal protein L19



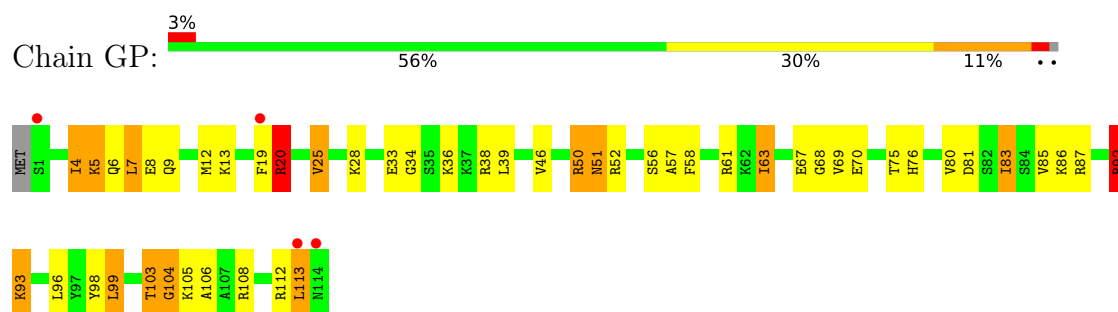
## • Molecule 16: 50S ribosomal protein L19



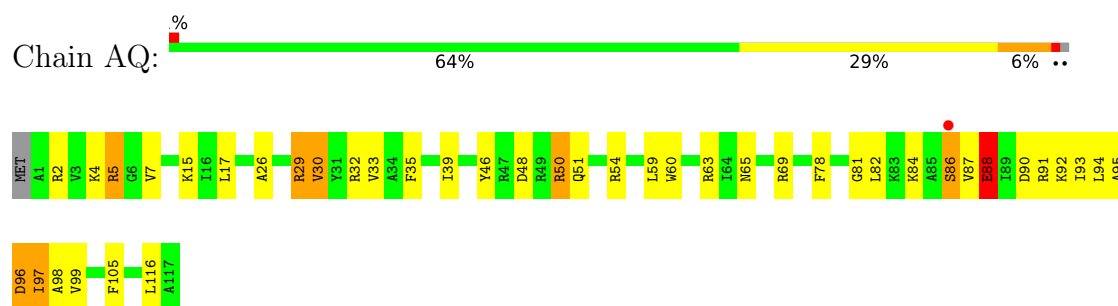
- Molecule 16: 50S ribosomal protein L19



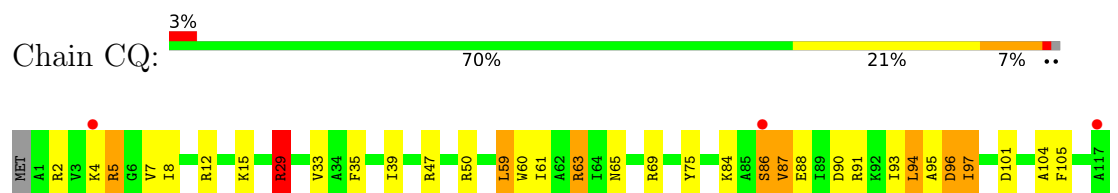
- Molecule 16: 50S ribosomal protein L19



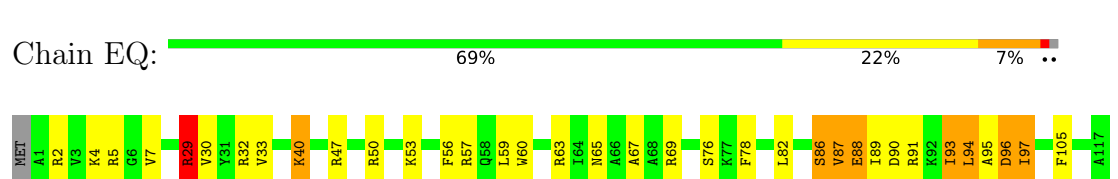
- Molecule 17: 50S ribosomal protein L20



- Molecule 17: 50S ribosomal protein L20



- Molecule 17: 50S ribosomal protein L20

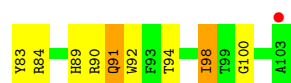
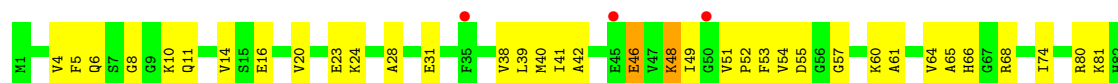


- Molecule 17: 50S ribosomal protein L20

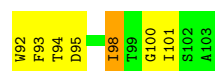
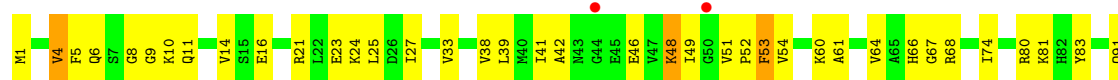




- Molecule 18: 50S ribosomal protein L21



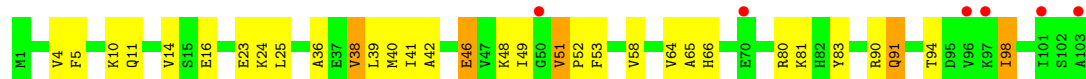
- Molecule 18: 50S ribosomal protein L21



- Molecule 18: 50S ribosomal protein L21



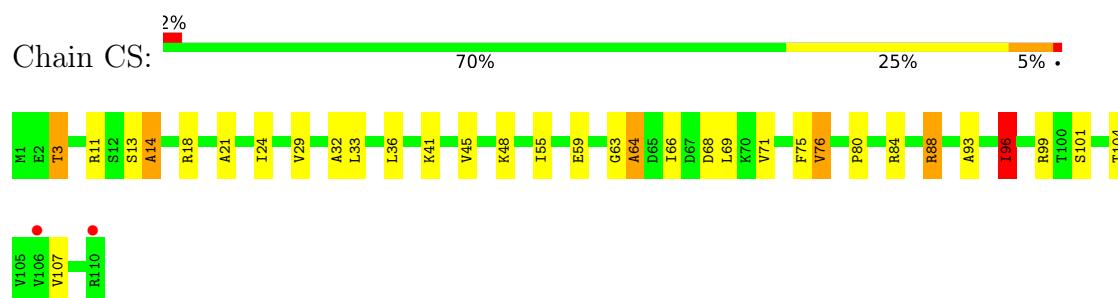
- Molecule 18: 50S ribosomal protein L21



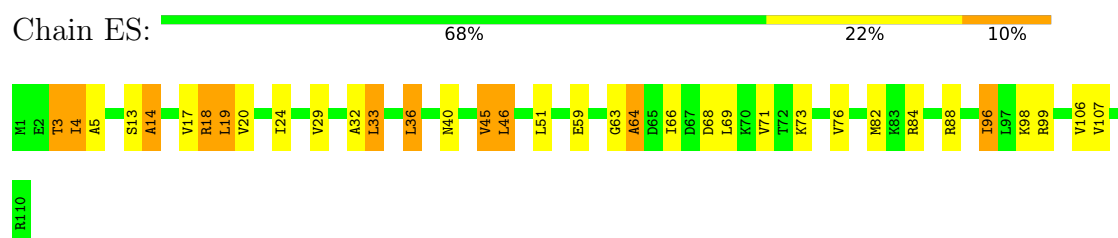
- Molecule 19: 50S ribosomal protein L22



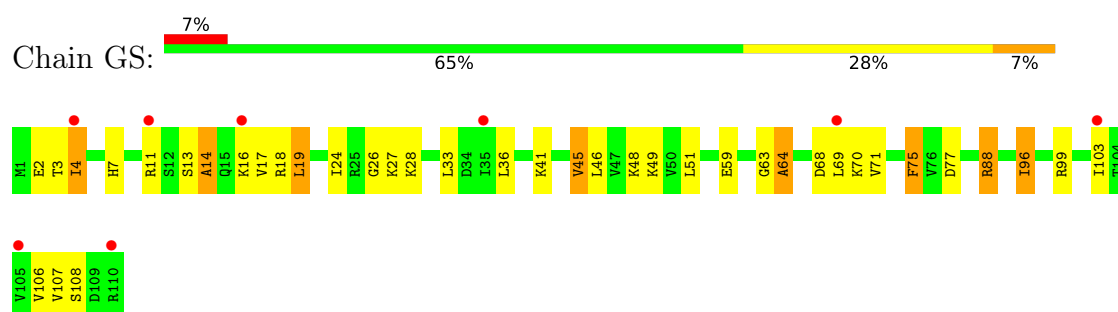
## • Molecule 19: 50S ribosomal protein L22



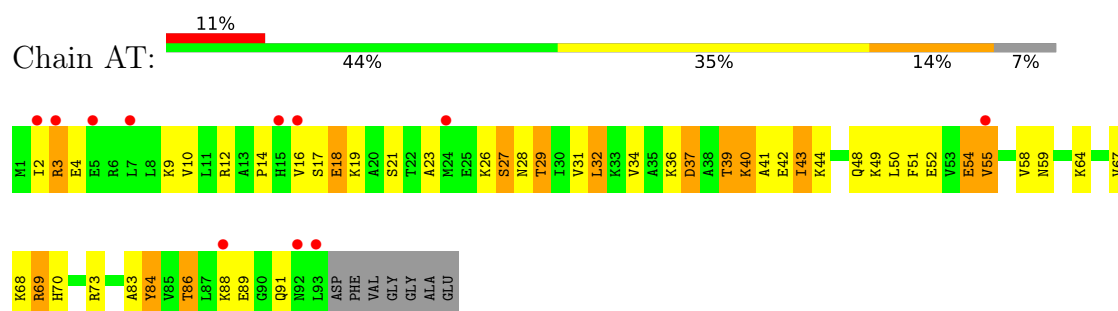
## • Molecule 19: 50S ribosomal protein L22



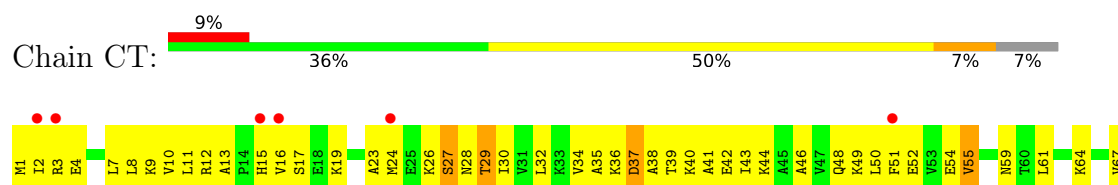
## • Molecule 19: 50S ribosomal protein L22

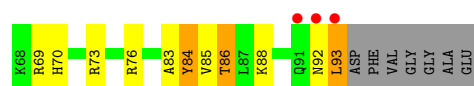


## • Molecule 20: 50S ribosomal protein L23

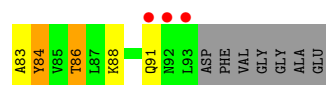
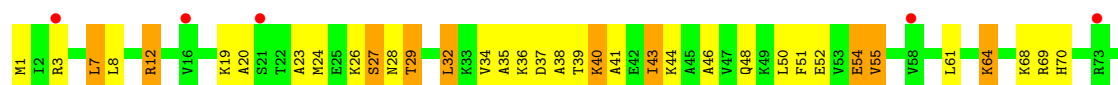


## • Molecule 20: 50S ribosomal protein L23

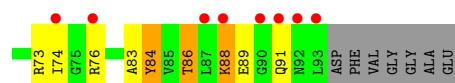
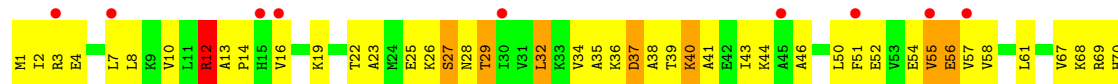




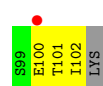
- Molecule 20: 50S ribosomal protein L23



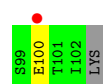
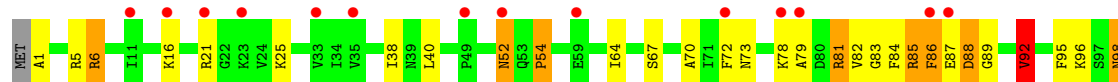
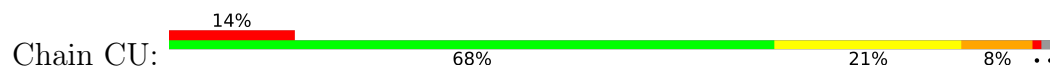
- Molecule 20: 50S ribosomal protein L23



- Molecule 21: 50S ribosomal protein L24

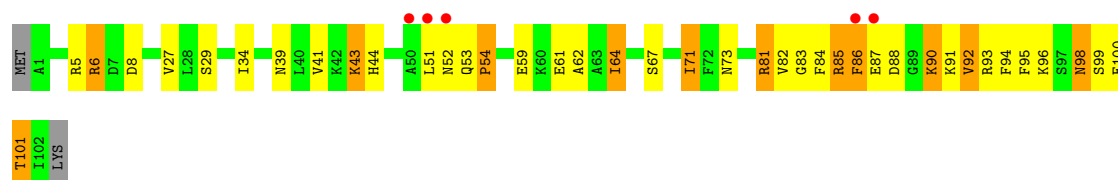


- Molecule 21: 50S ribosomal protein L24

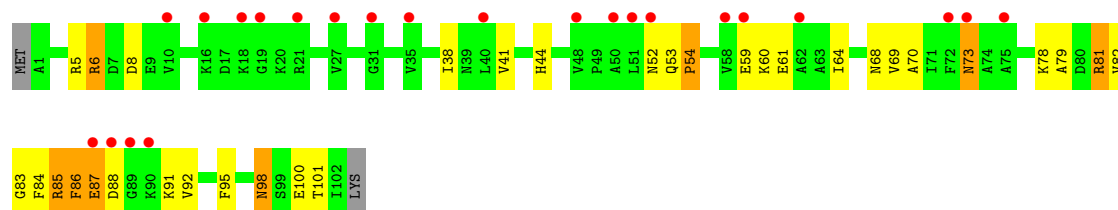


- Molecule 21: 50S ribosomal protein L24

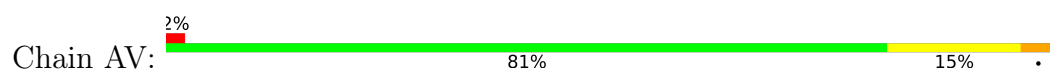




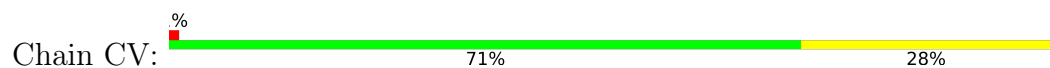
- Molecule 21: 50S ribosomal protein L24



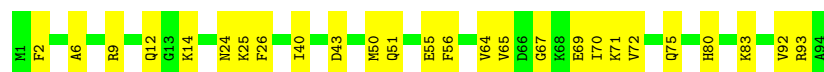
- Molecule 22: 50S ribosomal protein L25



- Molecule 22: 50S ribosomal protein L25



- Molecule 22: 50S ribosomal protein L25

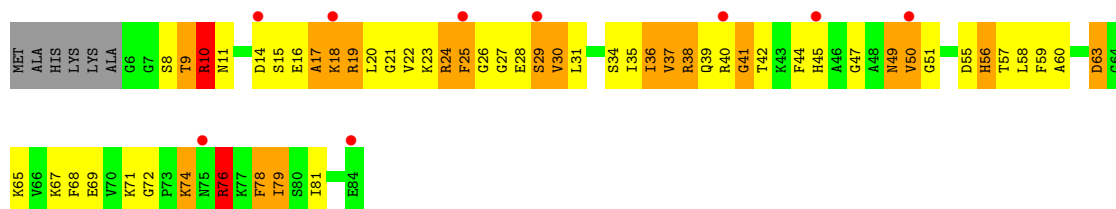


- Molecule 22: 50S ribosomal protein L25



- Molecule 23: 50S ribosomal protein L27





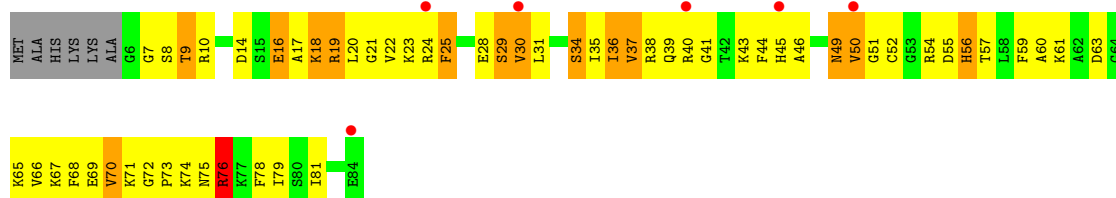
• Molecule 23: 50S ribosomal protein L27



• Molecule 23: 50S ribosomal protein L27



• Molecule 23: 50S ribosomal protein L27



• Molecule 24: 50S ribosomal protein L28



• Molecule 24: 50S ribosomal protein L28





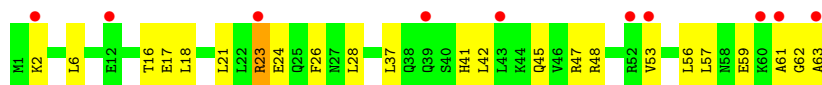
- Molecule 24: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L28



- Molecule 25: 50S ribosomal protein L29



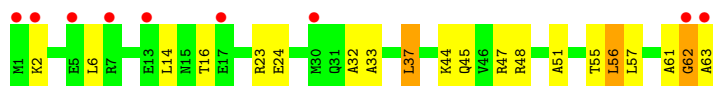
- Molecule 25: 50S ribosomal protein L29



- Molecule 25: 50S ribosomal protein L29

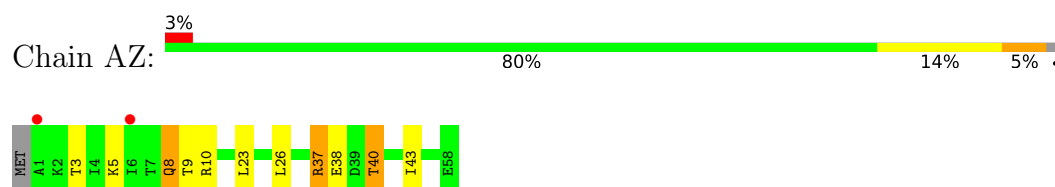


- Molecule 25: 50S ribosomal protein L29

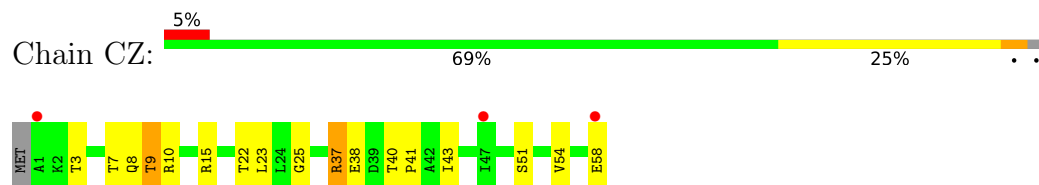


- Molecule 26: 50S ribosomal protein L30

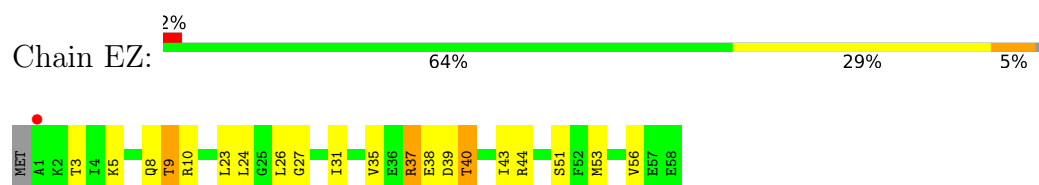




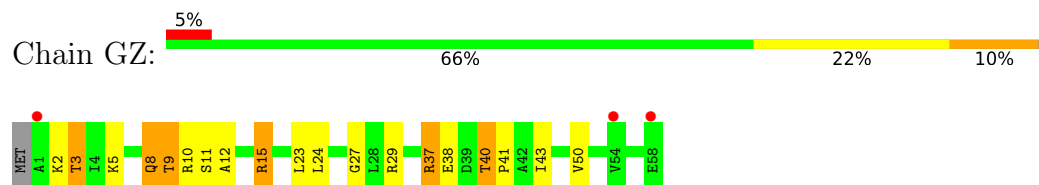
- Molecule 26: 50S ribosomal protein L30



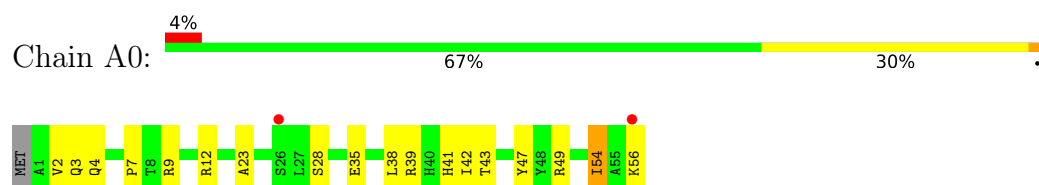
- Molecule 26: 50S ribosomal protein L30



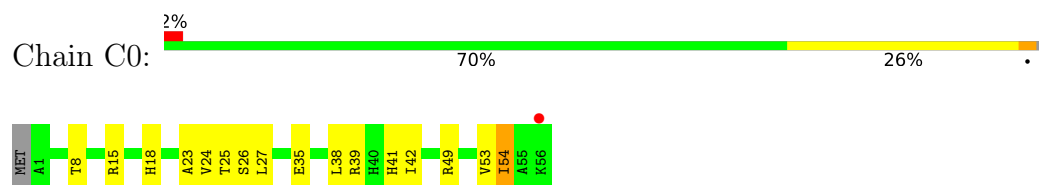
- Molecule 26: 50S ribosomal protein L30



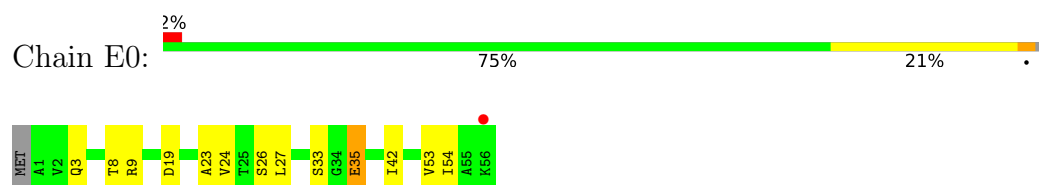
- Molecule 27: 50S ribosomal protein L32



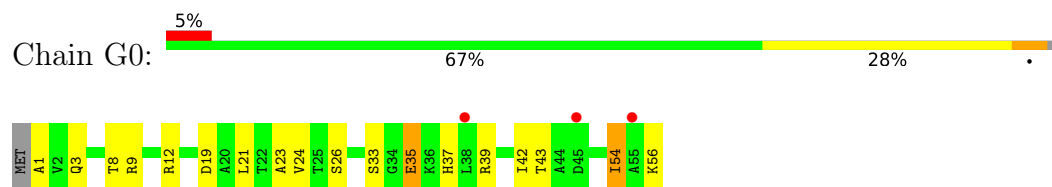
- Molecule 27: 50S ribosomal protein L32



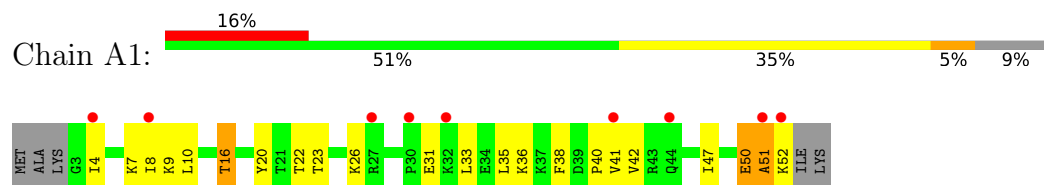
- Molecule 27: 50S ribosomal protein L32



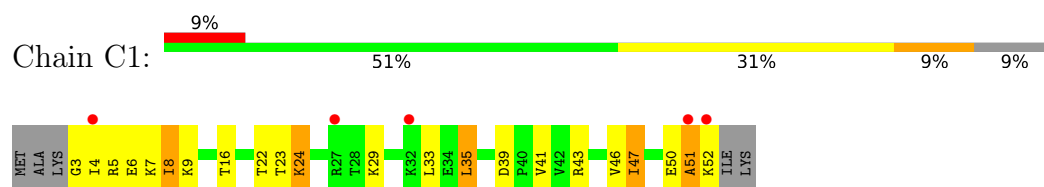
## • Molecule 27: 50S ribosomal protein L32



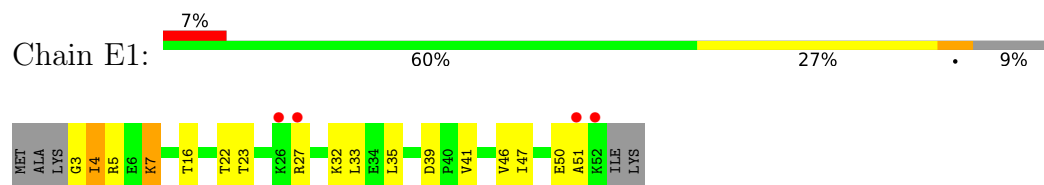
## • Molecule 28: 50S ribosomal protein L33



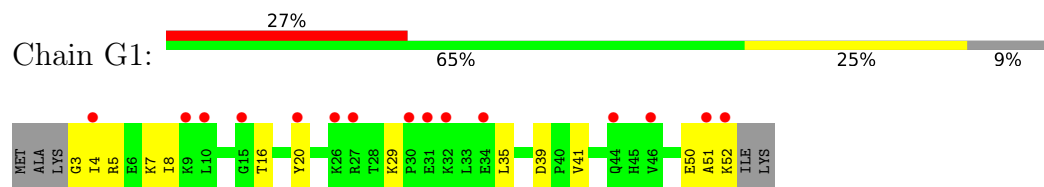
## • Molecule 28: 50S ribosomal protein L33



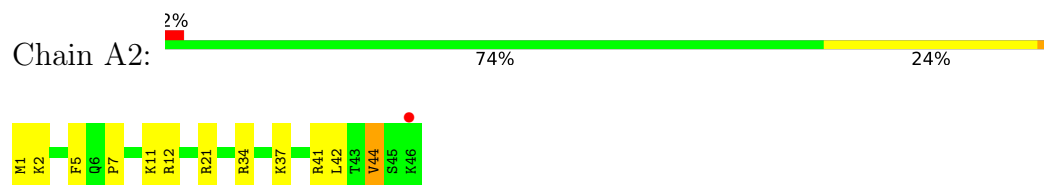
## • Molecule 28: 50S ribosomal protein L33



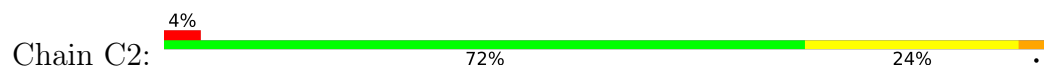
## • Molecule 28: 50S ribosomal protein L33



## • Molecule 29: 50S ribosomal protein L34



## • Molecule 29: 50S ribosomal protein L34

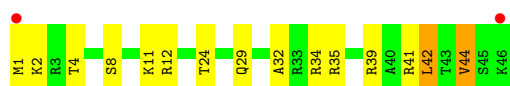




- Molecule 29: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L34



- Molecule 30: 50S ribosomal protein L35



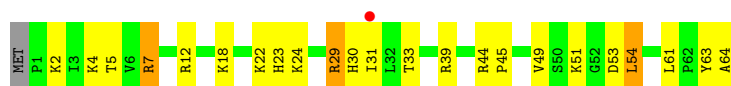
- Molecule 30: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L35

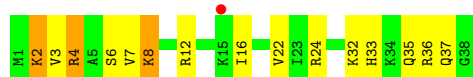


- Molecule 30: 50S ribosomal protein L35



- Molecule 31: 50S ribosomal protein L36





- Molecule 31: 50S ribosomal protein L36



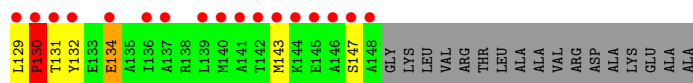
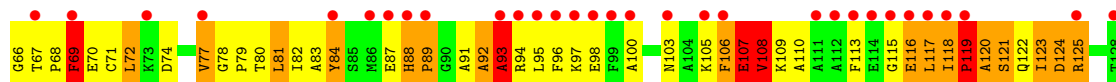
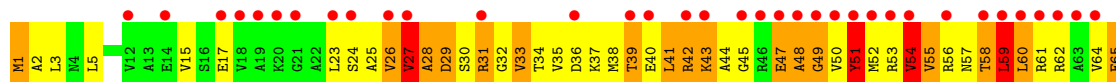
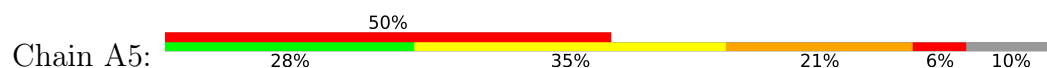
- Molecule 31: 50S ribosomal protein L36



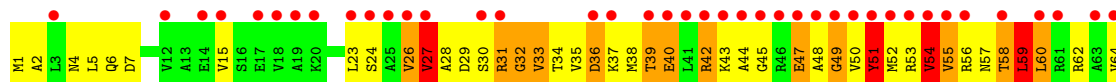
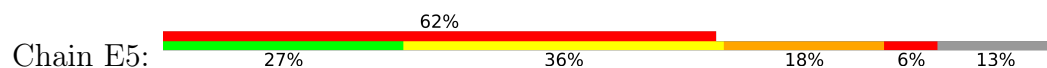
- Molecule 31: 50S ribosomal protein L36

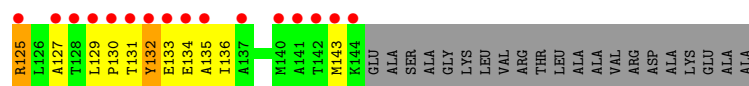


- Molecule 32: 50S ribosomal protein L10

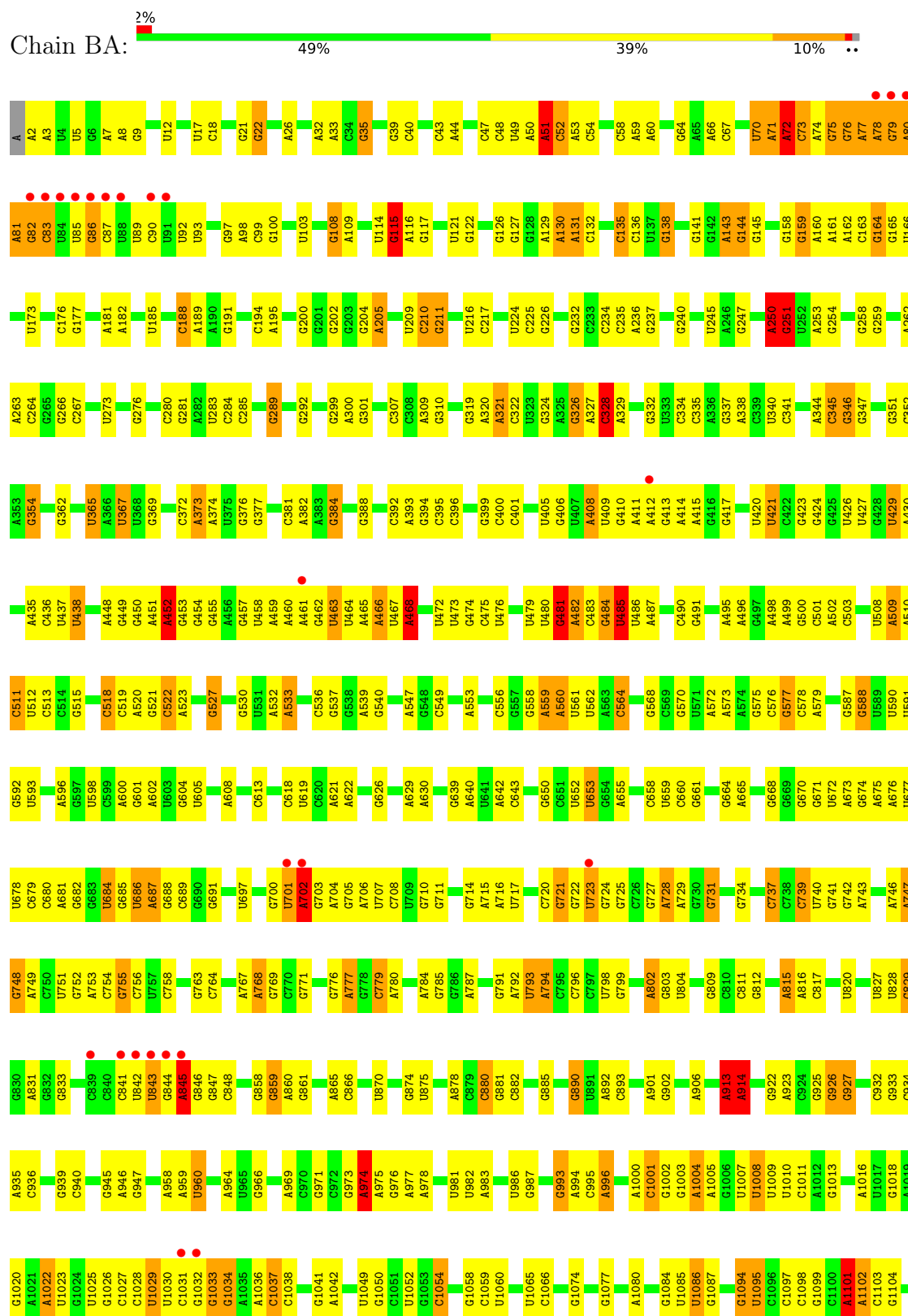


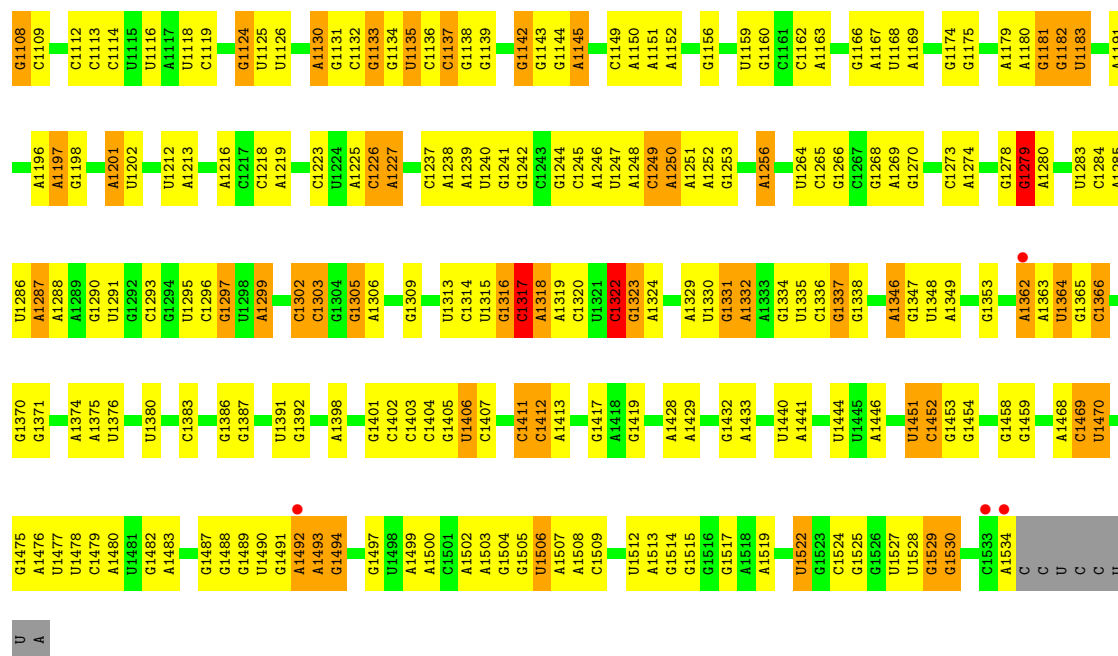
- Molecule 32: 50S ribosomal protein L10



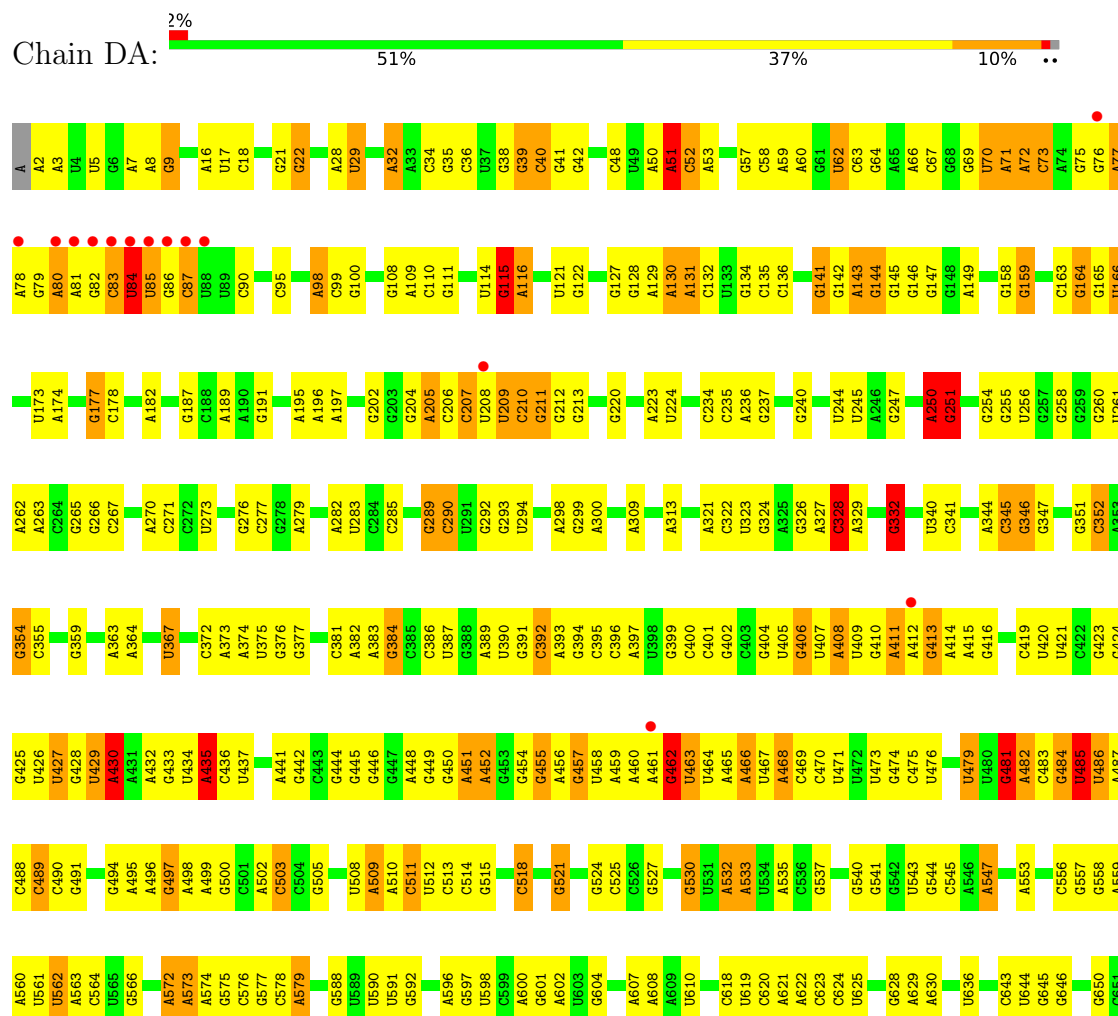


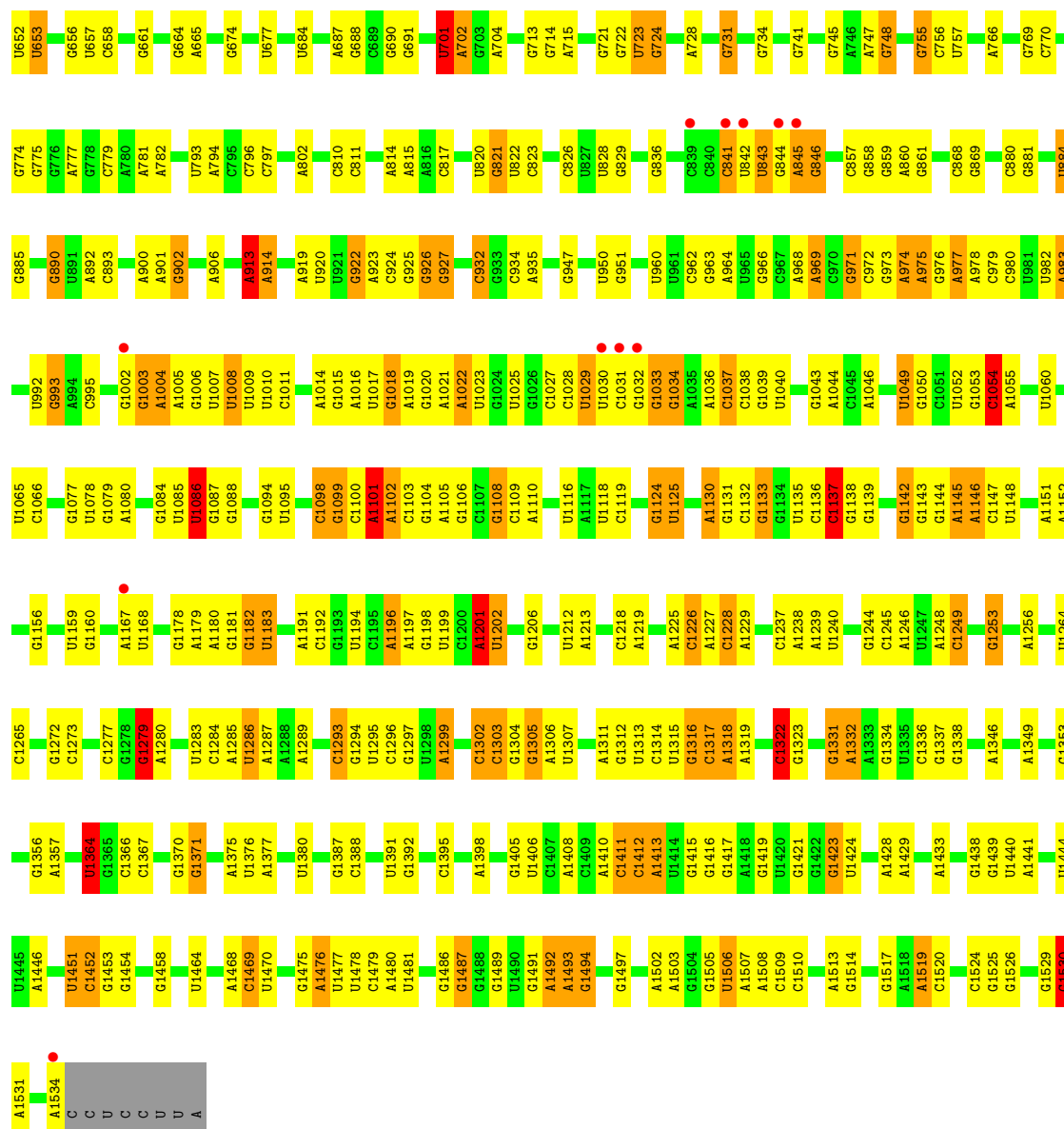
• Molecule 33: 16S rRNA



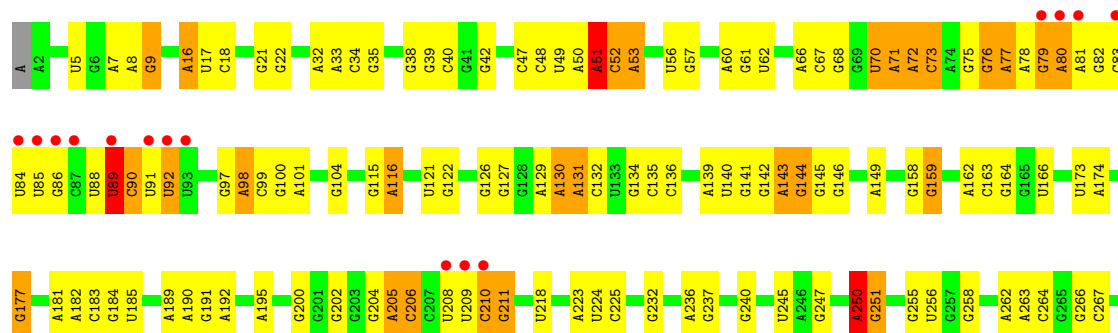


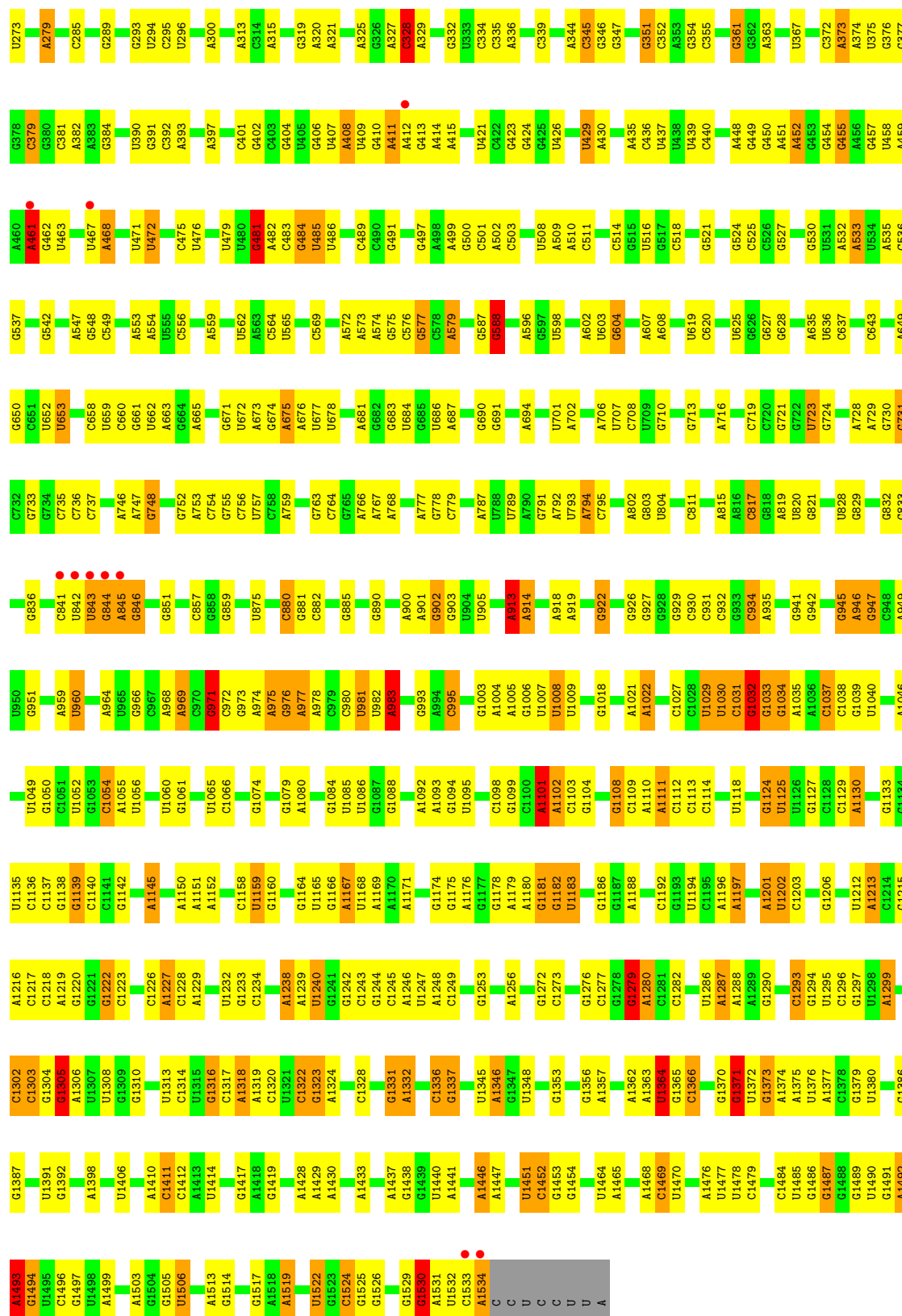
• Molecule 33: 16S rRNA



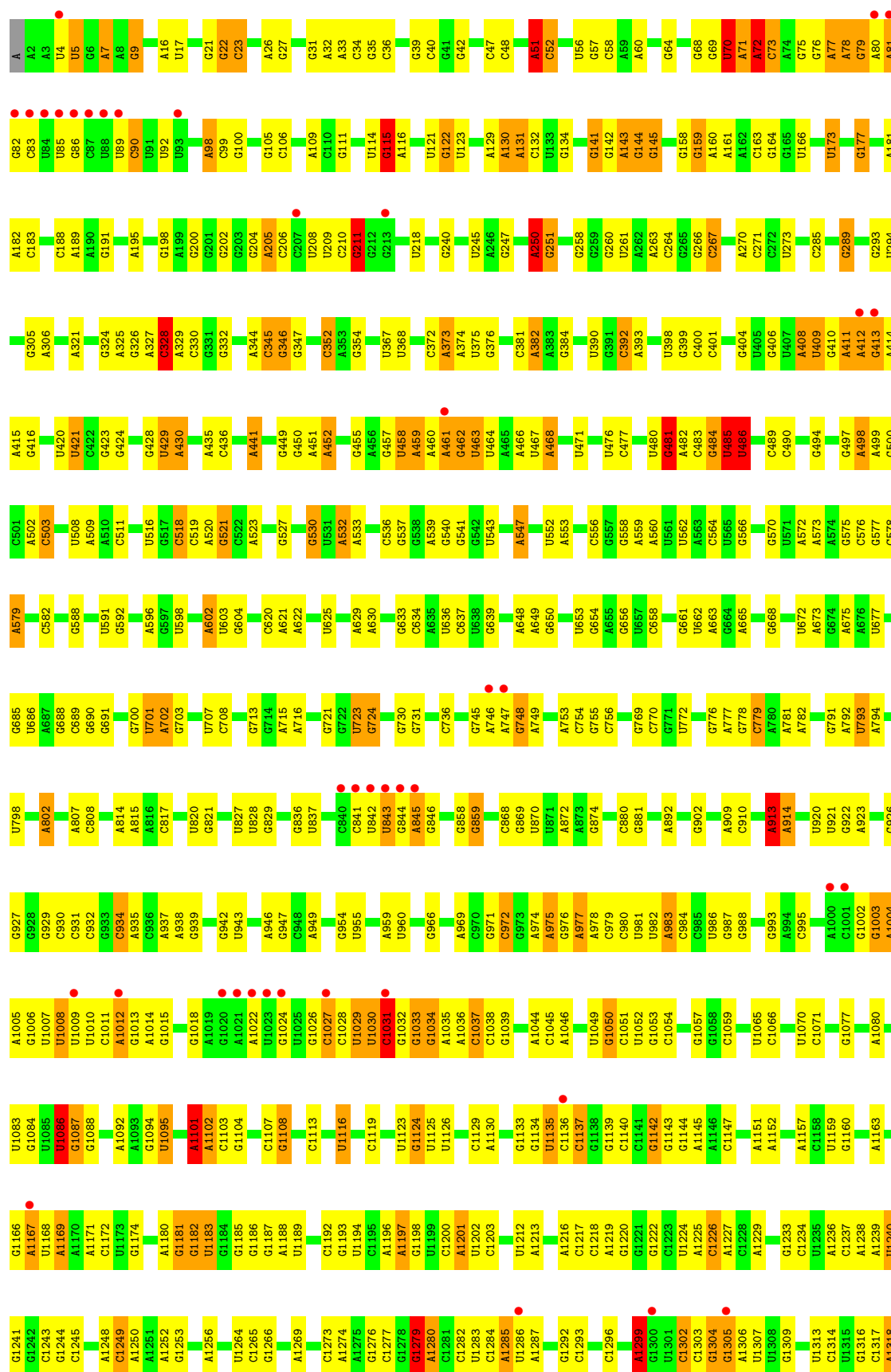


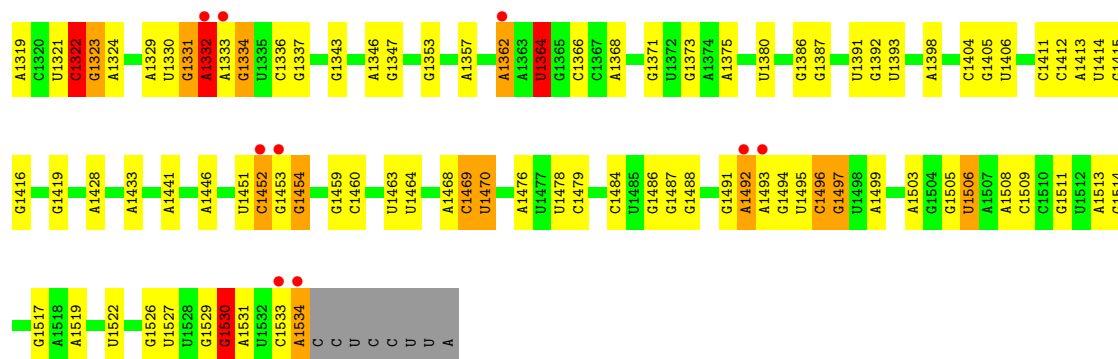
• Molecule 33: 16S rRNA



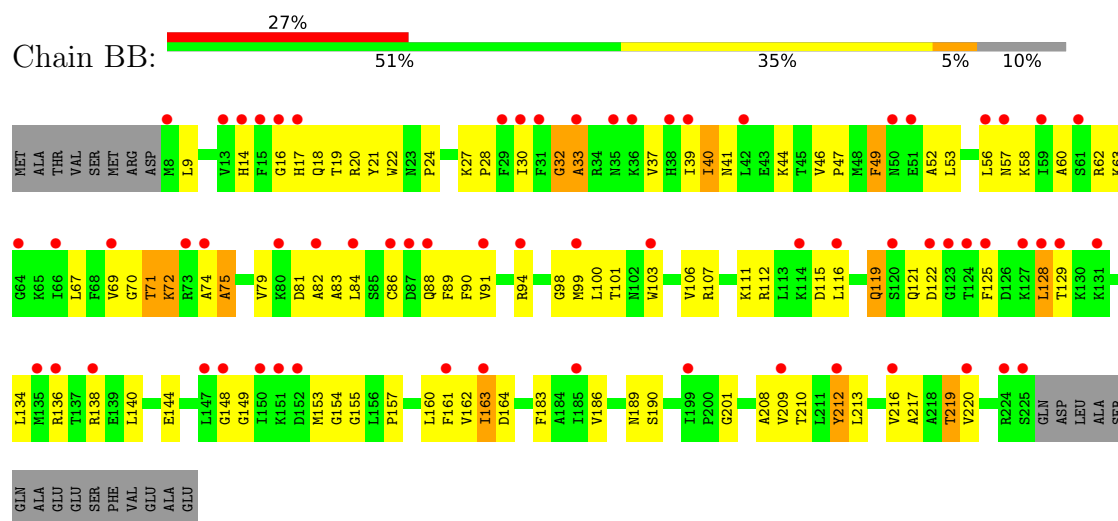




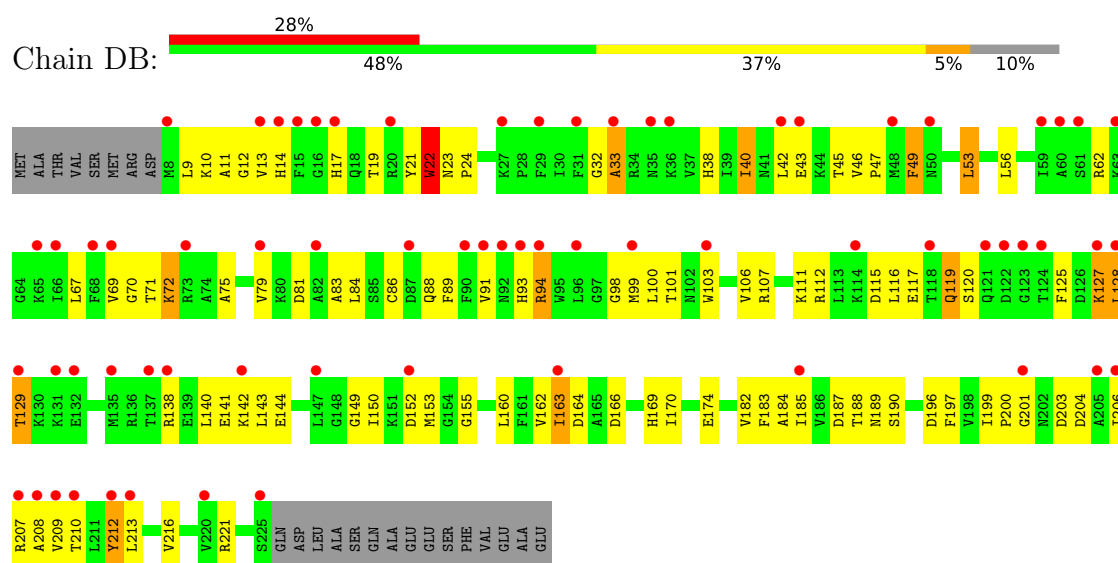




• Molecule 34: 30S ribosomal protein S2



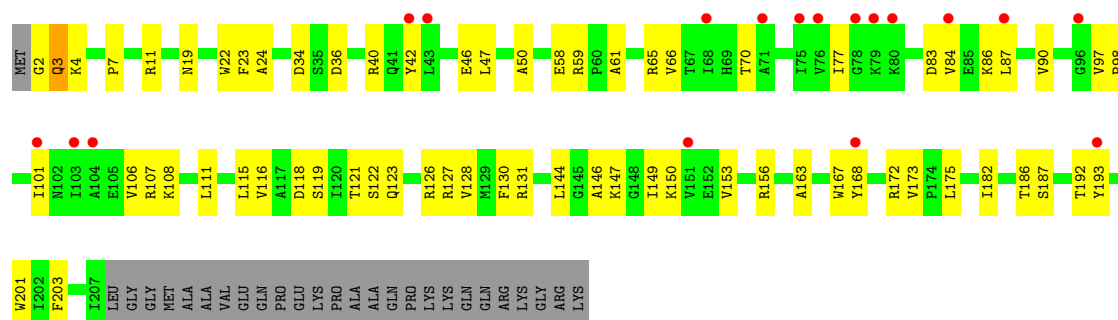
• Molecule 34: 30S ribosomal protein S2



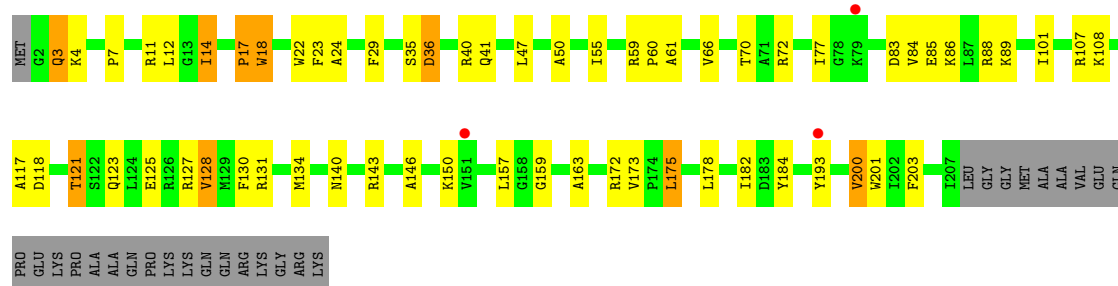
• Molecule 34: 30S ribosomal protein S2



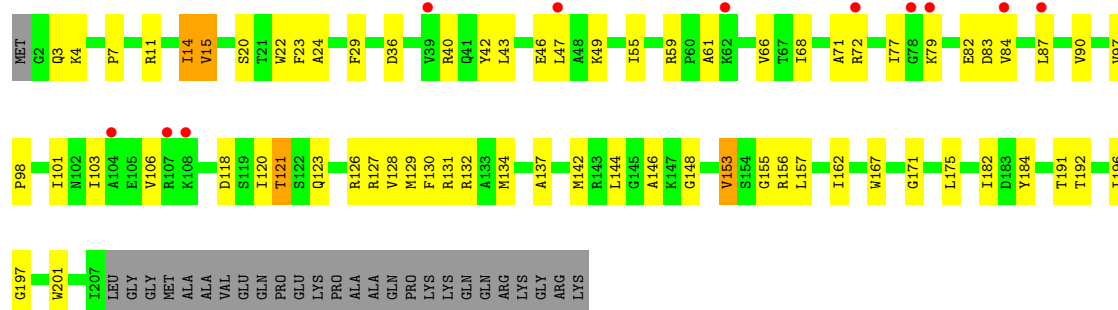




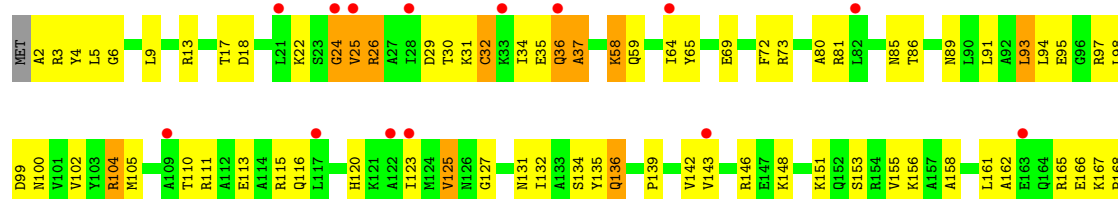
• Molecule 35: 30S ribosomal protein S3



• Molecule 35: 30S ribosomal protein S3

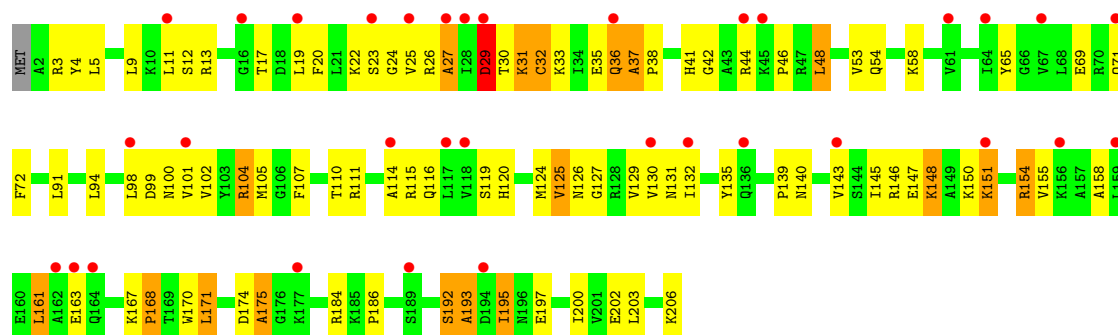


• Molecule 36: 30S ribosomal protein S4

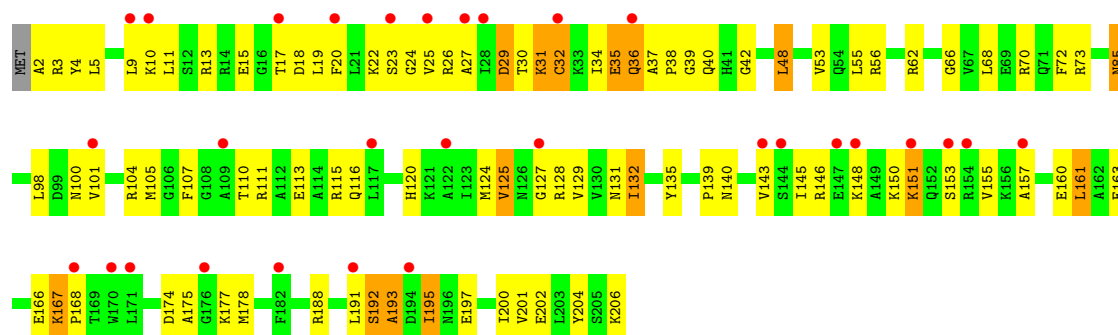




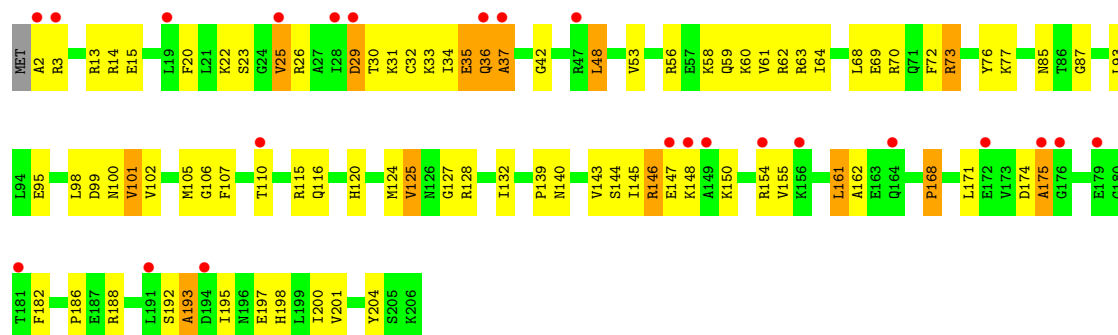
• Molecule 36: 30S ribosomal protein S4



• Molecule 36: 30S ribosomal protein S4

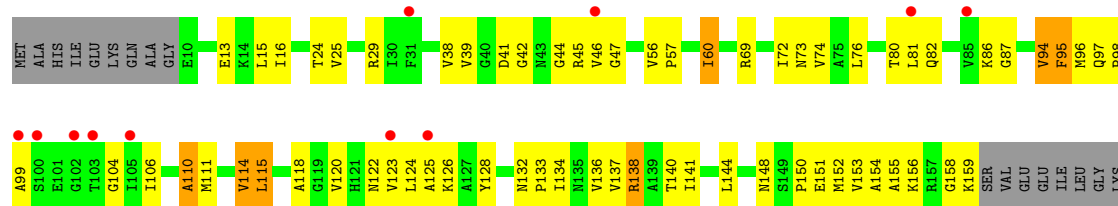


• Molecule 36: 30S ribosomal protein S4

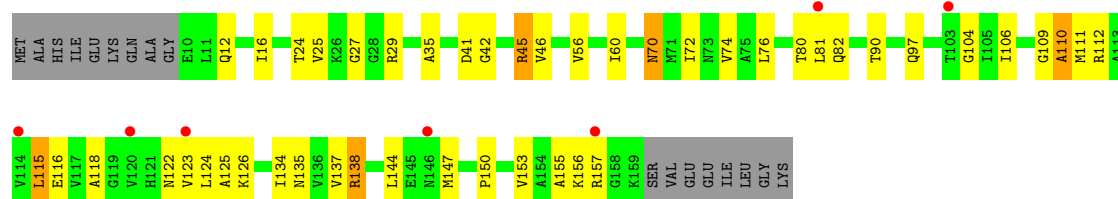


• Molecule 37: 30S ribosomal protein S5

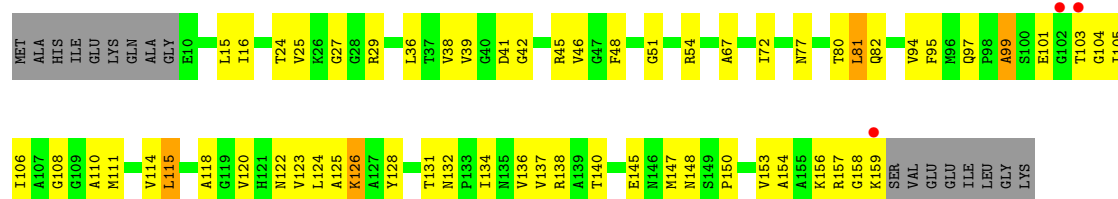




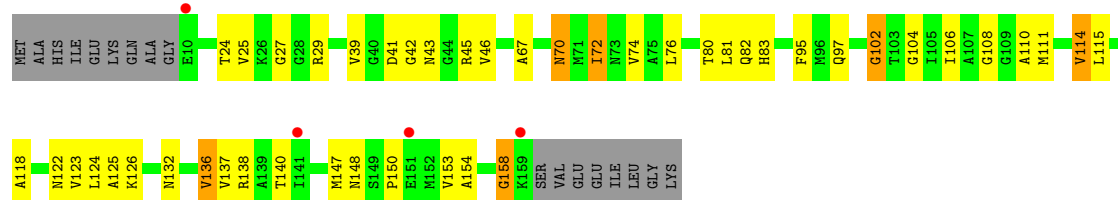
• Molecule 37: 30S ribosomal protein S5



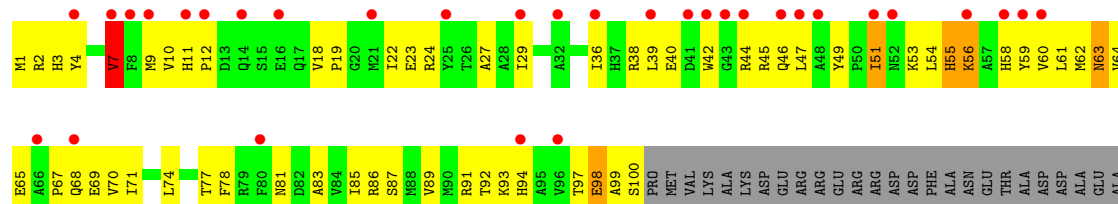
• Molecule 37: 30S ribosomal protein S5



• Molecule 37: 30S ribosomal protein S5

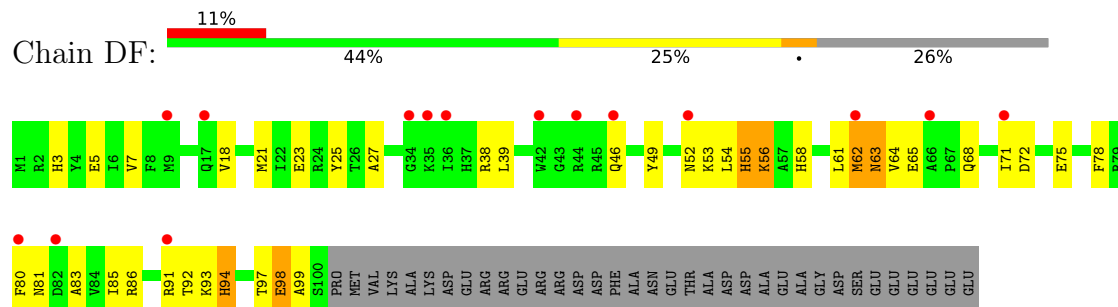


• Molecule 38: 30S ribosomal protein S6

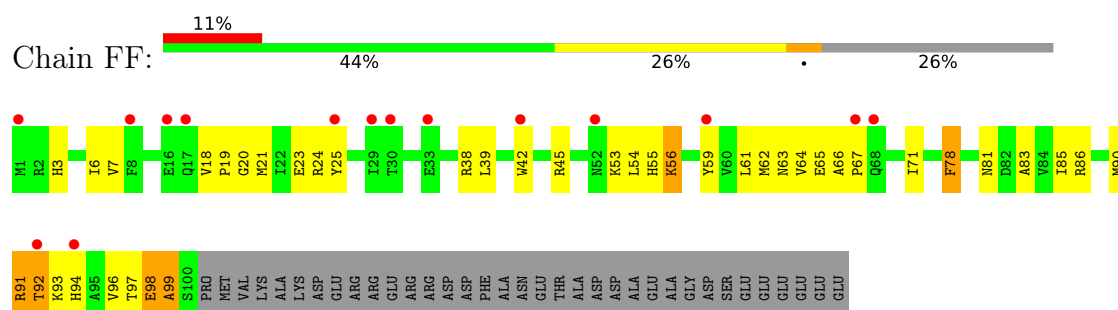


GLY  
ASP  
SER  
GLU  
GLU  
GLU  
GLU

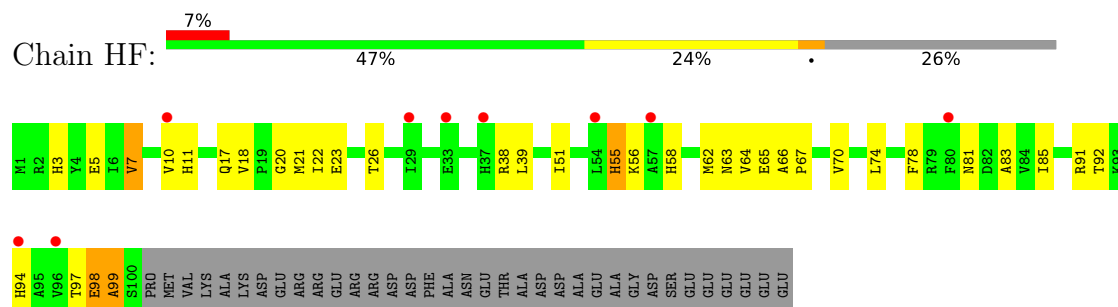
## • Molecule 38: 30S ribosomal protein S6



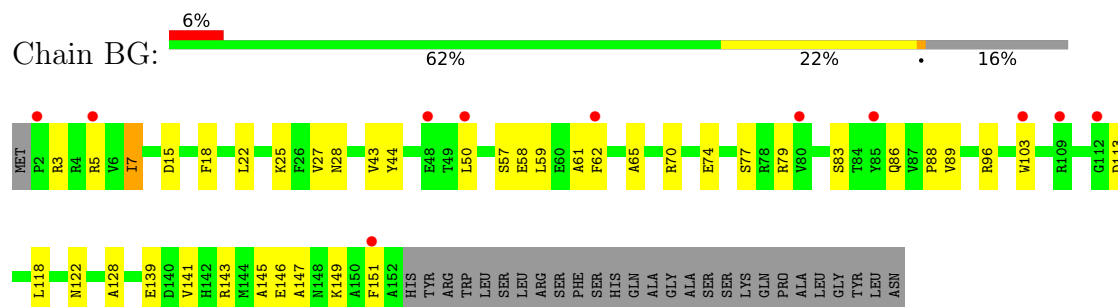
## • Molecule 38: 30S ribosomal protein S6



## • Molecule 38: 30S ribosomal protein S6

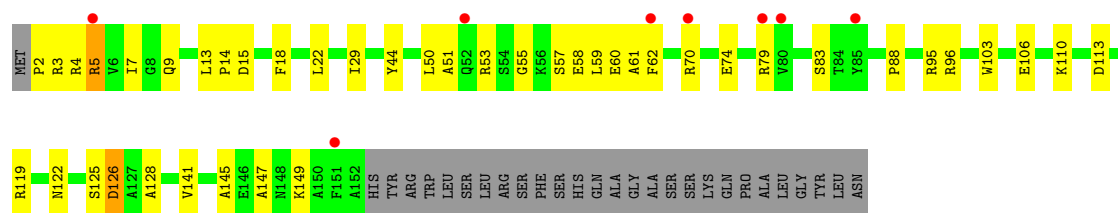


## • Molecule 39: 30S ribosomal protein S7

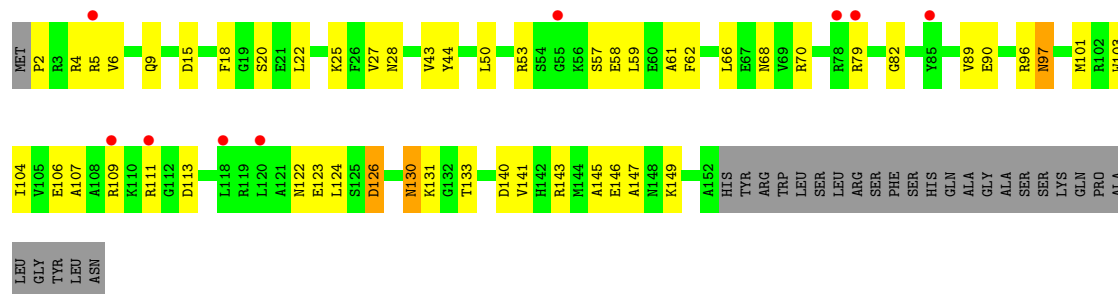


## • Molecule 39: 30S ribosomal protein S7

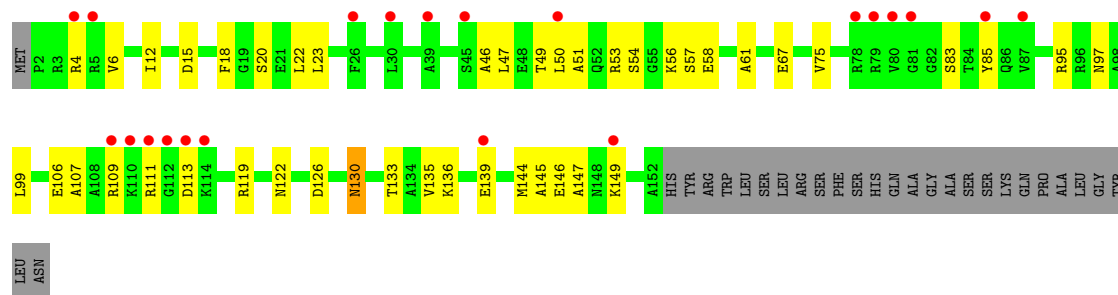




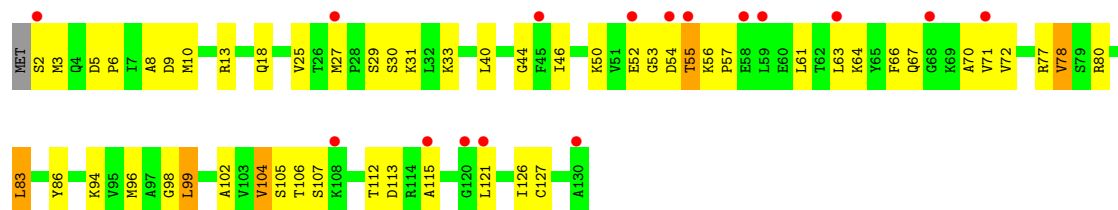
• Molecule 39: 30S ribosomal protein S7



• Molecule 39: 30S ribosomal protein S7



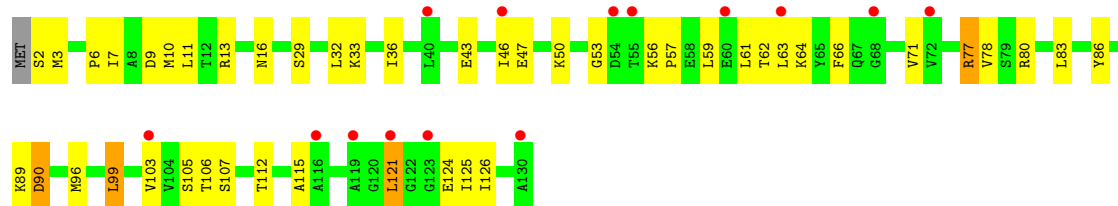
• Molecule 40: 30S ribosomal protein S8



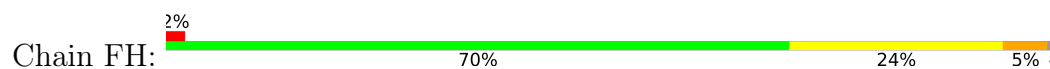
• Molecule 40: 30S ribosomal protein S8



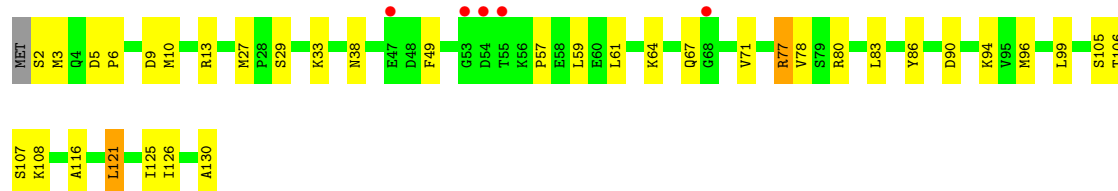
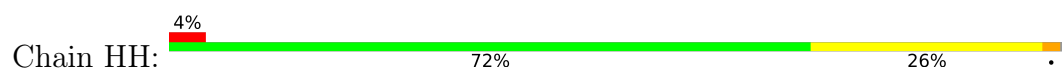




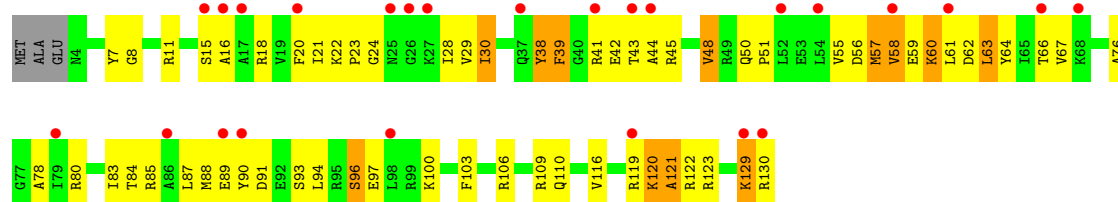
• Molecule 40: 30S ribosomal protein S8



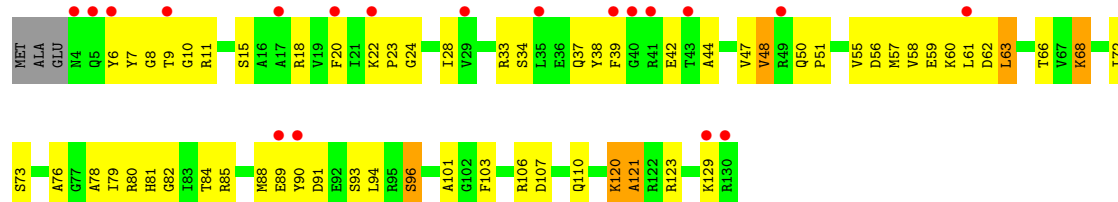
• Molecule 40: 30S ribosomal protein S8



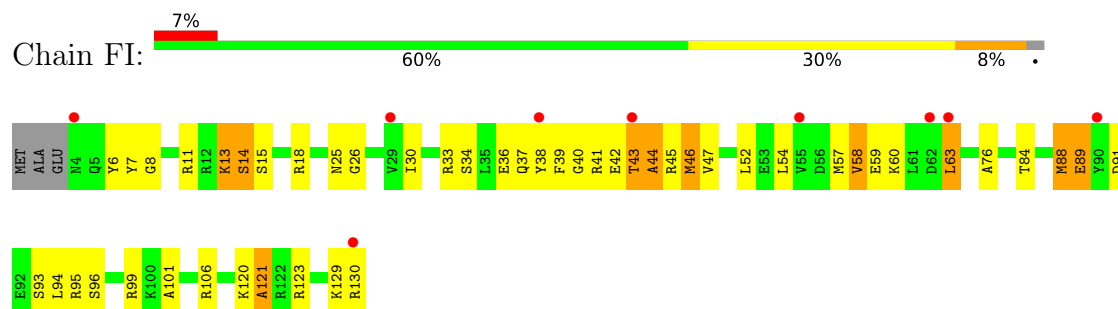
• Molecule 41: 30S ribosomal protein S9



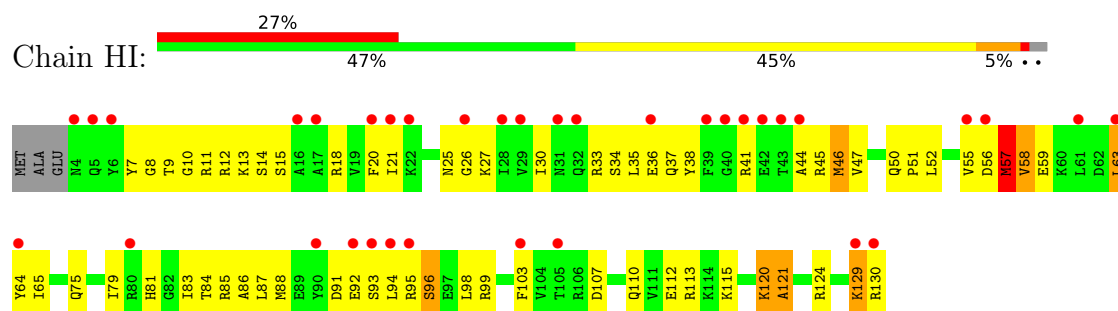
• Molecule 41: 30S ribosomal protein S9



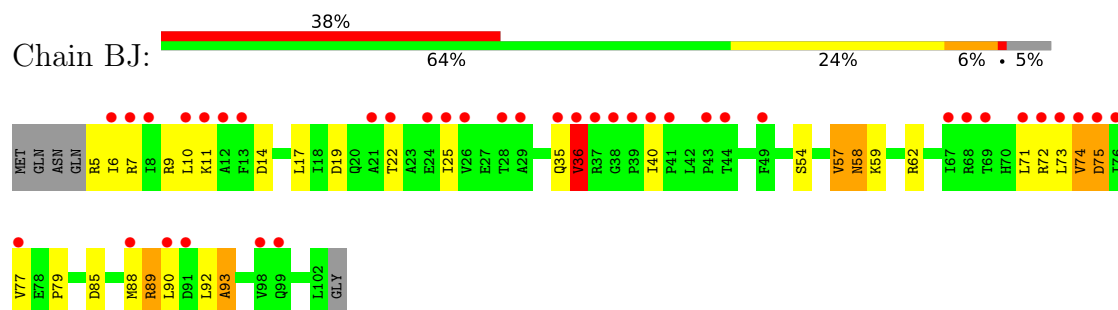
- Molecule 41: 30S ribosomal protein S9



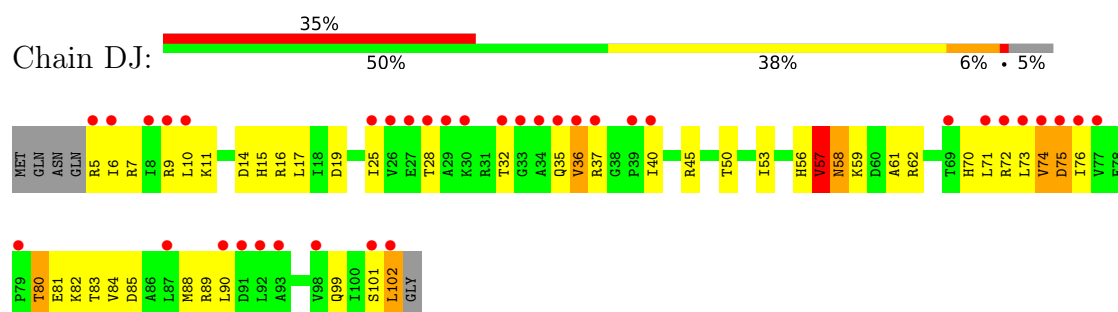
- Molecule 41: 30S ribosomal protein S9



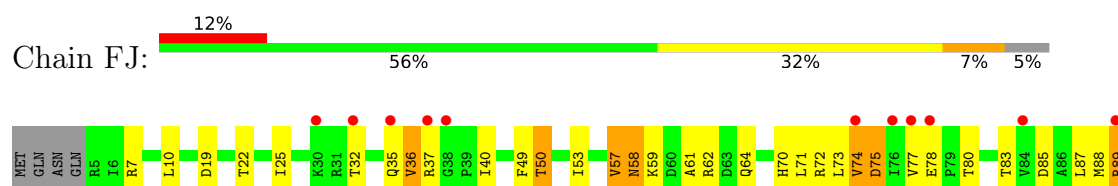
- Molecule 42: 30S ribosomal protein S10



- Molecule 42: 30S ribosomal protein S10

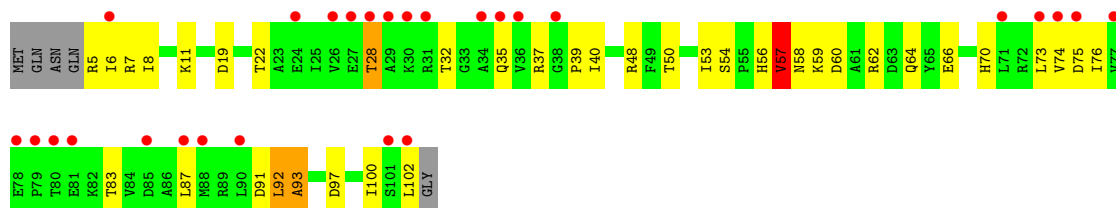


- Molecule 42: 30S ribosomal protein S10

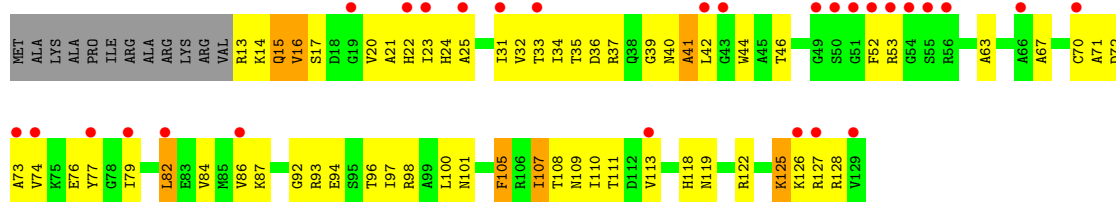
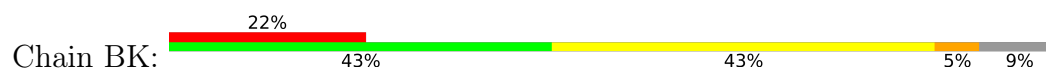




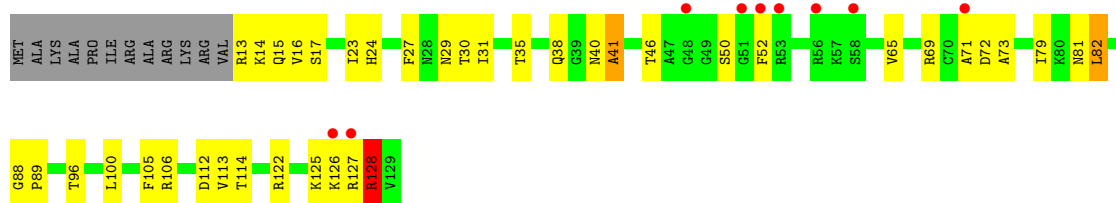
- Molecule 42: 30S ribosomal protein S10



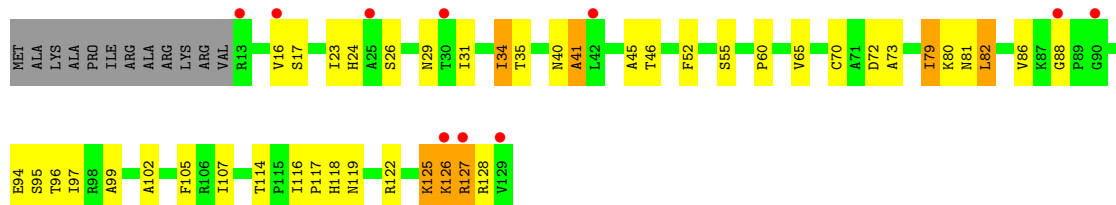
- Molecule 43: 30S ribosomal protein S11



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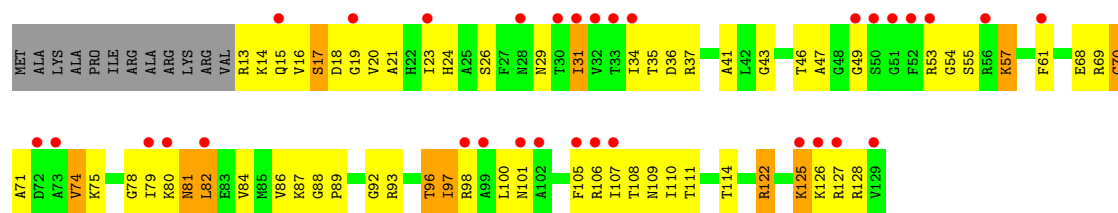


- Molecule 43: 30S ribosomal protein S11

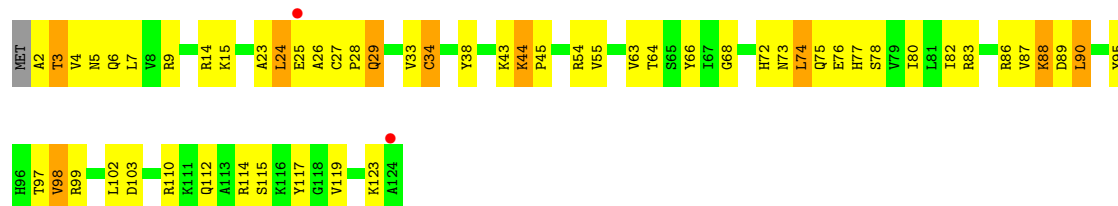


- Molecule 43: 30S ribosomal protein S11

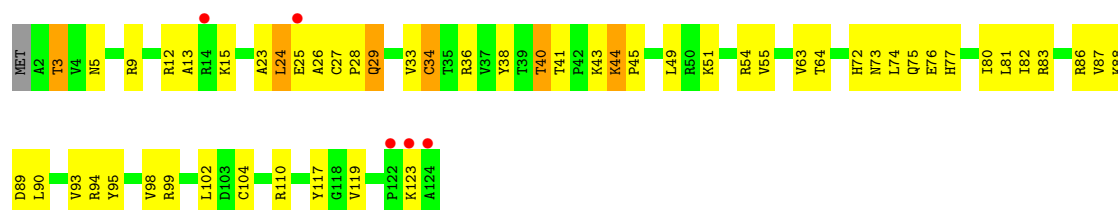




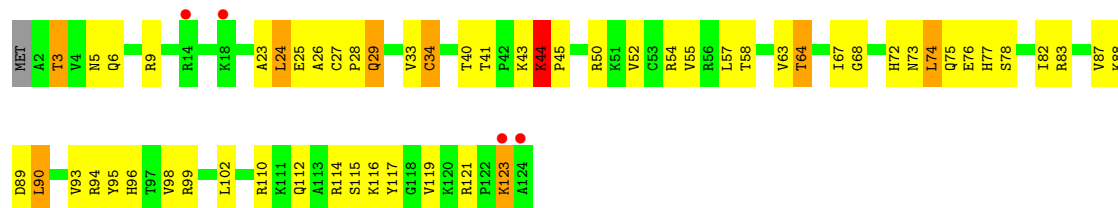
• Molecule 44: 30S ribosomal protein S12



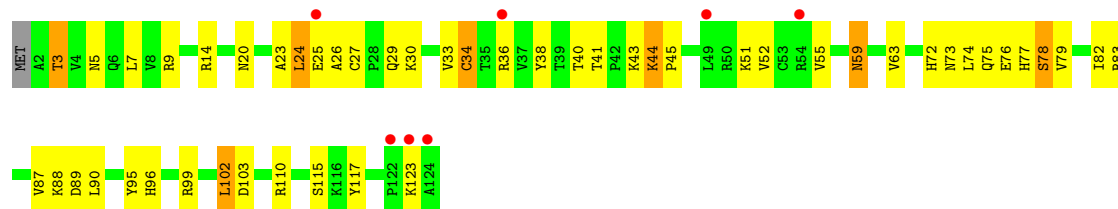
• Molecule 44: 30S ribosomal protein S12



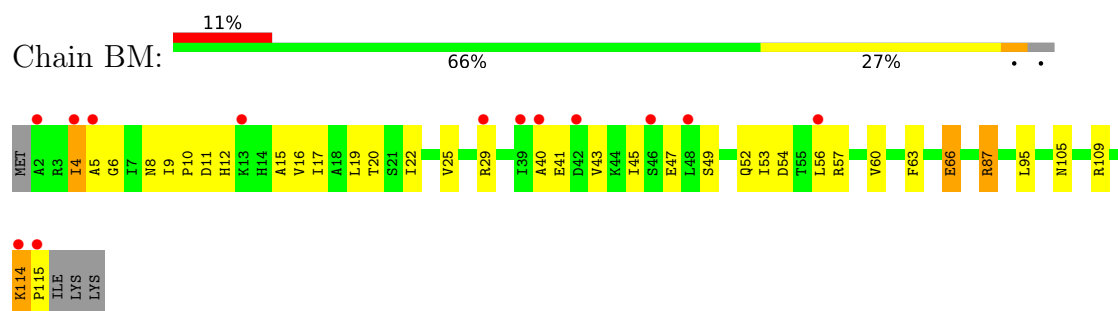
• Molecule 44: 30S ribosomal protein S12



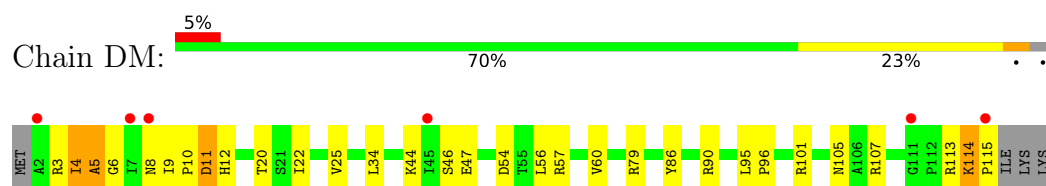
• Molecule 44: 30S ribosomal protein S12



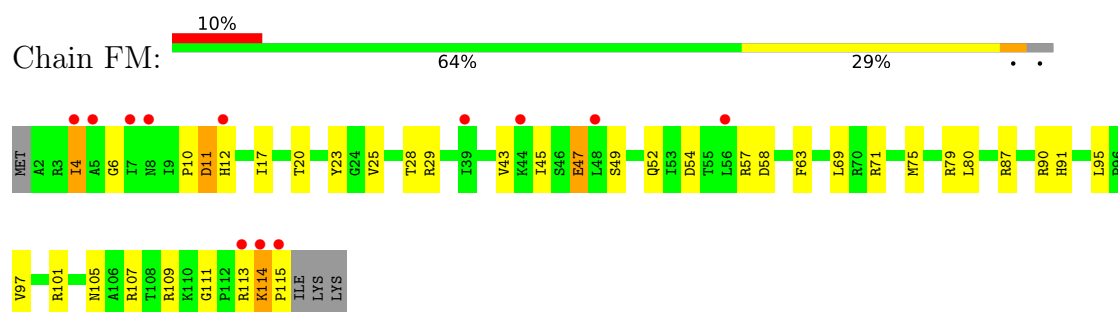
## • Molecule 45: 30S ribosomal protein S13



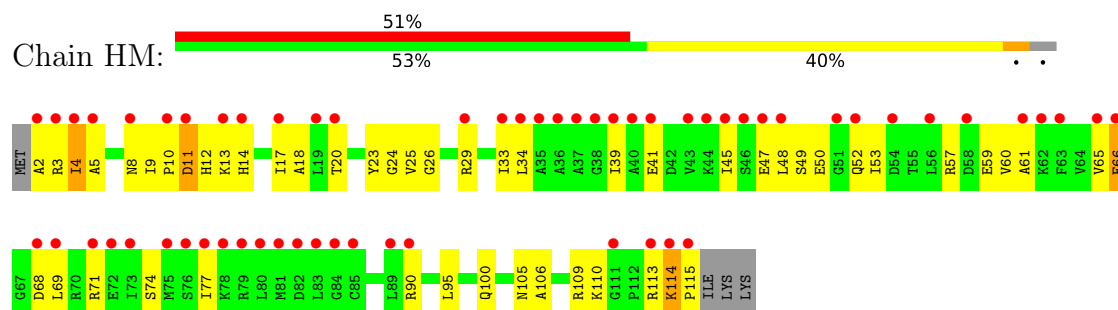
## • Molecule 45: 30S ribosomal protein S13



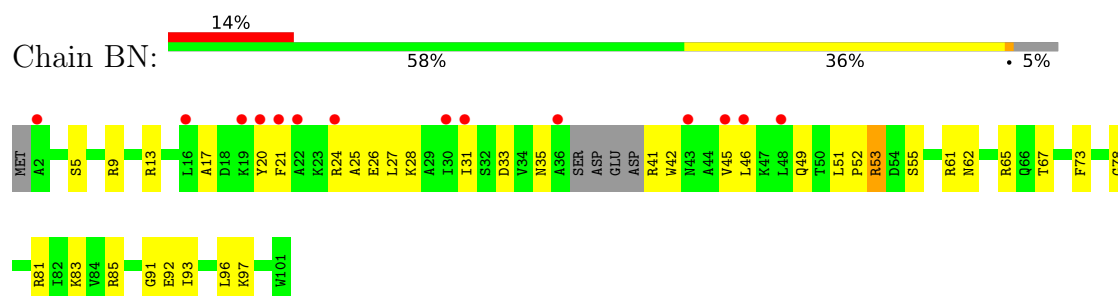
## • Molecule 45: 30S ribosomal protein S13



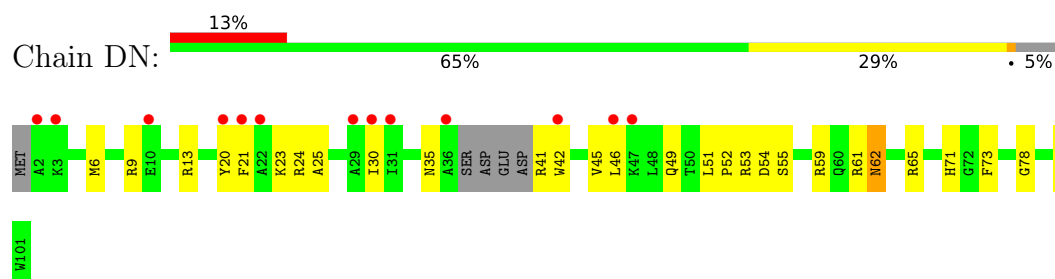
## • Molecule 45: 30S ribosomal protein S13



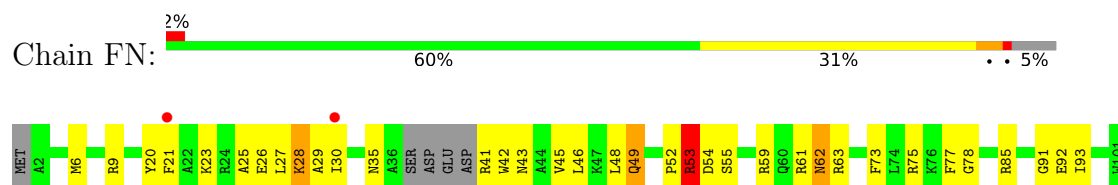
## • Molecule 46: 30S ribosomal protein S14



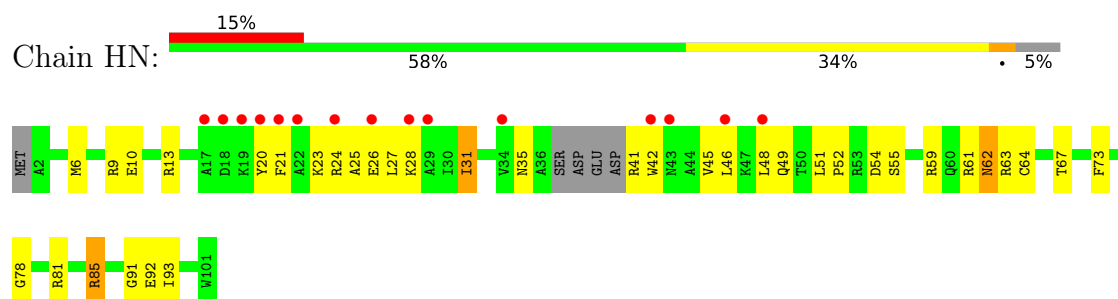
## • Molecule 46: 30S ribosomal protein S14



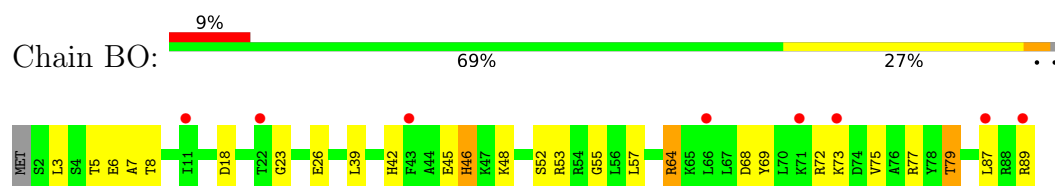
## • Molecule 46: 30S ribosomal protein S14



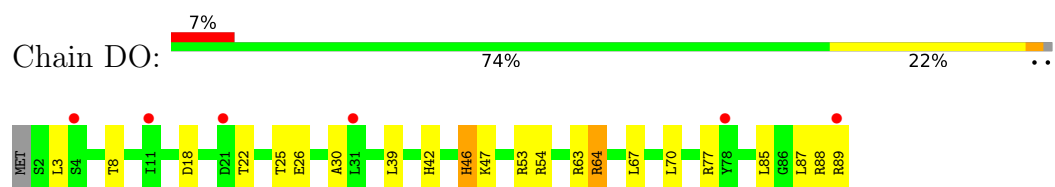
## • Molecule 46: 30S ribosomal protein S14



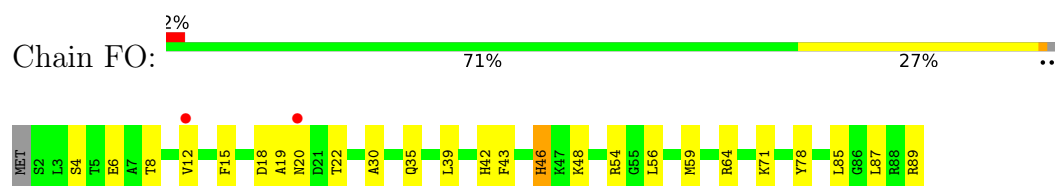
## • Molecule 47: 30S ribosomal protein S15



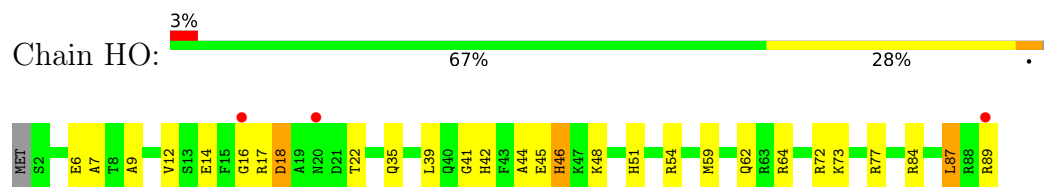
## • Molecule 47: 30S ribosomal protein S15



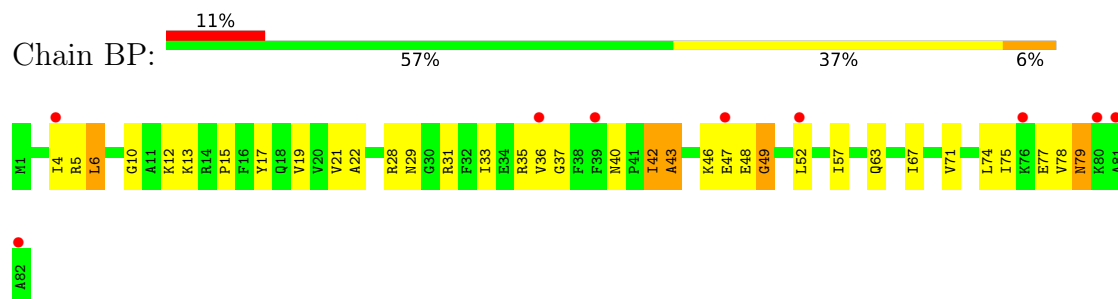
## • Molecule 47: 30S ribosomal protein S15



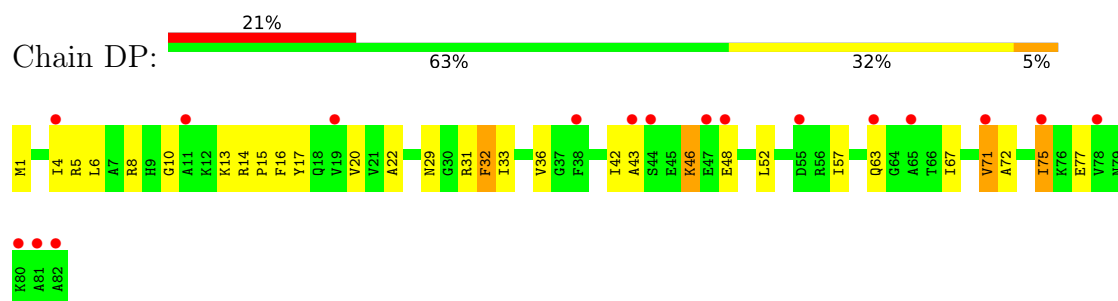
- Molecule 47: 30S ribosomal protein S15



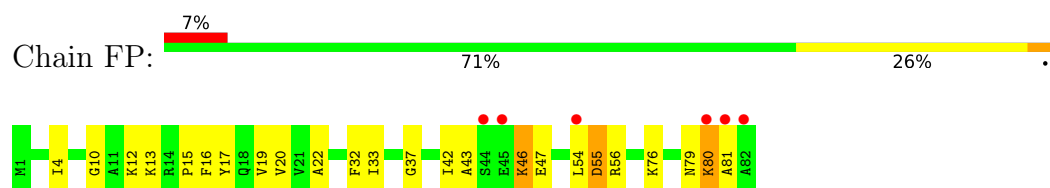
- Molecule 48: 30S ribosomal protein S16



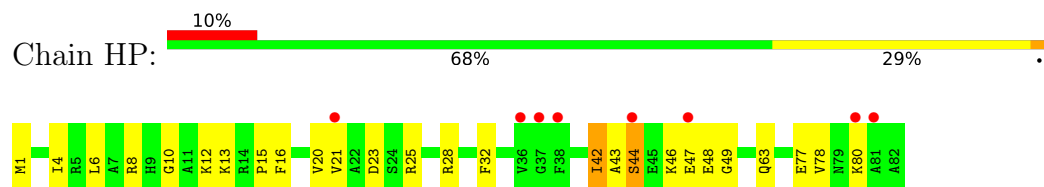
- Molecule 48: 30S ribosomal protein S16



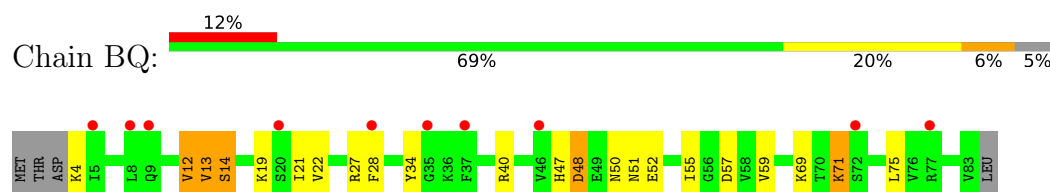
- Molecule 48: 30S ribosomal protein S16



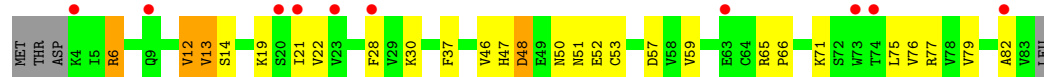
- Molecule 48: 30S ribosomal protein S16



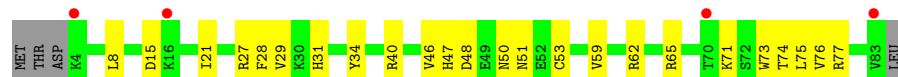
- Molecule 49: 30S ribosomal protein S17



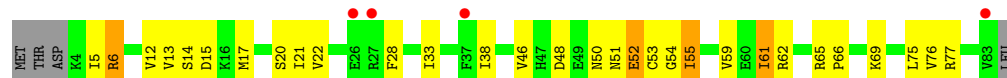
- Molecule 49: 30S ribosomal protein S17



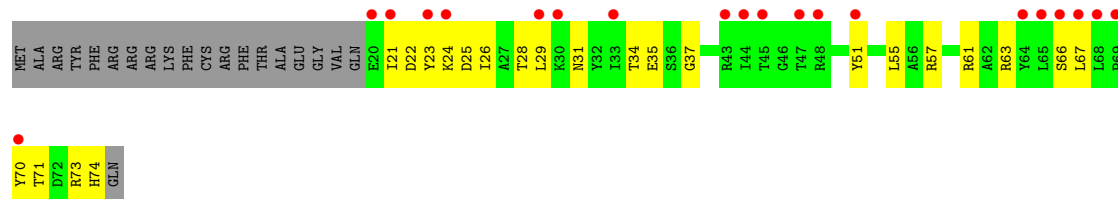
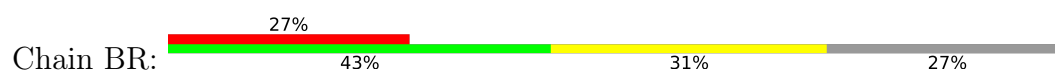
- Molecule 49: 30S ribosomal protein S17



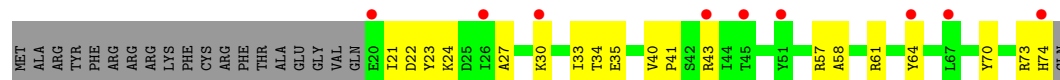
- Molecule 49: 30S ribosomal protein S17



- Molecule 50: 30S ribosomal protein S18



- Molecule 50: 30S ribosomal protein S18

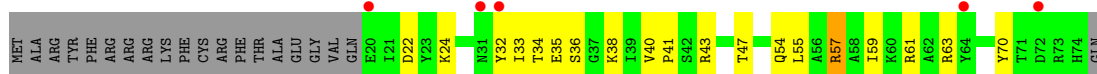


- Molecule 50: 30S ribosomal protein S18

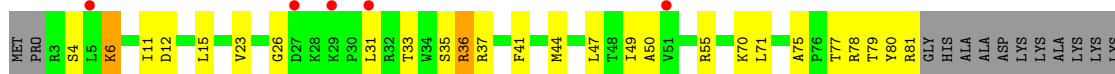


- Molecule 50: 30S ribosomal protein S18

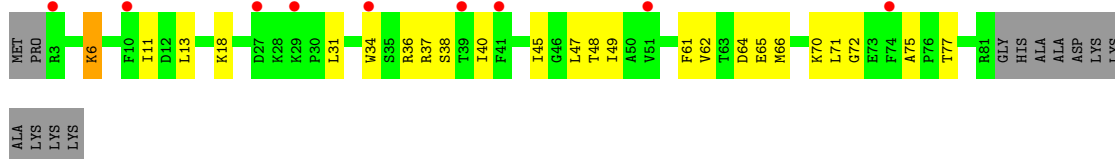




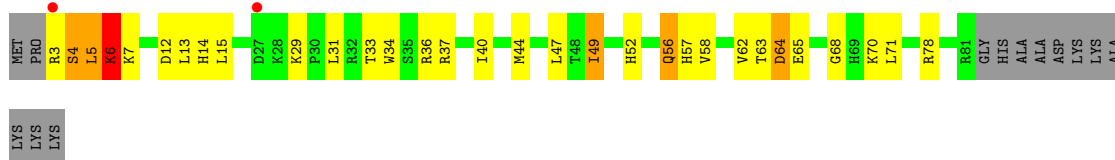
- Molecule 51: 30S ribosomal protein S19



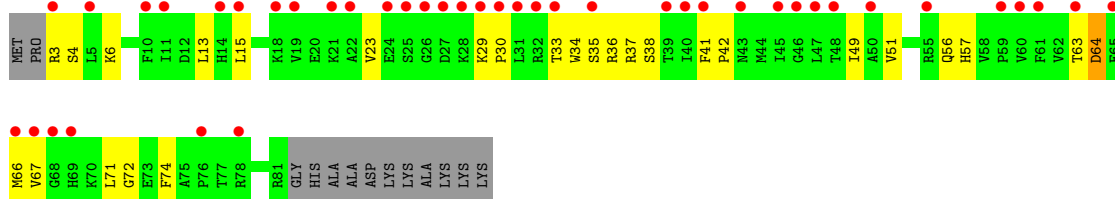
- Molecule 51: 30S ribosomal protein S19



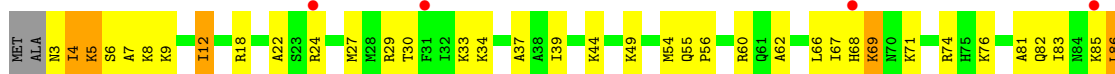
- Molecule 51: 30S ribosomal protein S19



- Molecule 51: 30S ribosomal protein S19



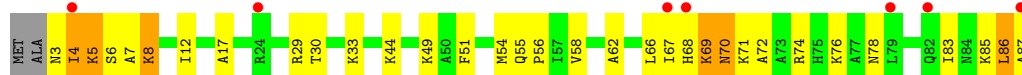
- Molecule 52: 30S ribosomal protein S20



A87

- Molecule 52: 30S ribosomal protein S20

Chain DT: 8% 60% 31% 7%



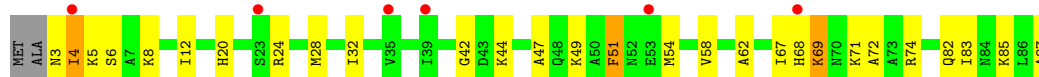
- Molecule 52: 30S ribosomal protein S20

Chain FT: 6% 60% 32% 6%



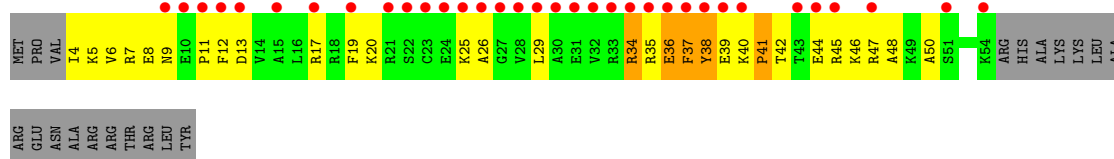
- Molecule 52: 30S ribosomal protein S20

Chain HT: 7% 66% 29%



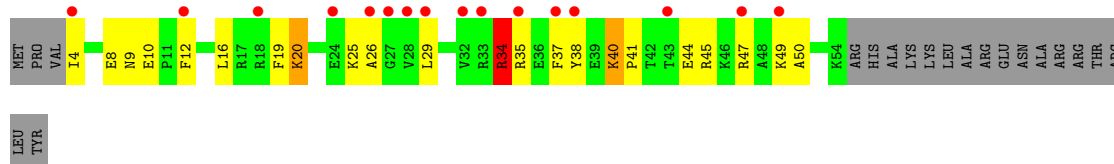
- Molecule 53: 30S ribosomal protein S21

Chain BU: 48% 30% 35% 7% 28%



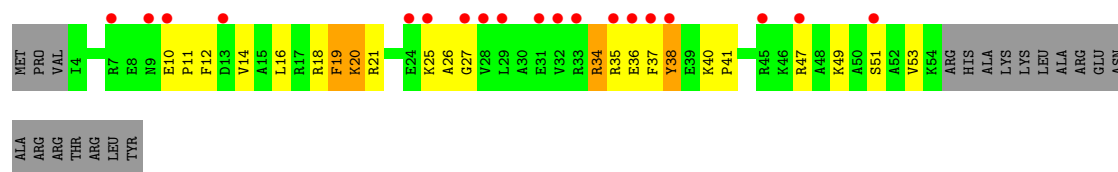
- Molecule 53: 30S ribosomal protein S21

Chain DU: 23% 41% 27% 28%



- Molecule 53: 30S ribosomal protein S21

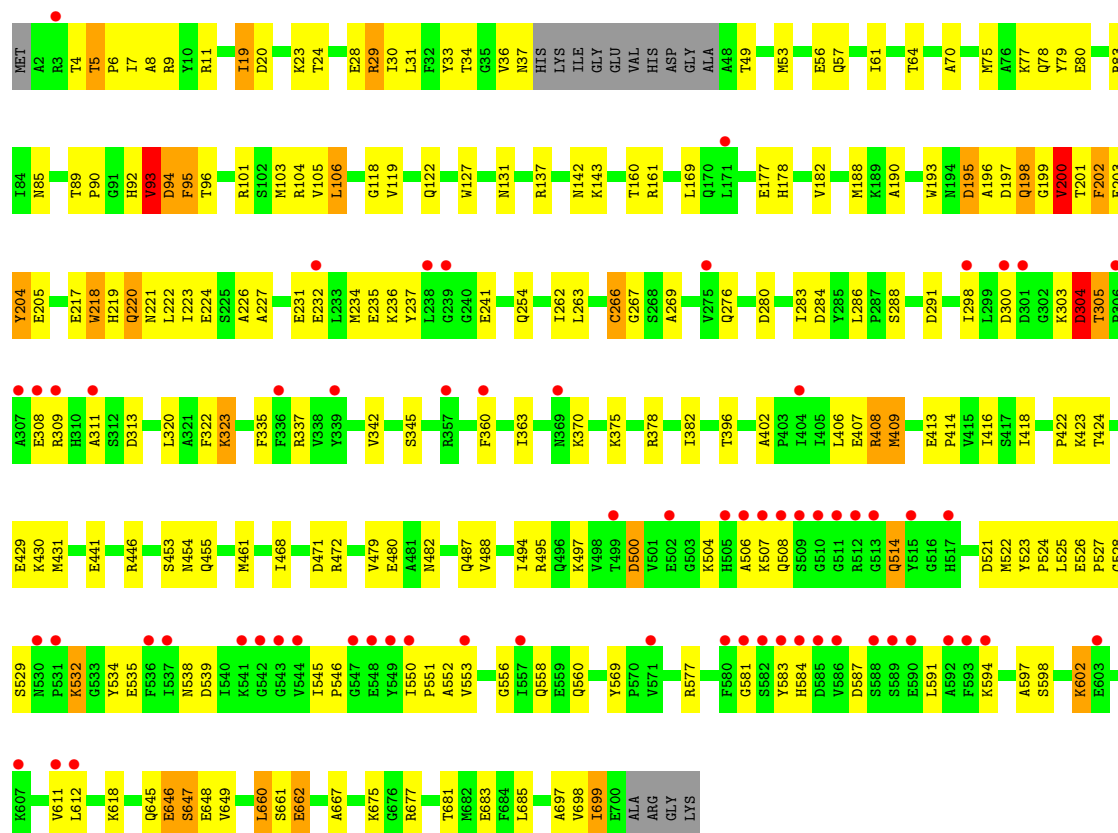
Chain FU: 27% 39% 27% 6% 28%



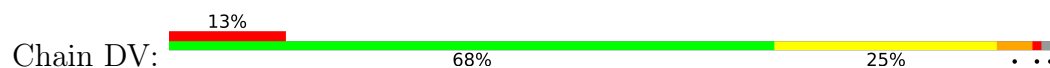
- Molecule 53: 30S ribosomal protein S21

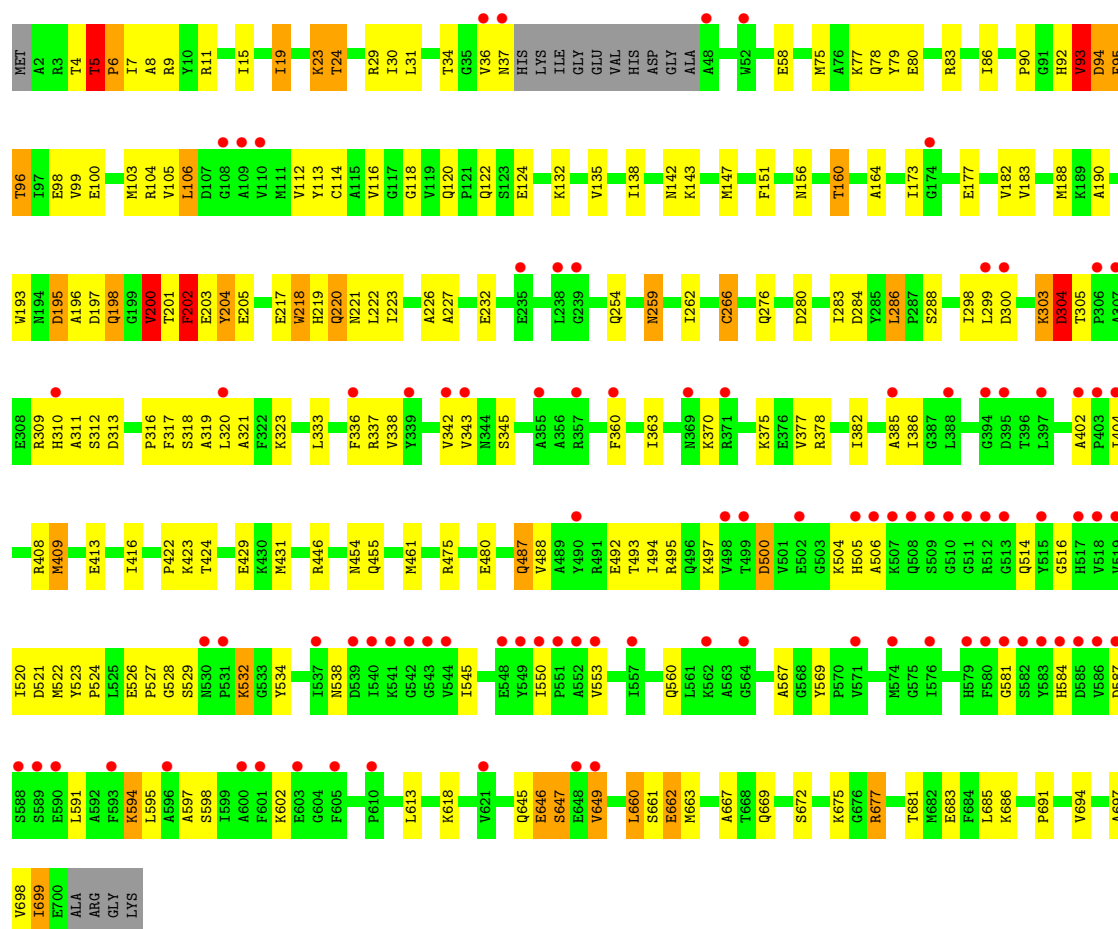


- Molecule 54: elongation factor G

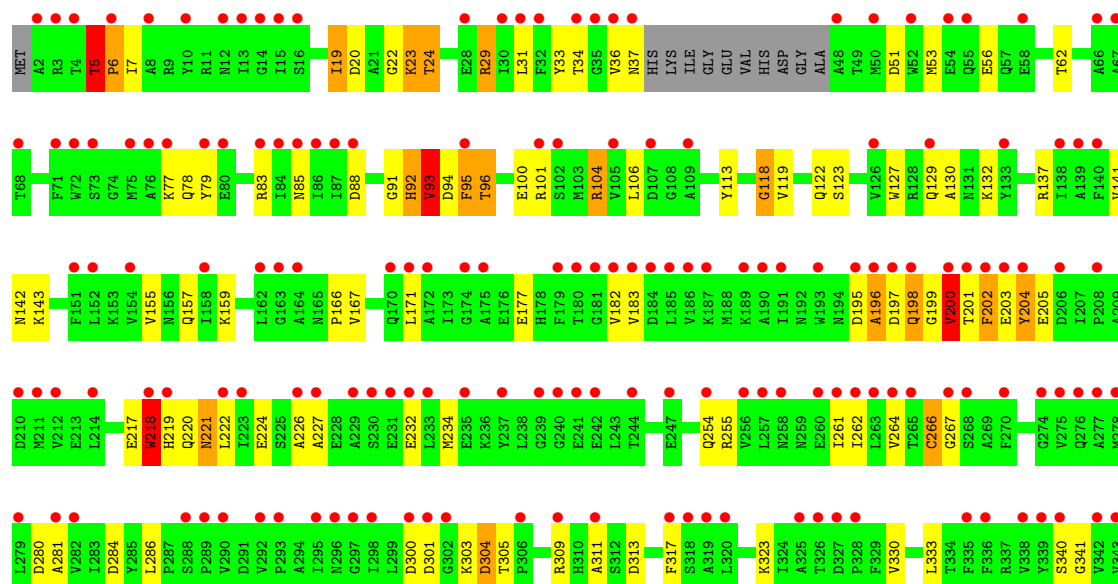


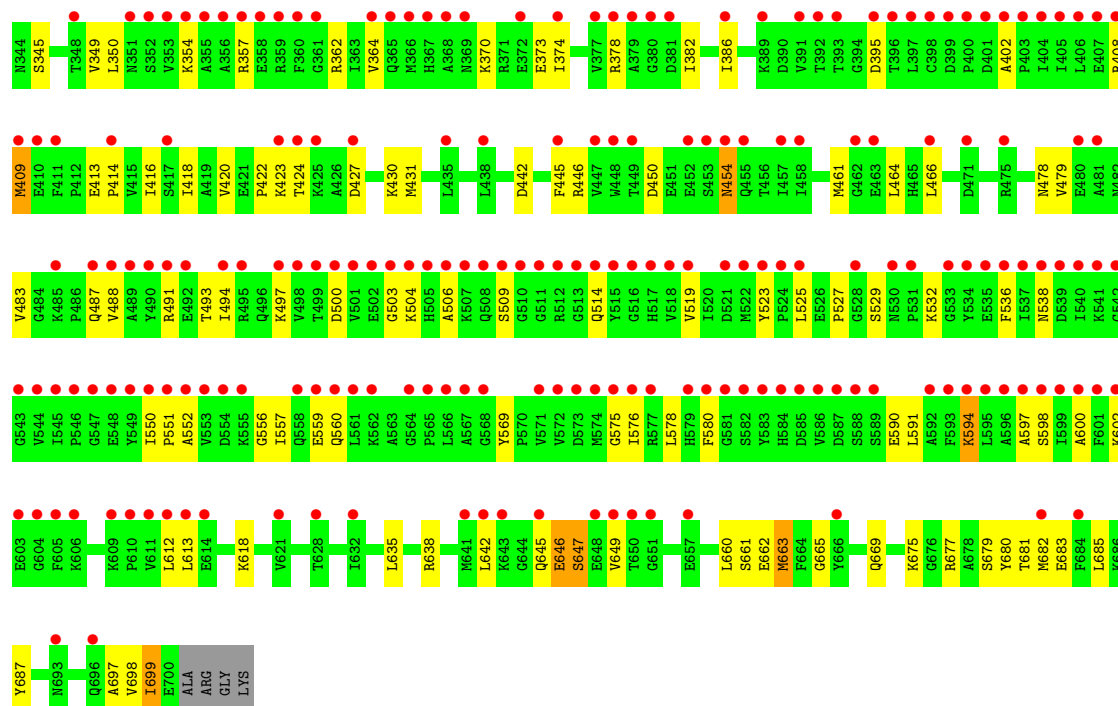
- Molecule 54: elongation factor G



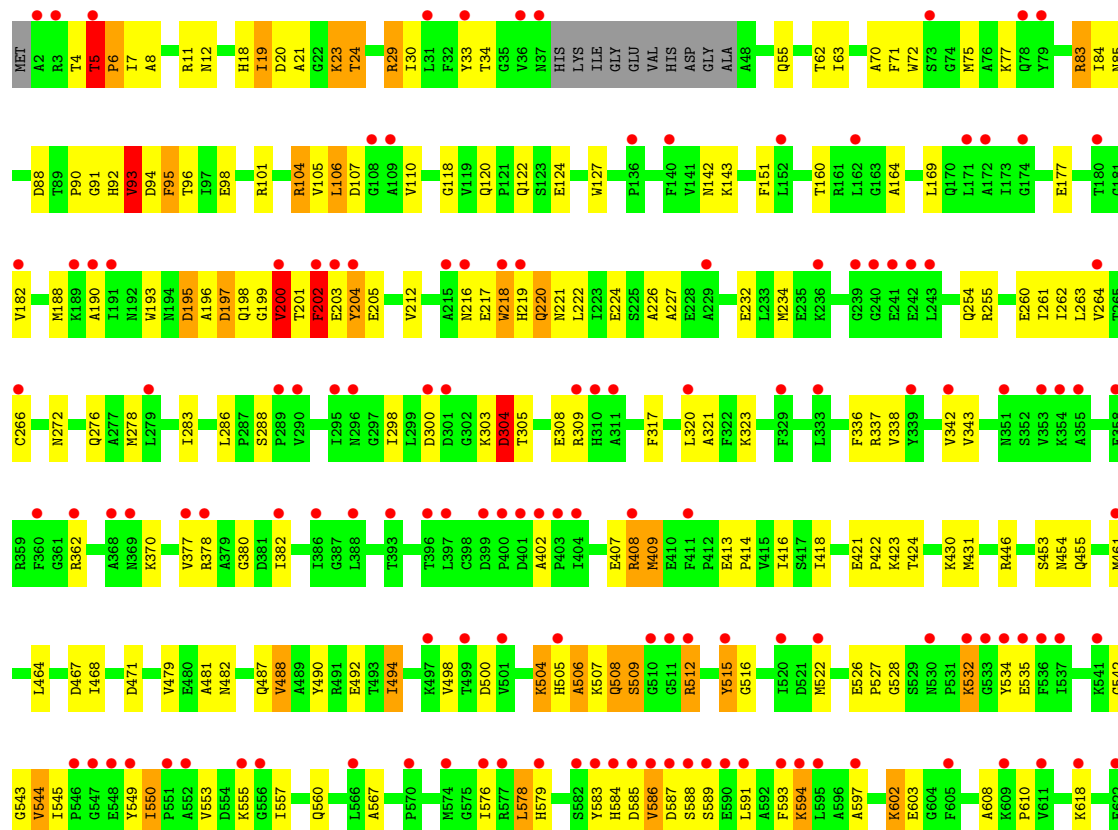


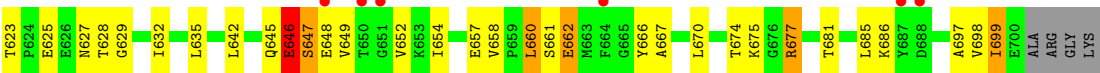
• Molecule 54: elongation factor G



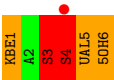
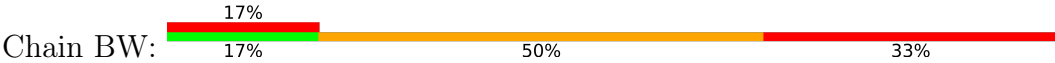


• Molecule 54: elongation factor G

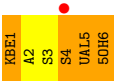




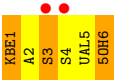
● Molecule 55: Viomycin



● Molecule 55: Viomycin



● Molecule 55: Viomycin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	54.5	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 39.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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(°)	Ideal(°)
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 ⓘ

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
40	FH	104	VAL
23	GW	19	ARG
47	FO	64	ARG
40	FH	99	LEU
4	GD	14	ILE

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

Mol	Chain	Res	Type
54	FV	122	GLN
34	HB	57	ASN
54	FV	310	HIS
4	GD	32	ASN
42	HJ	56	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
1	GA	1509	A
1	GA	1870	C
33	HA	1136	C
1	CA	1535	A
1	CA	1458	U

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

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

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	UAL	FW	5	55	-	0/3/7/9	-
55	5OH	FW	6	55	-	0/2/18/20	0/1/1/1
55	UAL	BW	5	55	-	1/3/7/9	-
55	DPP	DW	2	55	-	0/2/4/6	-
55	KBE	DW	1	55	-	5/7/7/8	-
55	DPP	FW	2	55	-	0/2/4/6	-
55	5OH	DW	6	55	-	1/2/18/20	0/1/1/1
55	DPP	BW	2	55	-	0/2/4/6	-
55	5OH	BW	6	55	-	2/2/18/20	0/1/1/1
55	UAL	DW	5	55	-	1/3/7/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	KBE	FW	1	55	-	2/7/7/8	-
55	KBE	BW	1	55	-	3/7/7/8	-

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(°)	Ideal(°)
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	BW	1	KBE	O-C-CA-CB
55	BW	1	KBE	C-CA-CB-N
55	BW	1	KBE	C-CA-CB-CG
55	BW	6	5OH	C-CA-CB-CR
55	DW	1	KBE	N-CB-CG-CD

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	BW	5	UAL	1	0
55	DW	2	DPP	1	0
55	DW	1	KBE	1	0
55	FW	2	DPP	1	0

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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	27,34,34	2.25	7 (25%)	34,54,54	1.97	7 (20%)
58	GCP	DV	801	56	27,34,34	2.36	6 (22%)	34,54,54	2.01	9 (26%)
58	GCP	BV	801	56	27,34,34	2.28	7 (25%)	34,54,54	1.99	9 (26%)
58	GCP	FV	801	56	27,34,34	1.53	6 (22%)	34,54,54	1.98	8 (23%)

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	-	3/15/38/38	0/3/3/3
58	GCP	DV	801	56	-	2/15/38/38	0/3/3/3
58	GCP	BV	801	56	-	3/15/38/38	0/3/3/3
58	GCP	FV	801	56	-	4/15/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	DV	801	GCP	C2'-C1'	-6.27	1.44	1.53
58	DV	801	GCP	C2-N2	5.82	1.45	1.33
58	BV	801	GCP	C2'-C1'	-5.79	1.45	1.53
58	HV	801	GCP	C2-N2	5.62	1.45	1.33
58	BV	801	GCP	C2-N2	5.60	1.45	1.33

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	DV	801	GCP	N3-C2-N1	-6.13	119.04	127.22
58	BV	801	GCP	N3-C2-N1	-5.85	119.41	127.22
58	DV	801	GCP	C2-N3-C4	5.48	121.61	115.36
58	HV	801	GCP	N3-C2-N1	-5.48	119.92	127.22
58	FV	801	GCP	C2-N3-C4	4.94	121.00	115.36

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	HV	801	GCP	PB-C3B-PG-O1G
58	HV	801	GCP	PB-C3B-PG-O3G

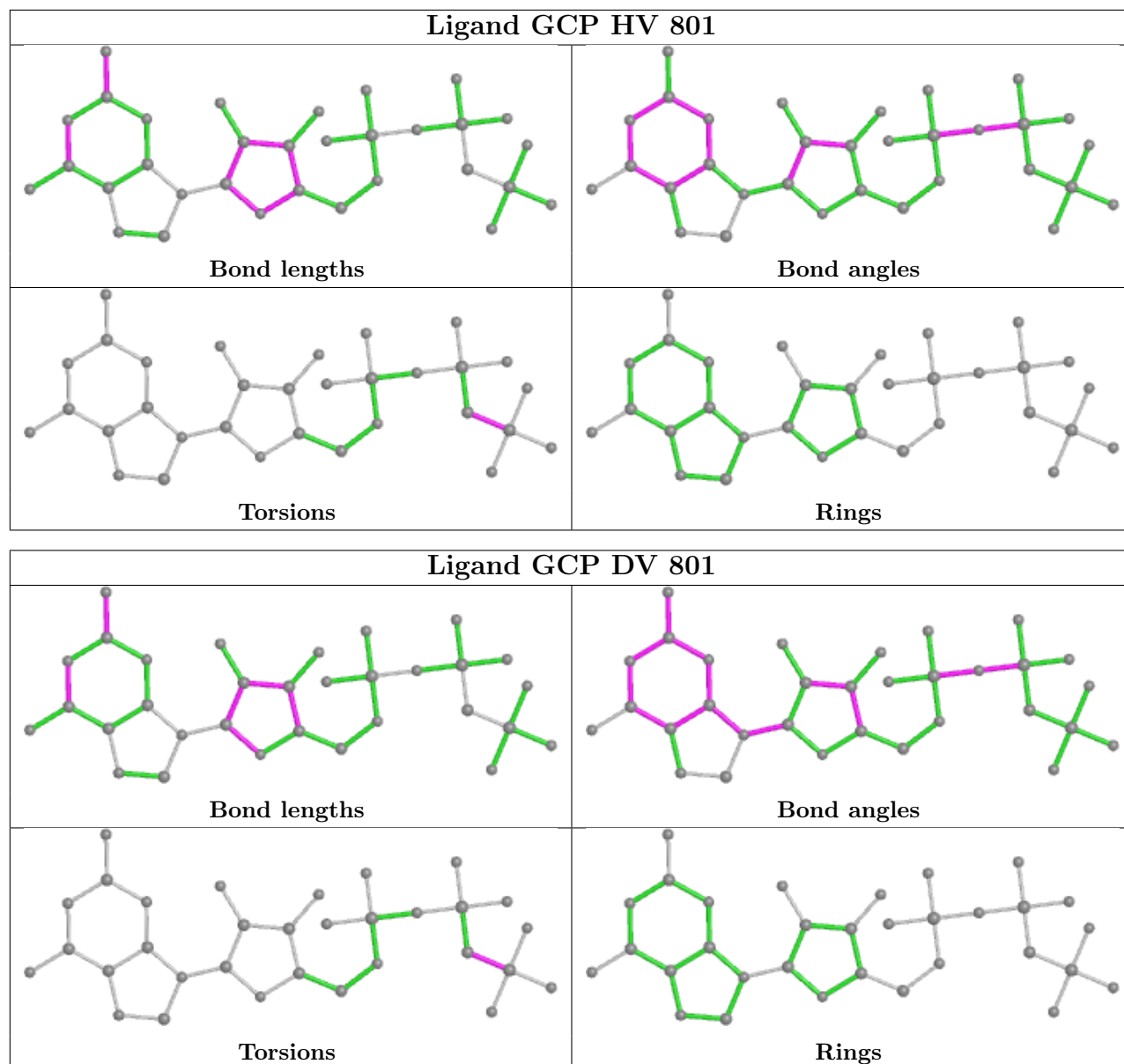
There are no ring outliers.

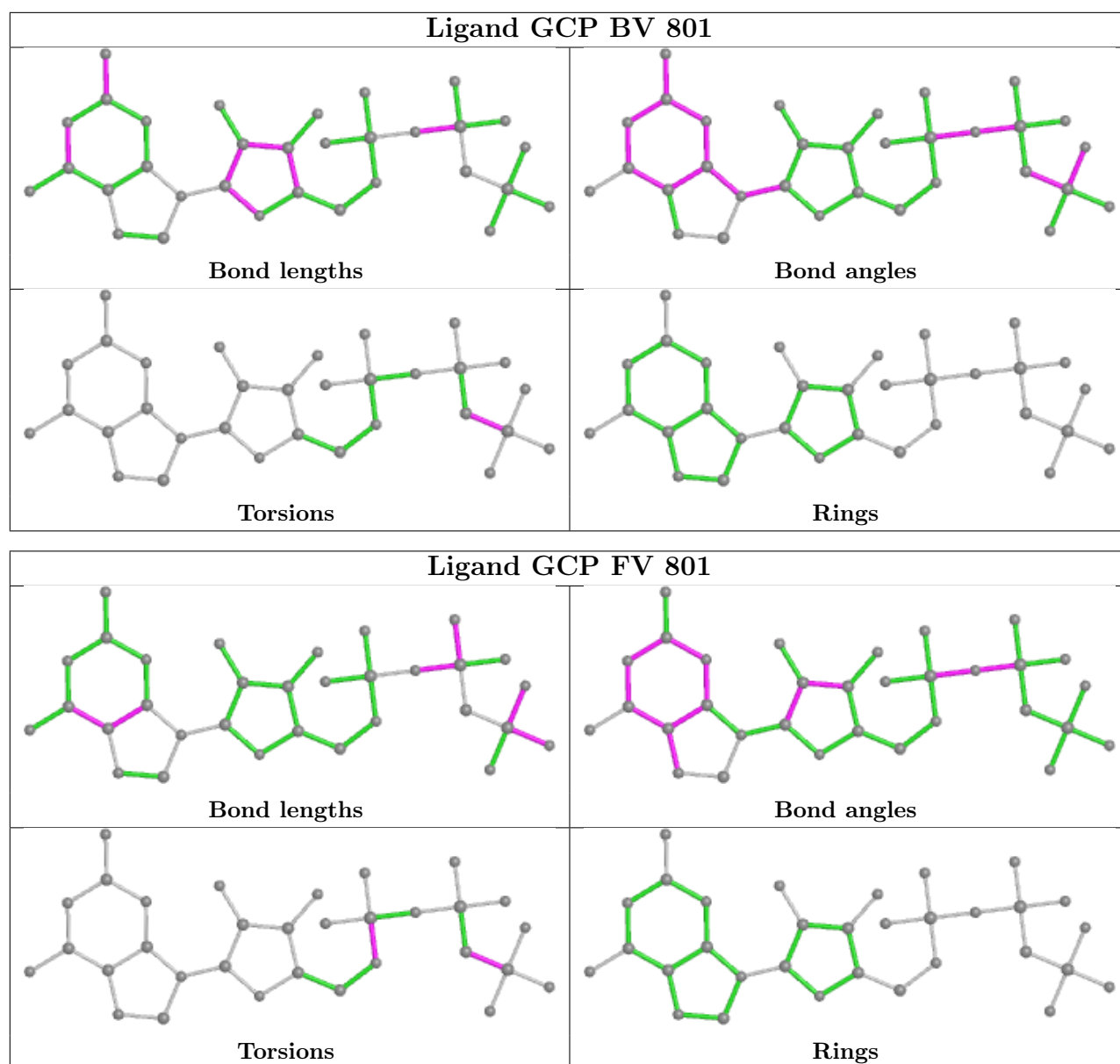
4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	HV	801	GCP	1	0
58	DV	801	GCP	1	0
58	BV	801	GCP	2	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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<sup>th</sup> 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 <sup>2</sup> )	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 <sup>2</sup> )	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, 18, 32, 61	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	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 <sup>2</sup> )	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 <sup>2</sup> )	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 <sup>2</sup> )	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 <sup>2</sup> )	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 <sup>2</sup> )	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, 95<sup>th</sup> 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 <sup>2</sup> )	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	BW	1	9/10	0.68	0.60	37,39,42,44	9
55	KBE	DW	1	9/10	0.68	0.37	32,33,40,41	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 ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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( $\text{\AA}^2$ )	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	BA	1614	1/1	0.82	0.38	26,26,26,26	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	GA	3069	1/1	0.82	0.07	63,63,63,63	0
56	MG	AA	3078	1/1	0.83	0.24	29,29,29,29	0
56	MG	HA	1613	1/1	0.83	0.47	41,41,41,41	0
56	MG	HA	1617	1/1	0.83	0.16	62,62,62,62	0
56	MG	BA	1609	1/1	0.84	0.11	38,38,38,38	0
56	MG	FA	1627	1/1	0.84	0.26	23,23,23,23	0
56	MG	HE	201	1/1	0.84	0.21	39,39,39,39	0
56	MG	EA	3087	1/1	0.86	0.59	30,30,30,30	0
56	MG	HT	101	1/1	0.86	0.46	41,41,41,41	0
56	MG	CA	3011	1/1	0.87	0.40	23,23,23,23	0
58	GCP	FV	801	32/32	0.87	0.20	43,58,69,87	0
56	MG	ED	301	1/1	0.88	0.22	7,7,7,7	0
56	MG	BE	201	1/1	0.88	0.14	43,43,43,43	0
56	MG	FA	1610	1/1	0.88	0.28	35,35,35,35	0
56	MG	EA	3109	1/1	0.88	0.17	8,8,8,8	0
56	MG	CA	3092	1/1	0.88	0.17	30,30,30,30	0
56	MG	FE	201	1/1	0.88	0.51	52,52,52,52	0
56	MG	CA	3118	1/1	0.89	0.33	29,29,29,29	0
56	MG	HC	401	1/1	0.89	0.32	49,49,49,49	0
56	MG	FU	101	1/1	0.89	0.14	24,24,24,24	0
56	MG	CA	3122	1/1	0.89	0.17	7,7,7,7	0
56	MG	EA	3130	1/1	0.89	0.21	29,29,29,29	0
56	MG	CA	3077	1/1	0.90	0.27	35,35,35,35	0
56	MG	GA	3059	1/1	0.90	0.48	44,44,44,44	0
56	MG	DA	1602	1/1	0.90	0.34	31,31,31,31	0
56	MG	CA	3091	1/1	0.91	0.21	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BL	201	1/1	0.91	0.23	51,51,51,51	0
56	MG	CA	3110	1/1	0.91	0.11	20,20,20,20	0
56	MG	GA	3073	1/1	0.91	0.47	20,20,20,20	0
56	MG	BU	101	1/1	0.91	0.26	39,39,39,39	0
56	MG	CA	3114	1/1	0.92	0.56	25,25,25,25	0
56	MG	HA	1637	1/1	0.92	0.10	47,47,47,47	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	GA	3082	1/1	0.92	0.11	35,35,35,35	0
56	MG	GA	3057	1/1	0.92	0.11	22,22,22,22	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	3087	1/1	0.93	0.15	31,31,31,31	0
56	MG	GA	3083	1/1	0.93	0.27	33,33,33,33	0
56	MG	GB	1201	1/1	0.93	0.09	38,38,38,38	0
56	MG	DA	1629	1/1	0.93	0.48	54,54,54,54	0
56	MG	EA	3010	1/1	0.93	0.16	11,11,11,11	0
56	MG	HA	1626	1/1	0.93	0.28	32,32,32,32	0
56	MG	EA	3057	1/1	0.93	0.11	15,15,15,15	0
56	MG	EA	3069	1/1	0.93	0.41	4,4,4,4	0
56	MG	AA	3011	1/1	0.93	0.17	18,18,18,18	0
56	MG	BA	1640	1/1	0.93	0.14	33,33,33,33	0
56	MG	AT	201	1/1	0.93	0.18	36,36,36,36	0
56	MG	CA	3120	1/1	0.94	0.15	3,3,3,3	0
56	MG	GA	3055	1/1	0.94	0.12	12,12,12,12	0
56	MG	AA	3005	1/1	0.94	0.16	23,23,23,23	0
56	MG	EA	3096	1/1	0.94	0.15	15,15,15,15	0
56	MG	GA	3060	1/1	0.94	0.28	23,23,23,23	0
56	MG	CA	3097	1/1	0.94	0.67	22,22,22,22	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	C4	101	1/1	0.94	0.06	22,22,22,22	0
56	MG	GA	3087	1/1	0.94	0.19	19,19,19,19	0
56	MG	GA	3103	1/1	0.94	0.24	12,12,12,12	0
56	MG	GA	3131	1/1	0.94	0.13	41,41,41,41	0
56	MG	GA	3133	1/1	0.94	0.23	4,4,4,4	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	HA	1601	1/1	0.94	0.16	38,38,38,38	0
56	MG	HA	1609	1/1	0.94	0.13	29,29,29,29	0
56	MG	AA	3090	1/1	0.94	0.10	23,23,23,23	0
56	MG	DA	1627	1/1	0.94	0.11	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	HA	1619	1/1	0.94	0.15	34,34,34,34	0
56	MG	FA	1601	1/1	0.94	0.14	28,28,28,28	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	CA	3111	1/1	0.94	0.16	13,13,13,13	0
56	MG	DA	1641	1/1	0.94	0.12	30,30,30,30	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	3023	1/1	0.95	0.17	7,7,7,7	0
56	MG	AC	301	1/1	0.95	0.35	10,10,10,10	0
56	MG	EA	3016	1/1	0.95	0.12	6,6,6,6	0
56	MG	AA	3093	1/1	0.95	0.26	34,34,34,34	0
56	MG	HA	1608	1/1	0.95	0.14	14,14,14,14	0
56	MG	EA	3068	1/1	0.95	0.12	35,35,35,35	0
56	MG	HA	1610	1/1	0.95	0.27	13,13,13,13	0
56	MG	GA	3061	1/1	0.95	0.21	10,10,10,10	0
56	MG	AA	3077	1/1	0.95	0.06	36,36,36,36	0
56	MG	EA	3079	1/1	0.95	0.23	0,0,0,0	0
56	MG	HA	1625	1/1	0.95	0.32	22,22,22,22	0
56	MG	GA	3077	1/1	0.95	0.10	33,33,33,33	0
56	MG	HA	1630	1/1	0.95	0.14	40,40,40,40	0
56	MG	DA	1610	1/1	0.95	0.04	48,48,48,48	0
56	MG	HA	1634	1/1	0.95	0.13	24,24,24,24	0
56	MG	DA	1614	1/1	0.95	0.12	44,44,44,44	0
56	MG	AB	1201	1/1	0.95	0.11	38,38,38,38	0
56	MG	AB	1202	1/1	0.95	0.24	44,44,44,44	0
56	MG	GA	3108	1/1	0.95	0.15	16,16,16,16	0
56	MG	BA	1624	1/1	0.95	0.12	28,28,28,28	0
56	MG	EA	3050	1/1	0.96	0.24	13,13,13,13	0
56	MG	BA	1612	1/1	0.96	0.22	5,5,5,5	0
56	MG	EA	3059	1/1	0.96	0.14	1,1,1,1	0
56	MG	CA	3061	1/1	0.96	0.12	3,3,3,3	0
56	MG	CA	3069	1/1	0.96	0.15	45,45,45,45	0
56	MG	GA	3075	1/1	0.96	0.15	7,7,7,7	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	AA	3059	1/1	0.96	0.50	12,12,12,12	0
56	MG	EA	3088	1/1	0.96	0.16	6,6,6,6	0
56	MG	GA	3093	1/1	0.96	0.49	28,28,28,28	0
56	MG	GA	3094	1/1	0.96	0.56	22,22,22,22	0
56	MG	EA	3090	1/1	0.96	0.07	29,29,29,29	0
56	MG	CA	3083	1/1	0.96	0.12	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	GA	3113	1/1	0.96	0.10	26,26,26,26	0
56	MG	CA	3087	1/1	0.96	0.06	29,29,29,29	0
56	MG	AA	3006	1/1	0.96	0.09	38,38,38,38	0
56	MG	DA	1606	1/1	0.96	0.11	26,26,26,26	0
56	MG	GB	1202	1/1	0.96	0.16	36,36,36,36	0
56	MG	BA	1631	1/1	0.96	0.07	28,28,28,28	0
56	MG	CA	3094	1/1	0.96	0.08	34,34,34,34	0
56	MG	HA	1604	1/1	0.96	0.17	27,27,27,27	0
56	MG	CA	3005	1/1	0.96	0.17	31,31,31,31	0
56	MG	DA	1628	1/1	0.96	0.33	37,37,37,37	0
56	MG	CA	3106	1/1	0.96	0.16	13,13,13,13	0
56	MG	DA	1639	1/1	0.96	0.10	40,40,40,40	0
56	MG	FA	1604	1/1	0.96	0.07	33,33,33,33	0
56	MG	AA	3069	1/1	0.96	0.17	6,6,6,6	0
56	MG	HA	1624	1/1	0.96	0.12	14,14,14,14	0
56	MG	DA	1642	1/1	0.96	0.16	29,29,29,29	0
56	MG	DU	101	1/1	0.96	0.27	36,36,36,36	0
56	MG	CA	3015	1/1	0.96	0.16	14,14,14,14	0
56	MG	EA	3011	1/1	0.96	0.86	17,17,17,17	0
56	MG	GA	3001	1/1	0.96	0.17	32,32,32,32	0
56	MG	GA	3018	1/1	0.96	0.26	36,36,36,36	0
56	MG	CA	3016	1/1	0.96	0.21	8,8,8,8	0
56	MG	GA	3037	1/1	0.96	0.19	19,19,19,19	0
56	MG	EA	3025	1/1	0.96	0.21	0,0,0,0	0
58	GCP	DV	801	32/32	0.96	0.14	20,38,49,52	0
56	MG	EA	3044	1/1	0.96	0.13	11,11,11,11	0
56	MG	DA	1618	1/1	0.97	0.09	33,33,33,33	0
56	MG	DA	1622	1/1	0.97	0.08	37,37,37,37	0
56	MG	DA	1624	1/1	0.97	0.17	48,48,48,48	0
56	MG	FA	1617	1/1	0.97	0.12	9,9,9,9	0
56	MG	FA	1618	1/1	0.97	0.10	28,28,28,28	0
56	MG	DA	1625	1/1	0.97	0.09	23,23,23,23	0
56	MG	FA	1628	1/1	0.97	0.18	19,19,19,19	0
56	MG	FA	1630	1/1	0.97	0.09	16,16,16,16	0
56	MG	DA	1626	1/1	0.97	0.08	24,24,24,24	0
56	MG	FA	1639	1/1	0.97	0.26	25,25,25,25	0
56	MG	FA	1641	1/1	0.97	0.17	18,18,18,18	0
56	MG	CA	3045	1/1	0.97	0.14	21,21,21,21	0
56	MG	CA	3057	1/1	0.97	0.11	1,1,1,1	0
56	MG	FV	802	1/1	0.97	0.12	48,48,48,48	0
56	MG	AA	3092	1/1	0.97	0.05	31,31,31,31	0
56	MG	GA	3006	1/1	0.97	0.12	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	1631	1/1	0.97	0.17	25,25,25,25	0
56	MG	DA	1636	1/1	0.97	0.29	41,41,41,41	0
56	MG	GA	3029	1/1	0.97	0.20	5,5,5,5	0
56	MG	AA	3002	1/1	0.97	0.10	20,20,20,20	0
56	MG	GA	3040	1/1	0.97	0.21	16,16,16,16	0
56	MG	GA	3046	1/1	0.97	0.07	35,35,35,35	0
56	MG	BA	1613	1/1	0.97	0.13	38,38,38,38	0
56	MG	AA	3098	1/1	0.97	0.23	5,5,5,5	0
56	MG	CA	3085	1/1	0.97	0.27	28,28,28,28	0
56	MG	EA	3005	1/1	0.97	0.12	27,27,27,27	0
56	MG	BA	1621	1/1	0.97	0.23	52,52,52,52	0
56	MG	BA	1623	1/1	0.97	0.10	24,24,24,24	0
56	MG	GA	3072	1/1	0.97	0.15	13,13,13,13	0
56	MG	AA	3100	1/1	0.97	0.12	6,6,6,6	0
56	MG	EA	3024	1/1	0.97	0.19	0,0,0,0	0
56	MG	BA	1629	1/1	0.97	0.15	41,41,41,41	0
56	MG	EA	3029	1/1	0.97	0.18	0,0,0,0	0
56	MG	AA	3111	1/1	0.97	0.16	21,21,21,21	0
56	MG	CA	3103	1/1	0.97	0.17	0,0,0,0	0
56	MG	GA	3091	1/1	0.97	0.14	11,11,11,11	0
56	MG	EA	3055	1/1	0.97	0.43	14,14,14,14	0
56	MG	EA	3056	1/1	0.97	0.08	2,2,2,2	0
56	MG	GA	3100	1/1	0.97	0.22	19,19,19,19	0
56	MG	GA	3102	1/1	0.97	0.35	40,40,40,40	0
56	MG	BA	1634	1/1	0.97	0.14	14,14,14,14	0
56	MG	BA	1635	1/1	0.97	0.23	29,29,29,29	0
56	MG	GA	3110	1/1	0.97	0.19	12,12,12,12	0
56	MG	GA	3111	1/1	0.97	0.17	11,11,11,11	0
56	MG	EA	3060	1/1	0.97	0.28	3,3,3,3	0
56	MG	GA	3118	1/1	0.97	0.29	9,9,9,9	0
56	MG	BA	1636	1/1	0.97	0.12	40,40,40,40	0
56	MG	AA	3063	1/1	0.97	0.08	9,9,9,9	0
56	MG	EA	3071	1/1	0.97	0.13	2,2,2,2	0
56	MG	AA	3086	1/1	0.97	0.07	35,35,35,35	0
56	MG	GB	1203	1/1	0.97	0.13	16,16,16,16	0
56	MG	EA	3080	1/1	0.97	0.20	3,3,3,3	0
56	MG	AA	3024	1/1	0.97	0.18	20,20,20,20	0
56	MG	AA	3088	1/1	0.97	0.13	14,14,14,14	0
56	MG	AC	302	1/1	0.97	0.23	19,19,19,19	0
56	MG	AA	3089	1/1	0.97	0.06	26,26,26,26	0
56	MG	CA	3007	1/1	0.97	0.09	15,15,15,15	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( $\text{\AA}^2$ )	Q<0.9
56	MG	EA	3102	1/1	0.97	0.21	0,0,0,0	0
56	MG	EA	3108	1/1	0.97	0.12	31,31,31,31	0
56	MG	HA	1621	1/1	0.97	0.28	29,29,29,29	0
56	MG	AD	301	1/1	0.97	0.14	6,6,6,6	0
56	MG	EA	3113	1/1	0.97	0.18	0,0,0,0	0
56	MG	EA	3117	1/1	0.97	0.10	11,11,11,11	0
56	MG	HA	1629	1/1	0.97	0.10	17,17,17,17	0
56	MG	EA	3125	1/1	0.97	0.10	3,3,3,3	0
56	MG	DA	1601	1/1	0.97	0.11	37,37,37,37	0
56	MG	AA	3044	1/1	0.97	0.14	17,17,17,17	0
56	MG	DA	1604	1/1	0.97	0.08	23,23,23,23	0
56	MG	BA	1604	1/1	0.97	0.12	20,20,20,20	0
56	MG	EB	1202	1/1	0.97	0.08	19,19,19,19	0
56	MG	CA	3020	1/1	0.97	0.16	19,19,19,19	0
56	MG	HV	802	1/1	0.97	0.13	38,38,38,38	0
58	GCP	BV	801	32/32	0.97	0.13	17,36,43,49	0
56	MG	DA	1611	1/1	0.97	0.10	15,15,15,15	0
56	MG	BA	1606	1/1	0.97	0.54	39,39,39,39	0
58	GCP	HV	801	32/32	0.97	0.11	24,48,54,56	0
56	MG	EA	3103	1/1	0.98	0.21	10,10,10,10	0
56	MG	BA	1620	1/1	0.98	0.05	20,20,20,20	0
56	MG	AA	3096	1/1	0.98	0.15	33,33,33,33	0
56	MG	BA	1622	1/1	0.98	0.21	32,32,32,32	0
56	MG	AA	3025	1/1	0.98	0.17	8,8,8,8	0
56	MG	EA	3120	1/1	0.98	0.22	0,0,0,0	0
56	MG	EA	3121	1/1	0.98	0.24	1,1,1,1	0
56	MG	EA	3122	1/1	0.98	0.19	0,0,0,0	0
56	MG	AA	3099	1/1	0.98	0.14	15,15,15,15	0
56	MG	BA	1625	1/1	0.98	0.20	21,21,21,21	0
56	MG	EA	3129	1/1	0.98	0.22	0,0,0,0	0
56	MG	CA	3123	1/1	0.98	0.17	8,8,8,8	0
56	MG	CA	3127	1/1	0.98	0.08	11,11,11,11	0
56	MG	CA	3132	1/1	0.98	0.17	2,2,2,2	0
56	MG	BA	1626	1/1	0.98	0.16	36,36,36,36	0
56	MG	EB	1204	1/1	0.98	0.06	12,12,12,12	0
56	MG	CB	1202	1/1	0.98	0.12	55,55,55,55	0
56	MG	BA	1627	1/1	0.98	0.08	25,25,25,25	0
56	MG	AA	3074	1/1	0.98	0.17	9,9,9,9	0
56	MG	BA	1630	1/1	0.98	0.11	25,25,25,25	0
56	MG	FA	1603	1/1	0.98	0.11	30,30,30,30	0
56	MG	AA	3105	1/1	0.98	0.19	12,12,12,12	0
56	MG	FA	1605	1/1	0.98	0.15	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	FA	1606	1/1	0.98	0.13	13,13,13,13	0
56	MG	FA	1607	1/1	0.98	0.10	18,18,18,18	0
56	MG	AA	3075	1/1	0.98	0.09	15,15,15,15	0
56	MG	FA	1611	1/1	0.98	0.23	0,0,0,0	0
56	MG	FA	1615	1/1	0.98	0.18	16,16,16,16	0
56	MG	AA	3112	1/1	0.98	0.11	7,7,7,7	0
56	MG	AA	3076	1/1	0.98	0.09	21,21,21,21	0
56	MG	FA	1621	1/1	0.98	0.18	10,10,10,10	0
56	MG	DA	1607	1/1	0.98	0.13	16,16,16,16	0
56	MG	DA	1608	1/1	0.98	0.14	14,14,14,14	0
56	MG	FA	1629	1/1	0.98	0.10	16,16,16,16	0
56	MG	AA	3116	1/1	0.98	0.18	3,3,3,3	0
56	MG	FA	1632	1/1	0.98	0.13	28,28,28,28	0
56	MG	FA	1633	1/1	0.98	0.11	28,28,28,28	0
56	MG	AA	3124	1/1	0.98	0.17	9,9,9,9	0
56	MG	FA	1638	1/1	0.98	0.10	33,33,33,33	0
56	MG	DA	1612	1/1	0.98	0.19	11,11,11,11	0
56	MG	FA	1640	1/1	0.98	0.18	23,23,23,23	0
56	MG	AA	3125	1/1	0.98	0.17	23,23,23,23	0
56	MG	DA	1615	1/1	0.98	0.15	24,24,24,24	0
56	MG	AA	3127	1/1	0.98	0.13	16,16,16,16	0
56	MG	DA	1620	1/1	0.98	0.08	22,22,22,22	0
56	MG	DA	1621	1/1	0.98	0.19	22,22,22,22	0
56	MG	GA	3002	1/1	0.98	0.17	14,14,14,14	0
56	MG	GA	3004	1/1	0.98	0.42	19,19,19,19	0
56	MG	AA	3050	1/1	0.98	0.09	7,7,7,7	0
56	MG	GA	3009	1/1	0.98	0.16	20,20,20,20	0
56	MG	GA	3010	1/1	0.98	0.26	15,15,15,15	0
56	MG	GA	3011	1/1	0.98	0.10	46,46,46,46	0
56	MG	GA	3014	1/1	0.98	0.28	8,8,8,8	0
56	MG	GA	3017	1/1	0.98	0.09	24,24,24,24	0
56	MG	CA	3003	1/1	0.98	0.13	12,12,12,12	0
56	MG	GA	3022	1/1	0.98	0.16	16,16,16,16	0
56	MG	AA	3054	1/1	0.98	0.12	11,11,11,11	0
56	MG	GA	3025	1/1	0.98	0.17	18,18,18,18	0
56	MG	GA	3026	1/1	0.98	0.16	6,6,6,6	0
56	MG	CA	3006	1/1	0.98	0.09	15,15,15,15	0
56	MG	GA	3030	1/1	0.98	0.24	11,11,11,11	0
56	MG	GA	3031	1/1	0.98	0.14	4,4,4,4	0
56	MG	GA	3033	1/1	0.98	0.24	12,12,12,12	0
56	MG	GA	3035	1/1	0.98	0.13	15,15,15,15	0
56	MG	GA	3036	1/1	0.98	0.14	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AB	1204	1/1	0.98	0.07	8,8,8,8	0
56	MG	CA	3008	1/1	0.98	0.17	15,15,15,15	0
56	MG	GA	3044	1/1	0.98	0.20	23,23,23,23	0
56	MG	GA	3045	1/1	0.98	0.17	7,7,7,7	0
56	MG	CA	3009	1/1	0.98	0.15	18,18,18,18	0
56	MG	GA	3047	1/1	0.98	0.18	27,27,27,27	0
56	MG	DA	1630	1/1	0.98	0.10	34,34,34,34	0
56	MG	AA	3080	1/1	0.98	0.18	7,7,7,7	0
56	MG	GA	3058	1/1	0.98	0.14	17,17,17,17	0
56	MG	DA	1632	1/1	0.98	0.15	28,28,28,28	0
56	MG	CA	3013	1/1	0.98	0.08	7,7,7,7	0
56	MG	DA	1638	1/1	0.98	0.04	40,40,40,40	0
56	MG	GA	3064	1/1	0.98	0.12	9,9,9,9	0
56	MG	GA	3066	1/1	0.98	0.17	4,4,4,4	0
56	MG	GA	3068	1/1	0.98	0.27	15,15,15,15	0
56	MG	AA	3082	1/1	0.98	0.03	29,29,29,29	0
56	MG	GA	3071	1/1	0.98	0.18	20,20,20,20	0
56	MG	AA	3085	1/1	0.98	0.08	30,30,30,30	0
56	MG	CA	3019	1/1	0.98	0.10	22,22,22,22	0
56	MG	AA	3057	1/1	0.98	0.09	18,18,18,18	0
56	MG	GA	3076	1/1	0.98	0.14	23,23,23,23	0
56	MG	EA	3003	1/1	0.98	0.14	6,6,6,6	0
56	MG	GA	3078	1/1	0.98	0.24	40,40,40,40	0
56	MG	GA	3079	1/1	0.98	0.12	18,18,18,18	0
56	MG	EA	3004	1/1	0.98	0.09	13,13,13,13	0
56	MG	CA	3024	1/1	0.98	0.19	2,2,2,2	0
56	MG	GA	3084	1/1	0.98	0.30	25,25,25,25	0
56	MG	EA	3006	1/1	0.98	0.12	19,19,19,19	0
56	MG	GA	3088	1/1	0.98	0.17	8,8,8,8	0
56	MG	GA	3089	1/1	0.98	0.13	14,14,14,14	0
56	MG	CA	3028	1/1	0.98	0.21	7,7,7,7	0
56	MG	CA	3030	1/1	0.98	0.21	11,11,11,11	0
56	MG	EA	3014	1/1	0.98	0.19	0,0,0,0	0
56	MG	GA	3095	1/1	0.98	0.18	2,2,2,2	0
56	MG	GA	3098	1/1	0.98	0.15	25,25,25,25	0
56	MG	CA	3037	1/1	0.98	0.20	1,1,1,1	0
56	MG	EA	3019	1/1	0.98	0.08	13,13,13,13	0
56	MG	EA	3020	1/1	0.98	0.24	4,4,4,4	0
56	MG	GA	3104	1/1	0.98	0.20	6,6,6,6	0
56	MG	GA	3106	1/1	0.98	0.21	3,3,3,3	0
56	MG	EA	3022	1/1	0.98	0.15	0,0,0,0	0
56	MG	AE	301	1/1	0.98	0.12	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	3026	1/1	0.98	0.07	10,10,10,10	0
56	MG	CA	3055	1/1	0.98	0.13	20,20,20,20	0
56	MG	GA	3114	1/1	0.98	0.17	10,10,10,10	0
56	MG	EA	3031	1/1	0.98	0.23	2,2,2,2	0
56	MG	GA	3120	1/1	0.98	0.21	5,5,5,5	0
56	MG	GA	3122	1/1	0.98	0.19	14,14,14,14	0
56	MG	GA	3126	1/1	0.98	0.09	18,18,18,18	0
56	MG	EA	3034	1/1	0.98	0.21	0,0,0,0	0
56	MG	A3	101	1/1	0.98	0.10	13,13,13,13	0
56	MG	CA	3060	1/1	0.98	0.22	13,13,13,13	0
56	MG	EA	3052	1/1	0.98	0.20	2,2,2,2	0
56	MG	EA	3053	1/1	0.98	0.18	1,1,1,1	0
56	MG	GB	1204	1/1	0.98	0.07	21,21,21,21	0
56	MG	GL	201	1/1	0.98	0.19	7,7,7,7	0
56	MG	EA	3054	1/1	0.98	0.13	5,5,5,5	0
56	MG	BA	1601	1/1	0.98	0.17	33,33,33,33	0
56	MG	HA	1602	1/1	0.98	0.37	48,48,48,48	0
56	MG	HA	1603	1/1	0.98	0.36	38,38,38,38	0
56	MG	CA	3068	1/1	0.98	0.13	13,13,13,13	0
56	MG	BA	1603	1/1	0.98	0.06	21,21,21,21	0
56	MG	EA	3058	1/1	0.98	0.13	6,6,6,6	0
56	MG	CA	3073	1/1	0.98	0.24	5,5,5,5	0
56	MG	HA	1611	1/1	0.98	0.23	20,20,20,20	0
56	MG	CA	3076	1/1	0.98	0.08	25,25,25,25	0
56	MG	HA	1615	1/1	0.98	0.27	38,38,38,38	0
56	MG	AA	3060	1/1	0.98	0.46	25,25,25,25	0
56	MG	HA	1618	1/1	0.98	0.08	19,19,19,19	0
56	MG	AA	3061	1/1	0.98	0.14	6,6,6,6	0
56	MG	AA	3029	1/1	0.98	0.09	21,21,21,21	0
56	MG	EA	3075	1/1	0.98	0.13	10,10,10,10	0
56	MG	EA	3076	1/1	0.98	0.10	18,18,18,18	0
56	MG	EA	3077	1/1	0.98	0.11	14,14,14,14	0
56	MG	EA	3078	1/1	0.98	0.18	3,3,3,3	0
56	MG	AA	3091	1/1	0.98	0.14	16,16,16,16	0
56	MG	AA	3064	1/1	0.98	0.13	20,20,20,20	0
56	MG	AA	3030	1/1	0.98	0.16	13,13,13,13	0
56	MG	HA	1636	1/1	0.98	0.05	21,21,21,21	0
56	MG	EA	3083	1/1	0.98	0.14	1,1,1,1	0
56	MG	HA	1638	1/1	0.98	0.09	26,26,26,26	0
56	MG	HA	1639	1/1	0.98	0.17	20,20,20,20	0
56	MG	EA	3086	1/1	0.98	0.07	34,34,34,34	0
56	MG	CA	3093	1/1	0.98	0.12	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	1616	1/1	0.98	0.22	35,35,35,35	0
56	MG	BA	1617	1/1	0.98	0.13	25,25,25,25	0
56	MG	EA	3094	1/1	0.98	0.11	15,15,15,15	0
56	MG	BA	1618	1/1	0.98	0.13	3,3,3,3	0
56	MG	CA	3105	1/1	0.98	0.17	6,6,6,6	0
56	MG	BA	1619	1/1	0.98	0.18	28,28,28,28	0
56	MG	EA	3035	1/1	0.99	0.17	0,0,0,0	0
56	MG	EA	3036	1/1	0.99	0.14	1,1,1,1	0
56	MG	EA	3038	1/1	0.99	0.11	2,2,2,2	0
56	MG	EA	3039	1/1	0.99	0.19	0,0,0,0	0
56	MG	EA	3041	1/1	0.99	0.10	2,2,2,2	0
56	MG	EA	3042	1/1	0.99	0.18	2,2,2,2	0
56	MG	EA	3043	1/1	0.99	0.10	4,4,4,4	0
56	MG	AA	3120	1/1	0.99	0.18	6,6,6,6	0
56	MG	EA	3045	1/1	0.99	0.13	1,1,1,1	0
56	MG	EA	3046	1/1	0.99	0.15	9,9,9,9	0
56	MG	EA	3047	1/1	0.99	0.09	6,6,6,6	0
56	MG	EA	3048	1/1	0.99	0.13	11,11,11,11	0
56	MG	EA	3049	1/1	0.99	0.23	8,8,8,8	0
56	MG	CA	3025	1/1	0.99	0.10	7,7,7,7	0
56	MG	CA	3026	1/1	0.99	0.09	5,5,5,5	0
56	MG	CA	3027	1/1	0.99	0.10	2,2,2,2	0
56	MG	AA	3121	1/1	0.99	0.10	20,20,20,20	0
56	MG	CA	3029	1/1	0.99	0.07	8,8,8,8	0
56	MG	AA	3122	1/1	0.99	0.16	2,2,2,2	0
56	MG	CA	3031	1/1	0.99	0.14	11,11,11,11	0
56	MG	CA	3032	1/1	0.99	0.17	3,3,3,3	0
56	MG	CA	3033	1/1	0.99	0.18	9,9,9,9	0
56	MG	CA	3034	1/1	0.99	0.19	18,18,18,18	0
56	MG	EA	3061	1/1	0.99	0.22	0,0,0,0	0
56	MG	EA	3062	1/1	0.99	0.17	0,0,0,0	0
56	MG	EA	3063	1/1	0.99	0.13	1,1,1,1	0
56	MG	EA	3064	1/1	0.99	0.19	0,0,0,0	0
56	MG	EA	3065	1/1	0.99	0.11	0,0,0,0	0
56	MG	EA	3066	1/1	0.99	0.19	0,0,0,0	0
56	MG	EA	3067	1/1	0.99	0.26	4,4,4,4	0
56	MG	CA	3035	1/1	0.99	0.16	3,3,3,3	0
56	MG	CA	3036	1/1	0.99	0.08	19,19,19,19	0
56	MG	AA	3123	1/1	0.99	0.17	14,14,14,14	0
56	MG	EA	3072	1/1	0.99	0.15	8,8,8,8	0
56	MG	EA	3073	1/1	0.99	0.19	0,0,0,0	0
56	MG	EA	3074	1/1	0.99	0.18	4,4,4,4	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	3038	1/1	0.99	0.18	7,7,7,7	0
56	MG	CA	3039	1/1	0.99	0.22	6,6,6,6	0
56	MG	CA	3040	1/1	0.99	0.19	12,12,12,12	0
56	MG	CA	3041	1/1	0.99	0.13	13,13,13,13	0
56	MG	CA	3042	1/1	0.99	0.11	8,8,8,8	0
56	MG	CA	3043	1/1	0.99	0.11	5,5,5,5	0
56	MG	EA	3081	1/1	0.99	0.15	3,3,3,3	0
56	MG	AA	3018	1/1	0.99	0.18	12,12,12,12	0
56	MG	AA	3058	1/1	0.99	0.19	9,9,9,9	0
56	MG	EA	3084	1/1	0.99	0.17	2,2,2,2	0
56	MG	EA	3085	1/1	0.99	0.19	4,4,4,4	0
56	MG	CA	3046	1/1	0.99	0.16	17,17,17,17	0
56	MG	CA	3047	1/1	0.99	0.10	31,31,31,31	0
56	MG	CA	3048	1/1	0.99	0.09	13,13,13,13	0
56	MG	CA	3049	1/1	0.99	0.18	9,9,9,9	0
56	MG	EA	3092	1/1	0.99	0.14	7,7,7,7	0
56	MG	EA	3093	1/1	0.99	0.09	21,21,21,21	0
56	MG	CA	3050	1/1	0.99	0.11	12,12,12,12	0
56	MG	EA	3095	1/1	0.99	0.17	5,5,5,5	0
56	MG	CA	3051	1/1	0.99	0.29	7,7,7,7	0
56	MG	CA	3052	1/1	0.99	0.10	10,10,10,10	0
56	MG	EA	3099	1/1	0.99	0.28	2,2,2,2	0
56	MG	EA	3100	1/1	0.99	0.14	0,0,0,0	0
56	MG	EA	3101	1/1	0.99	0.13	26,26,26,26	0
56	MG	CA	3054	1/1	0.99	0.17	6,6,6,6	0
56	MG	AA	3126	1/1	0.99	0.10	3,3,3,3	0
56	MG	EA	3105	1/1	0.99	0.14	4,4,4,4	0
56	MG	EA	3106	1/1	0.99	0.15	0,0,0,0	0
56	MG	CA	3056	1/1	0.99	0.11	7,7,7,7	0
56	MG	AA	3019	1/1	0.99	0.18	33,33,33,33	0
56	MG	EA	3110	1/1	0.99	0.11	24,24,24,24	0
56	MG	EA	3111	1/1	0.99	0.19	2,2,2,2	0
56	MG	CA	3059	1/1	0.99	0.17	3,3,3,3	0
56	MG	EA	3114	1/1	0.99	0.18	1,1,1,1	0
56	MG	EA	3116	1/1	0.99	0.15	0,0,0,0	0
56	MG	AA	3129	1/1	0.99	0.11	20,20,20,20	0
56	MG	EA	3118	1/1	0.99	0.19	1,1,1,1	0
56	MG	EA	3119	1/1	0.99	0.22	0,0,0,0	0
56	MG	AA	3130	1/1	0.99	0.15	27,27,27,27	0
56	MG	CA	3062	1/1	0.99	0.13	5,5,5,5	0
56	MG	CA	3063	1/1	0.99	0.16	2,2,2,2	0
56	MG	EA	3123	1/1	0.99	0.29	2,2,2,2	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	EA	3124	1/1	0.99	0.11	5,5,5,5	0
56	MG	CA	3064	1/1	0.99	0.10	1,1,1,1	0
56	MG	EA	3126	1/1	0.99	0.17	2,2,2,2	0
56	MG	CA	3065	1/1	0.99	0.11	1,1,1,1	0
56	MG	EA	3128	1/1	0.99	0.15	4,4,4,4	0
56	MG	CA	3066	1/1	0.99	0.17	2,2,2,2	0
56	MG	CA	3067	1/1	0.99	0.11	4,4,4,4	0
56	MG	EA	3131	1/1	0.99	0.20	5,5,5,5	0
56	MG	EA	3132	1/1	0.99	0.23	6,6,6,6	0
56	MG	AA	3020	1/1	0.99	0.13	24,24,24,24	0
56	MG	AA	3021	1/1	0.99	0.11	11,11,11,11	0
56	MG	CA	3070	1/1	0.99	0.15	4,4,4,4	0
56	MG	EB	1203	1/1	0.99	0.14	3,3,3,3	0
56	MG	CA	3071	1/1	0.99	0.14	2,2,2,2	0
56	MG	EC	301	1/1	0.99	0.14	1,1,1,1	0
56	MG	CA	3072	1/1	0.99	0.15	11,11,11,11	0
56	MG	ED	302	1/1	0.99	0.17	2,2,2,2	0
56	MG	AB	1203	1/1	0.99	0.12	14,14,14,14	0
56	MG	CA	3074	1/1	0.99	0.05	19,19,19,19	0
56	MG	CA	3075	1/1	0.99	0.22	20,20,20,20	0
56	MG	AA	3062	1/1	0.99	0.18	2,2,2,2	0
56	MG	AA	3022	1/1	0.99	0.11	8,8,8,8	0
56	MG	CA	3078	1/1	0.99	0.10	25,25,25,25	0
56	MG	CA	3079	1/1	0.99	0.22	12,12,12,12	0
56	MG	CA	3080	1/1	0.99	0.16	8,8,8,8	0
56	MG	FA	1608	1/1	0.99	0.18	14,14,14,14	0
56	MG	FA	1609	1/1	0.99	0.32	16,16,16,16	0
56	MG	CA	3081	1/1	0.99	0.15	10,10,10,10	0
56	MG	CA	3082	1/1	0.99	0.12	15,15,15,15	0
56	MG	FA	1612	1/1	0.99	0.31	17,17,17,17	0
56	MG	FA	1613	1/1	0.99	0.11	9,9,9,9	0
56	MG	AA	3004	1/1	0.99	0.07	34,34,34,34	0
56	MG	FA	1616	1/1	0.99	0.19	16,16,16,16	0
56	MG	CA	3084	1/1	0.99	0.21	4,4,4,4	0
56	MG	AA	3065	1/1	0.99	0.16	2,2,2,2	0
56	MG	FA	1619	1/1	0.99	0.10	25,25,25,25	0
56	MG	FA	1620	1/1	0.99	0.15	6,6,6,6	0
56	MG	CA	3086	1/1	0.99	0.19	20,20,20,20	0
56	MG	FA	1622	1/1	0.99	0.10	15,15,15,15	0
56	MG	FA	1623	1/1	0.99	0.21	7,7,7,7	0
56	MG	FA	1624	1/1	0.99	0.18	18,18,18,18	0
56	MG	FA	1625	1/1	0.99	0.09	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	FA	1626	1/1	0.99	0.16	15,15,15,15	0
56	MG	AA	3067	1/1	0.99	0.09	29,29,29,29	0
56	MG	CA	3088	1/1	0.99	0.10	28,28,28,28	0
56	MG	CA	3089	1/1	0.99	0.15	2,2,2,2	0
56	MG	CA	3090	1/1	0.99	0.13	20,20,20,20	0
56	MG	FA	1631	1/1	0.99	0.06	21,21,21,21	0
56	MG	AA	3008	1/1	0.99	0.12	15,15,15,15	0
56	MG	AA	3009	1/1	0.99	0.22	12,12,12,12	0
56	MG	FA	1634	1/1	0.99	0.07	19,19,19,19	0
56	MG	FA	1635	1/1	0.99	0.13	8,8,8,8	0
56	MG	AA	3072	1/1	0.99	0.16	7,7,7,7	0
56	MG	FA	1637	1/1	0.99	0.10	34,34,34,34	0
56	MG	AA	3073	1/1	0.99	0.16	8,8,8,8	0
56	MG	CA	3095	1/1	0.99	0.11	21,21,21,21	0
56	MG	CA	3096	1/1	0.99	0.21	10,10,10,10	0
56	MG	BA	1602	1/1	0.99	0.12	15,15,15,15	0
56	MG	CA	3098	1/1	0.99	0.21	10,10,10,10	0
56	MG	CA	3100	1/1	0.99	0.17	1,1,1,1	0
56	MG	CA	3101	1/1	0.99	0.15	10,10,10,10	0
56	MG	CA	3102	1/1	0.99	0.07	32,32,32,32	0
56	MG	AA	3027	1/1	0.99	0.15	8,8,8,8	0
56	MG	GA	3003	1/1	0.99	0.11	15,15,15,15	0
56	MG	CA	3104	1/1	0.99	0.14	4,4,4,4	0
56	MG	GA	3005	1/1	0.99	0.13	15,15,15,15	0
56	MG	AA	3028	1/1	0.99	0.28	2,2,2,2	0
56	MG	GA	3007	1/1	0.99	0.07	28,28,28,28	0
56	MG	GA	3008	1/1	0.99	0.20	12,12,12,12	0
56	MG	AA	3010	1/1	0.99	0.23	13,13,13,13	0
56	MG	CA	3108	1/1	0.99	0.12	3,3,3,3	0
56	MG	CA	3109	1/1	0.99	0.12	26,26,26,26	0
56	MG	GA	3012	1/1	0.99	0.19	2,2,2,2	0
56	MG	GA	3013	1/1	0.99	0.21	1,1,1,1	0
56	MG	BA	1607	1/1	0.99	0.26	8,8,8,8	0
56	MG	GA	3015	1/1	0.99	0.11	18,18,18,18	0
56	MG	GA	3016	1/1	0.99	0.15	9,9,9,9	0
56	MG	BA	1608	1/1	0.99	0.10	22,22,22,22	0
56	MG	CA	3112	1/1	0.99	0.14	4,4,4,4	0
56	MG	GA	3019	1/1	0.99	0.10	5,5,5,5	0
56	MG	GA	3020	1/1	0.99	0.21	3,3,3,3	0
56	MG	CA	3113	1/1	0.99	0.11	14,14,14,14	0
56	MG	AA	3001	1/1	0.99	0.09	11,11,11,11	0
56	MG	GA	3024	1/1	0.99	0.15	8,8,8,8	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	3115	1/1	0.99	0.16	12,12,12,12	0
56	MG	CA	3116	1/1	0.99	0.12	13,13,13,13	0
56	MG	GA	3027	1/1	0.99	0.17	6,6,6,6	0
56	MG	GA	3028	1/1	0.99	0.12	10,10,10,10	0
56	MG	CA	3117	1/1	0.99	0.08	7,7,7,7	0
56	MG	BA	1610	1/1	0.99	0.07	19,19,19,19	0
56	MG	CA	3119	1/1	0.99	0.21	3,3,3,3	0
56	MG	GA	3032	1/1	0.99	0.13	8,8,8,8	0
56	MG	BA	1611	1/1	0.99	0.13	15,15,15,15	0
56	MG	GA	3034	1/1	0.99	0.19	16,16,16,16	0
56	MG	CA	3121	1/1	0.99	0.21	3,3,3,3	0
56	MG	AA	3034	1/1	0.99	0.11	14,14,14,14	0
56	MG	AA	3035	1/1	0.99	0.20	3,3,3,3	0
56	MG	GA	3038	1/1	0.99	0.16	11,11,11,11	0
56	MG	CA	3124	1/1	0.99	0.15	0,0,0,0	0
56	MG	GA	3041	1/1	0.99	0.09	10,10,10,10	0
56	MG	GA	3043	1/1	0.99	0.10	8,8,8,8	0
56	MG	CA	3125	1/1	0.99	0.14	9,9,9,9	0
56	MG	AA	3081	1/1	0.99	0.14	16,16,16,16	0
56	MG	CA	3128	1/1	0.99	0.16	6,6,6,6	0
56	MG	CA	3129	1/1	0.99	0.17	9,9,9,9	0
56	MG	GA	3049	1/1	0.99	0.17	8,8,8,8	0
56	MG	GA	3050	1/1	0.99	0.15	9,9,9,9	0
56	MG	GA	3051	1/1	0.99	0.19	4,4,4,4	0
56	MG	GA	3052	1/1	0.99	0.18	8,8,8,8	0
56	MG	GA	3053	1/1	0.99	0.15	4,4,4,4	0
56	MG	GA	3054	1/1	0.99	0.14	1,1,1,1	0
56	MG	CA	3131	1/1	0.99	0.10	0,0,0,0	0
56	MG	BA	1615	1/1	0.99	0.20	22,22,22,22	0
56	MG	CA	3133	1/1	0.99	0.12	13,13,13,13	0
56	MG	CA	3134	1/1	0.99	0.18	23,23,23,23	0
56	MG	AA	3036	1/1	0.99	0.24	25,25,25,25	0
56	MG	AA	3083	1/1	0.99	0.27	33,33,33,33	0
56	MG	GA	3062	1/1	0.99	0.13	18,18,18,18	0
56	MG	GA	3063	1/1	0.99	0.27	3,3,3,3	0
56	MG	AA	3084	1/1	0.99	0.20	12,12,12,12	0
56	MG	GA	3065	1/1	0.99	0.15	3,3,3,3	0
56	MG	CD	301	1/1	0.99	0.17	3,3,3,3	0
56	MG	GA	3067	1/1	0.99	0.19	16,16,16,16	0
56	MG	AA	3037	1/1	0.99	0.19	9,9,9,9	0
56	MG	AA	3038	1/1	0.99	0.11	6,6,6,6	0
56	MG	GA	3070	1/1	0.99	0.23	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	3039	1/1	0.99	0.18	5,5,5,5	0
56	MG	AA	3040	1/1	0.99	0.12	24,24,24,24	0
56	MG	DA	1603	1/1	0.99	0.12	22,22,22,22	0
56	MG	GA	3074	1/1	0.99	0.14	2,2,2,2	0
56	MG	AA	3041	1/1	0.99	0.18	2,2,2,2	0
56	MG	DA	1605	1/1	0.99	0.12	28,28,28,28	0
56	MG	AA	3042	1/1	0.99	0.17	11,11,11,11	0
56	MG	AA	3013	1/1	0.99	0.16	5,5,5,5	0
56	MG	AA	3045	1/1	0.99	0.13	18,18,18,18	0
56	MG	GA	3080	1/1	0.99	0.26	5,5,5,5	0
56	MG	GA	3081	1/1	0.99	0.19	16,16,16,16	0
56	MG	DA	1609	1/1	0.99	0.16	16,16,16,16	0
56	MG	AA	3046	1/1	0.99	0.15	7,7,7,7	0
56	MG	BA	1628	1/1	0.99	0.12	26,26,26,26	0
56	MG	GA	3086	1/1	0.99	0.04	26,26,26,26	0
56	MG	AA	3094	1/1	0.99	0.06	20,20,20,20	0
56	MG	AA	3095	1/1	0.99	0.10	9,9,9,9	0
56	MG	AA	3047	1/1	0.99	0.10	30,30,30,30	0
56	MG	GA	3090	1/1	0.99	0.07	26,26,26,26	0
56	MG	DA	1616	1/1	0.99	0.27	26,26,26,26	0
56	MG	GA	3092	1/1	0.99	0.07	17,17,17,17	0
56	MG	DA	1617	1/1	0.99	0.13	45,45,45,45	0
56	MG	BA	1632	1/1	0.99	0.10	40,40,40,40	0
56	MG	DA	1619	1/1	0.99	0.12	33,33,33,33	0
56	MG	GA	3096	1/1	0.99	0.16	4,4,4,4	0
56	MG	GA	3097	1/1	0.99	0.17	26,26,26,26	0
56	MG	BA	1633	1/1	0.99	0.10	35,35,35,35	0
56	MG	GA	3099	1/1	0.99	0.13	12,12,12,12	0
56	MG	AA	3048	1/1	0.99	0.12	2,2,2,2	0
56	MG	GA	3101	1/1	0.99	0.10	15,15,15,15	0
56	MG	AA	3049	1/1	0.99	0.15	3,3,3,3	0
56	MG	DA	1623	1/1	0.99	0.07	12,12,12,12	0
56	MG	AA	3014	1/1	0.99	0.18	4,4,4,4	0
56	MG	GA	3105	1/1	0.99	0.15	3,3,3,3	0
56	MG	AA	3101	1/1	0.99	0.17	7,7,7,7	0
56	MG	GA	3107	1/1	0.99	0.12	27,27,27,27	0
56	MG	BA	1638	1/1	0.99	0.14	31,31,31,31	0
56	MG	GA	3109	1/1	0.99	0.09	9,9,9,9	0
56	MG	BA	1639	1/1	0.99	0.13	19,19,19,19	0
56	MG	AA	3102	1/1	0.99	0.24	0,0,0,0	0
56	MG	GA	3112	1/1	0.99	0.10	15,15,15,15	0
56	MG	AA	3103	1/1	0.99	0.17	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	3104	1/1	0.99	0.13	12,12,12,12	0
56	MG	GA	3115	1/1	0.99	0.23	23,23,23,23	0
56	MG	GA	3116	1/1	0.99	0.14	3,3,3,3	0
56	MG	GA	3117	1/1	0.99	0.07	22,22,22,22	0
56	MG	AA	3051	1/1	0.99	0.08	4,4,4,4	0
56	MG	GA	3119	1/1	0.99	0.16	5,5,5,5	0
56	MG	CA	3001	1/1	0.99	0.15	10,10,10,10	0
56	MG	GA	3121	1/1	0.99	0.14	4,4,4,4	0
56	MG	DA	1633	1/1	0.99	0.04	45,45,45,45	0
56	MG	GA	3123	1/1	0.99	0.20	11,11,11,11	0
56	MG	GA	3124	1/1	0.99	0.12	16,16,16,16	0
56	MG	GA	3125	1/1	0.99	0.11	5,5,5,5	0
56	MG	DA	1634	1/1	0.99	0.13	33,33,33,33	0
56	MG	GA	3127	1/1	0.99	0.12	1,1,1,1	0
56	MG	GA	3128	1/1	0.99	0.09	20,20,20,20	0
56	MG	GA	3129	1/1	0.99	0.22	19,19,19,19	0
56	MG	GA	3130	1/1	0.99	0.09	9,9,9,9	0
56	MG	DA	1635	1/1	0.99	0.08	38,38,38,38	0
56	MG	GA	3132	1/1	0.99	0.14	7,7,7,7	0
56	MG	CA	3002	1/1	0.99	0.14	17,17,17,17	0
56	MG	GA	3134	1/1	0.99	0.05	16,16,16,16	0
56	MG	DA	1637	1/1	0.99	0.11	23,23,23,23	0
56	MG	AA	3106	1/1	0.99	0.18	9,9,9,9	0
56	MG	CA	3004	1/1	0.99	0.08	6,6,6,6	0
56	MG	DA	1640	1/1	0.99	0.18	21,21,21,21	0
56	MG	GC	301	1/1	0.99	0.18	4,4,4,4	0
56	MG	AA	3107	1/1	0.99	0.19	18,18,18,18	0
56	MG	AA	3108	1/1	0.99	0.16	21,21,21,21	0
56	MG	AA	3109	1/1	0.99	0.21	6,6,6,6	0
56	MG	DV	802	1/1	0.99	0.11	34,34,34,34	0
56	MG	EA	3001	1/1	0.99	0.11	9,9,9,9	0
56	MG	AA	3110	1/1	0.99	0.21	4,4,4,4	0
56	MG	HA	1605	1/1	0.99	0.11	39,39,39,39	0
56	MG	HA	1606	1/1	0.99	0.16	17,17,17,17	0
56	MG	HA	1607	1/1	0.99	0.21	11,11,11,11	0
56	MG	AA	3052	1/1	0.99	0.12	2,2,2,2	0
56	MG	CA	3010	1/1	0.99	0.25	10,10,10,10	0
56	MG	AA	3053	1/1	0.99	0.10	6,6,6,6	0
56	MG	EA	3007	1/1	0.99	0.07	15,15,15,15	0
56	MG	HA	1612	1/1	0.99	0.19	8,8,8,8	0
56	MG	EA	3008	1/1	0.99	0.18	1,1,1,1	0
56	MG	HA	1614	1/1	0.99	0.12	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	EA	3009	1/1	0.99	0.20	0,0,0,0	0
56	MG	HA	1616	1/1	0.99	0.16	33,33,33,33	0
56	MG	CA	3012	1/1	0.99	0.12	3,3,3,3	0
56	MG	AA	3114	1/1	0.99	0.09	1,1,1,1	0
56	MG	EA	3012	1/1	0.99	0.17	1,1,1,1	0
56	MG	HA	1620	1/1	0.99	0.08	14,14,14,14	0
56	MG	EA	3013	1/1	0.99	0.14	0,0,0,0	0
56	MG	HA	1622	1/1	0.99	0.10	36,36,36,36	0
56	MG	HA	1623	1/1	0.99	0.11	18,18,18,18	0
56	MG	CA	3014	1/1	0.99	0.12	9,9,9,9	0
56	MG	EA	3015	1/1	0.99	0.51	1,1,1,1	0
56	MG	AA	3003	1/1	0.99	0.10	26,26,26,26	0
56	MG	HA	1627	1/1	0.99	0.14	24,24,24,24	0
56	MG	HA	1628	1/1	0.99	0.14	30,30,30,30	0
56	MG	EA	3017	1/1	0.99	0.16	3,3,3,3	0
56	MG	AA	3056	1/1	0.99	0.13	24,24,24,24	0
56	MG	HA	1631	1/1	0.99	0.10	28,28,28,28	0
56	MG	HA	1632	1/1	0.99	0.21	25,25,25,25	0
56	MG	CA	3017	1/1	0.99	0.18	2,2,2,2	0
56	MG	EA	3021	1/1	0.99	0.12	5,5,5,5	0
56	MG	HA	1635	1/1	0.99	0.15	17,17,17,17	0
56	MG	CA	3018	1/1	0.99	0.10	26,26,26,26	0
56	MG	EA	3023	1/1	0.99	0.17	2,2,2,2	0
56	MG	AA	3117	1/1	0.99	0.25	7,7,7,7	0
56	MG	AA	3118	1/1	0.99	0.11	11,11,11,11	0
56	MG	HA	1640	1/1	0.99	0.10	15,15,15,15	0
56	MG	EA	3026	1/1	0.99	0.10	28,28,28,28	0
56	MG	EA	3027	1/1	0.99	0.20	0,0,0,0	0
56	MG	EA	3028	1/1	0.99	0.18	1,1,1,1	0
56	MG	CA	3021	1/1	0.99	0.10	10,10,10,10	0
57	ZN	A4	101	1/1	0.99	0.09	63,63,63,63	0
57	ZN	C4	102	1/1	0.99	0.09	76,76,76,76	0
57	ZN	E4	101	1/1	0.99	0.09	54,54,54,54	0
57	ZN	G4	101	1/1	0.99	0.09	69,69,69,69	0
56	MG	EA	3030	1/1	0.99	0.16	0,0,0,0	0
56	MG	CA	3022	1/1	0.99	0.12	0,0,0,0	0
56	MG	EA	3032	1/1	0.99	0.16	0,0,0,0	0
56	MG	CA	3023	1/1	0.99	0.17	5,5,5,5	0
56	MG	AA	3032	1/1	1.00	0.16	14,14,14,14	0
56	MG	EA	3107	1/1	1.00	0.20	0,0,0,0	0
56	MG	AA	3066	1/1	1.00	0.17	6,6,6,6	0
56	MG	EA	3070	1/1	1.00	0.14	3,3,3,3	0

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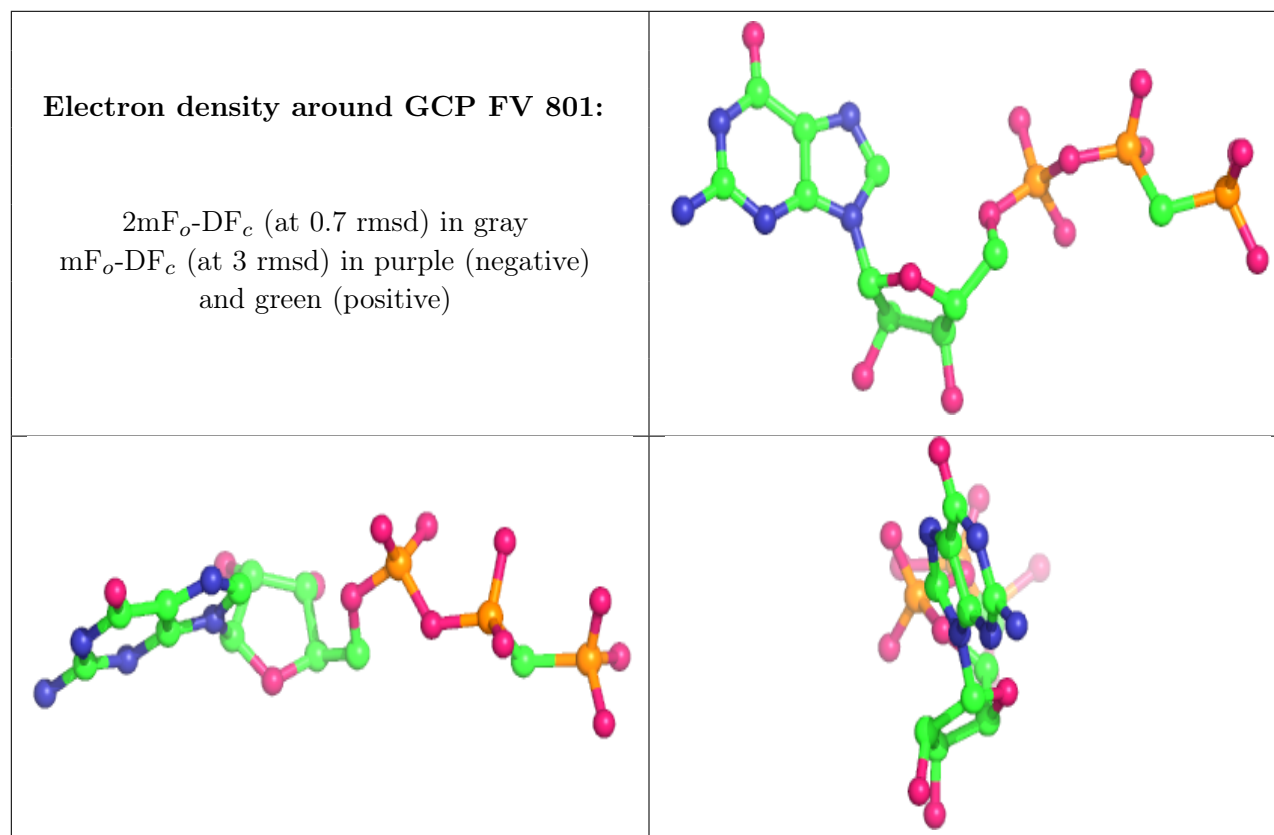
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	EA	3037	1/1	1.00	0.13	2,2,2,2	0
56	MG	CB	1203	1/1	1.00	0.11	6,6,6,6	0
56	MG	GA	3056	1/1	1.00	0.12	4,4,4,4	0
56	MG	EA	3112	1/1	1.00	0.15	5,5,5,5	0
56	MG	AA	3079	1/1	1.00	0.16	11,11,11,11	0
56	MG	FA	1614	1/1	1.00	0.13	5,5,5,5	0
56	MG	EA	3040	1/1	1.00	0.18	1,1,1,1	0
56	MG	EA	3115	1/1	1.00	0.13	2,2,2,2	0
56	MG	AA	3033	1/1	1.00	0.17	8,8,8,8	0
56	MG	AA	3023	1/1	1.00	0.17	3,3,3,3	0
56	MG	AA	3017	1/1	1.00	0.20	1,1,1,1	0
56	MG	AA	3070	1/1	1.00	0.13	11,11,11,11	0
56	MG	AA	3097	1/1	1.00	0.18	8,8,8,8	0
56	MG	CA	3053	1/1	1.00	0.12	5,5,5,5	0
56	MG	GA	3021	1/1	1.00	0.12	9,9,9,9	0
56	MG	AA	3128	1/1	1.00	0.14	2,2,2,2	0
56	MG	BA	1605	1/1	1.00	0.12	21,21,21,21	0
56	MG	AA	3071	1/1	1.00	0.13	3,3,3,3	0
56	MG	EA	3018	1/1	1.00	0.14	8,8,8,8	0
56	MG	EA	3051	1/1	1.00	0.15	0,0,0,0	0
56	MG	CA	3099	1/1	1.00	0.14	17,17,17,17	0
56	MG	AA	3113	1/1	1.00	0.11	8,8,8,8	0
56	MG	CA	3058	1/1	1.00	0.13	5,5,5,5	0
56	MG	EA	3089	1/1	1.00	0.10	5,5,5,5	0
56	MG	BV	802	1/1	1.00	0.17	27,27,27,27	0
56	MG	EA	3091	1/1	1.00	0.14	11,11,11,11	0
56	MG	CA	3126	1/1	1.00	0.14	7,7,7,7	0
56	MG	AA	3043	1/1	1.00	0.13	21,21,21,21	0
56	MG	DA	1613	1/1	1.00	0.10	12,12,12,12	0
56	MG	AA	3012	1/1	1.00	0.20	7,7,7,7	0
56	MG	AA	3016	1/1	1.00	0.12	10,10,10,10	0
56	MG	GA	3085	1/1	1.00	0.15	16,16,16,16	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	CA	3130	1/1	1.00	0.17	1,1,1,1	0
56	MG	AA	3031	1/1	1.00	0.17	8,8,8,8	0
56	MG	GA	3042	1/1	1.00	0.14	24,24,24,24	0
56	MG	CA	3107	1/1	1.00	0.20	6,6,6,6	0
56	MG	EA	3002	1/1	1.00	0.17	4,4,4,4	0
56	MG	AA	3055	1/1	1.00	0.17	18,18,18,18	0
56	MG	EA	3033	1/1	1.00	0.17	1,1,1,1	0
56	MG	EA	3104	1/1	1.00	0.16	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	GA	3048	1/1	1.00	0.19	6,6,6,6	0
56	MG	AA	3119	1/1	1.00	0.15	13,13,13,13	0

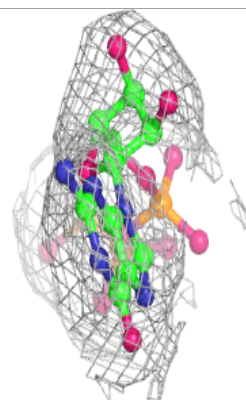
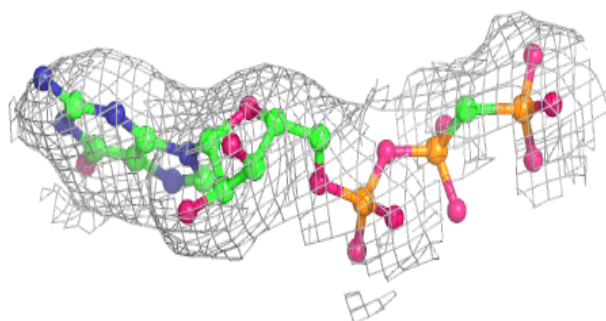
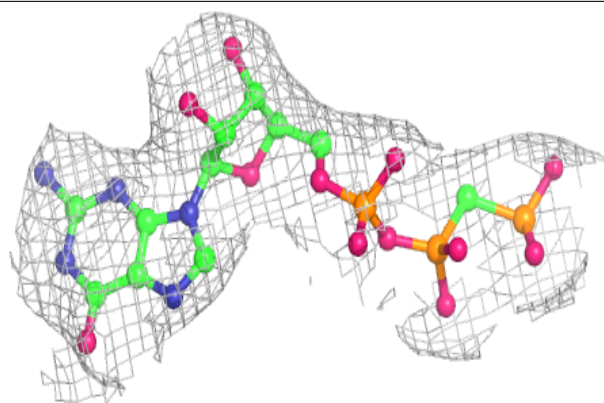
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



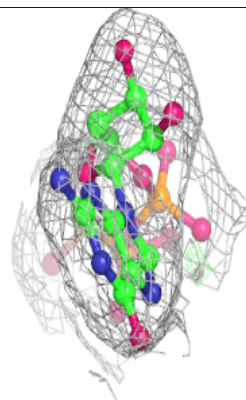
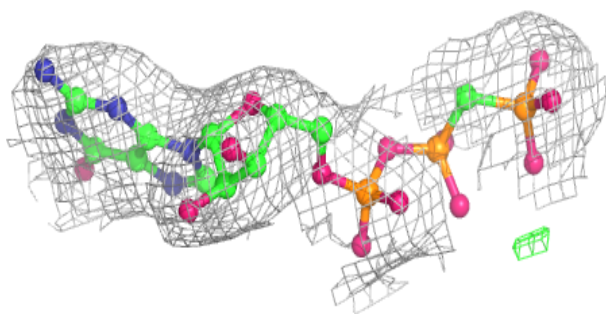
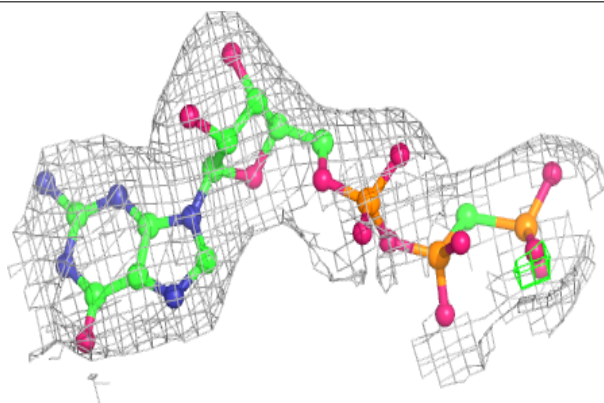


**Electron density around GCP DV 801:**

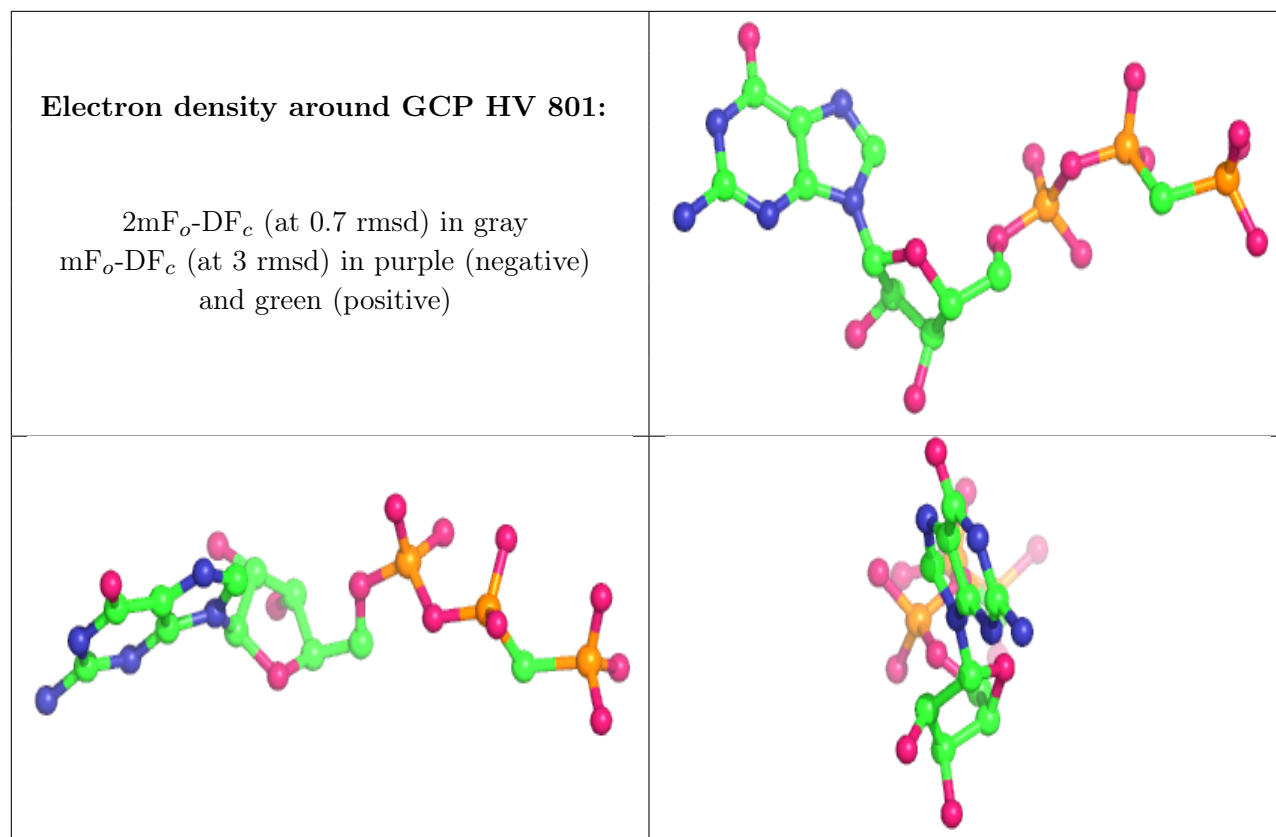
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**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)







## 6.5 Other polymers [i](#)

There are no such residues in this entry.