



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 09:16 am GMT

PDB ID : 4V9O  
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28972

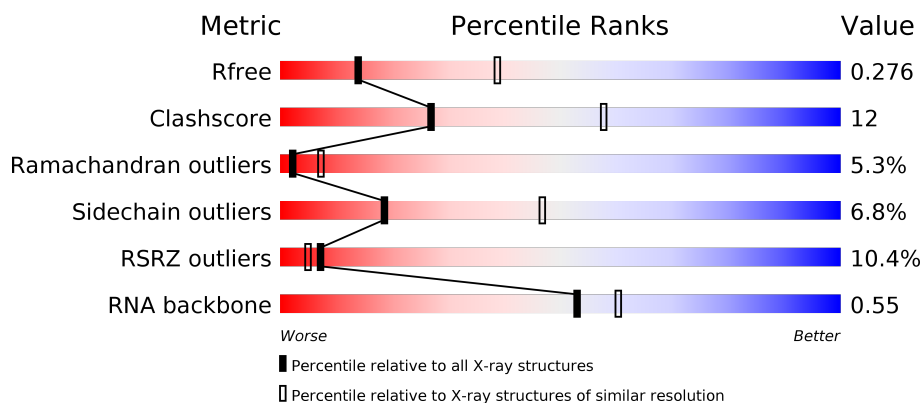
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 Å.

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



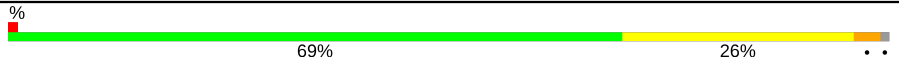



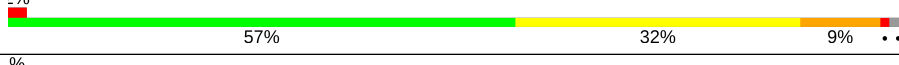
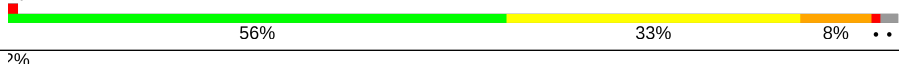
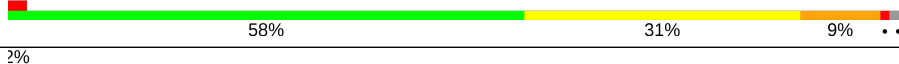
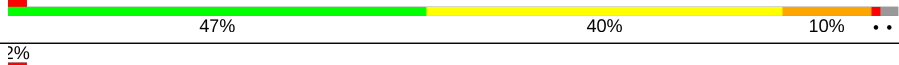
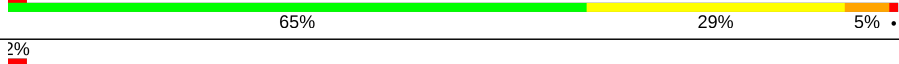


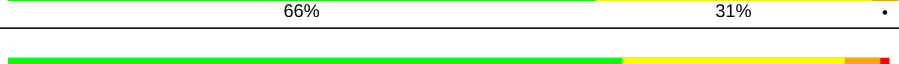

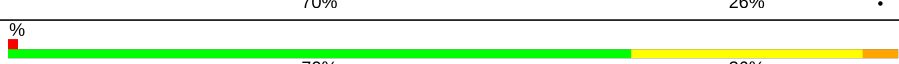

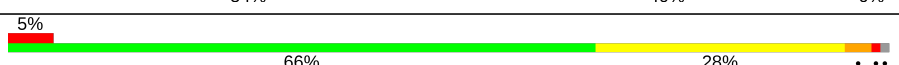
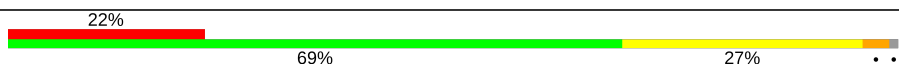
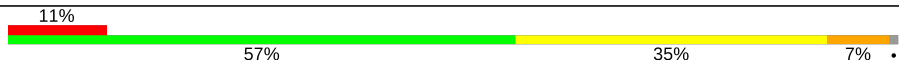



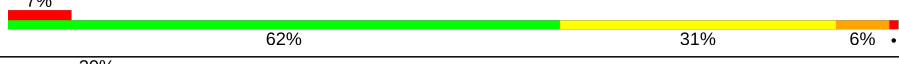
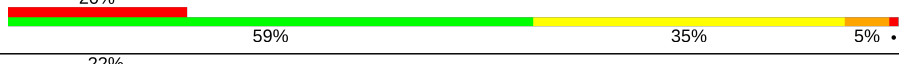


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)
RNA backbone	2435	1004 (3.20-2.60)

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

Mol	Chain	Length	Quality of chain
1	AB	120	 66% 26% 7% •
1	CB	120	 60% 32% 7% •
1	EB	120	 63% 24% 9% • •
1	GB	120	 36% 51% 10% • •

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Mol	Chain	Length	Quality of chain
2	AC	273	
2	CC	273	
2	EC	273	
2	GC	273	
3	AA	2904	
3	CA	2904	
3	EA	2904	
3	GA	2904	
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	C5	165	
32	E5	165	
33	A6	121	
34	BB	241	

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Mol	Chain	Length	Quality of chain
34	DB	241	
34	FB	241	
34	HB	241	
35	BA	1542	
35	DA	1542	
35	FA	1542	
35	HA	1542	
36	BC	233	
36	DC	233	
36	FC	233	
36	HC	233	
37	BD	206	
37	DD	206	
37	FD	206	
37	HD	206	
38	BE	167	
38	DE	167	
38	FE	167	
38	HE	167	
39	BF	135	
39	DF	135	
39	FF	135	
39	HF	135	
40	BG	179	
40	DG	179	

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Mol	Chain	Length	Quality of chain
40	FG	179	
40	HG	179	
41	BH	130	
41	DH	130	
41	FH	130	
41	HH	130	
42	BI	130	
42	DI	130	
42	FI	130	
42	HI	130	
43	BJ	103	
43	DJ	103	
43	FJ	103	
43	HJ	103	
44	BK	129	
44	DK	129	
44	FK	129	
44	HK	129	
45	BL	124	
45	DL	124	
45	FL	124	
45	HL	124	
46	BM	118	
46	DM	118	
46	FM	118	

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Mol	Chain	Length	Quality of chain
46	HM	118	
47	BN	101	
47	DN	101	
47	FN	101	
47	HN	101	
48	BO	89	
48	DO	89	
48	FO	89	
48	HO	89	
49	BP	82	
49	DP	82	
49	FP	82	
49	HP	82	
50	BQ	84	
50	DQ	84	
50	FQ	84	
50	HQ	84	
51	BR	75	
51	DR	75	
51	FR	75	
51	HR	75	
52	BS	92	
52	DS	92	
52	FS	92	
52	HS	92	

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Mol	Chain	Length	Quality of chain
53	BT	87	
53	DT	87	
53	FT	87	
53	HT	87	
54	BU	71	
54	DU	71	
54	FU	71	
54	HU	71	
55	BV	704	
55	DV	704	
55	FV	704	
55	HV	704	
56	BW	6	
56	DW	6	
56	FW	6	
56	HW	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
57	MG	AA	3026	-	-	-	X
57	MG	AA	3029	-	-	-	X
57	MG	AA	3037	-	-	-	X
57	MG	AA	3041	-	-	-	X
57	MG	AA	3047	-	-	-	X
57	MG	AA	3050	-	-	-	X
57	MG	AA	3068	-	-	-	X
57	MG	AA	3078	-	-	-	X
57	MG	AA	3090	-	-	-	X
57	MG	AA	3095	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	AA	3097	-	-	-	X
57	MG	AA	3100	-	-	-	X
57	MG	AA	3106	-	-	-	X
57	MG	AA	3107	-	-	-	X
57	MG	AA	3108	-	-	-	X
57	MG	AA	3111	-	-	-	X
57	MG	AA	3115	-	-	-	X
57	MG	AA	3129	-	-	-	X
57	MG	AA	3135	-	-	-	X
57	MG	BA	1607	-	-	-	X
57	MG	BA	1616	-	-	-	X
57	MG	BA	1627	-	-	-	X
57	MG	CA	3040	-	-	-	X
57	MG	CA	3046	-	-	-	X
57	MG	CA	3068	-	-	-	X
57	MG	CA	3105	-	-	-	X
57	MG	CA	3109	-	-	-	X
57	MG	CA	3112	-	-	-	X
57	MG	CA	3120	-	-	-	X
57	MG	CA	3131	-	-	-	X
57	MG	CA	3136	-	-	-	X
57	MG	DA	1628	-	-	-	X
57	MG	DA	1642	-	-	-	X
57	MG	DV	802	-	-	-	X
57	MG	EA	3005	-	-	-	X
57	MG	EA	3023	-	-	-	X
57	MG	EA	3025	-	-	-	X
57	MG	EA	3038	-	-	-	X
57	MG	EA	3040	-	-	-	X
57	MG	EA	3042	-	-	-	X
57	MG	EA	3046	-	-	-	X
57	MG	EA	3096	-	-	-	X
57	MG	EA	3100	-	-	-	X
57	MG	EA	3103	-	-	-	X
57	MG	EA	3104	-	-	-	X
57	MG	EA	3123	-	-	-	X
57	MG	FA	1609	-	-	-	X
57	MG	FA	1611	-	-	-	X
57	MG	FA	1613	-	-	-	X
57	MG	FA	1626	-	-	-	X
57	MG	FA	1635	-	-	-	X
57	MG	GA	3009	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	GA	3021	-	-	-	X
57	MG	GA	3023	-	-	-	X
57	MG	GA	3030	-	-	-	X
57	MG	GA	3050	-	-	-	X
57	MG	GA	3055	-	-	-	X
57	MG	GA	3100	-	-	-	X
57	MG	GA	3104	-	-	-	X
57	MG	GA	3107	-	-	-	X
57	MG	GA	3115	-	-	-	X
57	MG	GA	3119	-	-	-	X
57	MG	GA	3131	-	-	-	X
57	MG	HA	1613	-	-	-	X
57	MG	HA	1628	-	-	-	X

## 2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 592086 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 5S rRNA.

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

- Molecule 2 is a protein called 50S ribosomal protein L2.

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

- Molecule 3 is a RNA chain called 23S rRNA.

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

- 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	C5	148	Total	C	N	O	S	0	0	0
			1117	705	196	209	7			
32	E5	145	Total	C	N	O	S	0	0	0
			1101	696	193	205	7			

- Molecule 33 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	A6	30	Total	C	N	O	S	0	0	0
			227	144	33	47	3			

- 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 RNA chain called 16S rRNA.

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

- Molecule 36 is a protein called 30S ribosomal protein S3.

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

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

- Molecule 37 is a protein called 30S ribosomal protein S4.

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

- Molecule 38 is a protein called 30S ribosomal protein S5.

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

- Molecule 39 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BF	102	Total	C	N	O	S	0	0	0
			832	525	150	150	7			
39	DF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			
39	FF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			
39	HF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			



- Molecule 40 is a protein called 30S ribosomal protein S7.

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

- Molecule 41 is a protein called 30S ribosomal protein S8.

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

- Molecule 42 is a protein called 30S ribosomal protein S9.

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

- Molecule 43 is a protein called 30S ribosomal protein S10.

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

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

- Molecule 44 is a protein called 30S ribosomal protein S11.

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

- Molecule 45 is a protein called 30S ribosomal protein S12.

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

- Molecule 46 is a protein called 30S ribosomal protein S13.

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

- Molecule 47 is a protein called 30S ribosomal protein S14.

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

- Molecule 48 is a protein called 30S ribosomal protein S15.

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

- Molecule 49 is a protein called 30S ribosomal protein S16.

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

- Molecule 50 is a protein called 30S ribosomal protein S17.

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

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

- Molecule 51 is a protein called 30S ribosomal protein S18.

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

- Molecule 52 is a protein called 30S ribosomal protein S19.

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

- Molecule 53 is a protein called 30S ribosomal protein S20.

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

- Molecule 54 is a protein called 30S ribosomal protein S21.

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

- Molecule 55 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	BV	690	Total	C	N	O	S	0	0	0
			5345	3369	920	1031	25			
55	DV	689	Total	C	N	O	S	0	0	0
			5340	3366	919	1030	25			
55	FV	689	Total	C	N	O	S	0	0	0
			5340	3366	919	1030	25			
55	HV	689	Total	C	N	O	S	0	0	0
			5340	3366	919	1030	25			

- Molecule 56 is a protein called Viomycin.

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

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	FA	39	Total	Mg	0	0
			39	39		
57	BA	40	Total	Mg	0	0
			40	40		
57	CA	136	Total	Mg	0	0
			136	136		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	HE	1	Total 1	Mg 1	0	0
57	AB	4	Total 4	Mg 4	0	0
57	BE	1	Total 1	Mg 1	0	0
57	GA	136	Total 136	Mg 136	0	0
57	HA	41	Total 41	Mg 41	0	0
57	EB	4	Total 4	Mg 4	0	0
57	FU	1	Total 1	Mg 1	0	0
57	FV	1	Total 1	Mg 1	0	0
57	C4	1	Total 1	Mg 1	0	0
57	AE	1	Total 1	Mg 1	0	0
57	AA	136	Total 136	Mg 136	0	0
57	FE	1	Total 1	Mg 1	0	0
57	DV	1	Total 1	Mg 1	0	0
57	EA	137	Total 137	Mg 137	0	0
57	BU	1	Total 1	Mg 1	0	0
57	HK	1	Total 1	Mg 1	0	0
57	CN	1	Total 1	Mg 1	0	0
57	BN	1	Total 1	Mg 1	0	0
57	EE	1	Total 1	Mg 1	0	0
57	GL	1	Total 1	Mg 1	0	0
57	A4	1	Total 1	Mg 1	0	0

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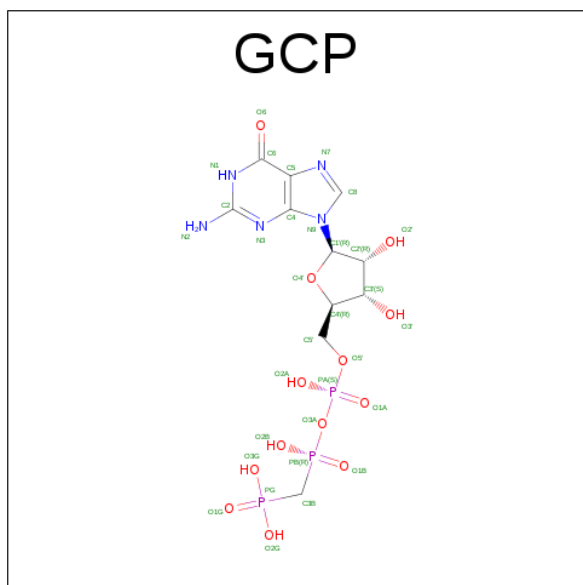
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	DA	43	Total 43	Mg 43	0	0
57	GC	2	Total 2	Mg 2	0	0
57	BV	1	Total 1	Mg 1	0	0
57	CB	4	Total 4	Mg 4	0	0
57	FN	2	Total 2	Mg 2	0	0
57	AC	1	Total 1	Mg 1	0	0
57	ED	1	Total 1	Mg 1	0	0
57	GB	4	Total 4	Mg 4	0	0
57	CE	1	Total 1	Mg 1	0	0
57	HV	1	Total 1	Mg 1	0	0

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 59 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: C<sub>11</sub>H<sub>18</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



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

- Molecule 60 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	AB	18	Total O 18 18	0	0
60	AC	6	Total O 6 6	0	0
60	AA	614	Total O 614 614	0	0
60	AD	4	Total O 4 4	0	0
60	AE	1	Total O 1 1	0	0
60	AF	1	Total O 1 1	0	0
60	AJ	1	Total O 1 1	0	0
60	AL	5	Total O 5 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AN	2	Total 2	O 2	0	0
60	AP	1	Total 1	O 1	0	0
60	AQ	2	Total 2	O 2	0	0
60	AS	1	Total 1	O 1	0	0
60	A0	2	Total 2	O 2	0	0
60	A2	1	Total 1	O 1	0	0
60	A3	1	Total 1	O 1	0	0
60	A4	1	Total 1	O 1	0	0
60	BA	202	Total 202	O 202	0	0
60	BL	1	Total 1	O 1	0	0
60	BN	2	Total 2	O 2	0	0
60	BT	2	Total 2	O 2	0	0
60	BV	1	Total 1	O 1	0	0
60	CB	21	Total 21	O 21	0	0
60	CA	607	Total 607	O 607	0	0
60	CC	8	Total 8	O 8	0	0
60	CD	3	Total 3	O 3	0	0
60	CE	1	Total 1	O 1	0	0
60	CJ	2	Total 2	O 2	0	0
60	CL	5	Total 5	O 5	0	0
60	CN	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	CQ	1	Total 1	O 1	0	0
60	CS	2	Total 2	O 2	0	0
60	CT	2	Total 2	O 2	0	0
60	CU	1	Total 1	O 1	0	0
60	C0	1	Total 1	O 1	0	0
60	C2	1	Total 1	O 1	0	0
60	C3	1	Total 1	O 1	0	0
60	C4	2	Total 2	O 2	0	0
60	DA	186	Total 186	O 186	0	0
60	DC	2	Total 2	O 2	0	0
60	DD	1	Total 1	O 1	0	0
60	DE	1	Total 1	O 1	0	0
60	DG	1	Total 1	O 1	0	0
60	DK	1	Total 1	O 1	0	0
60	DL	2	Total 2	O 2	0	0
60	DN	8	Total 8	O 8	0	0
60	DQ	1	Total 1	O 1	0	0
60	DT	4	Total 4	O 4	0	0
60	DU	1	Total 1	O 1	0	0
60	DV	1	Total 1	O 1	0	0
60	EA	610	Total 610	O 610	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	EB	18	Total 18	O 18	0	0
60	EC	9	Total 9	O 9	0	0
60	ED	3	Total 3	O 3	0	0
60	EE	2	Total 2	O 2	0	0
60	EL	4	Total 4	O 4	0	0
60	EN	3	Total 3	O 3	0	0
60	ER	1	Total 1	O 1	0	0
60	ET	2	Total 2	O 2	0	0
60	EV	2	Total 2	O 2	0	0
60	E0	1	Total 1	O 1	0	0
60	E2	1	Total 1	O 1	0	0
60	E3	2	Total 2	O 2	0	0
60	E4	2	Total 2	O 2	0	0
60	FA	197	Total 197	O 197	0	0
60	FC	1	Total 1	O 1	0	0
60	FE	2	Total 2	O 2	0	0
60	FN	3	Total 3	O 3	0	0
60	FT	4	Total 4	O 4	0	0
60	FU	1	Total 1	O 1	0	0
60	FV	1	Total 1	O 1	0	0
60	GB	19	Total 19	O 19	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	GA	606	Total 606	O 606	0	0
60	GC	10	Total 10	O 10	0	0
60	GD	3	Total 3	O 3	0	0
60	GE	2	Total 2	O 2	0	0
60	GJ	1	Total 1	O 1	0	0
60	GL	4	Total 4	O 4	0	0
60	GN	4	Total 4	O 4	0	0
60	GQ	1	Total 1	O 1	0	0
60	GR	2	Total 2	O 2	0	0
60	GS	2	Total 2	O 2	0	0
60	GU	1	Total 1	O 1	0	0
60	GV	1	Total 1	O 1	0	0
60	G2	2	Total 2	O 2	0	0
60	G3	1	Total 1	O 1	0	0
60	G4	1	Total 1	O 1	0	0
60	HA	193	Total 193	O 193	0	0
60	HD	3	Total 3	O 3	0	0
60	HE	3	Total 3	O 3	0	0
60	HN	7	Total 7	O 7	0	0
60	HQ	1	Total 1	O 1	0	0
60	HT	1	Total 1	O 1	0	0

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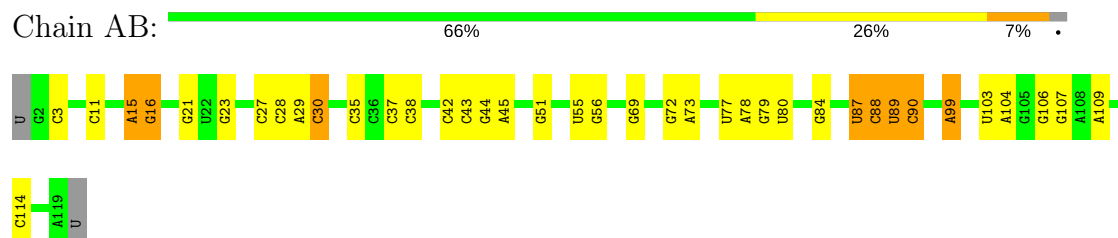
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	HV	1	Total	O	0	0
			1	1		

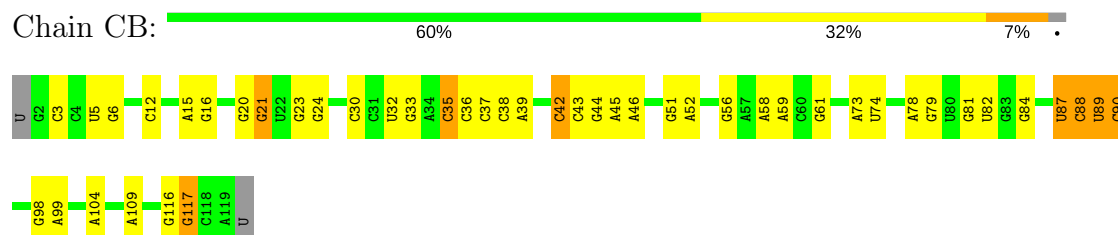
### 3 Residue-property plots [i](#)

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

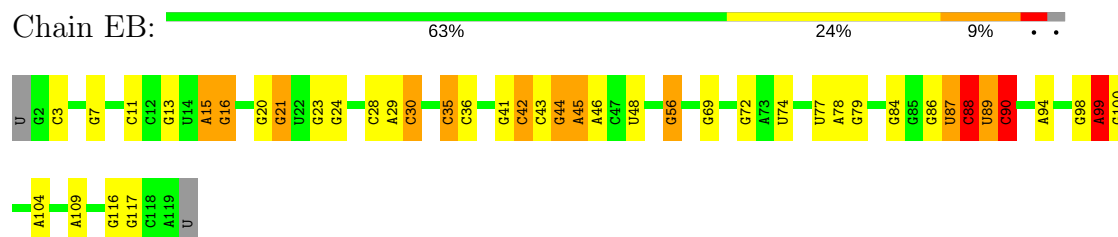
#### • Molecule 1: 5S rRNA



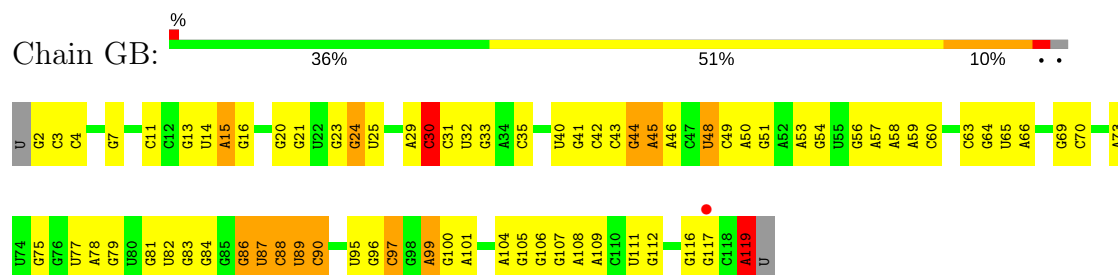
#### • Molecule 1: 5S rRNA



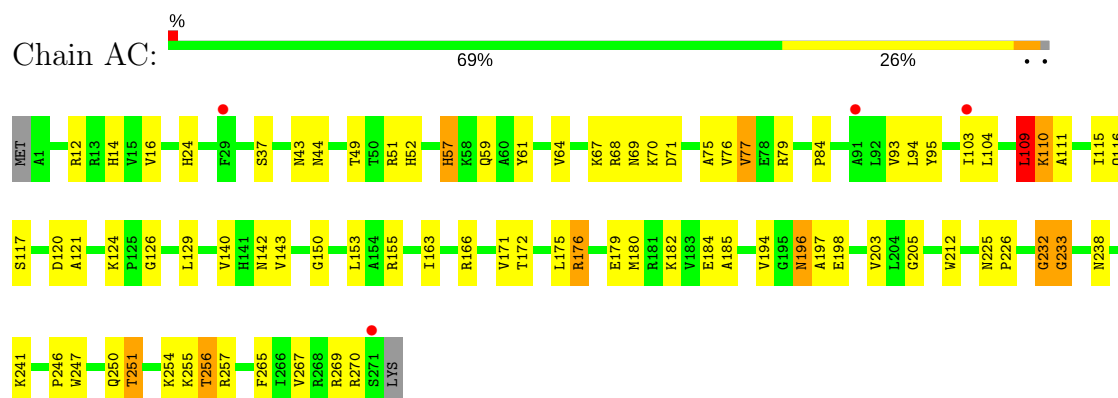
#### • Molecule 1: 5S rRNA



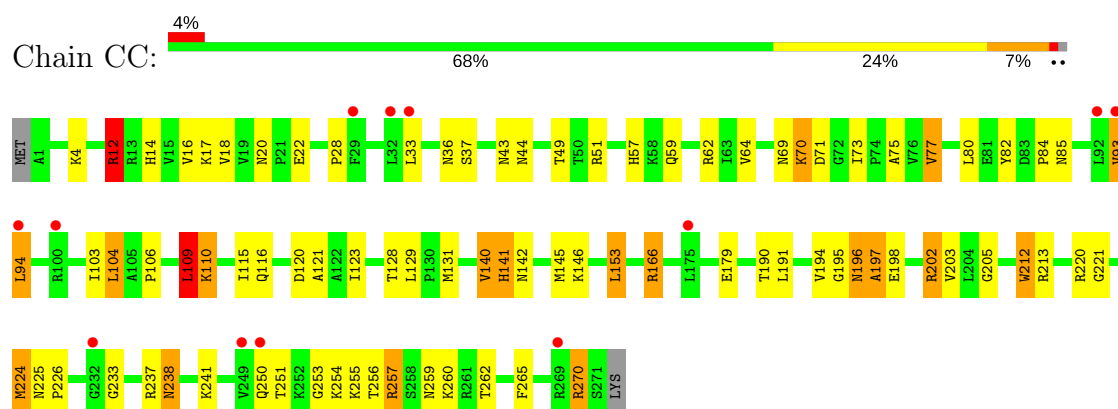
#### • Molecule 1: 5S rRNA



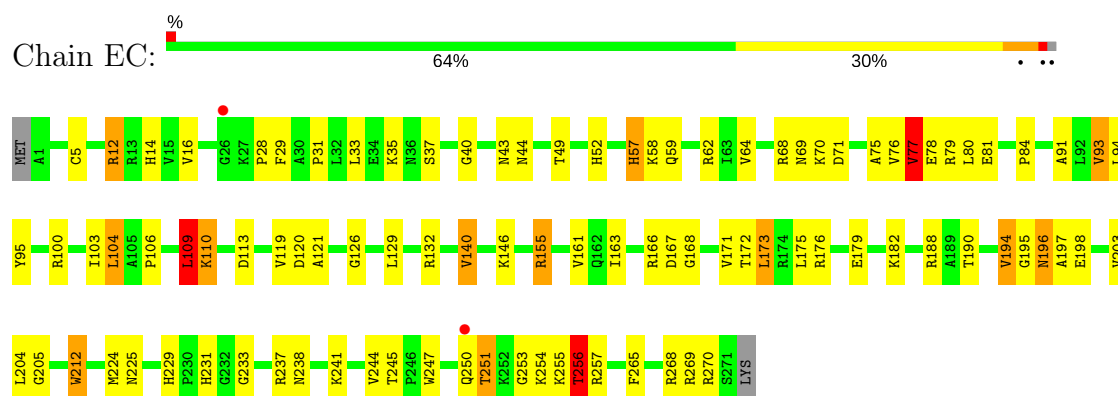
• Molecule 2: 50S ribosomal protein L2



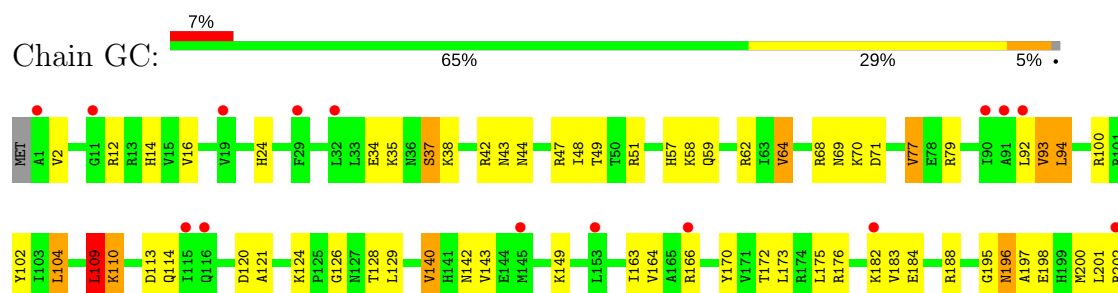
• Molecule 2: 50S ribosomal protein L2



• Molecule 2: 50S ribosomal protein L2

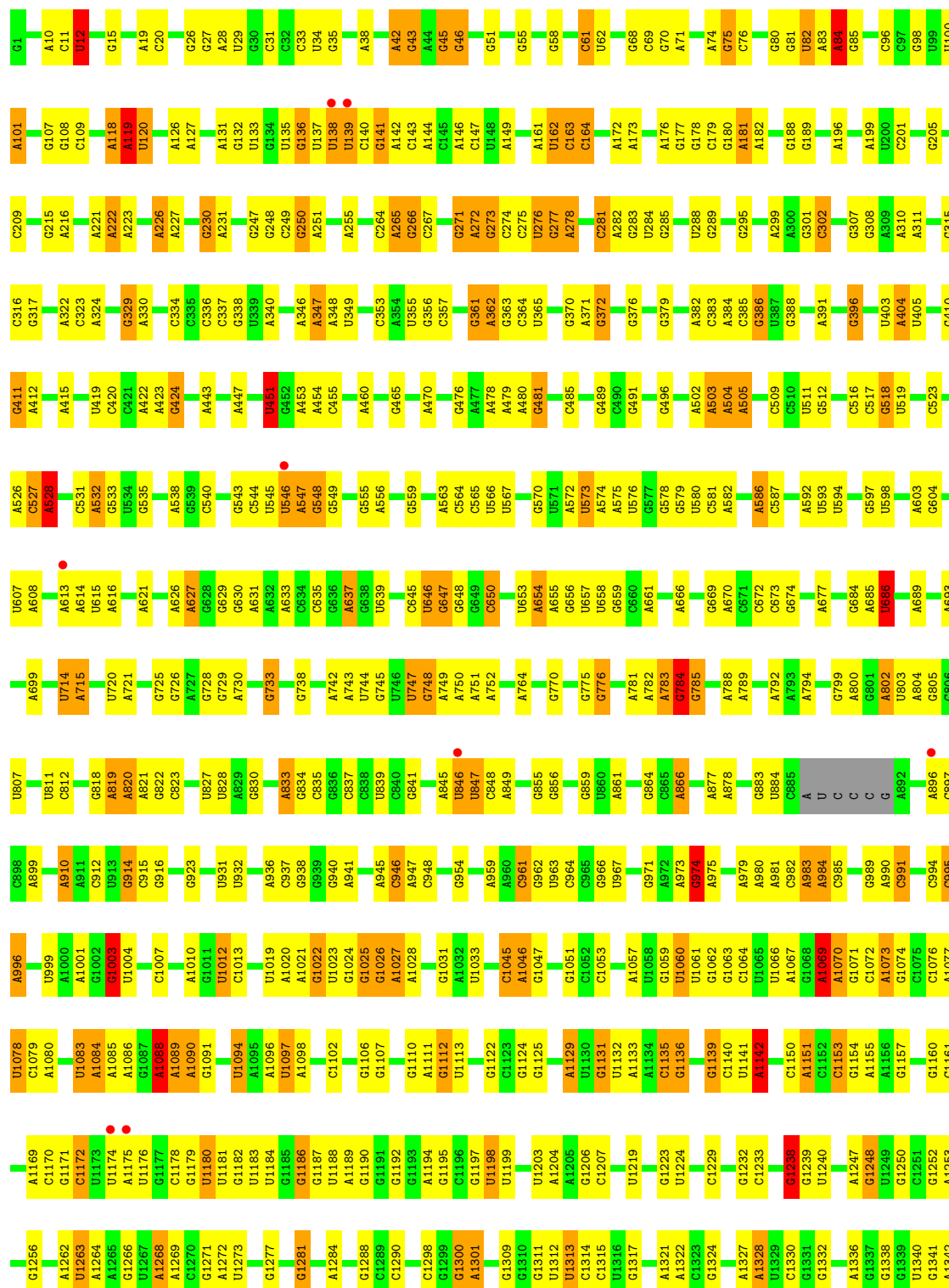


• Molecule 2: 50S ribosomal protein L2



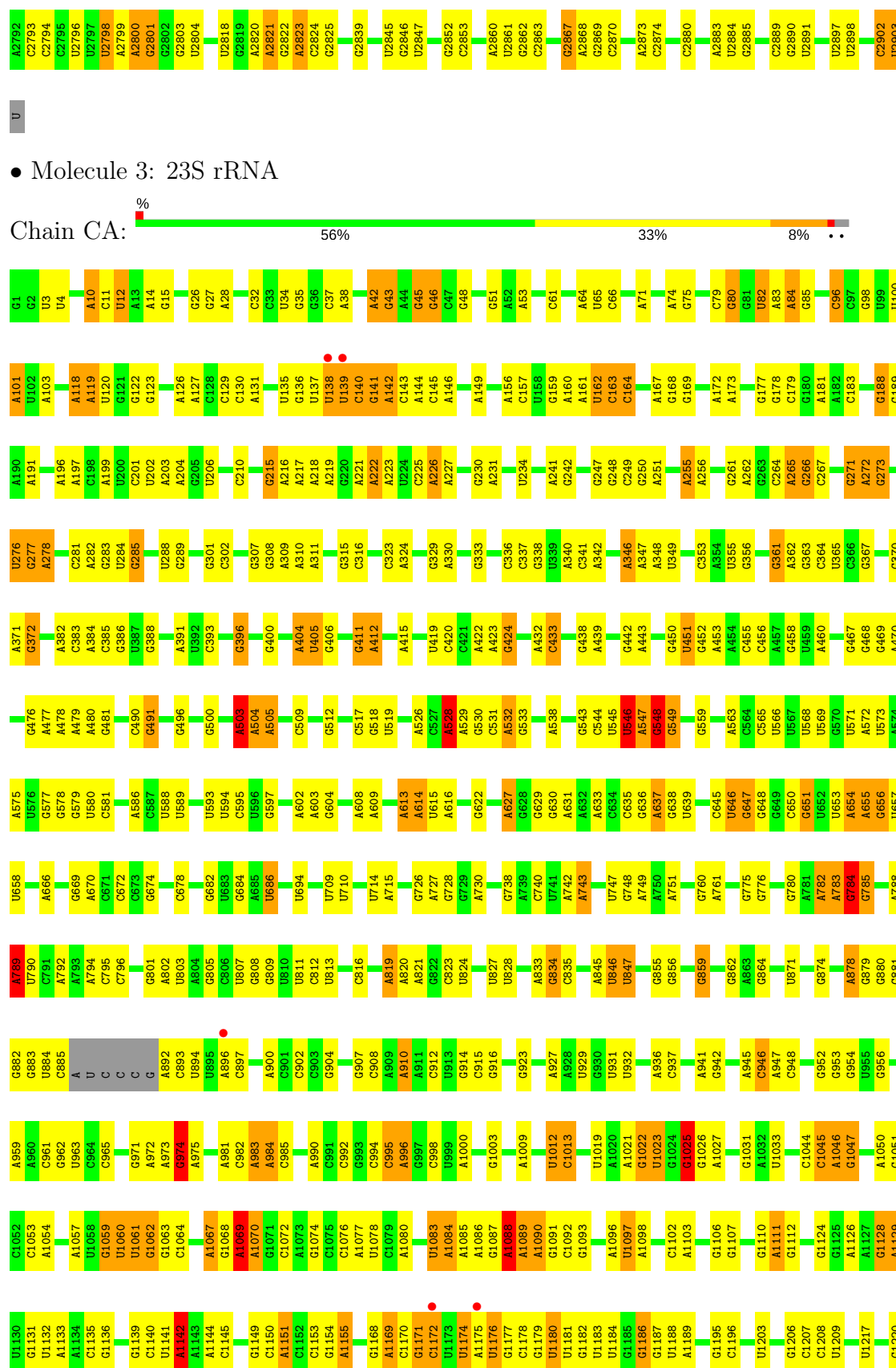


### • Molecule 3: 23S rRNA

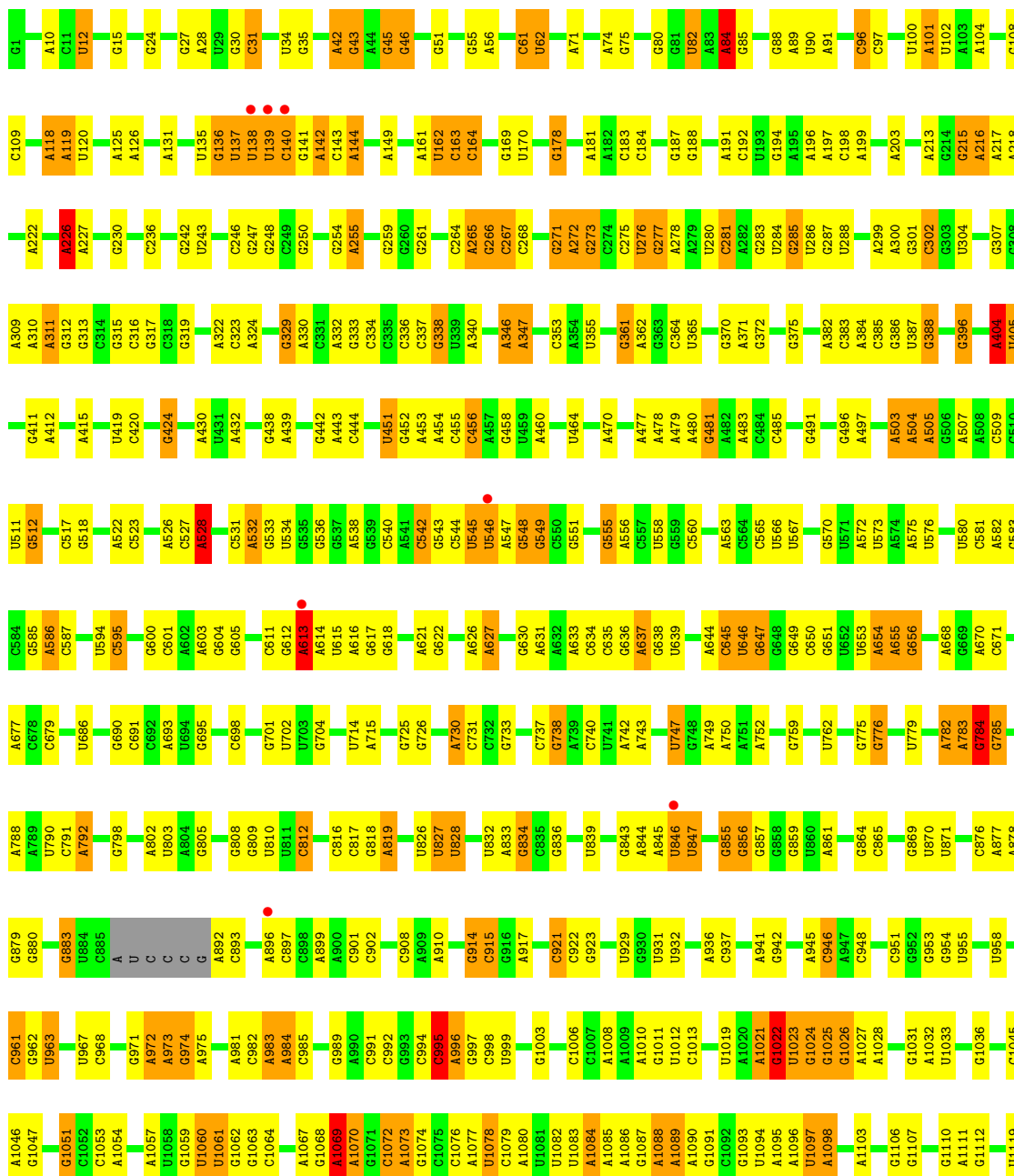




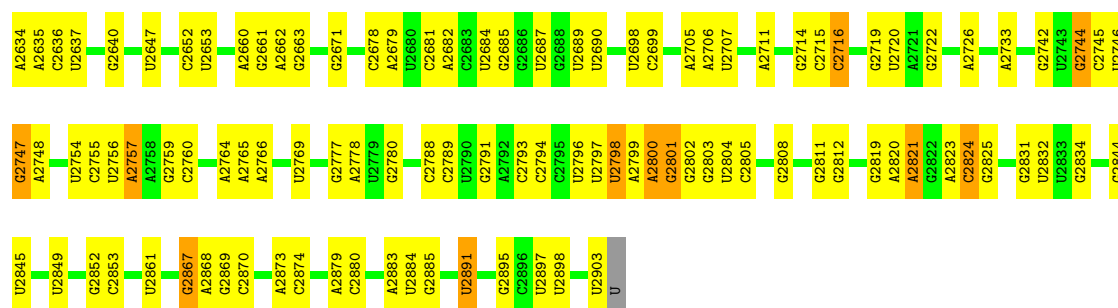
C2699	C2601	C2507	G2409	G2318	U2213	G2144	G2061	A1966	C1837	C1761	A1652	A1553	A1439	G1343
A2700	A2602	A2516	G2410	G2319	C2214	C2145	A2062	C1967	C1838	A1762	G1653	C1653	U1440	U1344
G2702	G2603	C2517	G2415	U2320	A2225	C2146	G2069	A1968	G1839	C1763	A1654	C1655	G1441	C1348
C2703	C2703	A2518	G2421	U2321	C2226	G2147	G2069	A1969	C1843	G1770	C1658	G1658	U1442	C1349
C2704	G2608	G2526	C2422	A2322	G2230	U2149	A2071	U1970	C1943	G1771	G1659	A1868	G1443	C1350
U2707	U2609	C2527	U2423	U2324	U2231	C2150	C2072	G1972	C1844	A1847	G1659	A1868	G1444	C1351
C2710	C2610	U2528	C2424	G2325	U2232	G2151	C2073	U1979	A1848	A1772	U1662	A1570	U1352	U1352
C2711	C2611	G2529	A2425	C2326	G2233	U2152	U2074	G1980	A1848	A1773	A1669	A1571	C1451	C1353
G2714	U2613	U2533	A2426	G2327	G2238	C2154	U2075	G1983	G1857	C1774	A1670	A1572	G1450	G1355
C2715	A2614	A2534	C2427	U2328	U2239	U2155	C2091	U1991	A1858	U1775	C1670	U1579	G1452	G1358
C2716	U2615	U2534	G2428	U2240	U2240	U2156	U2092	U1992	U1864	U1776	C1670	A1580	U1458	A1359
G2719	C2616	U2537	A2430	A2241	A2241	G2157	G2093	U1993	U1867	U1777	G1674	A1581	U1459	A1365
U2720	U2617	C2538	U2244	U2244	U2244	A	A2094	U1992	G1867	U1778	C1674	A1582	U1466	A1366
C2723	C2618	A2542	A2435	A2332	A2247	G	U2099	U1993	G1868	U1779	C1675	A1583	U1466	A1367
U2724	G2619	G2543	G2436	U2334	A2247	C	G2102	C1996	G1869	A1783	A1676	U1584	U1466	G1368
U2725	U2629	G2544	U2437	A2335	G2280	G	G2103	C1997	C1870	A1784	A1677	U1585	U1466	G1368
A2726	C2636	A2547	U2343	U2344	U2259	C	C2104	C1997	A1871	U1785	A1678	A1586	A1469	G1371
A2727	U2637	U2548	G2344	U2345	U2262	U	U2105	C2006	G1872	A1789	G1684	A1591	U1474	A1378
U2728	G2638	G2551	C2442	G2345	C2263	C	U2106	G1873	G1884	C1790	C1685	A1592	U1475	U1379
G2733	U2647	U2552	C2443	A2346	U2263	U	G2107	U2011	U1884	A1791	C1686	A1593	U1476	G1380
A2740	G2648	G2553	G2446	C2347	A2267	A	U2109	A2015	C1805	C1795	C1691	U1594	U1477	G1381
A2741	U2649	U2554	G2447	A2268	A2268	A	G2110	U2016	G1906	C1796	U1692	A1603	U1478	A1383
G2742	U2650	U2555	A2448	G2269	G2275	U	U	U2017	G1906	U1797	U1692	A1604	U1482	A1384
U2743	A2657	U2556	G2455	A2352	A2270	A	G	G2018	A1913	U1798	G1703	C1605	U1485	A1385
G2744	A2667	C2557	G2455	C2354	G2271	C	A	A2019	C1914	U1799	C1704	C1606	U1486	C1386
C2745	A2660	U2558	G2467	G2355	A2274	C	G	A2020	U1915	C1800	A1705	C1607	U1487	A1387
U2746	G2661	A2564	A2468	G2361	C2275	A	G	U2022	A1927	A1802	G1714	C1608	A1392	A1392
A2747	G2662	G2565	A2469	G2365	G2276	C	A	C2023	A1928	C1803	U1715	A1609	C1493	A1393
A2748	G2663	U2566	G2470	G2365	G2277	C	U	G2024	G1929	C1804	G1715	A1610	U1494	U1394
U2754	G2664	G2567	A2476	G2368	A2278	C2179	G	C2025	G1930	A1805	A1722	C1611	A1495	A1395
C2755	U2571	U2572	U2477	C2368	G2279	U2180	A	A2030	G1835	G1807	G1723	C1612	A1504	U1396
A2757	C2573	C2573	U2478	G2373	G2282	U2181	U	A2031	A1936	A1808	G1723	G1613	A1504	C1398
G2758	G2674	G2576	U2479	G2383	A2284	A2183	G	G2032	A1937	G1811	U1729	A1614	A1508	C1398
G2759	A2675	G2576	A2482	U2384	G2285	A2184	G	A2033	A1938	U1812	C1730	C1615	A1509	A1403
C2760	U2579	C2579	C2486	C2385	G2286	G2186	A	A2037	U1939	G1813	G1731	A1616	G1510	C1404
A2764	C2678	U2580	A2486	A2386	A2287	U2187	G	G2038	C1942	G1814	G1737	A1617	G1514	C1414
A2765	A2679	G2581	U2491	A2387	A2288	U2194	G	U2039	U1943	A1815	G1738	A1618	U1415	U1415
A2766	U2680	G2582	U2492	G2389	G2289	U2195	C	G2040	G1945	C1816	A1739	G1622	G1515	G1416
G2770	C2681	G2583	G2495	G2393	A2297	U2197	U	C2043	U1946	U1817	A1744	G1627	U1523	C1417
U2777	U2682	U2584	A2498	U2396	A2298	A2198	G	C2047	G1950	A1819	U1747	C1638	G1524	G1418
A2778	G2683	U2585	C2499	G2396	U2305	C2199	A2134	G2048	U1955	U1820	C1748	C1639	C1533	A1419
U2779	G2684	U2588	U2500	G2396	C2306	G2200	A2135	G2048	U1956	G1824	A1749	C1639	U1534	A1420
G2780	C2685	G2589	G2501	U2402	G2307	U2202	G2136	C2053	C1957	G1828	G1750	C1643	C1536	C1428
U2788	U2689	G2595	G2502	G2404	G2308	U2203	U2137	C2054	C1957	A1829	G1753	G1645	G1537	G1429
U2789	U2690	U2599	A2503	G2405	A2311	G2204	U2139	G2056	G1959	C1830	U1754	C1646	G1538	G1430
G2791	U2691	U2599	U2504	A2406	C2312	U2210	G2140	C2057	A1960	G1831	A1758	U1647	U1542	G1435
	U2790	U2599	U2505	A2407	U2313	A2211	G2142	A2058	U1963	C1832	A1759	G1649	U1543	G1436
				U2408	A2314	A2212	C2143	A2060		C1833	C1760			U1438



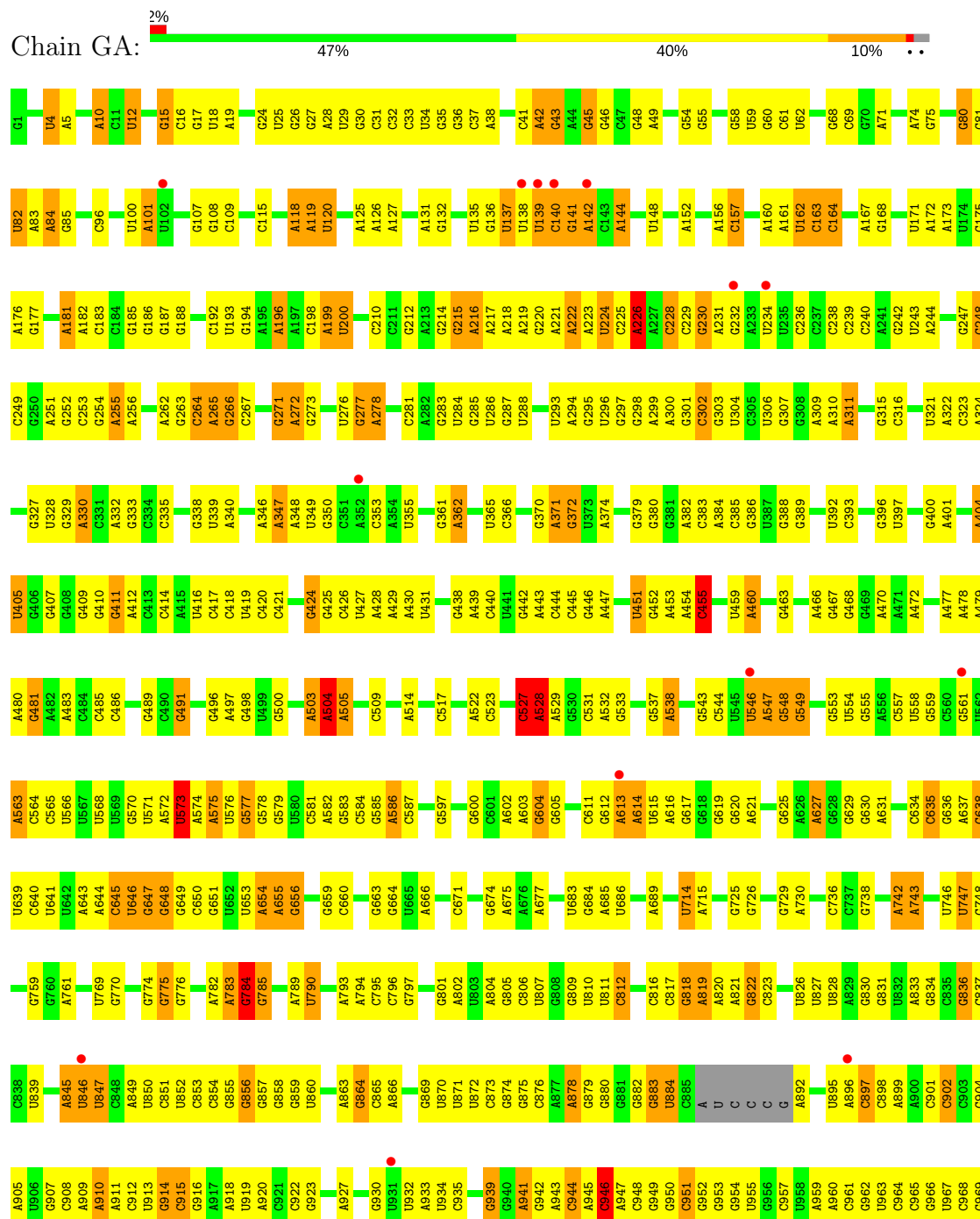
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C2501	U2500	C2403	G2318	G2204	A2134	G2055	G1968	G1842	A1759	U1647	U1647	U1415	U1316	G1225
G2592	C2501	G2319	G2320	G2209	G2136	G2056	A1969	C1843	C1760	U1648	U1533	G1416	G1317	A1230
G2595	G2502	U2321	U2320	U2210	U2137	A2060	G1972	A1847	C1761	G1649	U1534	C1417	U1318	U1231
G2596	U2503	A2406	A2322	A2212	G2138	G2061	G1973	A1848	U1762	A1652	A1535	G1418	A1322	G1238
G2602	U2504	U2407	G2323	A2211	U2139	A2062	G1974	A1858	C1764	G1653	C1536	A1419	A1327	G1239
G2603	G2505	G2408	U2324	U2213	G2140	C2063	G1975	U1864	U1774	A1654	A1548	A1420	U1328	U1243
G2606	U2506	C2412	G2325	U2214	A2142	C2064	U1976	U1865	G1775	A1655	C1549	C1428	U1242	U1243
G2607	G2507	G2413	C2326	G2215	C2143	G2065	A1977	U1869	U1776	G1658	A1553	G1435	U1329	A1244
G2608	A2518	G2414	A2327	G2216	G2144	A2070	A1978	C1870	G1776	A1664	A1563	A1439	G1332	G1245
G2609	C2521	C2416	U2329	U2219	C2145	A2071	G1983	A1871	U1779	U1668	U1563	A1439	G1332	G1248
A2614	U2522	G2330	G2331	U2220	A2147	C2072	G1989	A1872	U1780	A1668	C1564	G1444	A1342	U1249
U2615	G2523	C2332	C2333	G2221	U2148	U2079	U1990	G1873	U1781	A1669	C1565	G1445	U1343	G1250
G2618	G2524	A2333	A2334	A2225	U2149	A2080	U1991	C1874	U1782	A1673	A1566	G1446	U1344	C1251
C2619	U2525	U2334	U2335	C2226	U2151	U2081	U1992	G1875	U1783	G1674	G1567	C1447	U1352	G1252
U2629	U2526	A2336	A2335	U2233	U2152	C2091	U1993	U1883	A1784	G1675	A1570	G1448	A1352	A1253
A2632	C2527	U2343	U2344	G2234	C2153	U2092	C1997	G1884	A1785	A1676	A1570	G1449	G1360	G1256
C2636	U2528	C2347	C2348	G2235	U2154	U2093	A1998	U1889	A1786	A1677	G1573	C1451	G1361	A1262
U2637	G2529	A2346	U2347	U2236	U2155	A2094	C1999	A1899	U1789	G1681	A1578	U1452	C1362	A1265
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U2647	U2535	G2357	G2358	G2241	C	A2097	G2010	U1914	A1794	C1685	A1583	U1469	G1368	A1268
G2649	U2536	C2361	C2362	U2242	C	U2101	U2016	U1915	C1795	G1707	U1584	U1476	G1369	A1269
U2653	U2537	A2364	A2365	U2243	G	C2102	U2017	G1930	U1796	C1708	C1585	U1477	C1370	C1270
A2654	U2538	G2366	G2367	U2244	U	U2103	G2018	U1931	G1797	U1713	A1593	G1479	U1372	A1272
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G2660	U2540	U2373	U2374	U2246	A	U2105	A2020	A1937	A1808	U1722	C1595	C1483	A1378	A1276
A2662	U2541	C2374	C2375	U2247	A	U2106	C2021	A1938	A1809	G1723	U1484	U1485	U1379	G1277
G2663	U2542	A2376	A2377	U2248	U	U2107	U2022	A1939	A1810	C1726	C1603	U1486	G1380	G1280
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G2671	U2544	C2380	C2381	U2250	A	G2109	G2024	G1945	G1812	U1728	C1606	G1492	A1383	A1286
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	U2555	U2402	U2403	U2261	U2187	G	C2043	A1960	C1837	U1747	U1629	U1513	U1405	G1309
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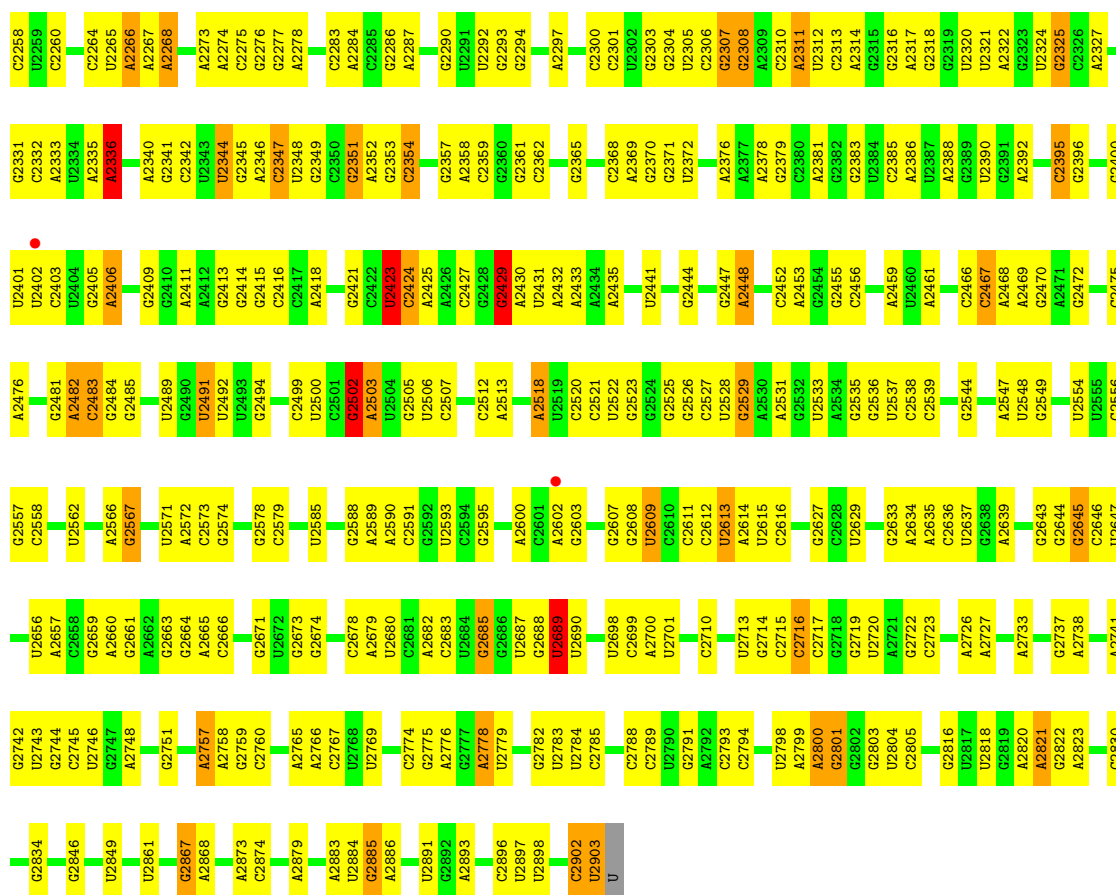




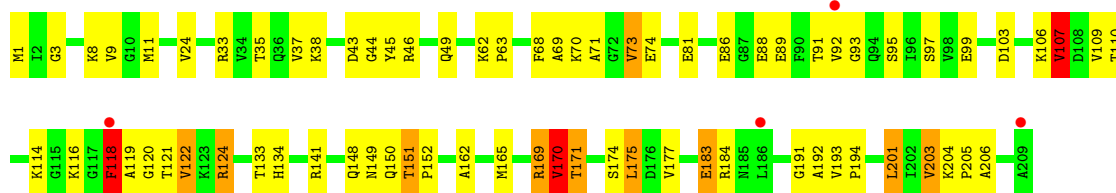
### • Molecule 3: 23S rRNA



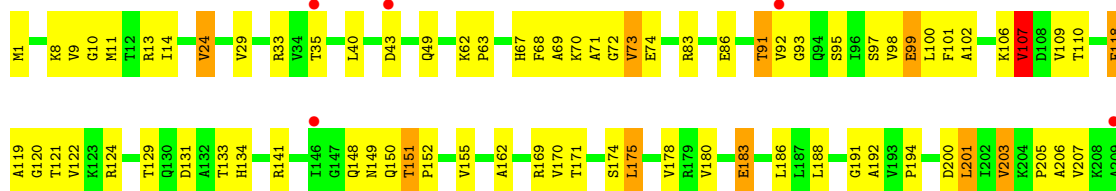




• Molecule 4: 50S ribosomal protein L3



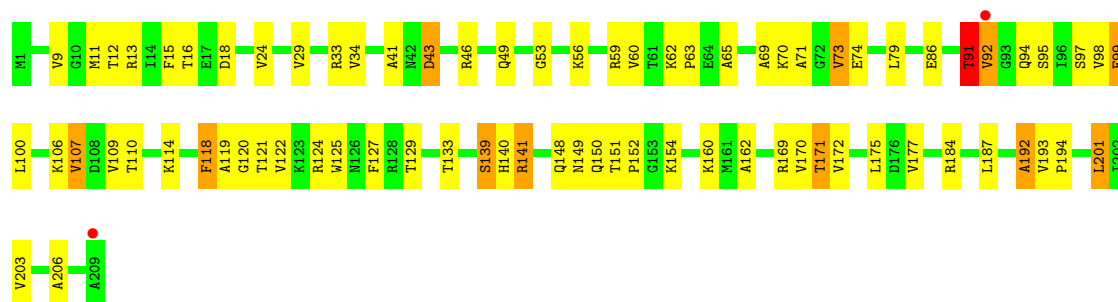
• Molecule 4: 50S ribosomal protein L3



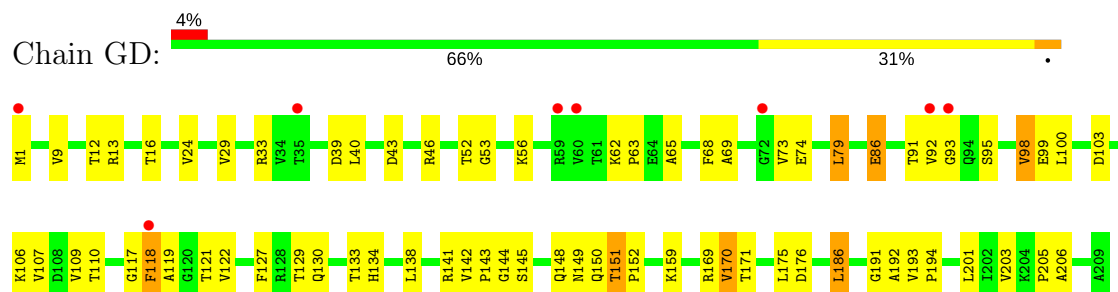
• Molecule 4: 50S ribosomal protein L3



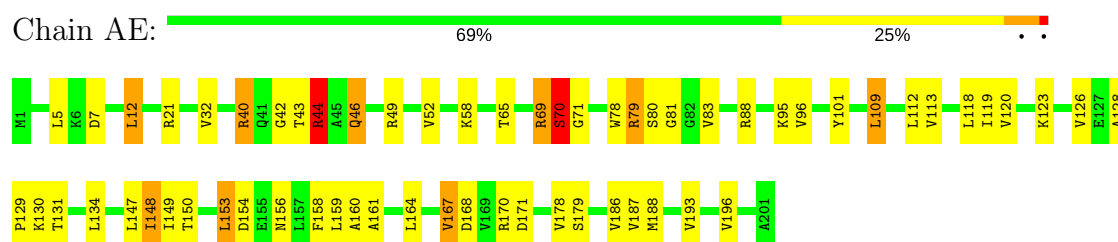




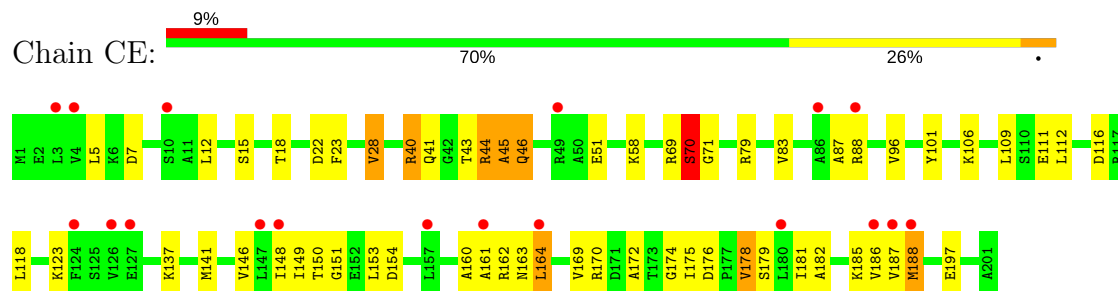
- Molecule 4: 50S ribosomal protein L3



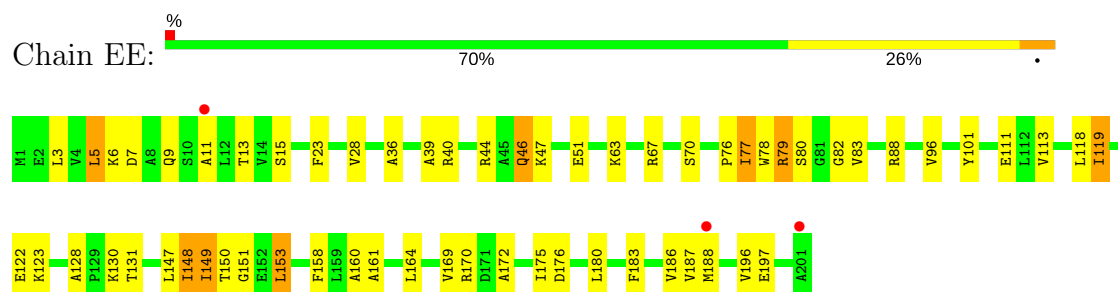
- Molecule 5: 50S ribosomal protein L4



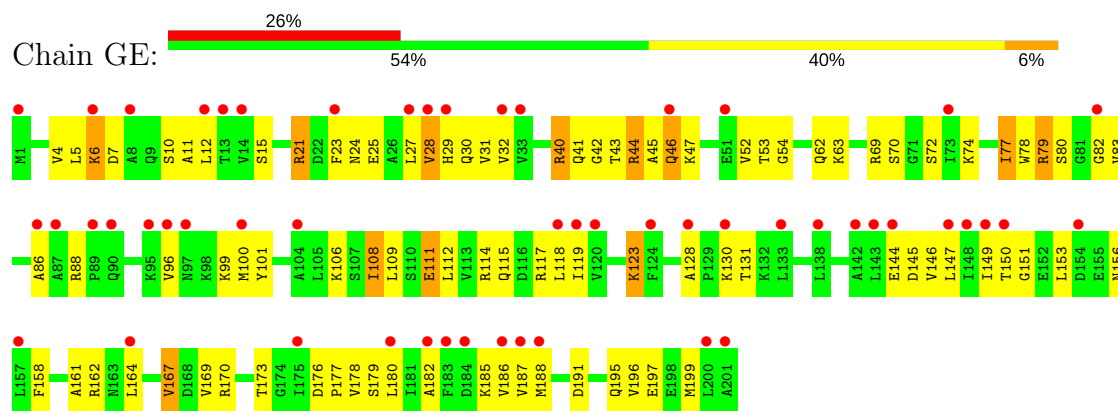
- Molecule 5: 50S ribosomal protein L4



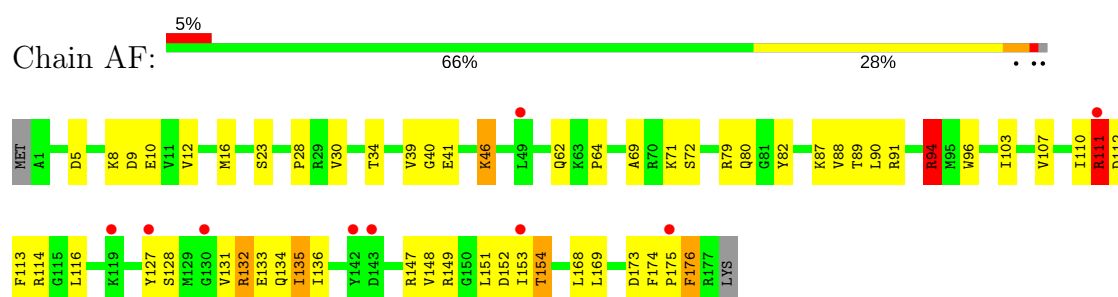
- Molecule 5: 50S ribosomal protein L4



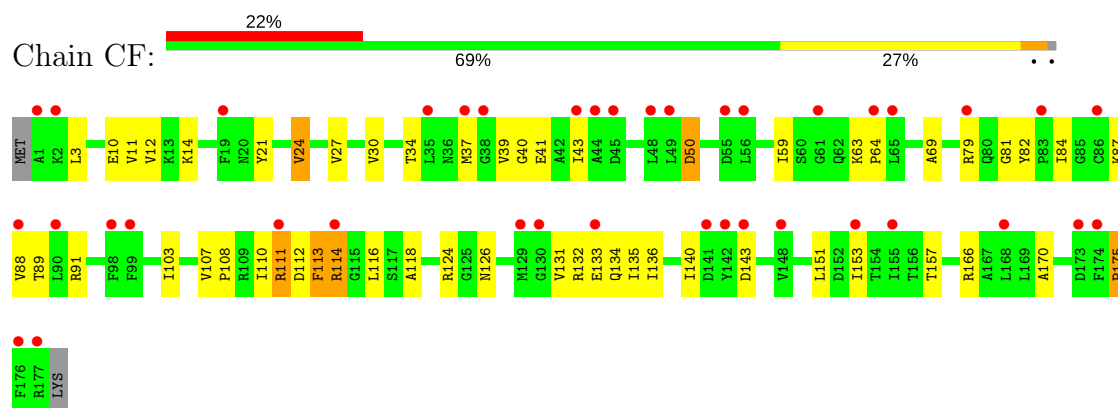
- Molecule 5: 50S ribosomal protein L4



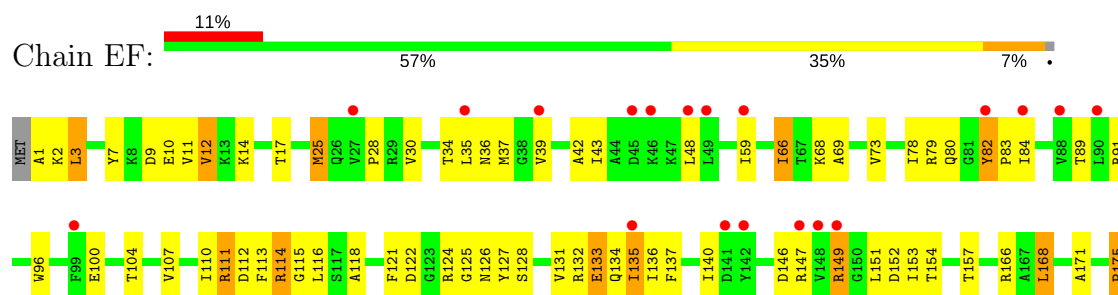
- Molecule 6: 50S ribosomal protein L5



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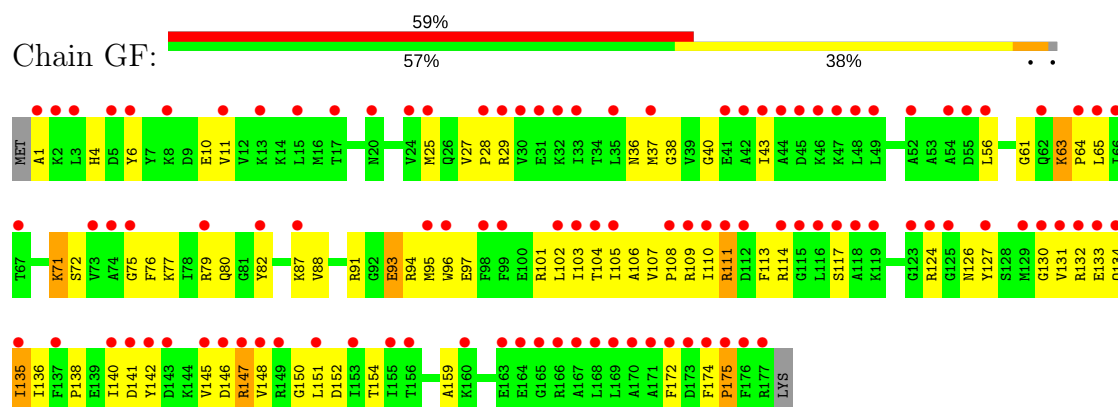


- Molecule 6: 50S ribosomal protein L5

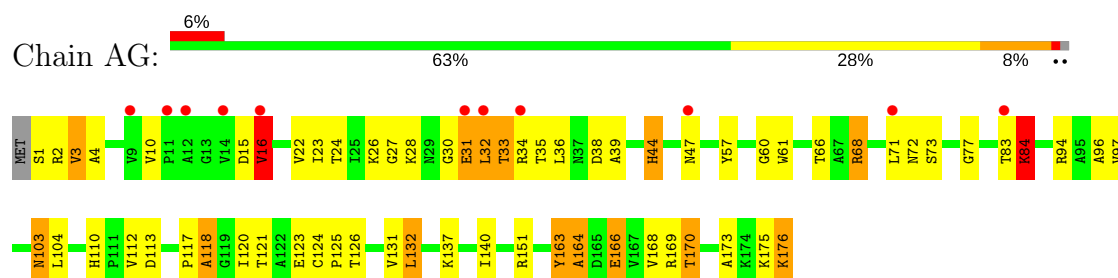




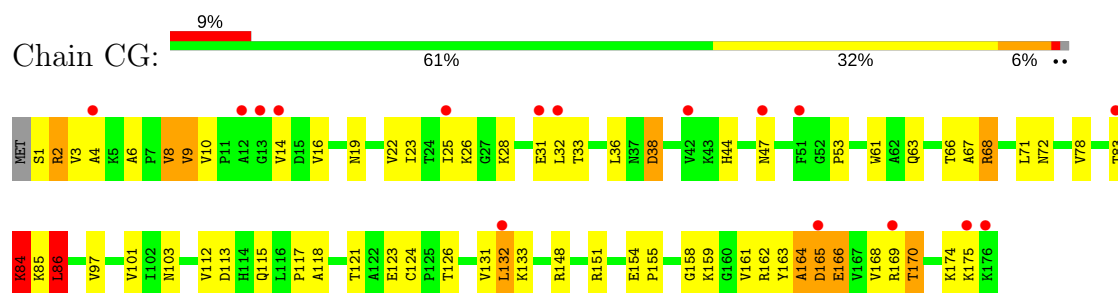
- Molecule 6: 50S ribosomal protein L5



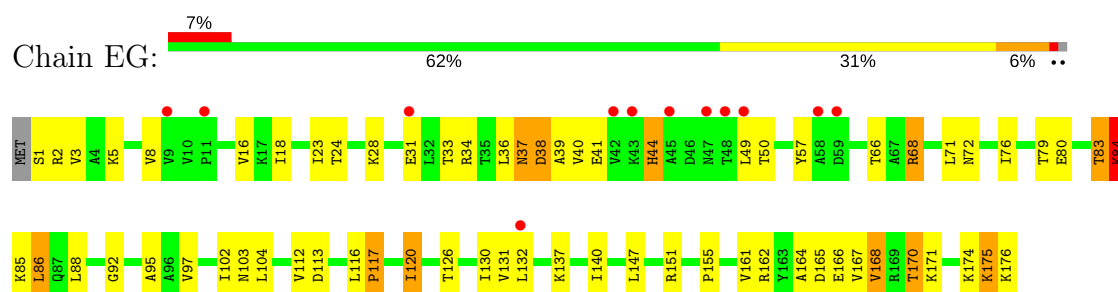
- Molecule 7: 50S ribosomal protein L6



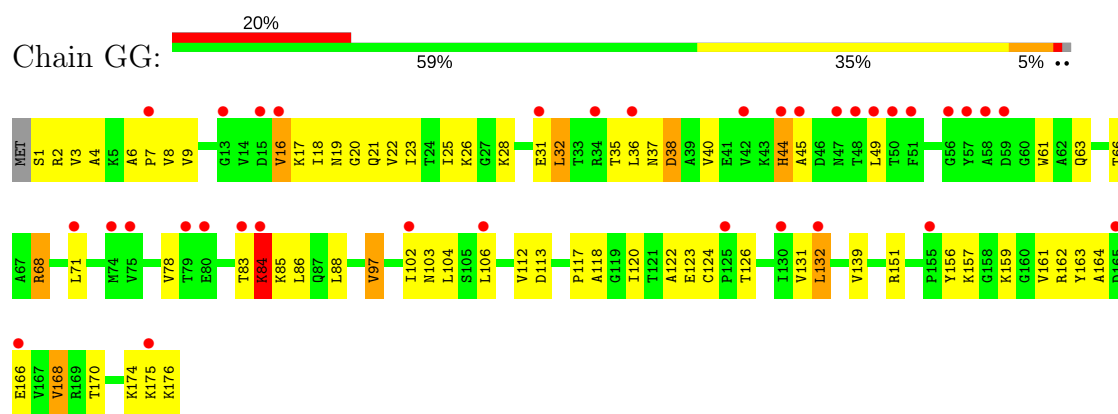
- Molecule 7: 50S ribosomal protein L6



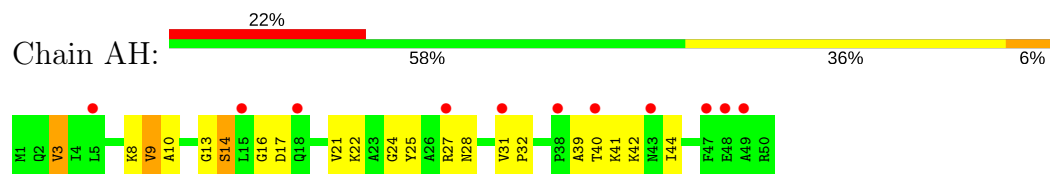
- Molecule 7: 50S ribosomal protein L6



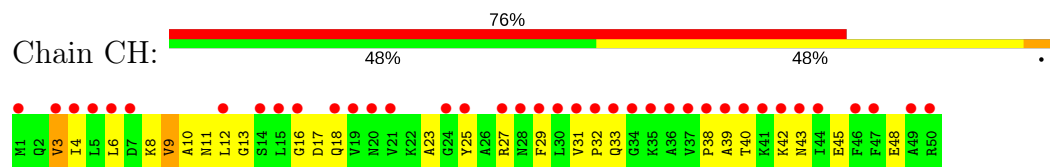
- Molecule 7: 50S ribosomal protein L6



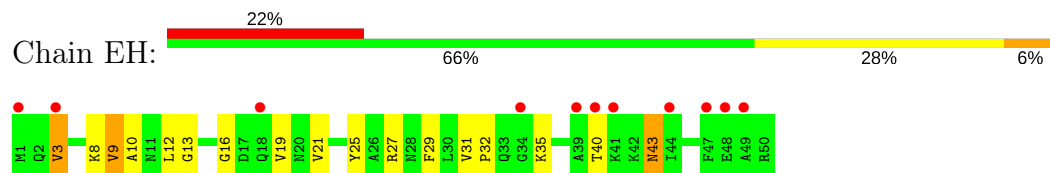
- Molecule 8: 50S ribosomal protein L9



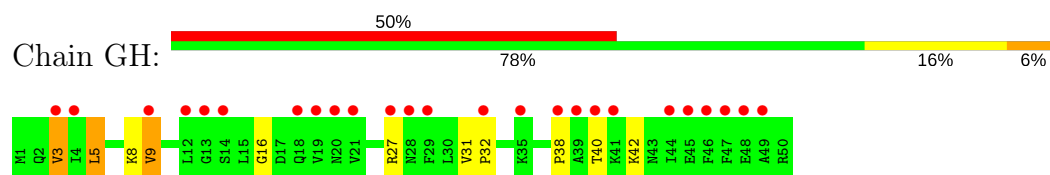
- Molecule 8: 50S ribosomal protein L9



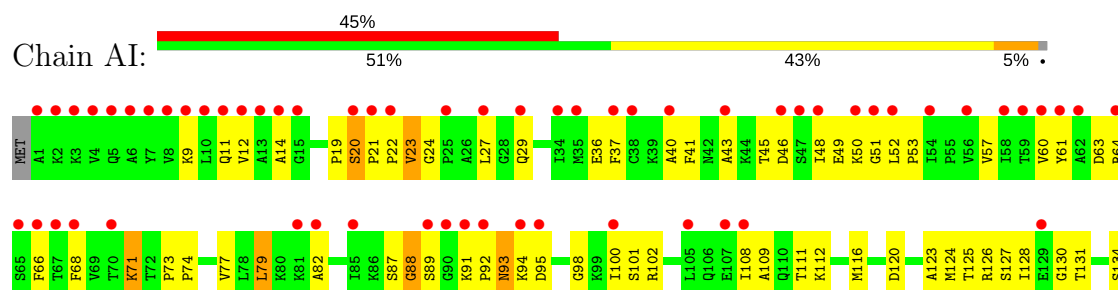
- Molecule 8: 50S ribosomal protein L9

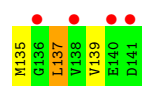


- Molecule 8: 50S ribosomal protein L9

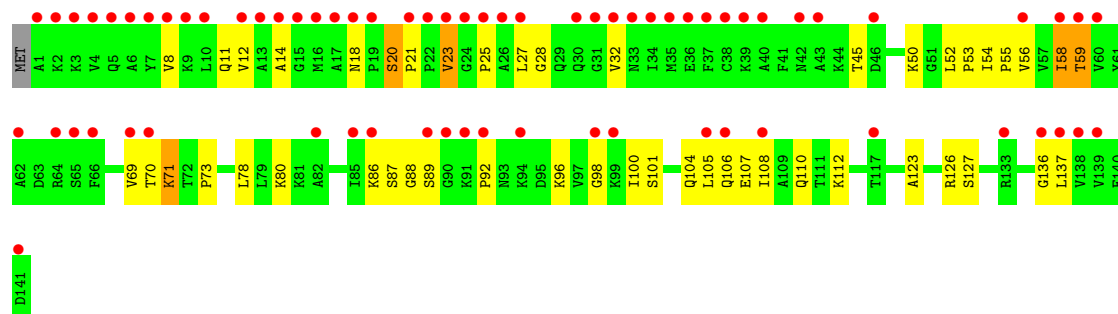


- Molecule 9: 50S ribosomal protein L11

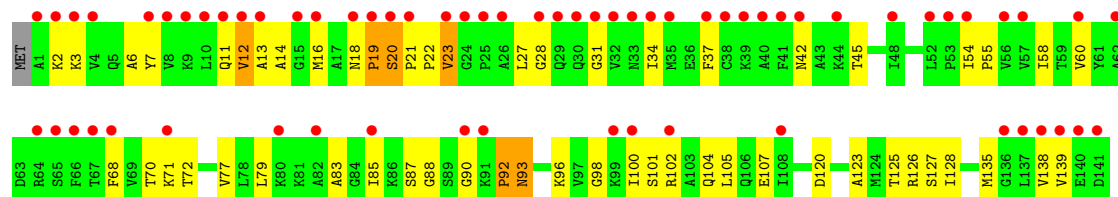




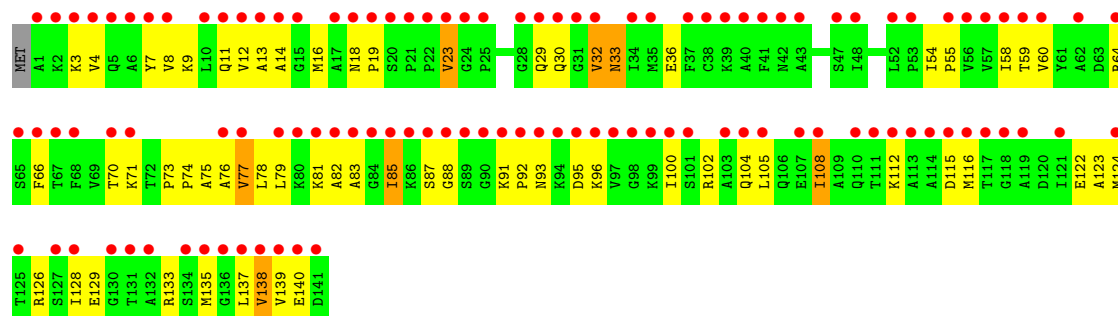
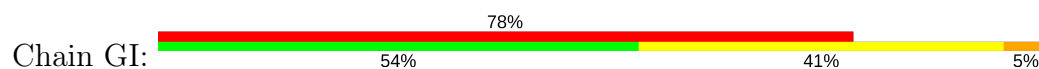
• Molecule 9: 50S ribosomal protein L11



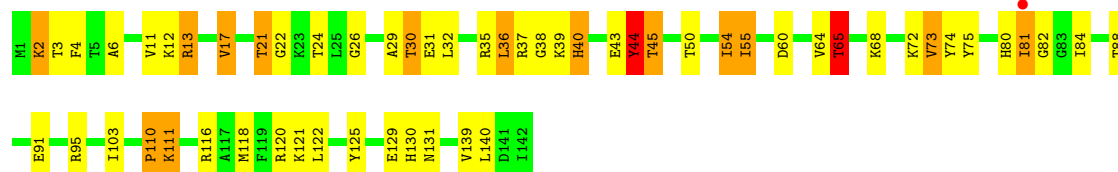
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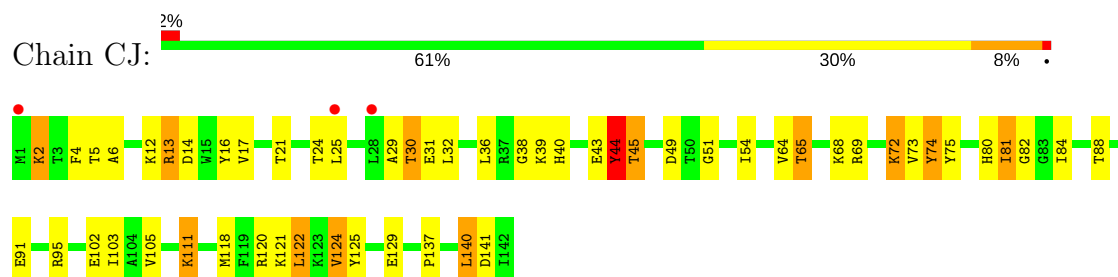
• Molecule 9: 50S ribosomal protein L11



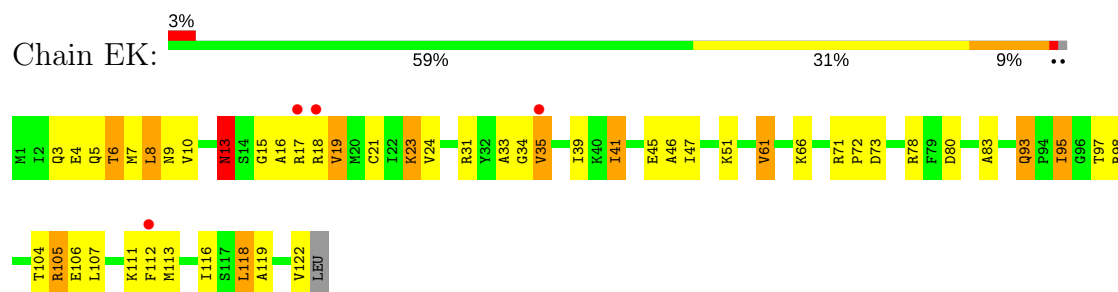
• Molecule 10: 50S ribosomal protein L13



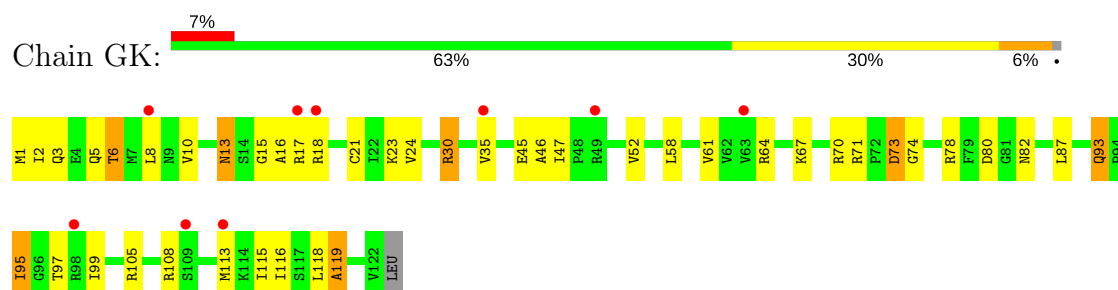
- Molecule 10: 50S ribosomal protein L13



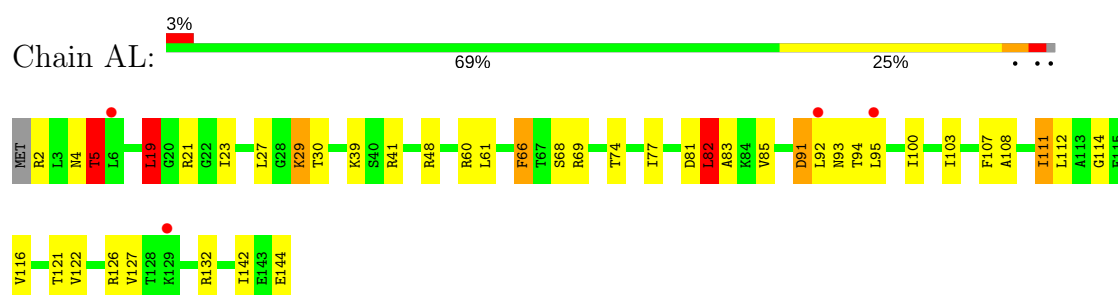
- Molecule 11: 50S ribosomal protein L14



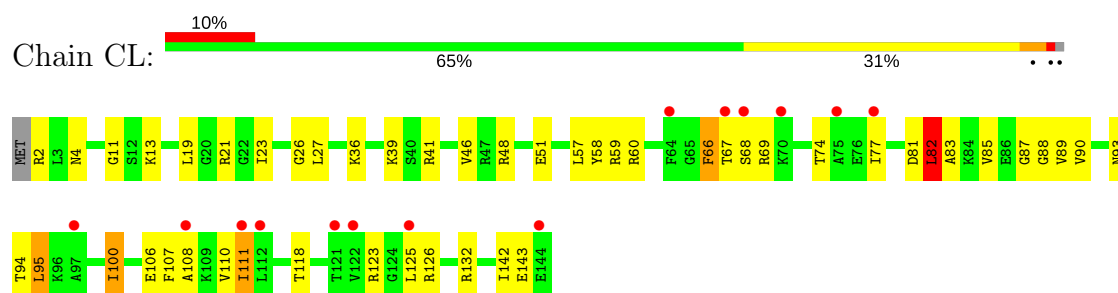
- Molecule 11: 50S ribosomal protein L14



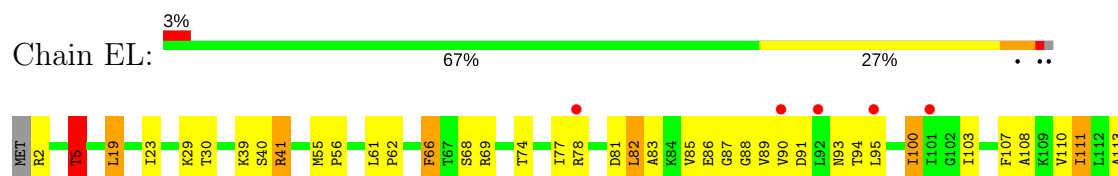
- Molecule 12: 50S ribosomal protein L15



- Molecule 12: 50S ribosomal protein L15

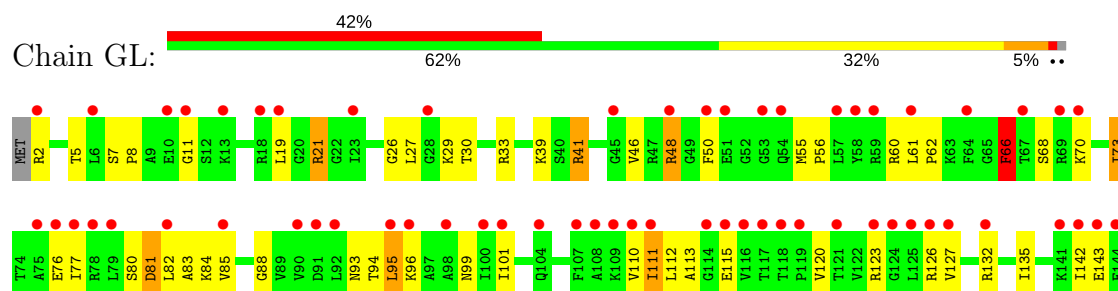


- Molecule 12: 50S ribosomal protein L15

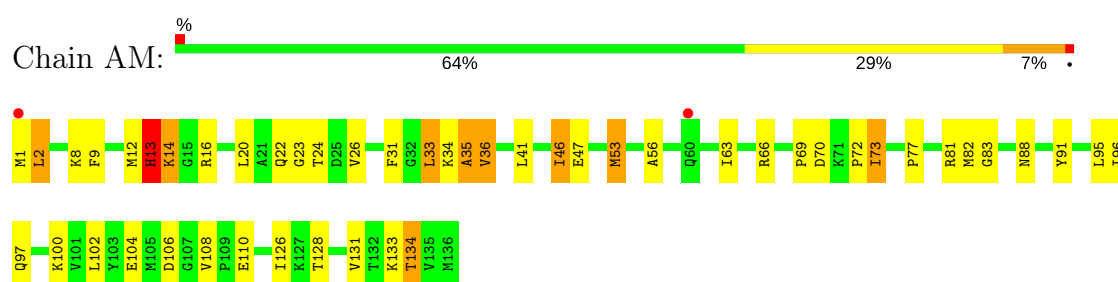




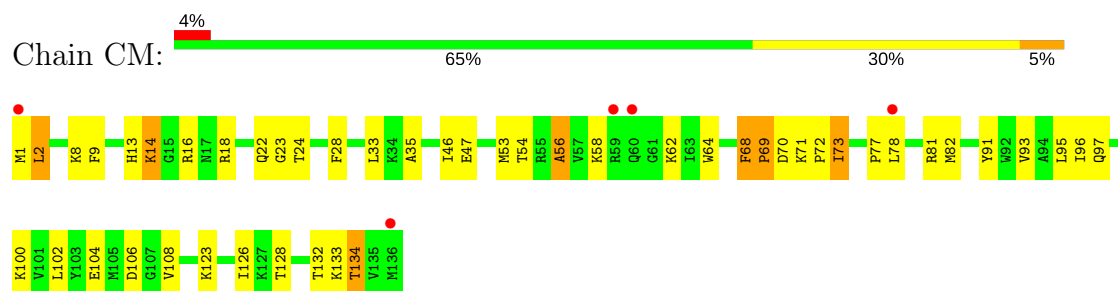
- Molecule 12: 50S ribosomal protein L15



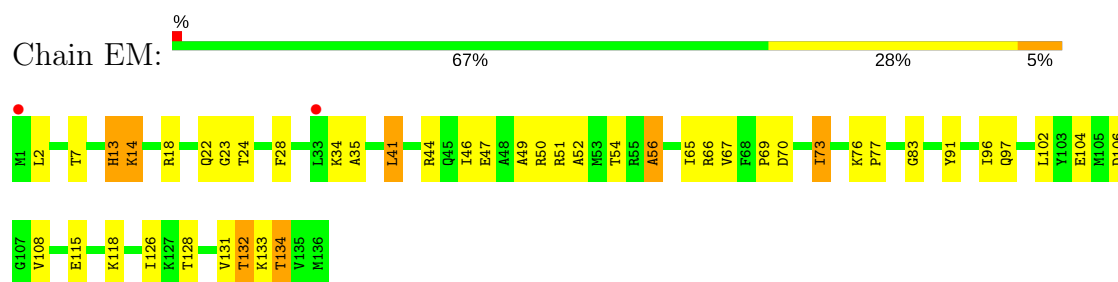
- Molecule 13: 50S ribosomal protein L16



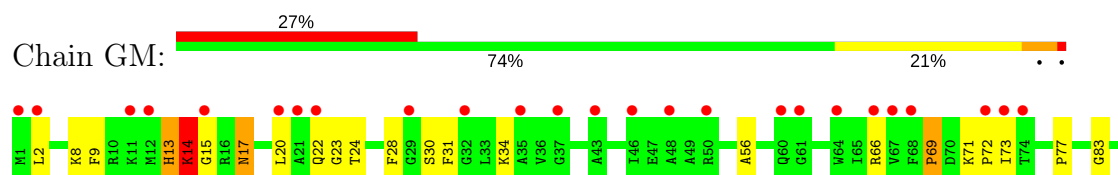
- Molecule 13: 50S ribosomal protein L16



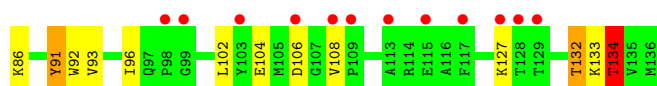
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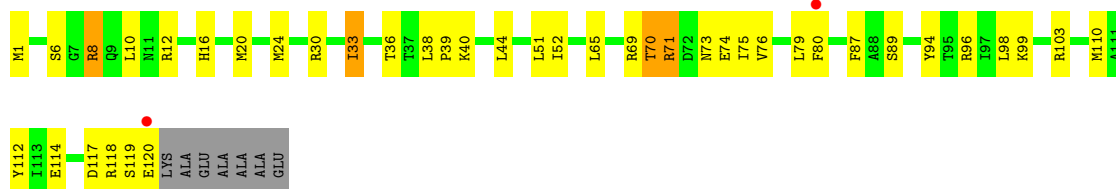
- Molecule 13: 50S ribosomal protein L16



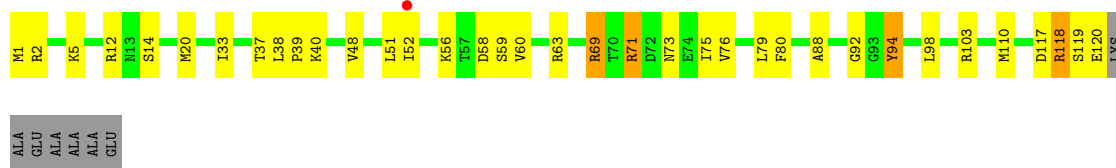




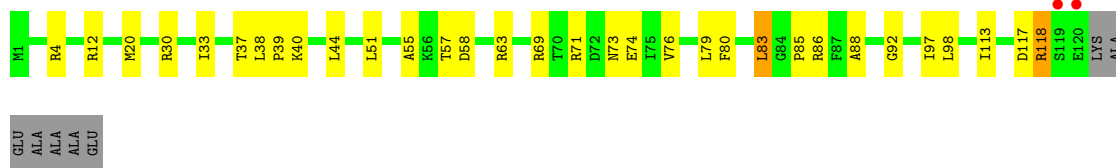
- Molecule 14: 50S ribosomal protein L17



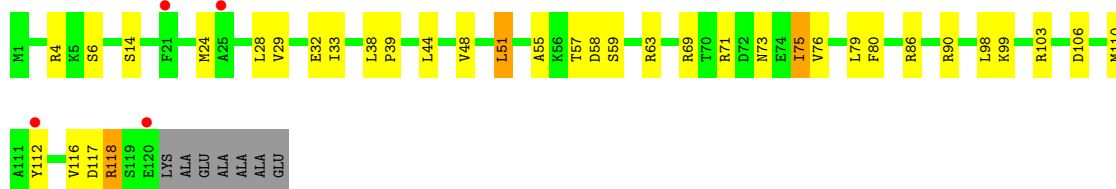
- Molecule 14: 50S ribosomal protein L17



- Molecule 14: 50S ribosomal protein L17



- Molecule 14: 50S ribosomal protein L17

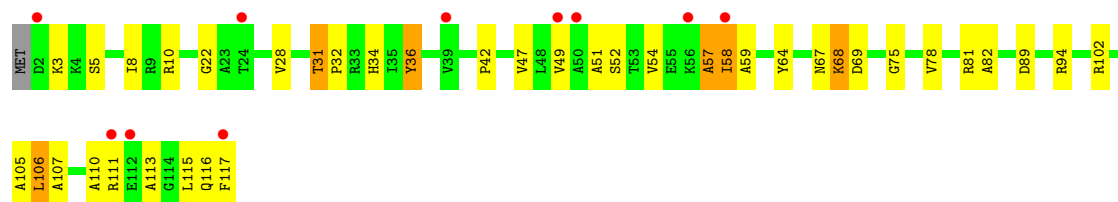


- Molecule 15: 50S ribosomal protein L18

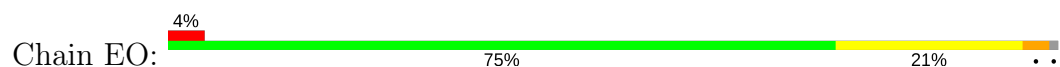




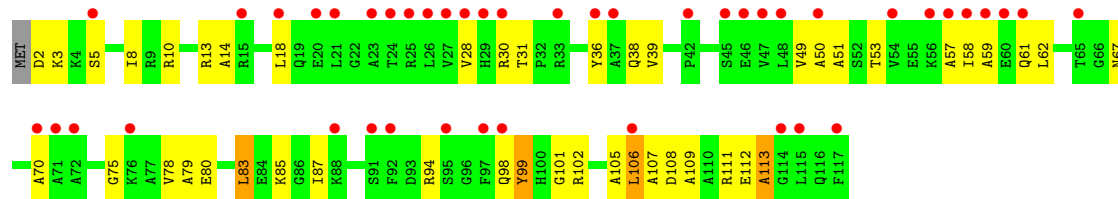
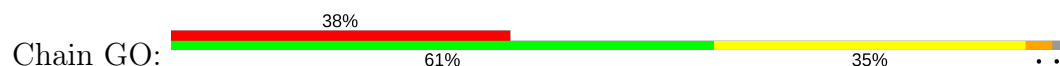
- Molecule 15: 50S ribosomal protein L18



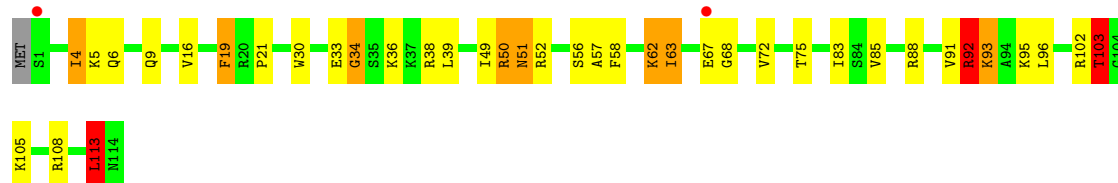
- Molecule 15: 50S ribosomal protein L18



- Molecule 15: 50S ribosomal protein L18



- Molecule 16: 50S ribosomal protein L19

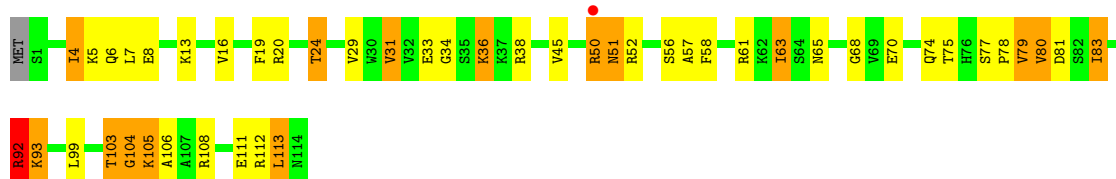


- Molecule 16: 50S ribosomal protein L19

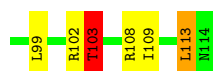




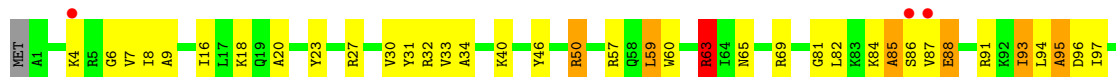
- Molecule 16: 50S ribosomal protein L19



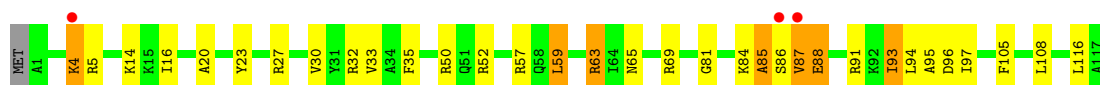
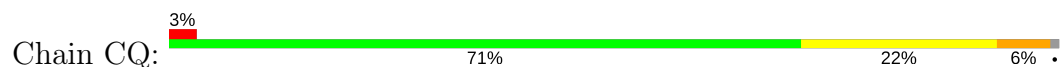
- Molecule 16: 50S ribosomal protein L19



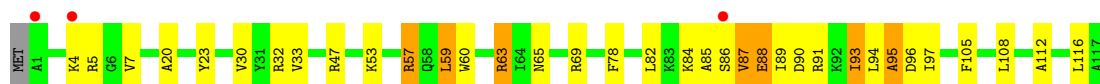
- Molecule 17: 50S ribosomal protein L20



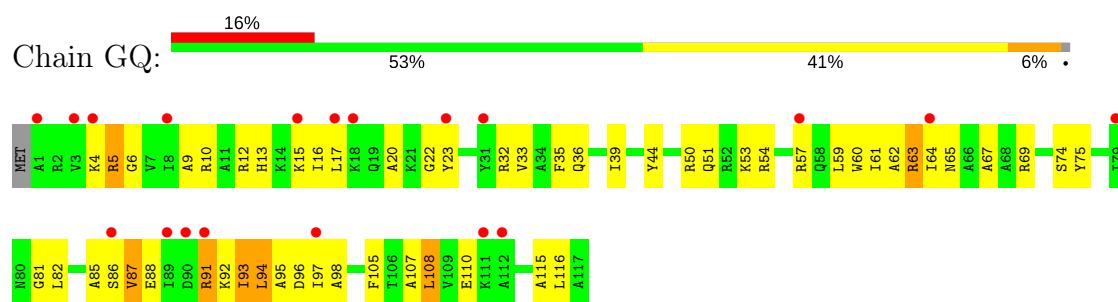
- Molecule 17: 50S ribosomal protein L20



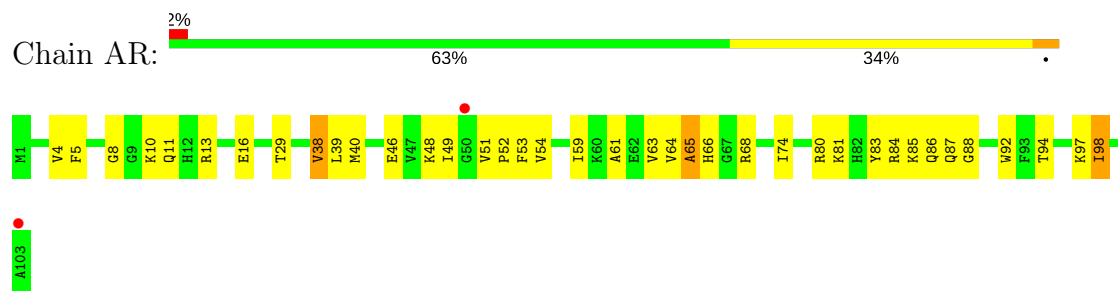
- Molecule 17: 50S ribosomal protein L20



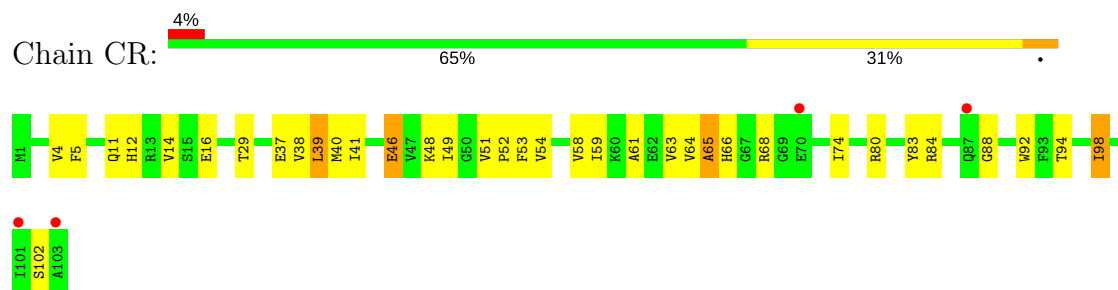
- Molecule 17: 50S ribosomal protein L20



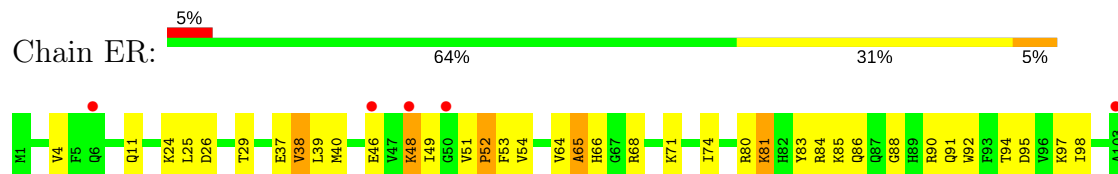
- Molecule 18: 50S ribosomal protein L21



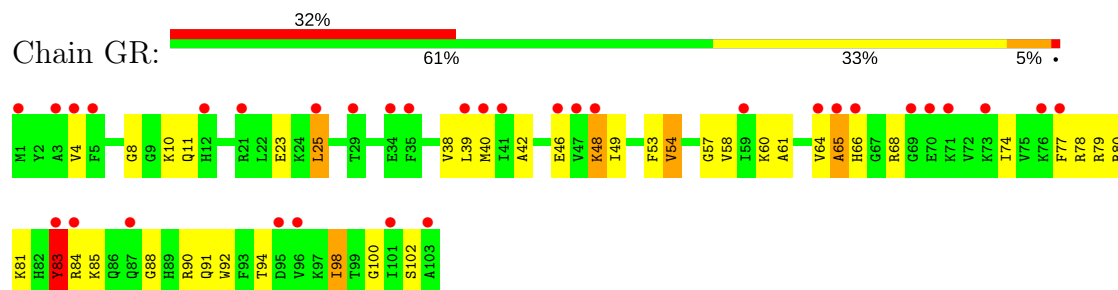
- Molecule 18: 50S ribosomal protein L21



- Molecule 18: 50S ribosomal protein L21

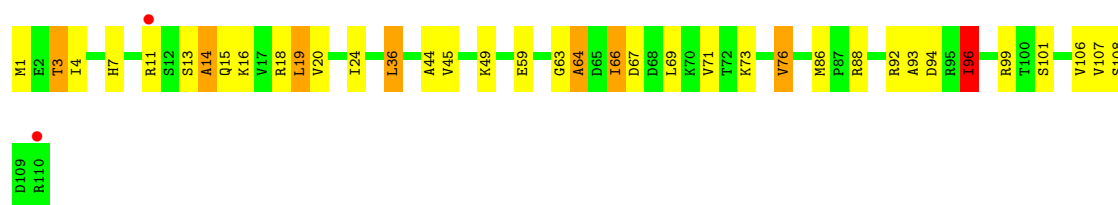


- Molecule 18: 50S ribosomal protein L21

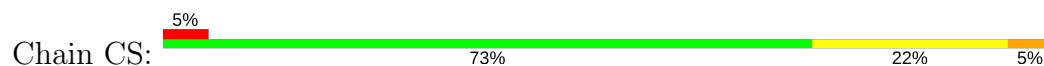


- Molecule 19: 50S ribosomal protein L22





- Molecule 19: 50S ribosomal protein L22



- Molecule 19: 50S ribosomal protein L22



- Molecule 19: 50S ribosomal protein L22

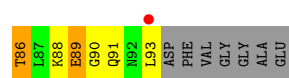


- Molecule 20: 50S ribosomal protein L23

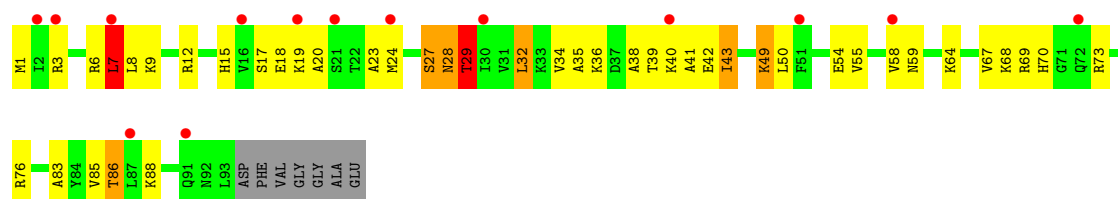


- Molecule 20: 50S ribosomal protein L23

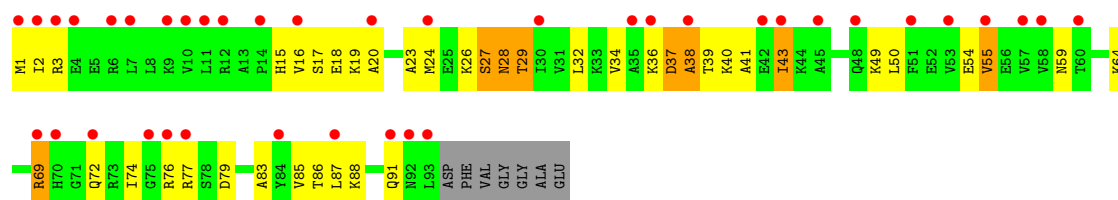
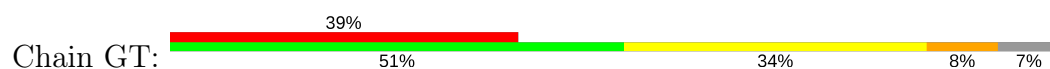




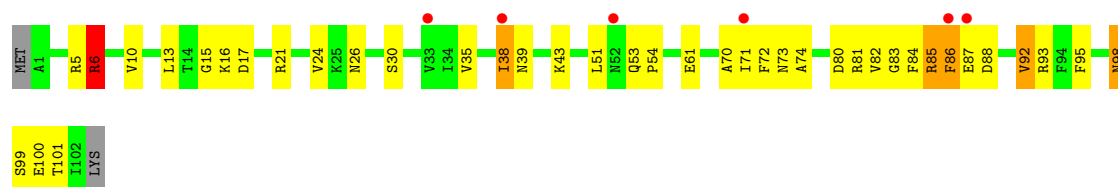
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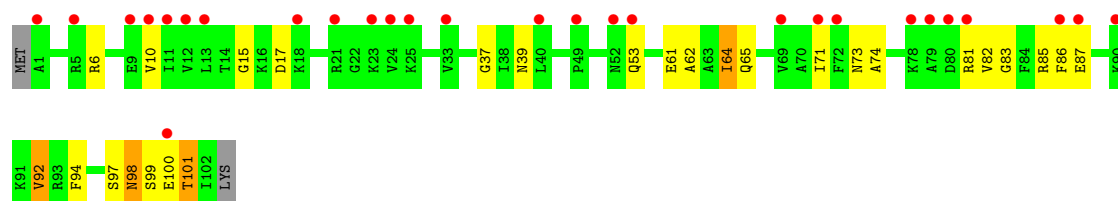
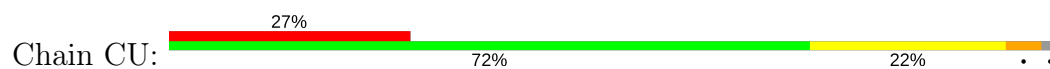
• Molecule 20: 50S ribosomal protein L23



• Molecule 21: 50S ribosomal protein L24

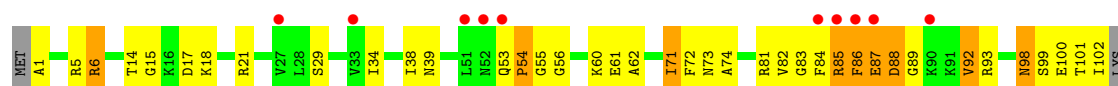


• Molecule 21: 50S ribosomal protein L24

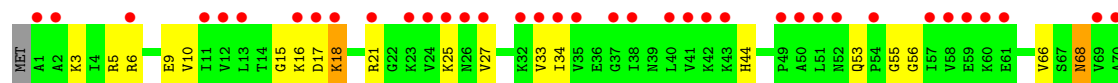


• Molecule 21: 50S ribosomal protein L24

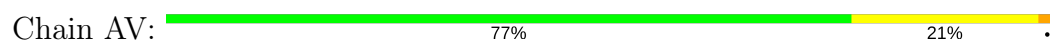




- Molecule 21: 50S ribosomal protein L24



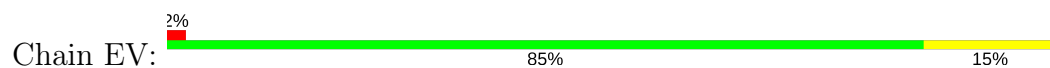
- Molecule 22: 50S ribosomal protein L25



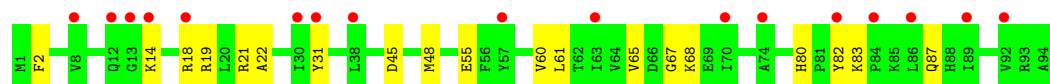
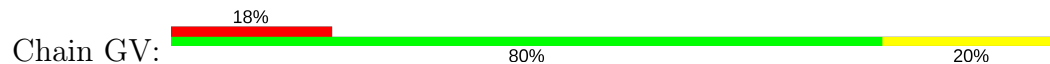
- Molecule 22: 50S ribosomal protein L25



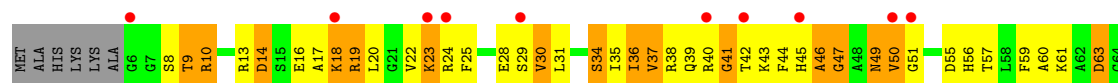
- Molecule 22: 50S ribosomal protein L25



- Molecule 22: 50S ribosomal protein L25

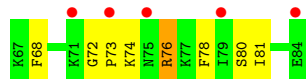


- Molecule 23: 50S ribosomal protein L27

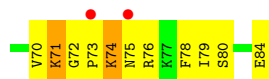
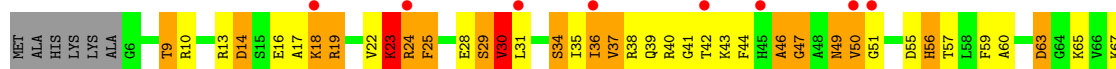




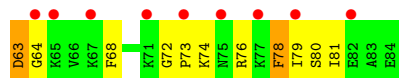
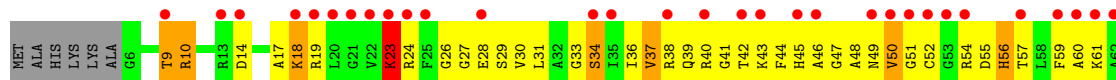
- Molecule 23: 50S ribosomal protein L27



- Molecule 23: 50S ribosomal protein L27



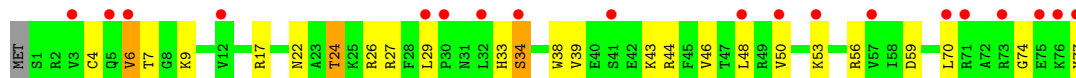
- Molecule 23: 50S ribosomal protein L27



- Molecule 24: 50S ribosomal protein L28



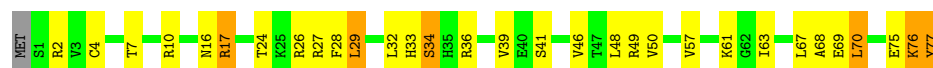
- Molecule 24: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L28

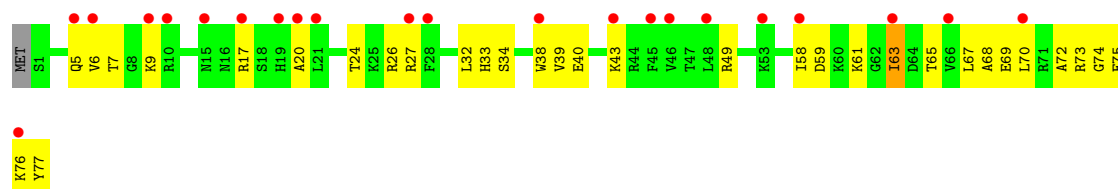


Chain EX: 



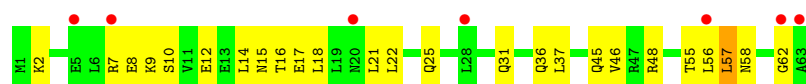
- Molecule 24: 50S ribosomal protein L28

Chain GX: 




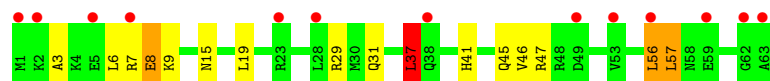
- Molecule 25: 50S ribosomal protein L29

Chain AY: 



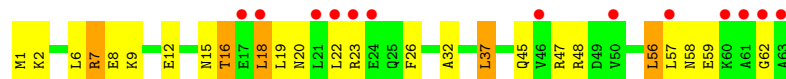
- Molecule 25: 50S ribosomal protein L29

Chain CY: 



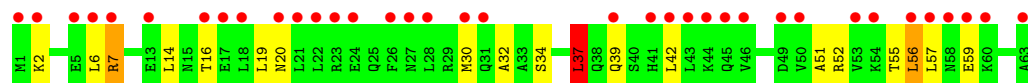
- Molecule 25: 50S ribosomal protein L29

Chain EY: 



- Molecule 25: 50S ribosomal protein L29

Chain GY: 

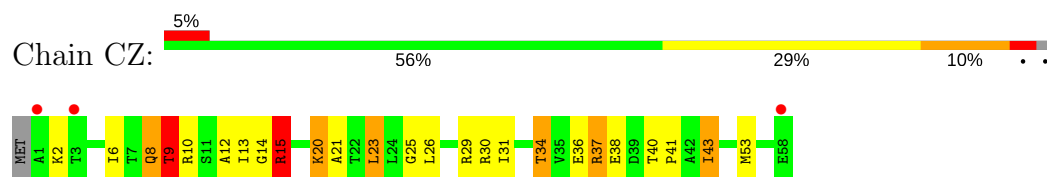


- Molecule 26: 50S ribosomal protein L30

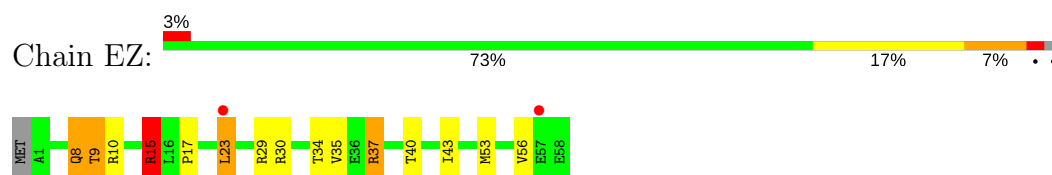
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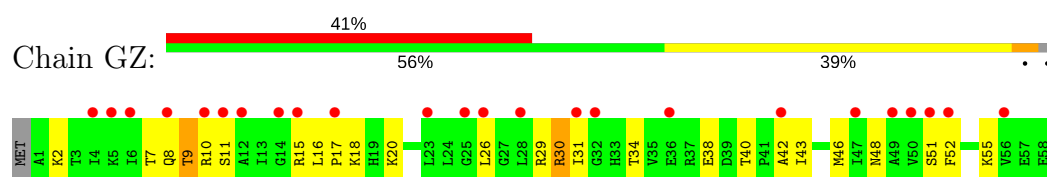
- Molecule 26: 50S ribosomal protein L30



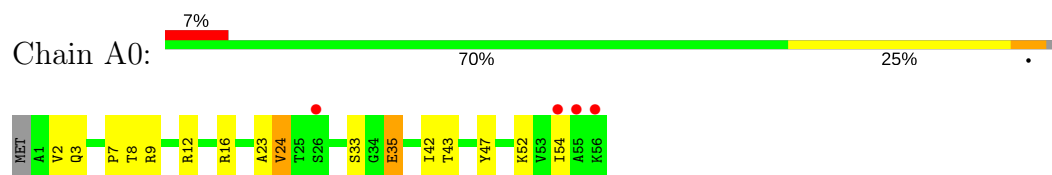
- Molecule 26: 50S ribosomal protein L30



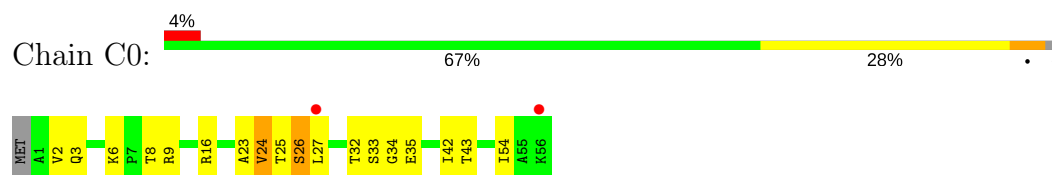
- Molecule 26: 50S ribosomal protein L30



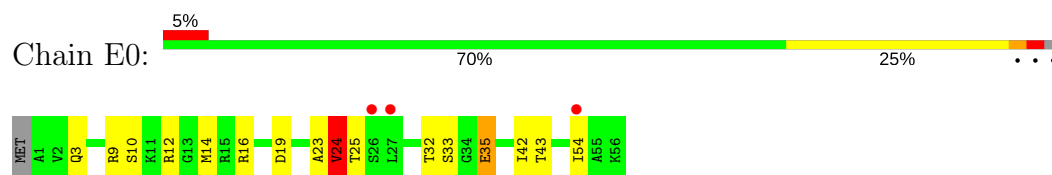
- Molecule 27: 50S ribosomal protein L32



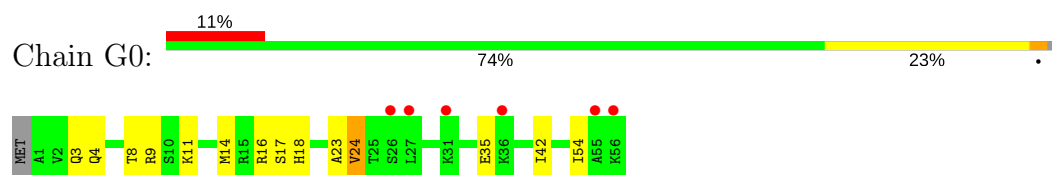
- Molecule 27: 50S ribosomal protein L32



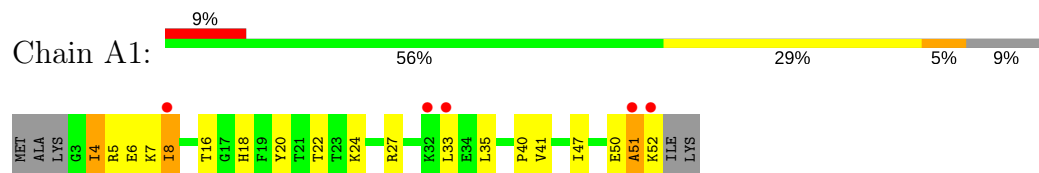
- Molecule 27: 50S ribosomal protein L32



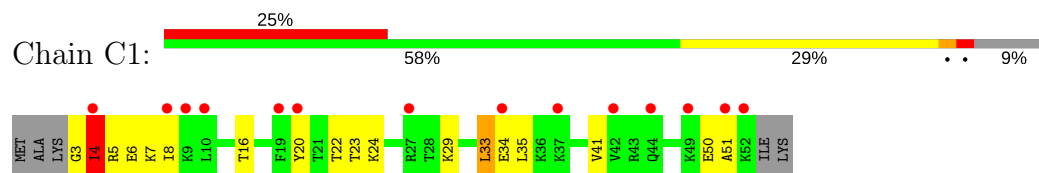
- Molecule 27: 50S ribosomal protein L32



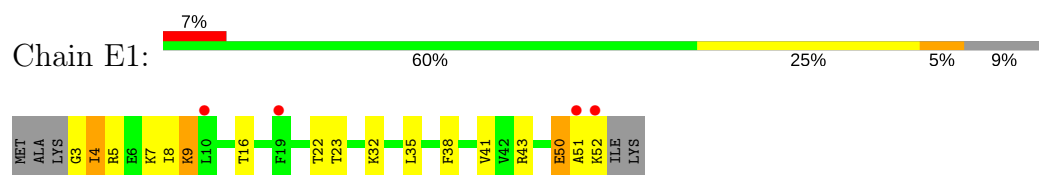
- Molecule 28: 50S ribosomal protein L33



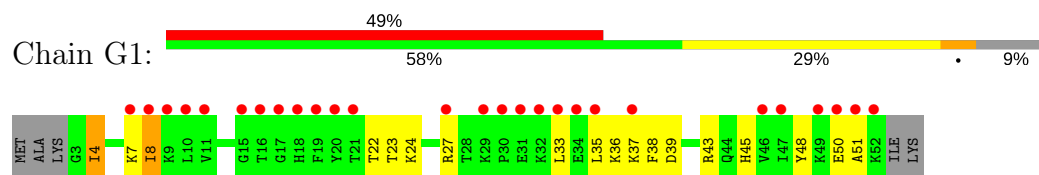
- Molecule 28: 50S ribosomal protein L33



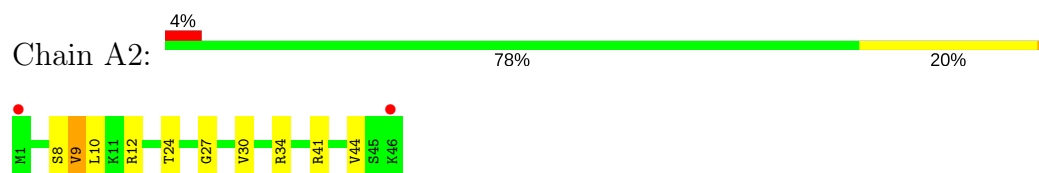
- Molecule 28: 50S ribosomal protein L33



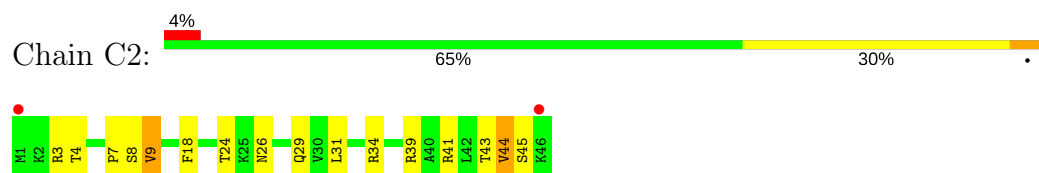
- Molecule 28: 50S ribosomal protein L33



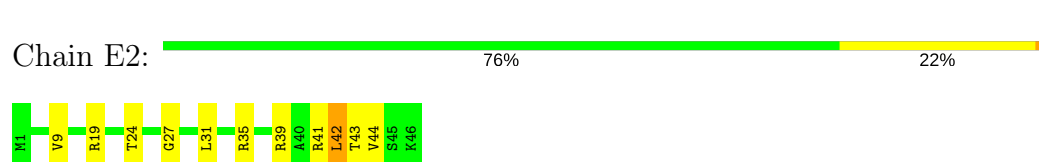
- Molecule 29: 50S ribosomal protein L34



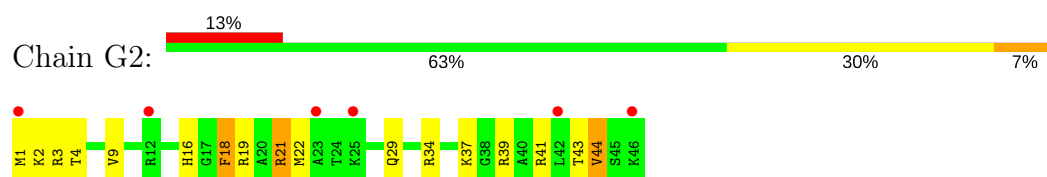
- Molecule 29: 50S ribosomal protein L34



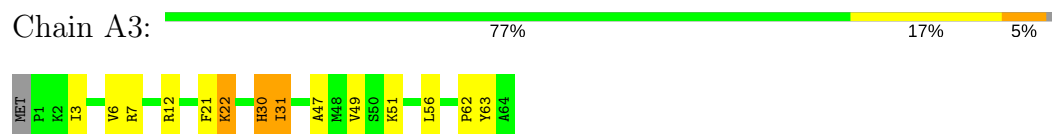
- Molecule 29: 50S ribosomal protein L34



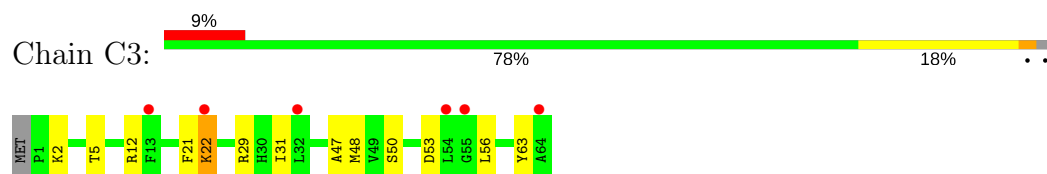
- Molecule 29: 50S ribosomal protein L34



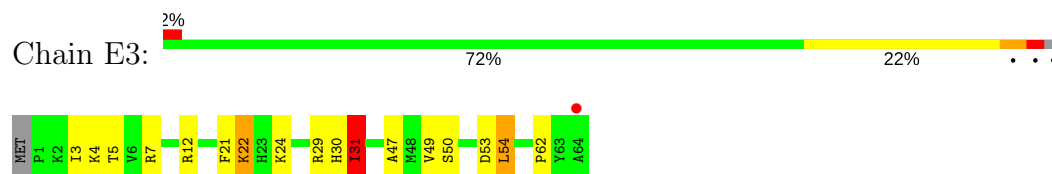
- Molecule 30: 50S ribosomal protein L35



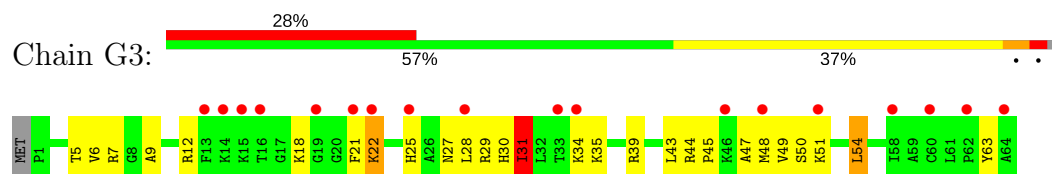
- Molecule 30: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L35



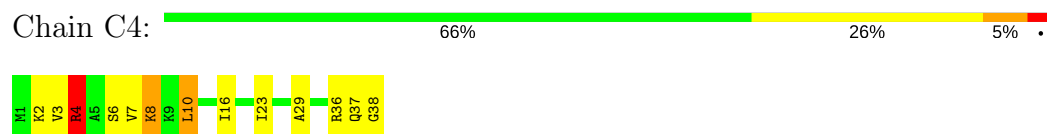
- Molecule 30: 50S ribosomal protein L35



- Molecule 31: 50S ribosomal protein L36

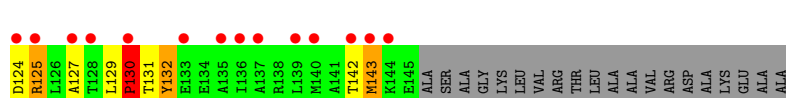


- Molecule 31: 50S ribosomal protein L36



- Molecule 31: 50S ribosomal protein L36



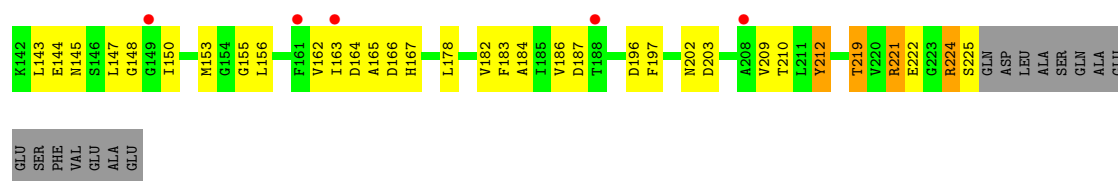


- Chain A6:
- 
- Sequence logo for Chain A6. The y-axis represents frequency in bits (0.00 to 0.15). The x-axis lists amino acids. A bar chart above the sequence shows the percentage of each amino acid in the chain: MET (12%), S1 (15%), I7 (7%), T8 (12%), E9 (15%), A10 (7%), V11 (12%), A12 (15%), A13 (7%), M14 (12%), S15 (15%), V16 (7%), M17 (12%), D18 (15%), V19 (7%), P20 (12%), E21 (15%), L22 (7%), I23 (12%), S24 (15%), A25 (7%), K26 (12%), E27 (15%), E28 (7%), K29 (12%), F30 (15%), GLY (7%), VAL (12%), SER (15%), ALA (7%), ALA (12%), ALA (15%), GLY (7%), VAL (12%), VAL (15%), SER (7%), LYS (12%), ASP (15%), ASP (7%), ALA (12%), ALA (15%), PRO (7%), VAL (12%), VAL (15%), GLU (7%), ALA (12%), ALA (15%), GLU (7%), GLY (12%), LYS (15%), THR (7%), PHE (12%), ASP (15%), VAL (7%), ILE (12%), LEU (15%), LYS (7%), ALA (12%), ALA (15%), GLY (7%), ALA (12%).

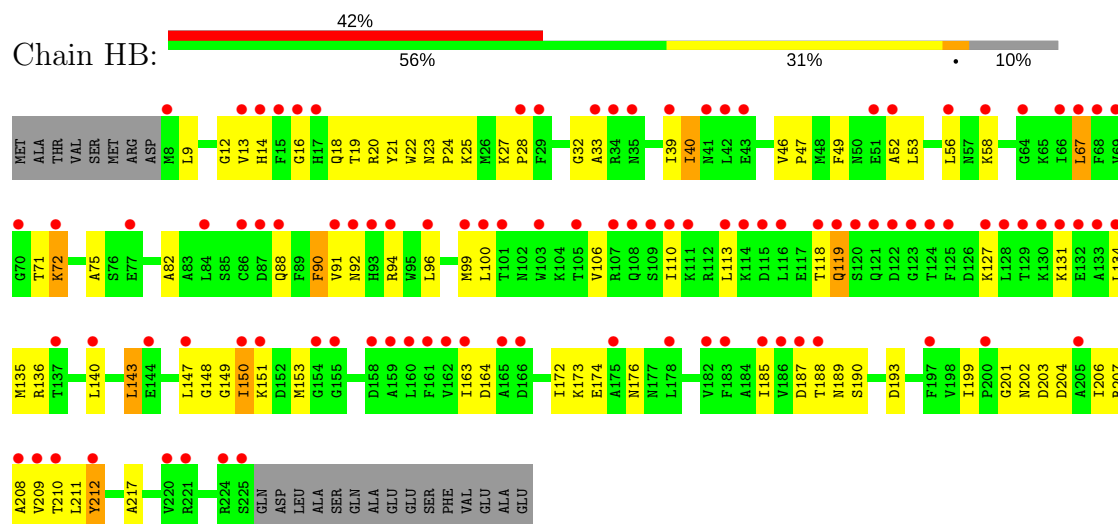
- Chain BB:
- 
- | Category | Percentage |
|----------|------------|
| Red      | 12%        |
| Green    | 56%        |
| Yellow   | 29%        |
| Orange   | 5%         |
| Grey     | 10%        |

- Chain DB:

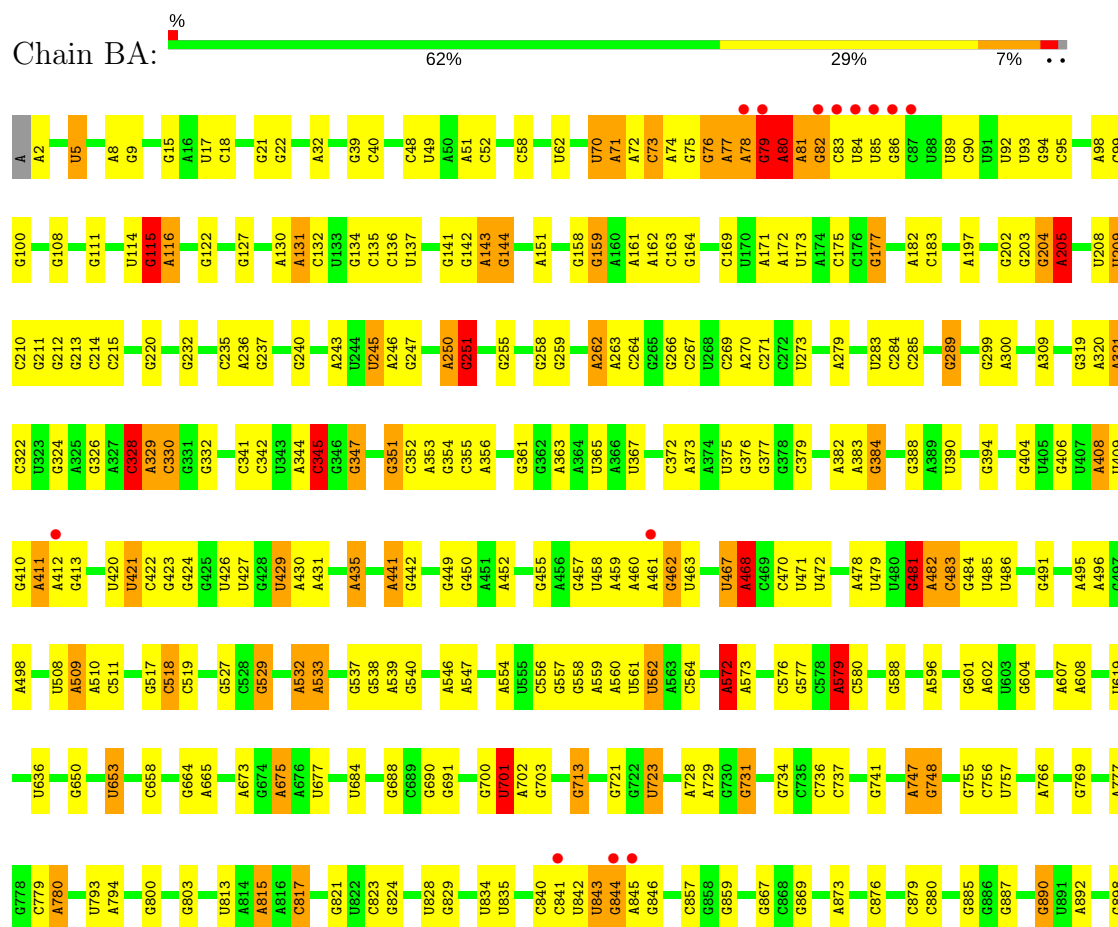
- Chain FB:
- 
- 13% 52% 34% 5% 10%
- Chain FB categories (from top to bottom): MET, THR, ALA, VAL, SER, MET, ARG, ASP, P8, L9, H14, F15, G16, H17, O18, T19, R20, Y21, W22, N23, P24, G25, K26, K27, P28, F29, G32, A33, R34, H38, I39, T40, H41, L42, E43, K44, T45, V46, P47, H48, F49, N50, E51, A52, L53, N57, K58, T59, A60, K63, G64, R65, F68, H69.

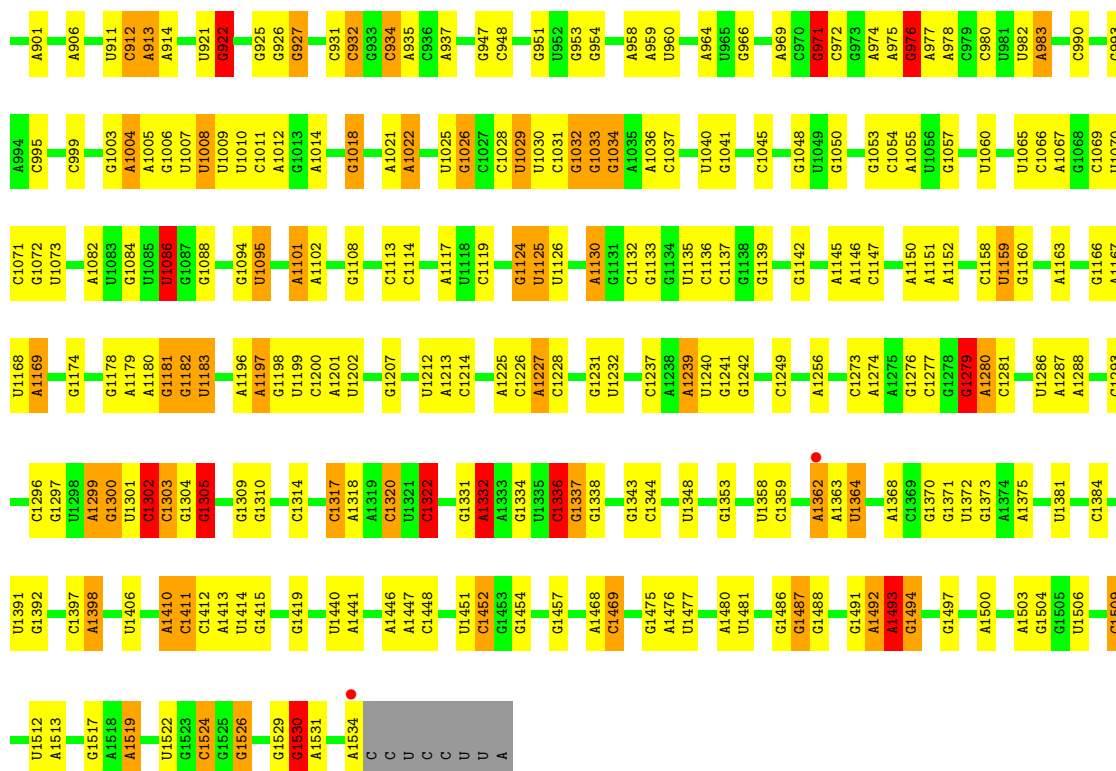


• Molecule 34: 30S ribosomal protein S2

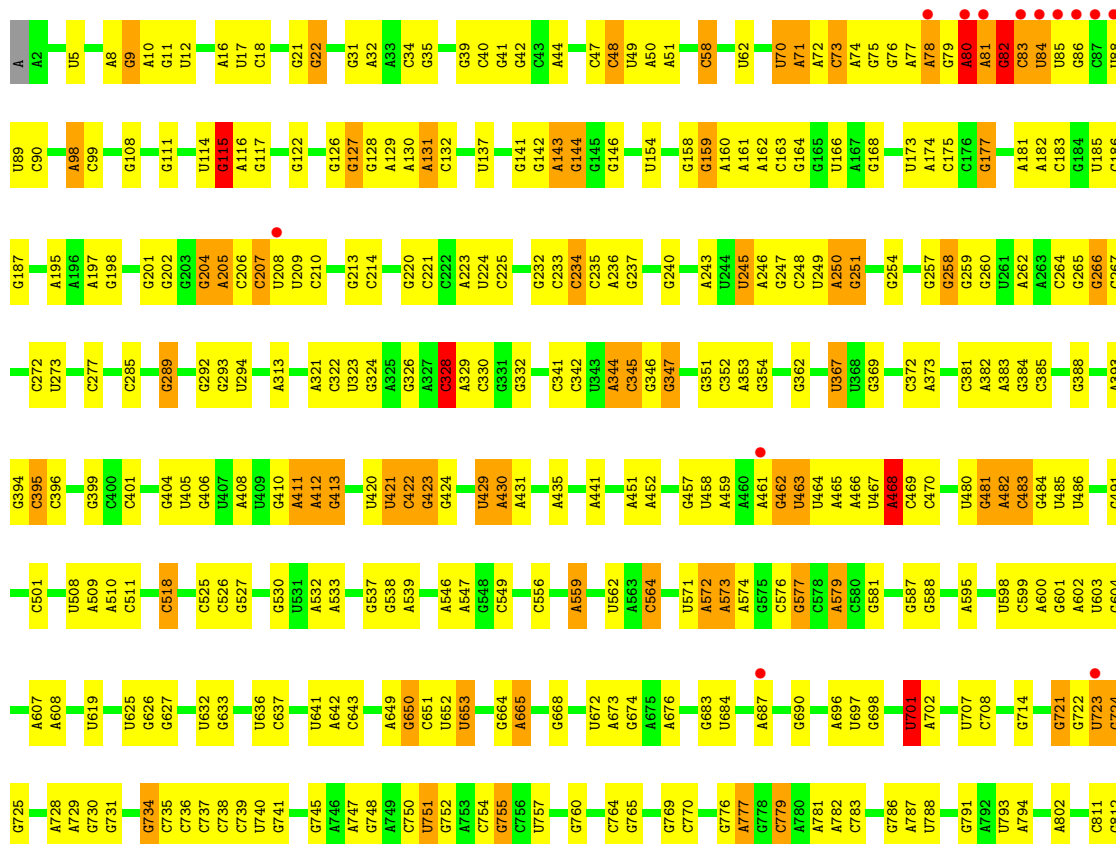


• Molecule 35: 16S rRNA

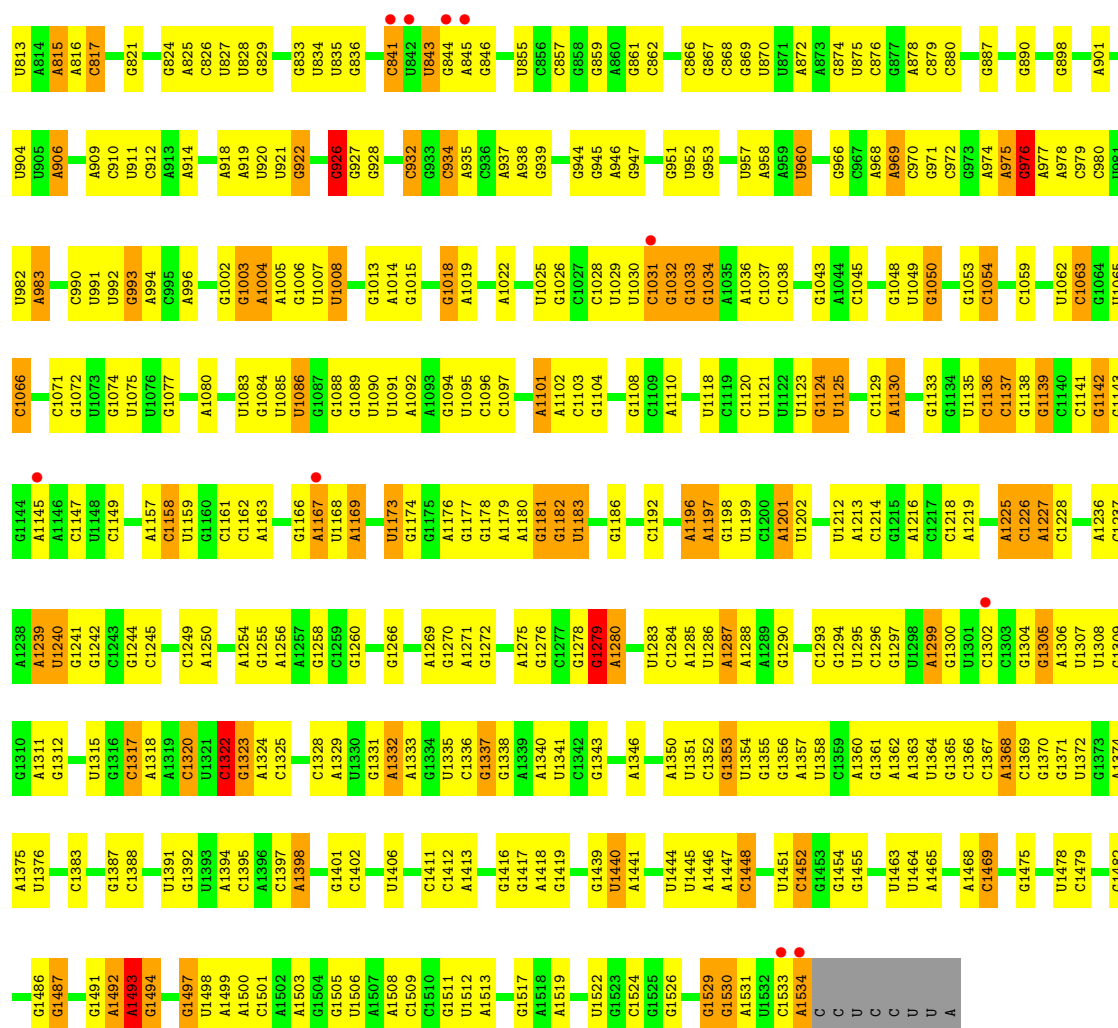




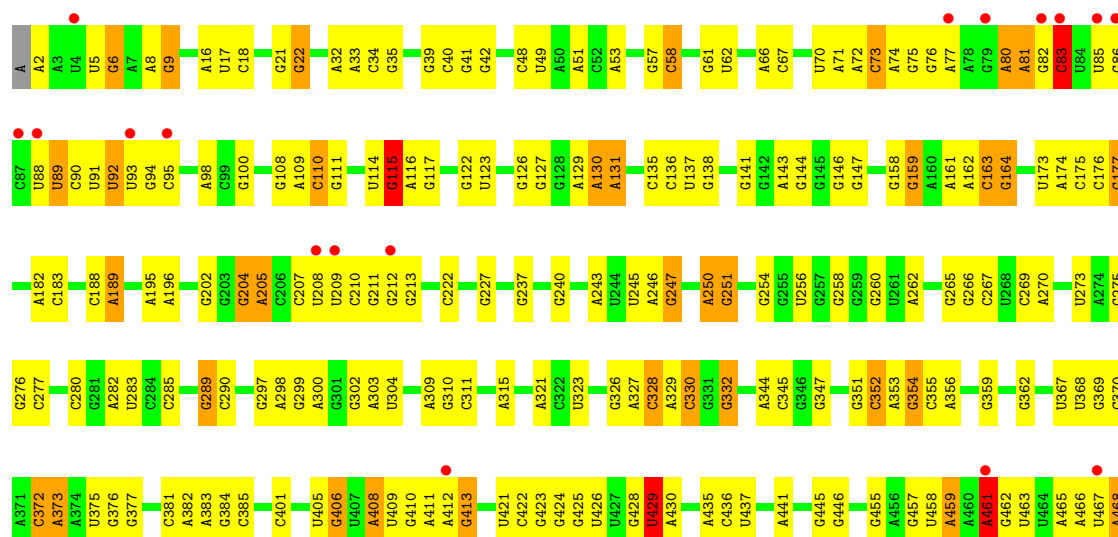
• Molecule 35: 16S rRNA







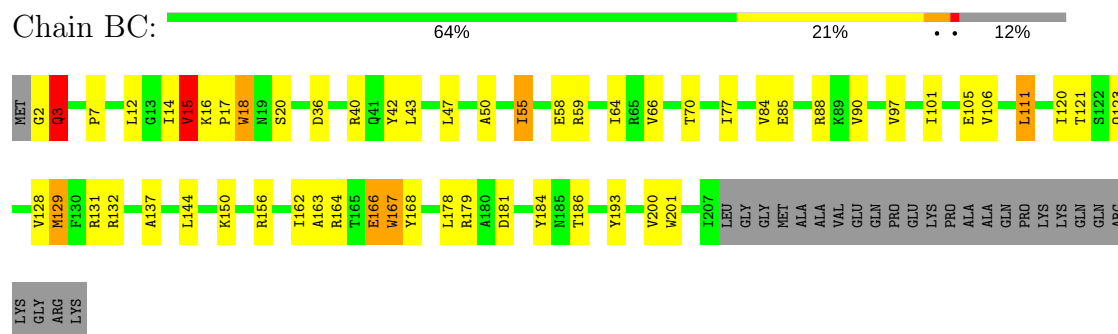
### • Molecule 35: 16S rRNA



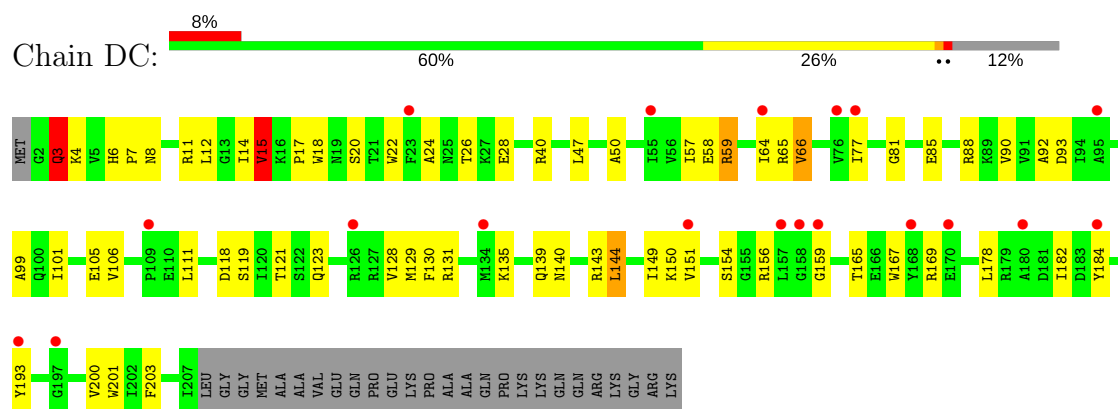


G1486	G1487	G1488	G1491	A1492	G1493	G1494	G1496	G1497	A1503	G1504	G1505	G1506	G1509	G1510	G1511	G1512	A1513	G1517	A1518	A1519	G1520	G1521	G1522	G1523	G1524	G1525	G1526	G1527	G1528	G1529	G1530	A1531	G1532	G1533	A1534	C	C	U	U	C	U	U	U	A																																																																																																																																																																																																																																																																																																																																																																																																																																																								
U1376	A1377	C1378	G1379	U1380	U1381	U1382	U1383	U1384	U1385	U1386	U1387	U1388	U1389	U1390	U1391	U1392	U1393	U1394	U1395	U1396	U1397	U1398	U1399	U1400	U1401	U1402	U1403	U1404	U1405	U1406	U1407	U1408	U1409	U1410	U1411	U1412	U1413	U1414	U1415	U1416	U1417	U1418	U1419	U1420	U1421	U1422	U1423	U1424	U1425	U1426	U1427	U1428	U1429	U1430	U1431	U1432	U1433	U1434	U1435	U1436	U1437	U1438	U1439	U1440	U1441	U1442	U1443	U1444	U1445	U1446	U1447	U1448	U1449	U1450	U1451	U1452	C1453	U1454	U1455	U1456	U1457	U1458	U1459	U1460	U1461	U1462	U1463	U1464	U1465	U1466	U1467																																																																																																																																																																																																																																																																																																																																																																																																									
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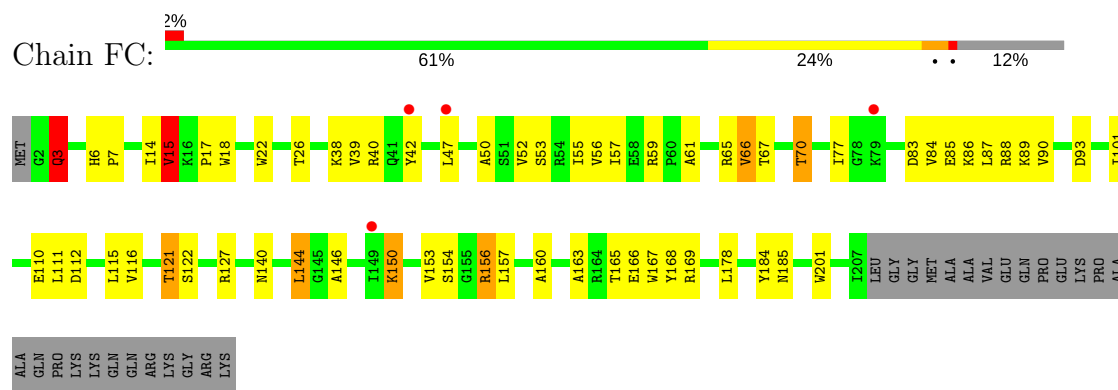
- Molecule 36: 30S ribosomal protein S3



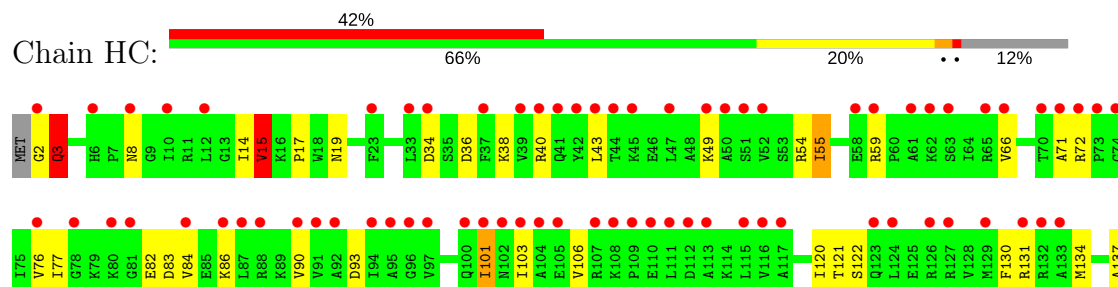
- Molecule 36: 30S ribosomal protein S3

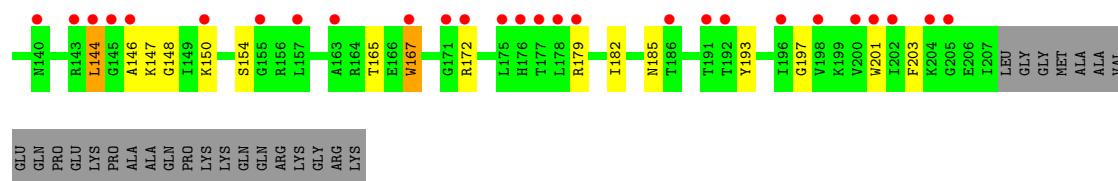


- Molecule 36: 30S ribosomal protein S3

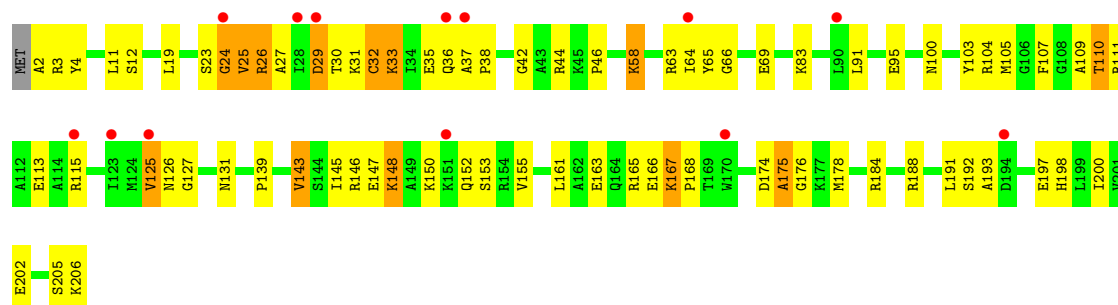


- Molecule 36: 30S ribosomal protein S3

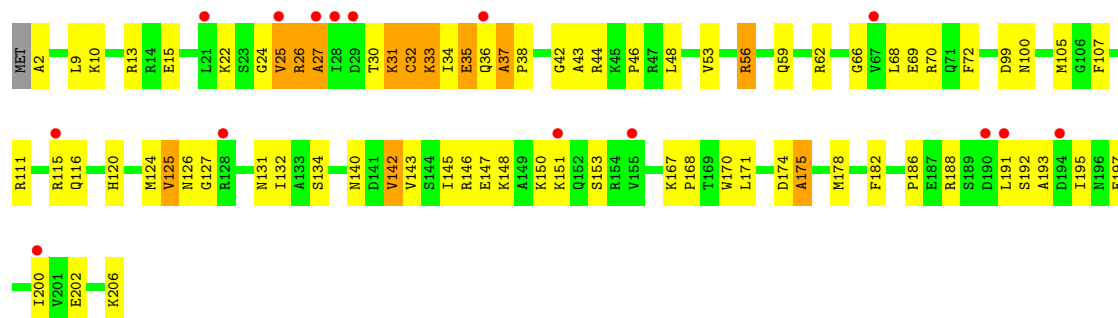




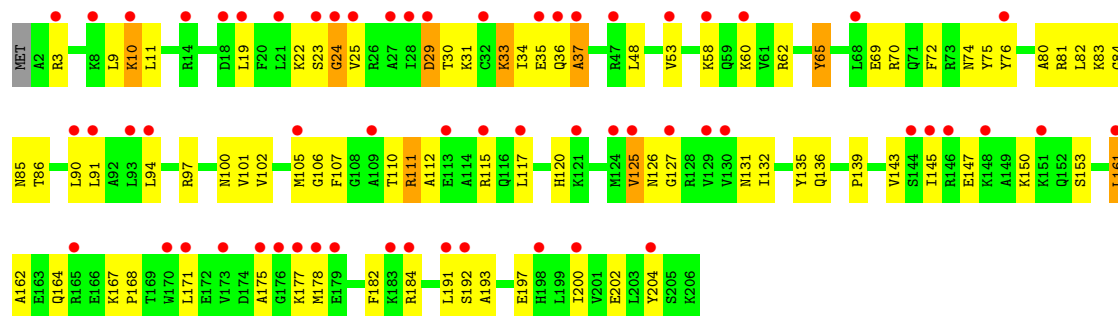
• Molecule 37: 30S ribosomal protein S4



• Molecule 37: 30S ribosomal protein S4

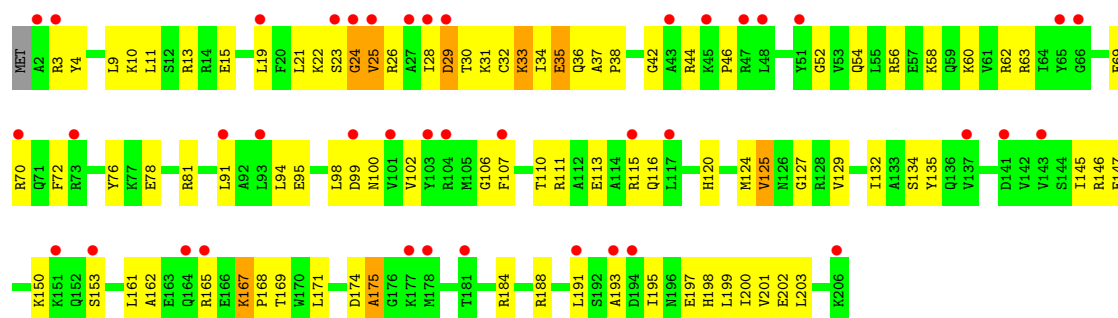


• Molecule 37: 30S ribosomal protein S4

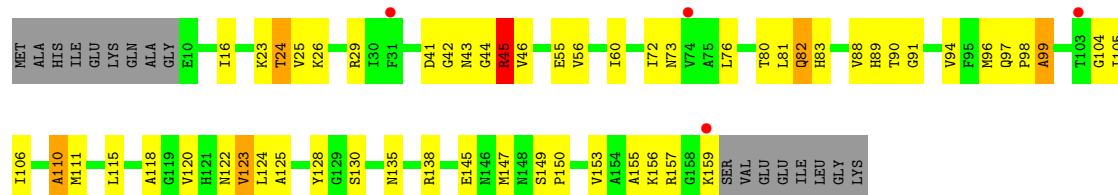


• Molecule 37: 30S ribosomal protein S4

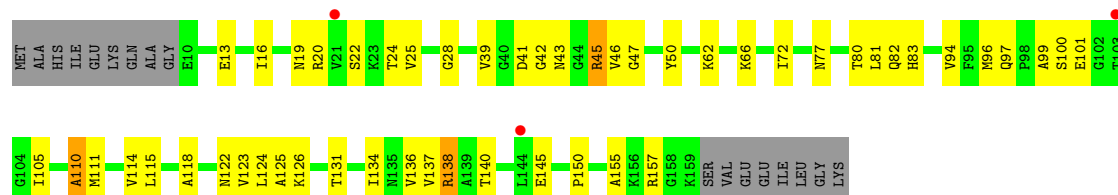




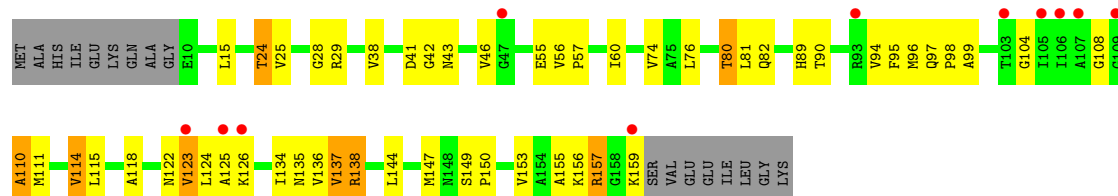
• Molecule 38: 30S ribosomal protein S5



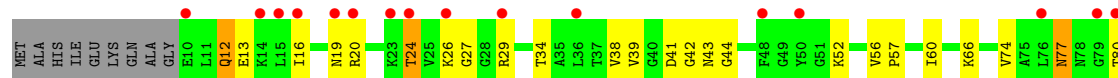
• Molecule 38: 30S ribosomal protein S5

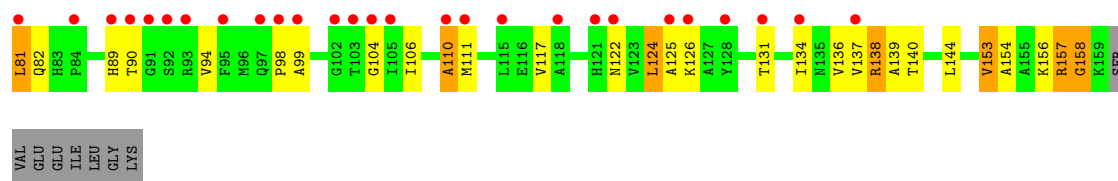


• Molecule 38: 30S ribosomal protein S5

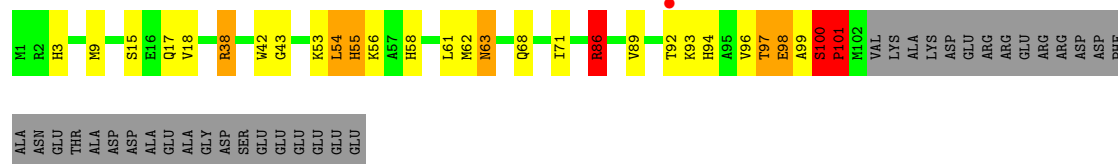


• Molecule 38: 30S ribosomal protein S5

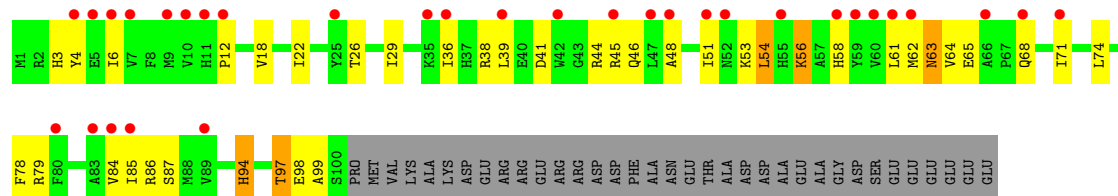




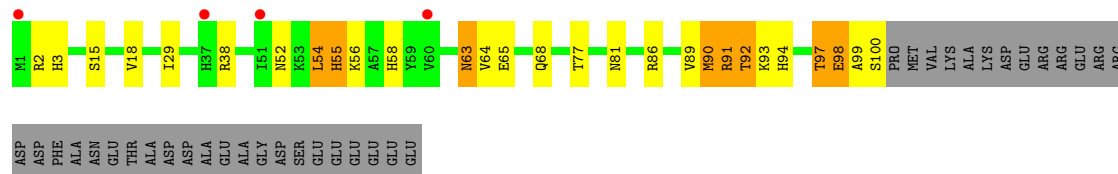
• Molecule 39: 30S ribosomal protein S6



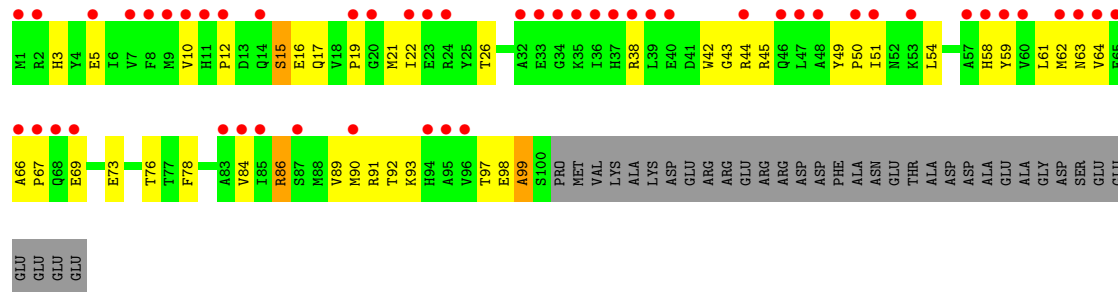
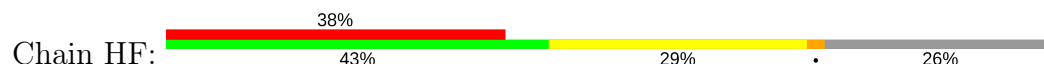
• Molecule 39: 30S ribosomal protein S6



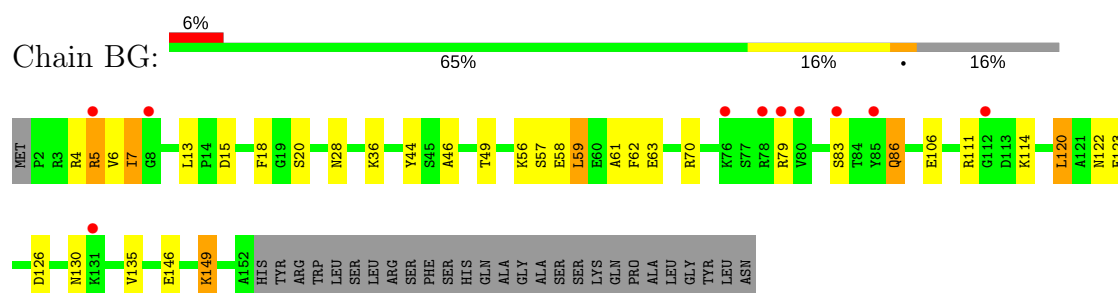
• Molecule 39: 30S ribosomal protein S6



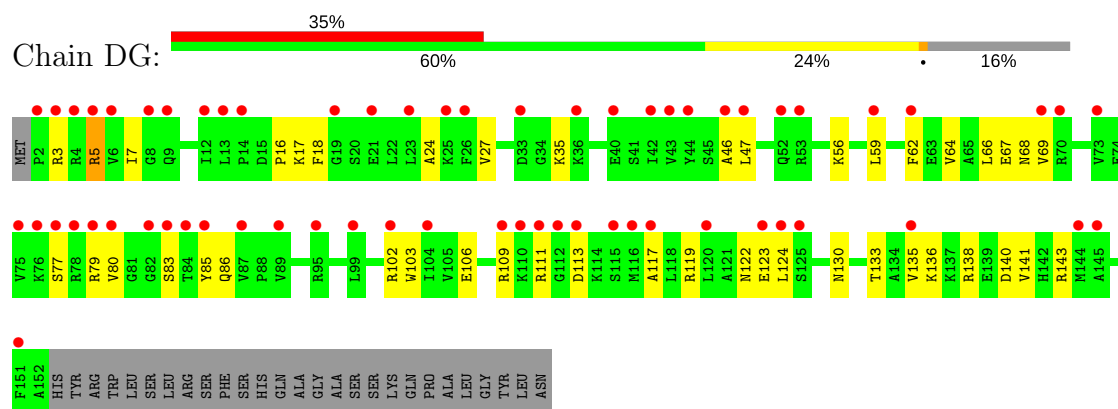
• Molecule 39: 30S ribosomal protein S6



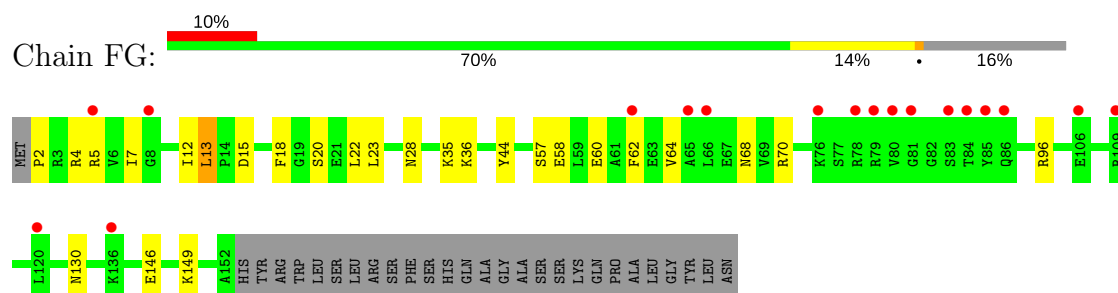
• Molecule 40: 30S ribosomal protein S7



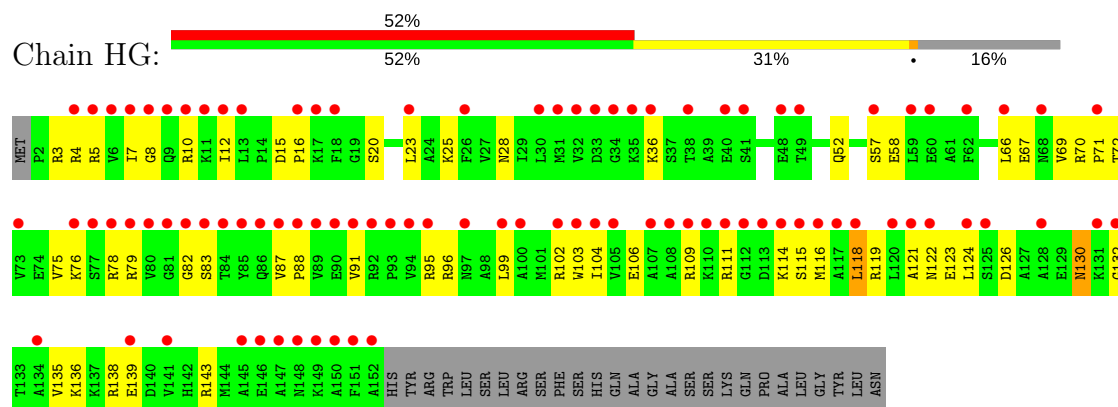
- Molecule 40: 30S ribosomal protein S7



- Molecule 40: 30S ribosomal protein S7



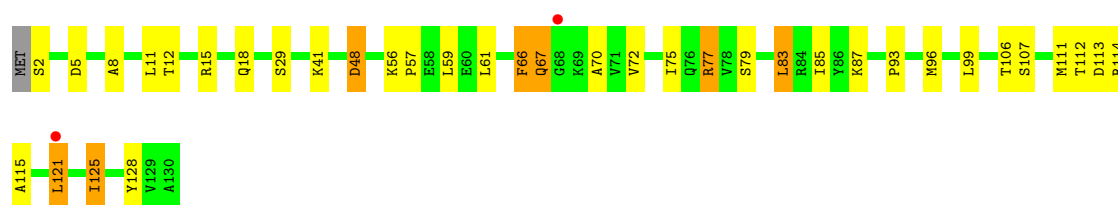
- Molecule 40: 30S ribosomal protein S7



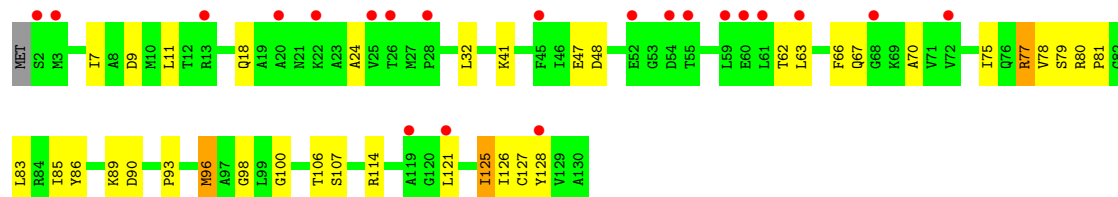
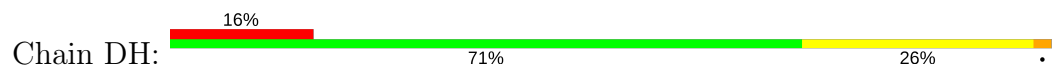
- Molecule 41: 30S ribosomal protein S8



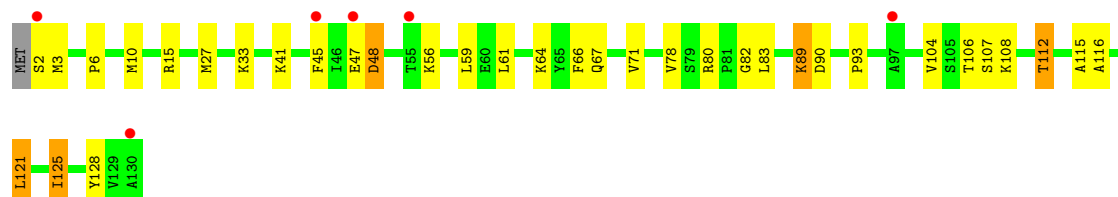
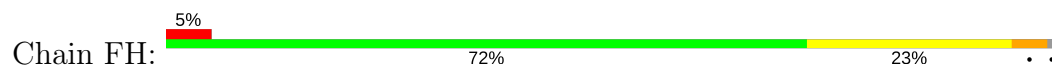




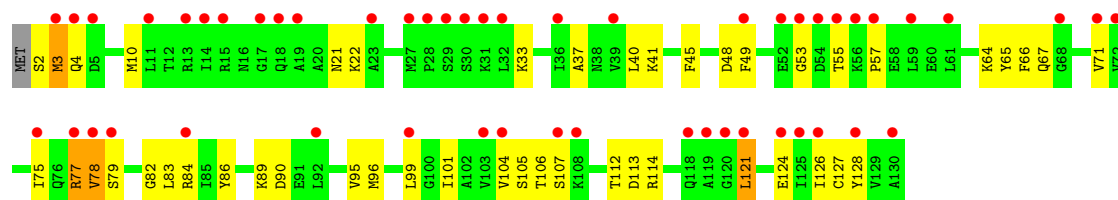
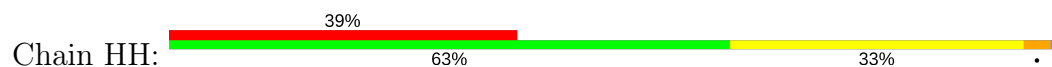
- Molecule 41: 30S ribosomal protein S8



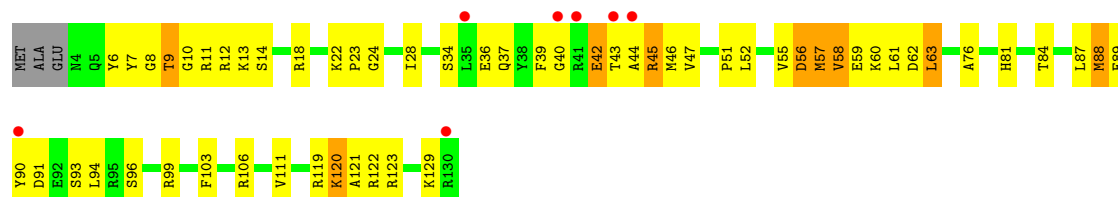
- Molecule 41: 30S ribosomal protein S8



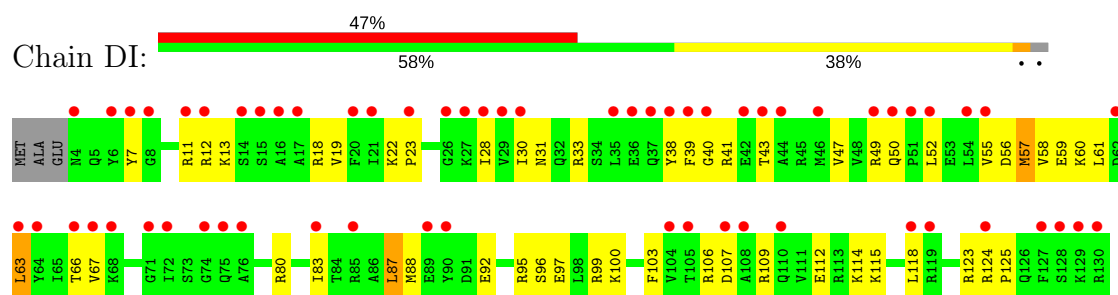
- Molecule 41: 30S ribosomal protein S8



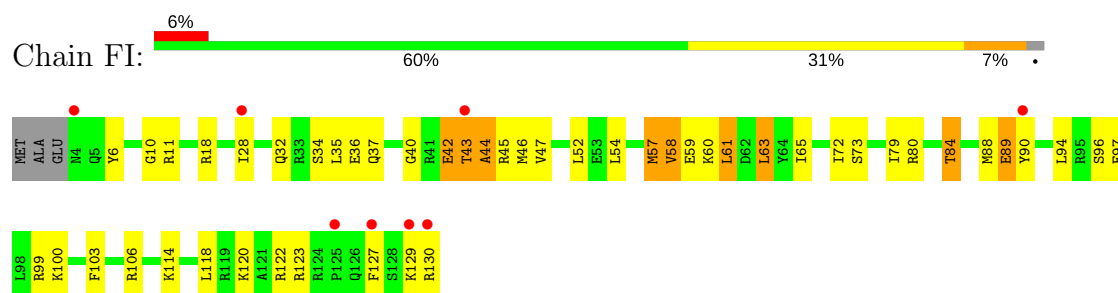
- Molecule 42: 30S ribosomal protein S9



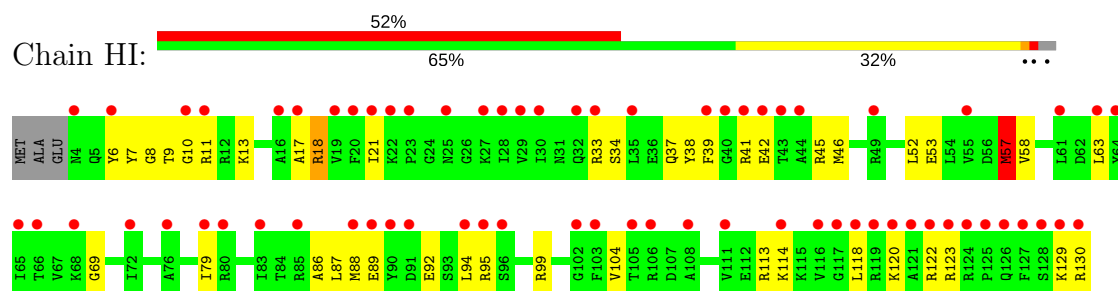
- Molecule 42: 30S ribosomal protein S9



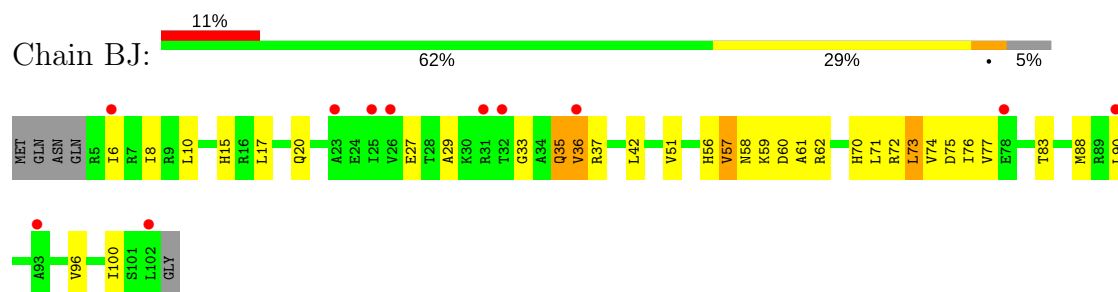
- Molecule 42: 30S ribosomal protein S9



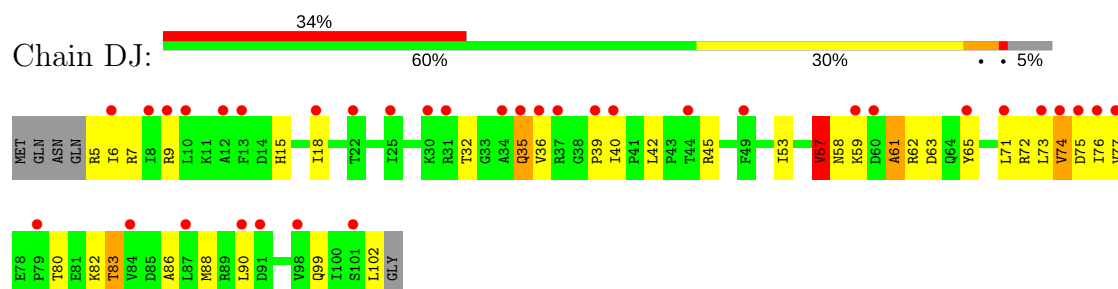
- Molecule 42: 30S ribosomal protein S9



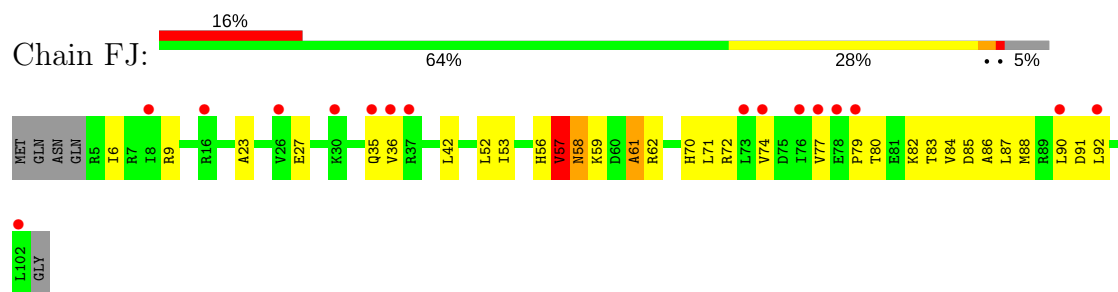
- Molecule 43: 30S ribosomal protein S10



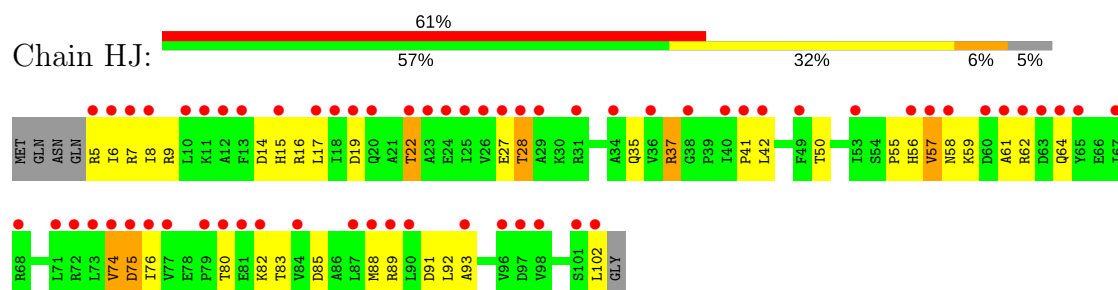
- Molecule 43: 30S ribosomal protein S10



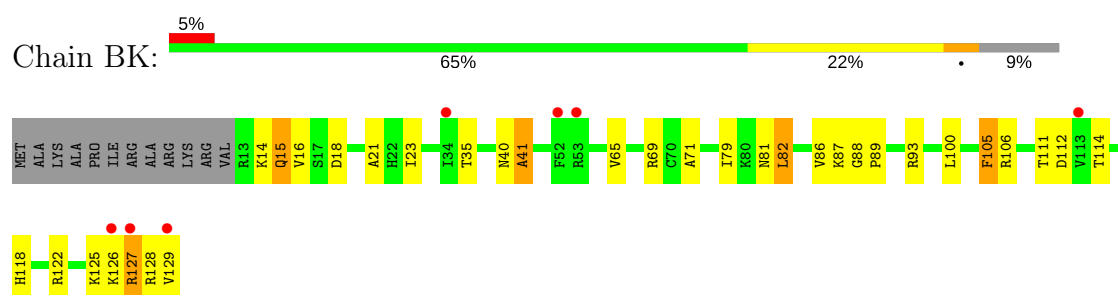
## • Molecule 43: 30S ribosomal protein S10



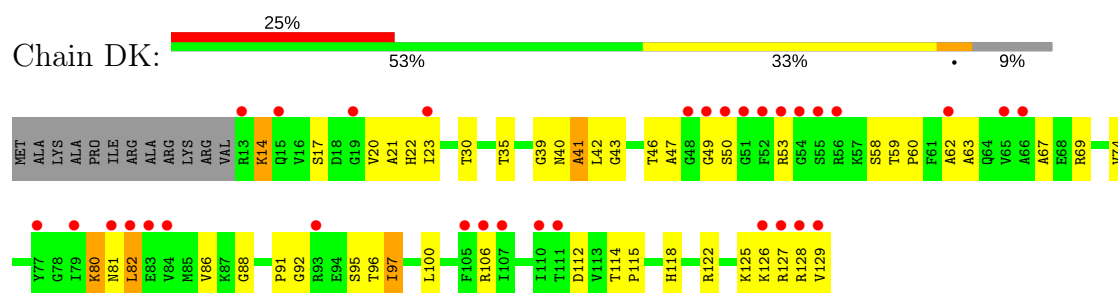
## • Molecule 43: 30S ribosomal protein S10



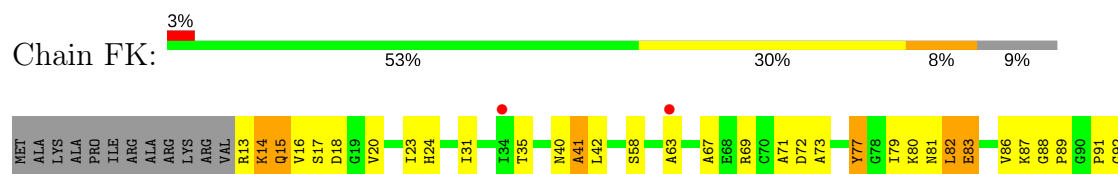
## • Molecule 44: 30S ribosomal protein S11



## • Molecule 44: 30S ribosomal protein S11

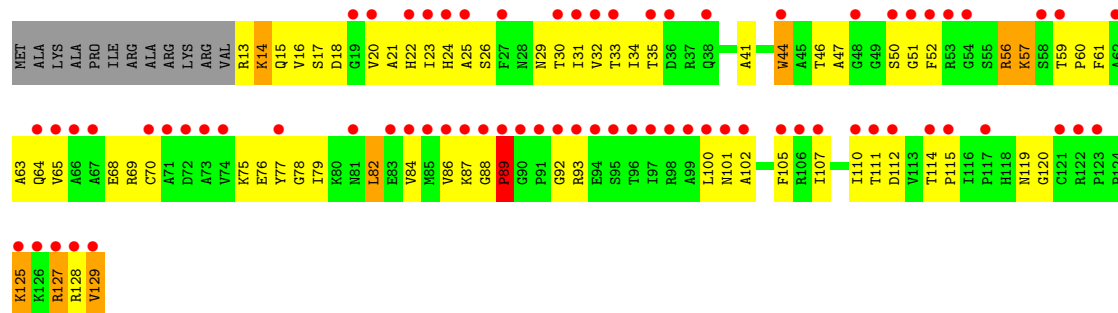
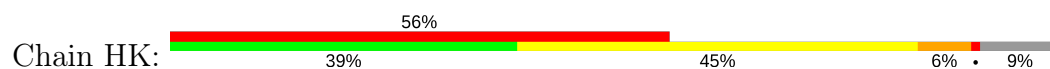


## • Molecule 44: 30S ribosomal protein S11

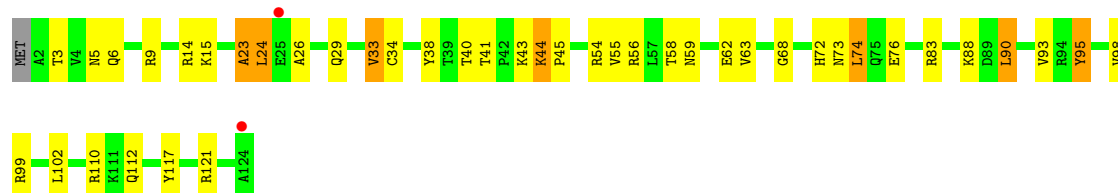




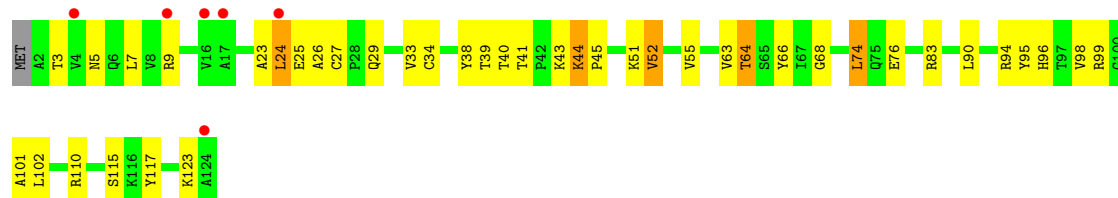
- Molecule 44: 30S ribosomal protein S11



- Molecule 45: 30S ribosomal protein S12



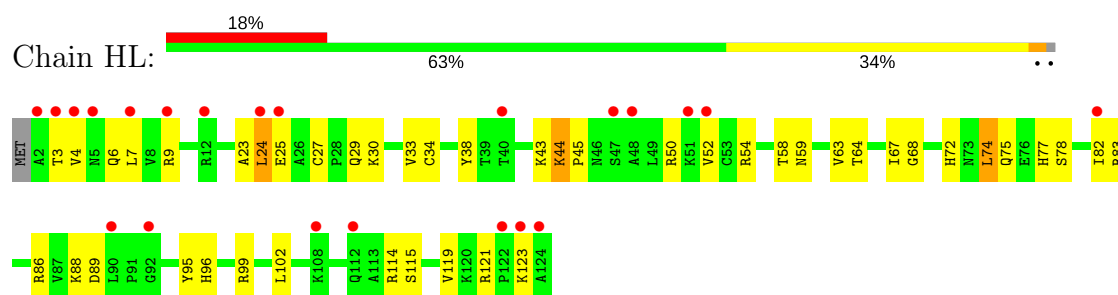
- Molecule 45: 30S ribosomal protein S12



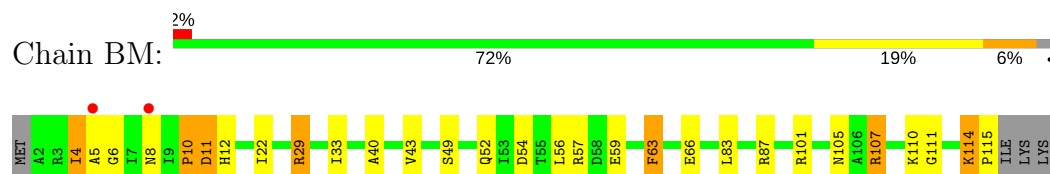
- Molecule 45: 30S ribosomal protein S12



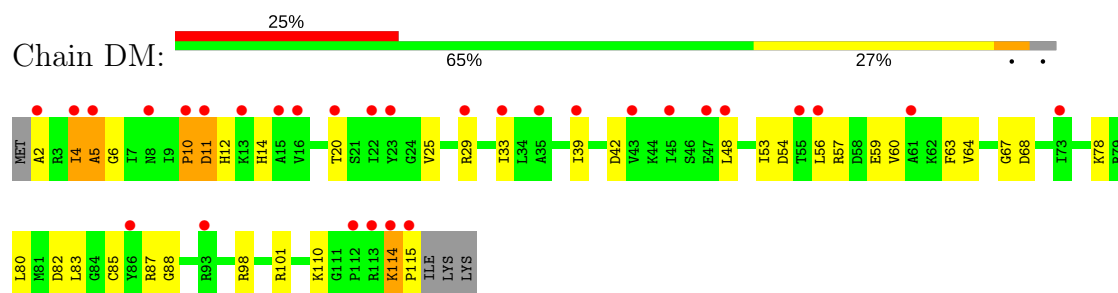
- Molecule 45: 30S ribosomal protein S12



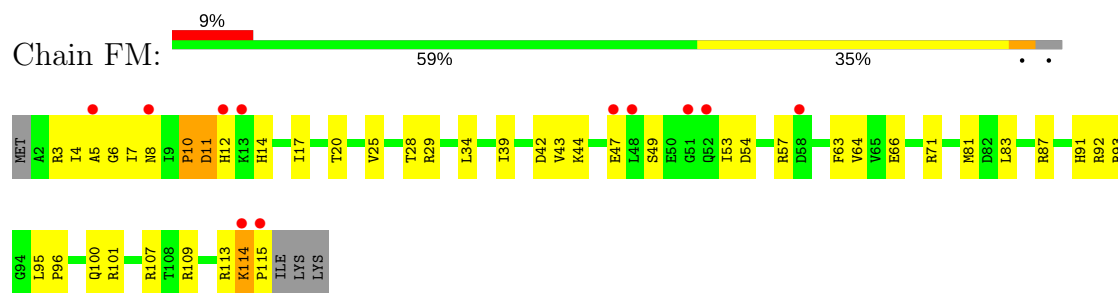
- Molecule 46: 30S ribosomal protein S13



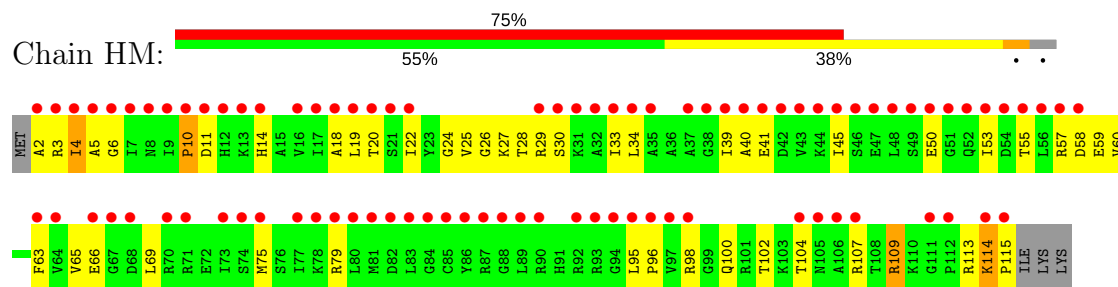
- Molecule 46: 30S ribosomal protein S13



- Molecule 46: 30S ribosomal protein S13

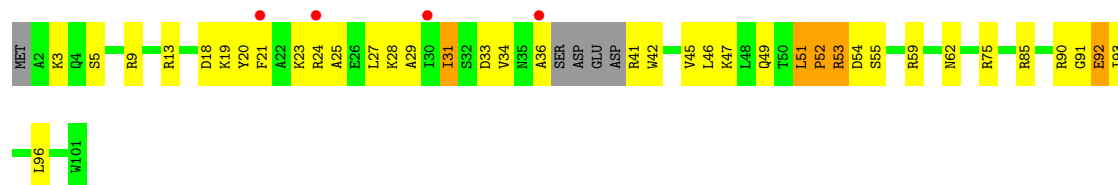


- Molecule 46: 30S ribosomal protein S13

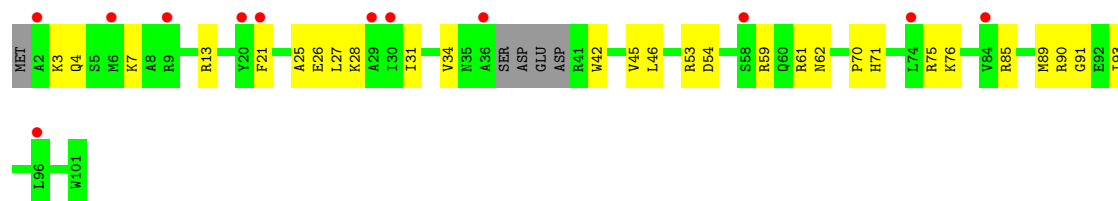


- Molecule 47: 30S ribosomal protein S14

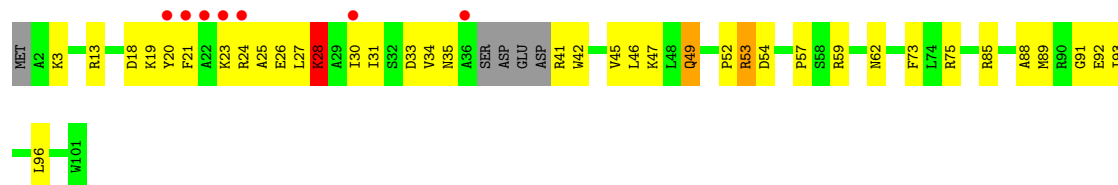




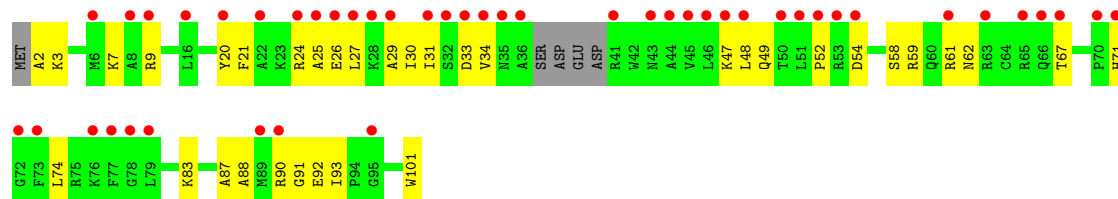
- Molecule 47: 30S ribosomal protein S14



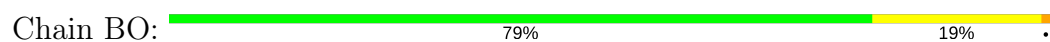
- Molecule 47: 30S ribosomal protein S14



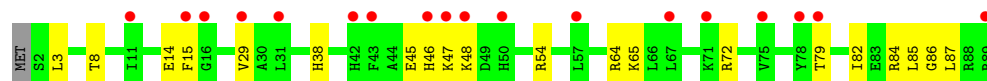
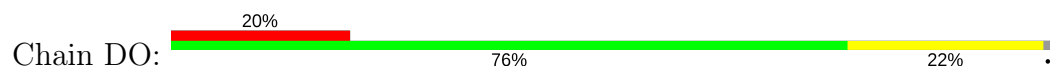
- Molecule 47: 30S ribosomal protein S14



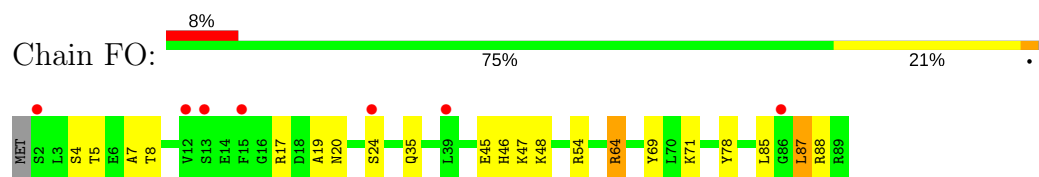
- Molecule 48: 30S ribosomal protein S15



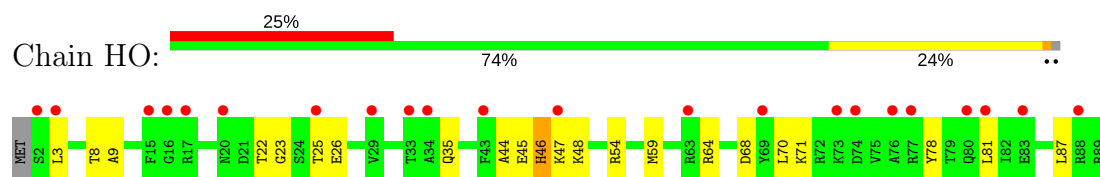
- Molecule 48: 30S ribosomal protein S15



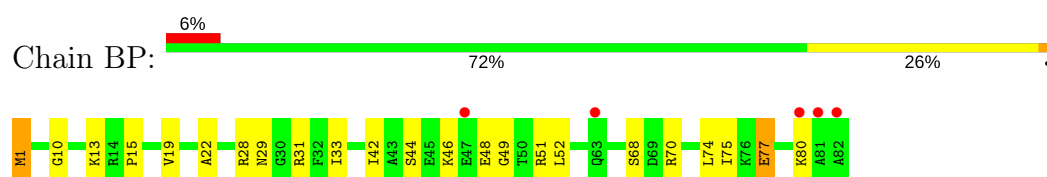
## • Molecule 48: 30S ribosomal protein S15



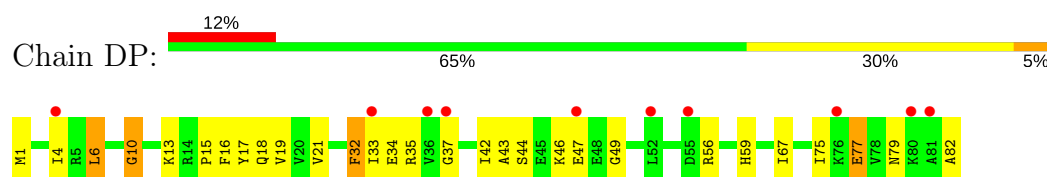
## • Molecule 48: 30S ribosomal protein S15



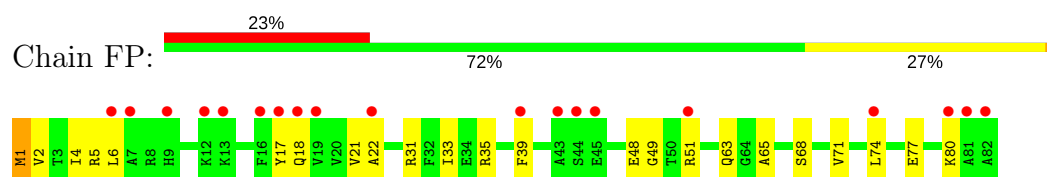
## • Molecule 49: 30S ribosomal protein S16



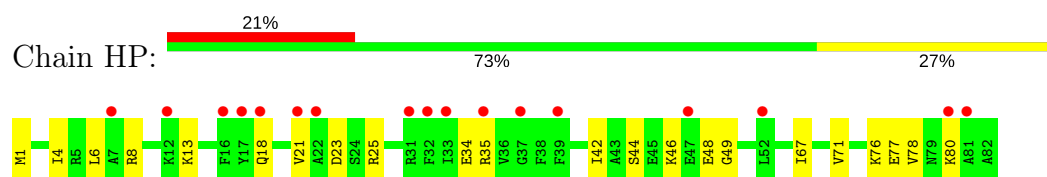
## • Molecule 49: 30S ribosomal protein S16



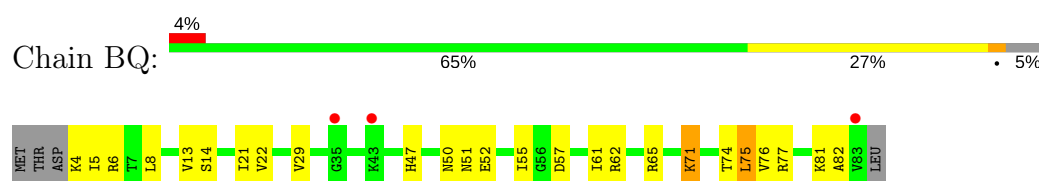
## • Molecule 49: 30S ribosomal protein S16



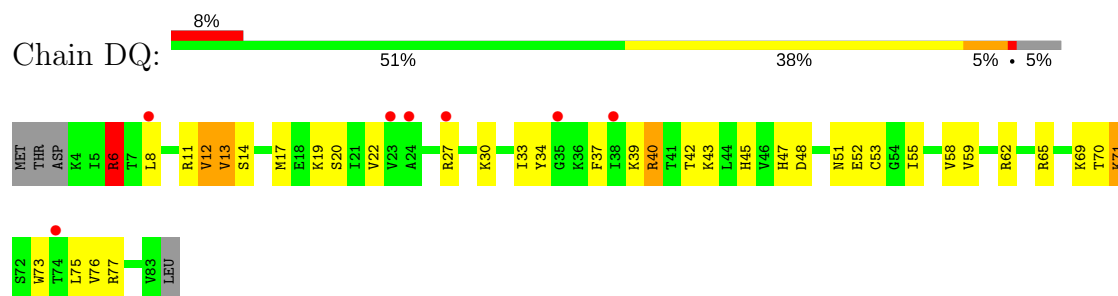
## • Molecule 49: 30S ribosomal protein S16



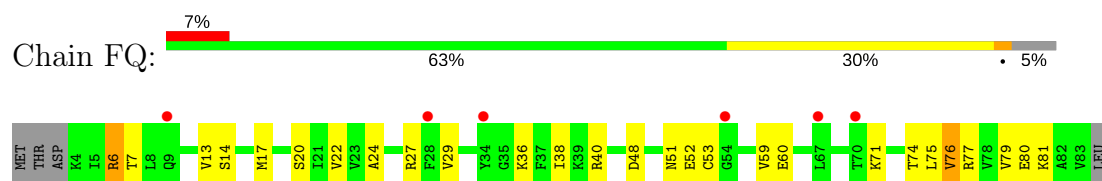
## • Molecule 50: 30S ribosomal protein S17



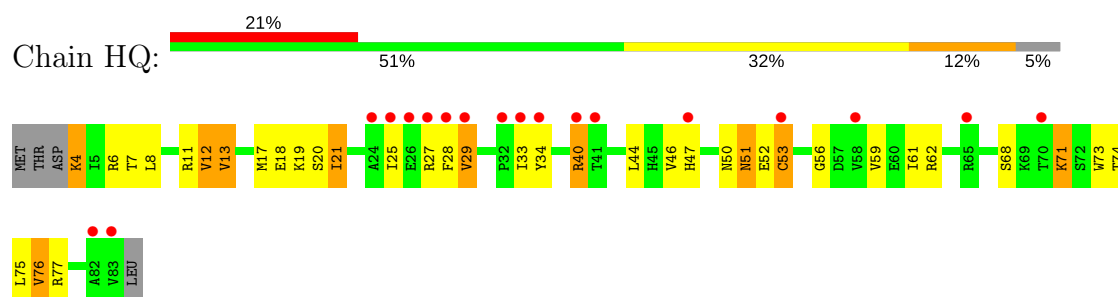
## • Molecule 50: 30S ribosomal protein S17



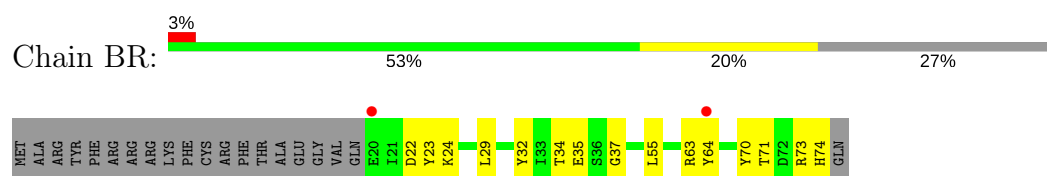
## • Molecule 50: 30S ribosomal protein S17



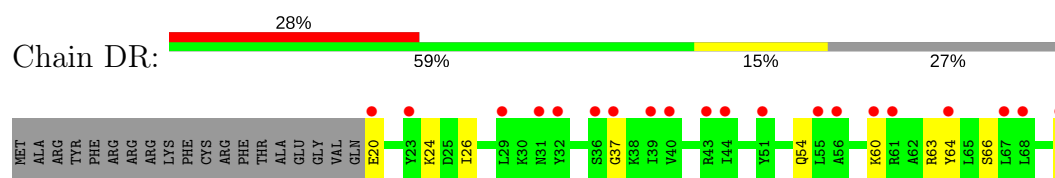
## • Molecule 50: 30S ribosomal protein S17



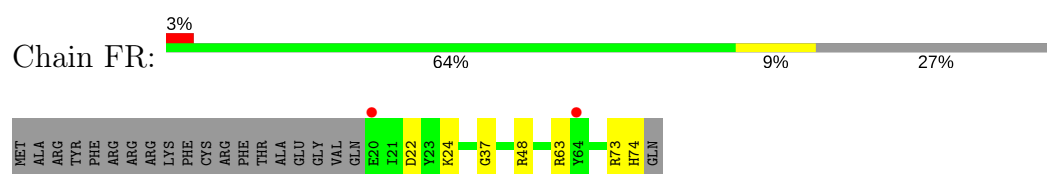
## • Molecule 51: 30S ribosomal protein S18



## • Molecule 51: 30S ribosomal protein S18

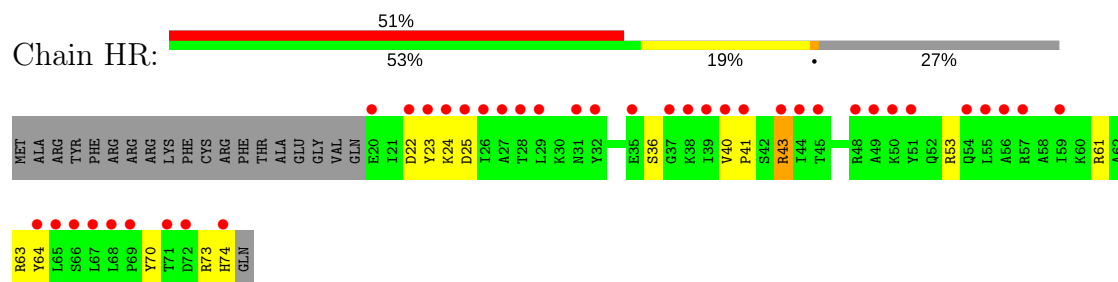


## • Molecule 51: 30S ribosomal protein S18

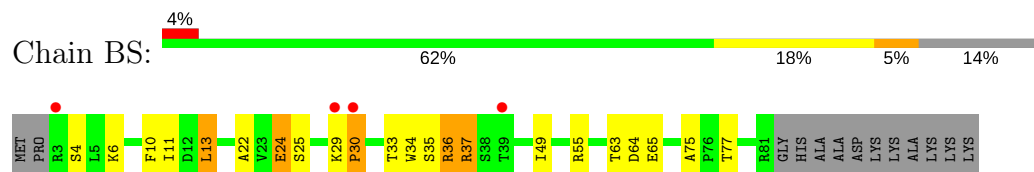




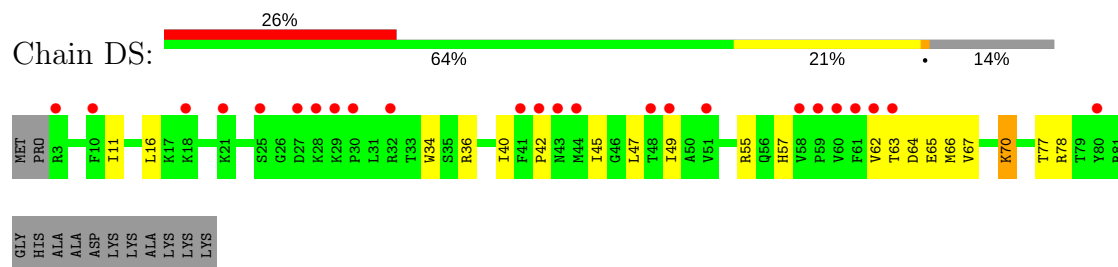
- Molecule 51: 30S ribosomal protein S18



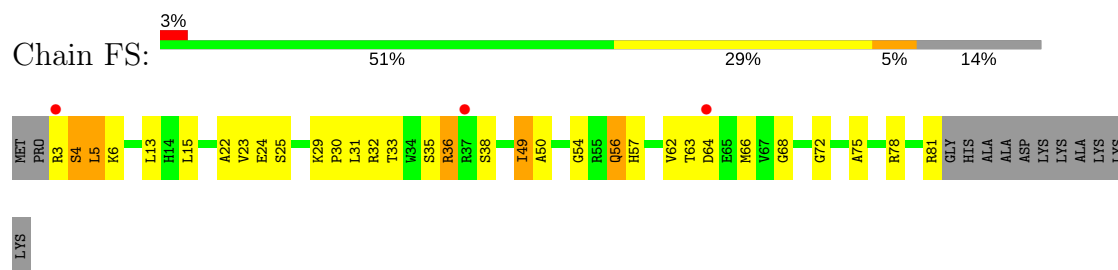
- Molecule 52: 30S ribosomal protein S19



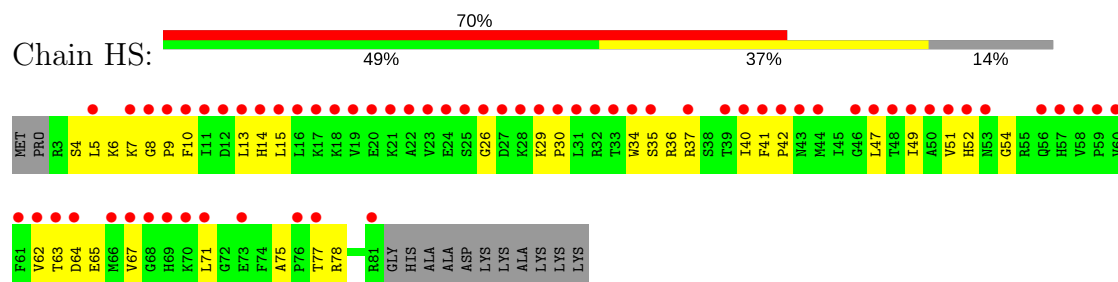
- Molecule 52: 30S ribosomal protein S19



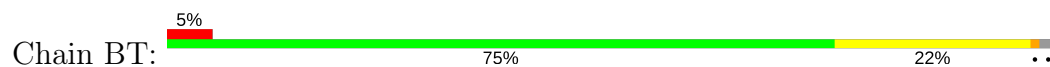
- Molecule 52: 30S ribosomal protein S19

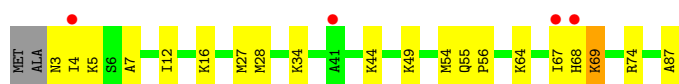


- Molecule 52: 30S ribosomal protein S19

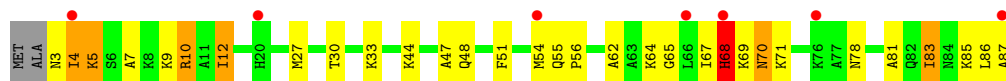


- Molecule 53: 30S ribosomal protein S20

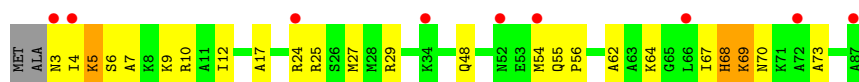




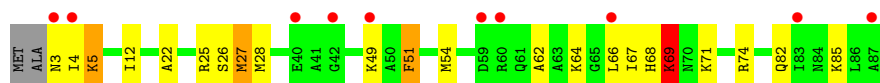
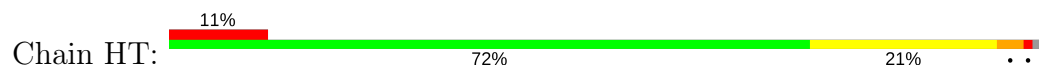
- Molecule 53: 30S ribosomal protein S20



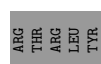
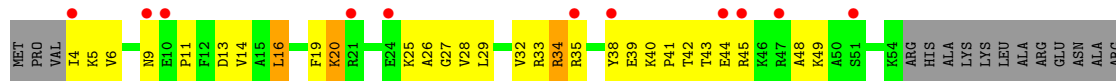
- Molecule 53: 30S ribosomal protein S20



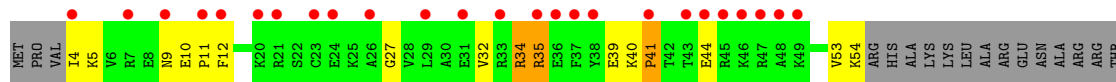
- Molecule 53: 30S ribosomal protein S20



- Molecule 54: 30S ribosomal protein S21

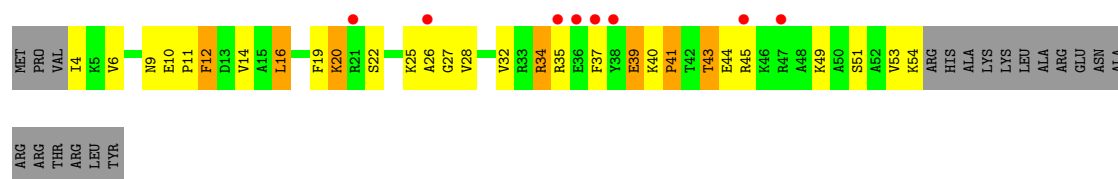


- Molecule 54: 30S ribosomal protein S21

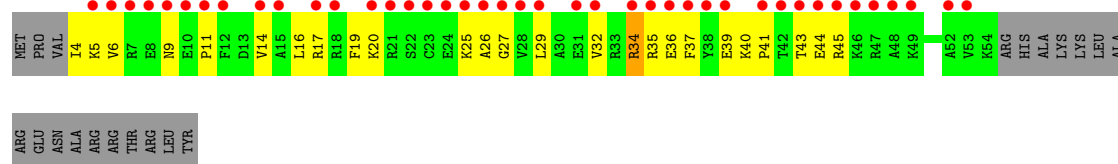
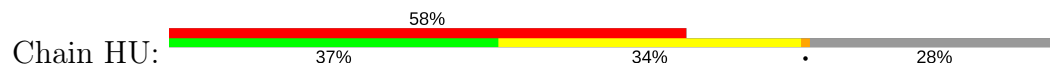


- Molecule 54: 30S ribosomal protein S21

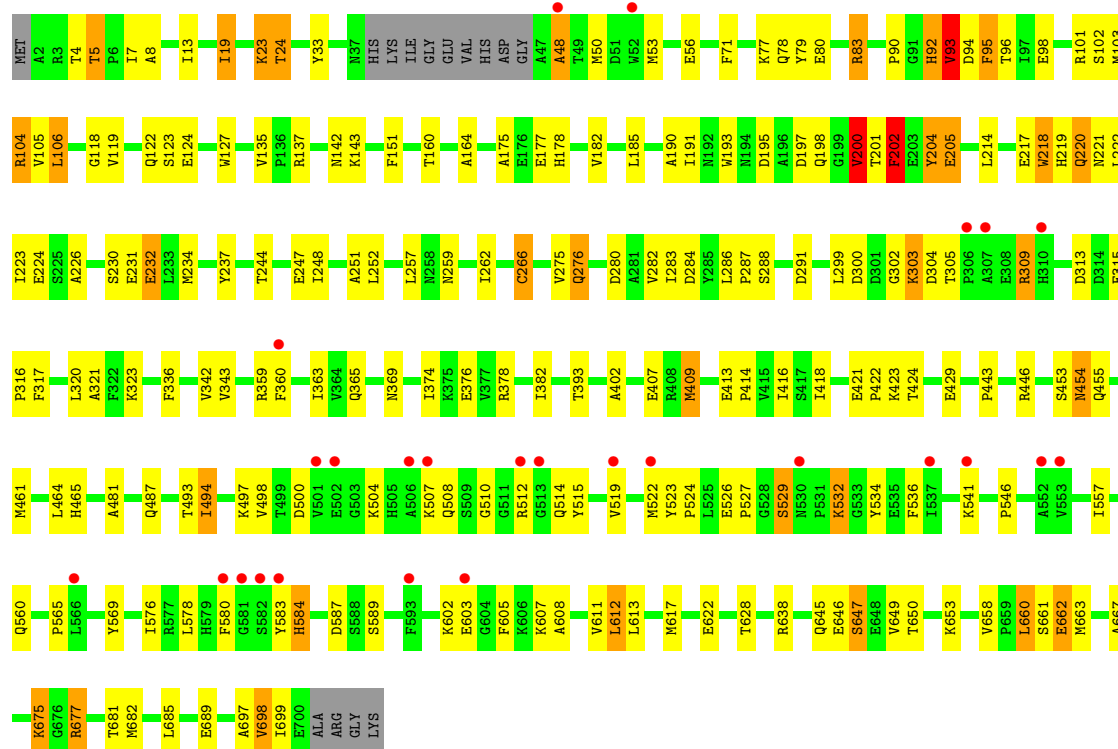




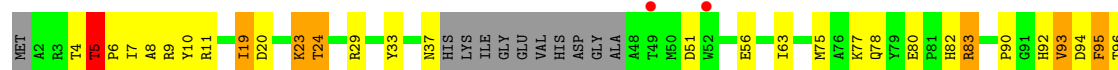
• Molecule 54: 30S ribosomal protein S21

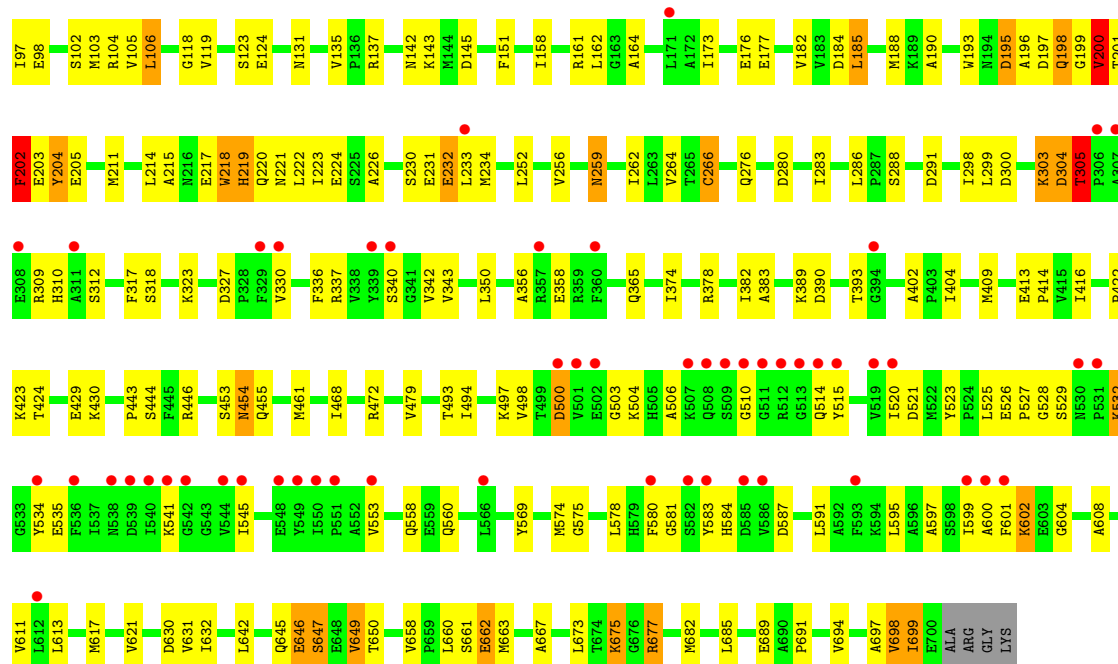


• Molecule 55: Elongation factor G

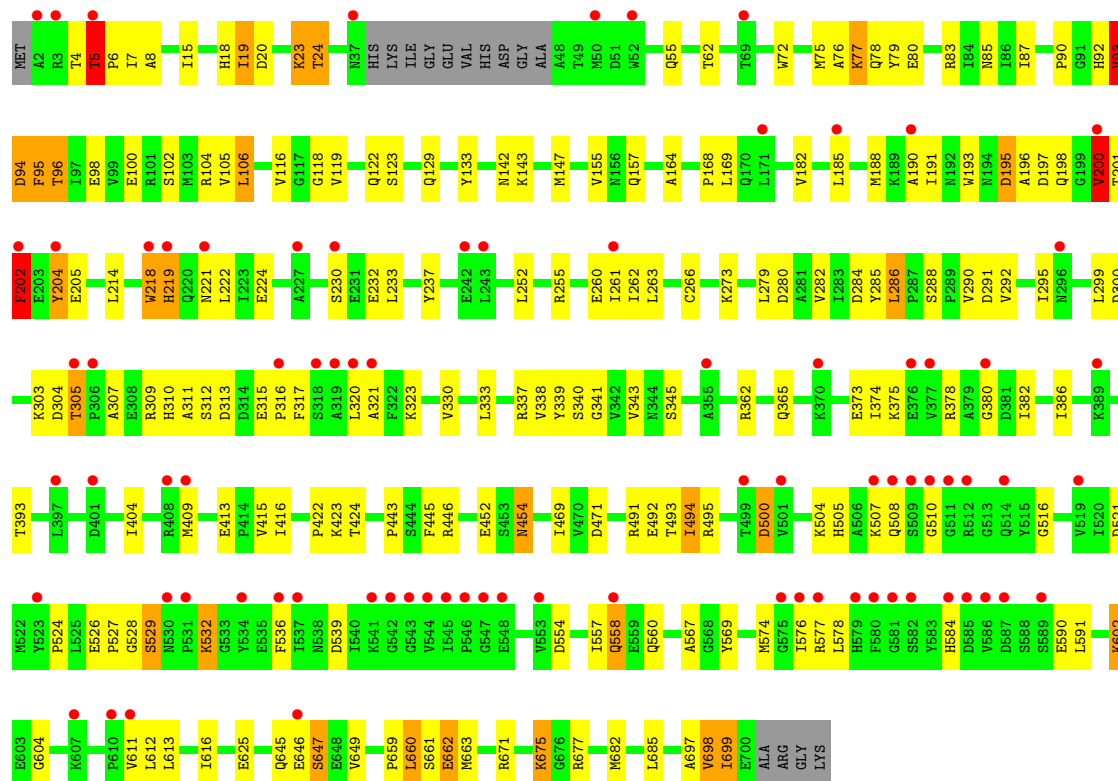


• Molecule 55: Elongation factor G



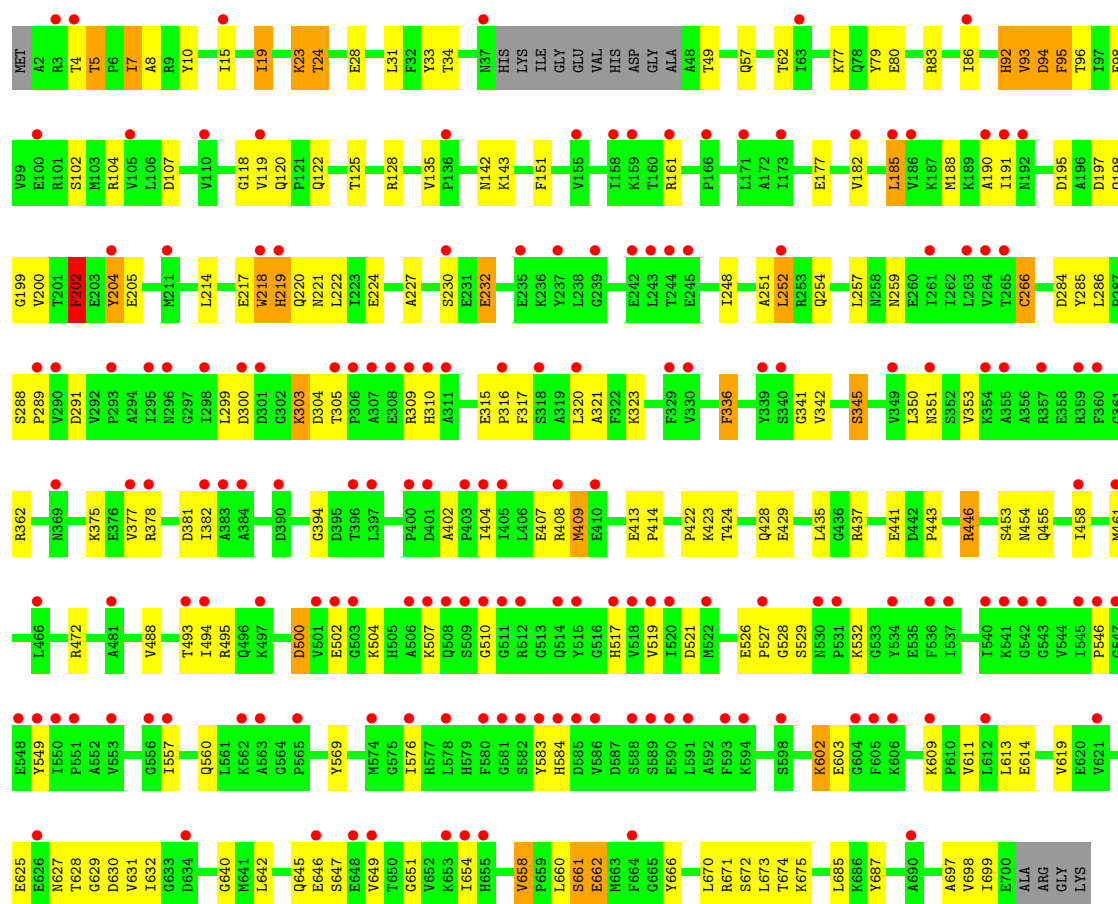


### • Molecule 55: Elongation factor G

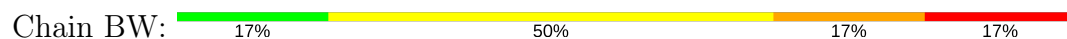


### • Molecule 55: Elongation factor G

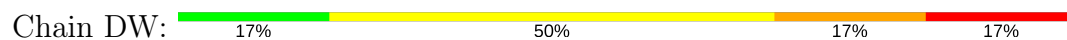




• Molecule 56: Viomycin



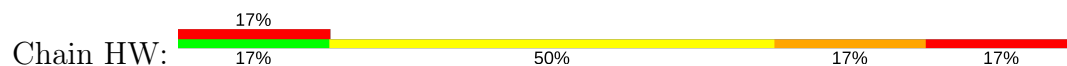
• Molecule 56: Viomycin



• Molecule 56: Viomycin



• Molecule 56: Viomycin



?	A	S	S	?	?
1	2	3	4	5	6

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	361.60Å 361.77Å 433.20Å 90.00° 103.57° 90.00°	Depositor
Resolution (Å)	70.00 – 2.90 69.05 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (70.00-2.90) 78.9 (69.05-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.35 (at 2.91Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.223 , 0.272 0.230 , 0.276	Depositor DCC
$R_{free}$ test set	8388 reflections (0.45%)	DCC
Wilson B-factor (Å <sup>2</sup> )	73.3	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 28.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	592086	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	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 29.65 % 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 1.4952e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	AB	0.66	0/2828	1.10	2/4410 (0.0%)
1	CB	0.53	0/2828	1.02	1/4410 (0.0%)
1	EB	0.63	0/2828	1.15	8/4410 (0.2%)
1	GB	0.75	0/2828	1.13	10/4410 (0.2%)
2	AC	0.54	0/2121	0.79	2/2852 (0.1%)
2	CC	0.46	0/2121	0.72	2/2852 (0.1%)
2	EC	0.52	0/2121	0.76	2/2852 (0.1%)
2	GC	0.46	0/2121	0.74	1/2852 (0.0%)
3	AA	0.81	17/68626 (0.0%)	1.22	304/107056 (0.3%)
3	CA	0.62	4/68626 (0.0%)	1.08	117/107056 (0.1%)
3	EA	0.76	17/68626 (0.0%)	1.22	292/107056 (0.3%)
3	GA	0.64	0/68626	1.14	193/107056 (0.2%)
4	AD	0.57	0/1586	0.77	1/2134 (0.0%)
4	CD	0.51	0/1586	0.75	1/2134 (0.0%)
4	ED	0.55	0/1586	0.74	0/2134
4	GD	0.48	0/1586	0.72	1/2134 (0.0%)
5	AE	0.53	0/1571	0.76	2/2113 (0.1%)
5	CE	0.43	0/1571	0.66	0/2113
5	EE	0.51	0/1571	0.72	0/2113
5	GE	0.54	0/1571	0.75	2/2113 (0.1%)
6	AF	0.49	0/1434	0.71	1/1926 (0.1%)
6	CF	0.48	0/1434	0.70	0/1926
6	EF	0.50	0/1434	0.73	0/1926
6	GF	0.60	0/1434	0.75	0/1926
7	AG	0.55	0/1343	0.73	0/1816
7	CG	0.49	0/1343	0.73	1/1816 (0.1%)
7	EG	0.50	0/1343	0.75	0/1816
7	GG	0.51	0/1343	0.68	0/1816
8	AH	0.53	0/389	0.73	0/523
8	CH	0.61	0/389	0.74	0/523
8	EH	0.50	0/389	0.73	0/523
8	GH	0.55	0/389	0.69	0/523



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
9	AI	0.62	0/1046	0.84	1/1410 (0.1%)
9	CI	0.57	0/1046	0.72	0/1410
9	EI	0.53	0/1046	0.72	0/1410
9	GI	0.71	0/1046	0.80	0/1410
10	AJ	0.63	1/1152 (0.1%)	0.78	0/1551
10	CJ	0.52	1/1152 (0.1%)	0.72	0/1551
10	EJ	0.63	1/1152 (0.1%)	0.78	0/1551
10	GJ	0.48	0/1152	0.71	1/1551 (0.1%)
11	AK	0.65	1/947 (0.1%)	0.77	0/1268
11	CK	0.55	0/947	0.78	0/1268
11	EK	0.53	0/947	0.74	0/1268
11	GK	0.49	0/947	0.77	0/1268
12	AL	0.56	0/1054	0.79	2/1403 (0.1%)
12	CL	0.44	0/1054	0.74	1/1403 (0.1%)
12	EL	0.55	0/1054	0.77	1/1403 (0.1%)
12	GL	0.53	0/1054	0.73	0/1403
13	AM	0.61	0/1093	0.77	0/1460
13	CM	0.47	0/1093	0.67	0/1460
13	EM	0.55	0/1093	0.72	0/1460
13	GM	0.48	0/1093	0.68	0/1460
14	AN	0.51	0/973	0.68	0/1301
14	CN	0.45	0/973	0.64	0/1301
14	EN	0.48	0/973	0.65	0/1301
14	GN	0.45	0/973	0.65	0/1301
15	AO	0.46	0/902	0.70	0/1209
15	CO	0.42	0/902	0.70	0/1209
15	EO	0.44	0/902	0.74	0/1209
15	GO	0.55	0/902	0.82	1/1209 (0.1%)
16	AP	0.52	0/929	0.78	1/1242 (0.1%)
16	CP	0.51	0/929	0.80	0/1242
16	EP	0.55	0/929	0.80	0/1242
16	GP	0.51	0/929	0.81	2/1242 (0.2%)
17	AQ	0.62	0/960	0.71	1/1278 (0.1%)
17	CQ	0.50	0/960	0.67	0/1278
17	EQ	0.58	0/960	0.68	0/1278
17	GQ	0.49	0/960	0.69	1/1278 (0.1%)
18	AR	0.61	1/829 (0.1%)	0.76	0/1107
18	CR	0.50	0/829	0.70	0/1107
18	ER	0.57	1/829 (0.1%)	0.77	0/1107
18	GR	0.55	0/829	0.78	1/1107 (0.1%)
19	AS	0.54	0/864	0.73	0/1156
19	CS	0.46	0/864	0.66	0/1156
19	ES	0.52	0/864	0.75	0/1156

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
19	GS	0.45	0/864	0.75	2/1156 (0.2%)
20	AT	0.54	0/744	0.85	1/994 (0.1%)
20	CT	0.49	0/744	0.74	0/994
20	ET	0.59	0/744	0.87	3/994 (0.3%)
20	GT	0.54	0/744	0.76	0/994
21	AU	0.56	0/787	0.78	0/1051
21	CU	0.47	0/787	0.69	0/1051
21	EU	0.48	0/787	0.79	0/1051
21	GU	0.56	0/787	0.73	0/1051
22	AV	0.48	0/766	0.67	1/1025 (0.1%)
22	CV	0.44	0/766	0.62	0/1025
22	EV	0.49	0/766	0.67	0/1025
22	GV	0.55	0/766	0.70	0/1025
23	AW	0.69	0/603	1.00	1/797 (0.1%)
23	CW	0.63	0/603	0.88	0/797
23	EW	0.69	0/603	0.97	0/797
23	GW	0.63	0/603	0.87	0/797
24	AX	0.50	0/635	0.79	1/848 (0.1%)
24	CX	0.41	0/635	0.71	0/848
24	EX	0.51	0/635	0.78	0/848
24	GX	0.45	0/635	0.68	0/848
25	AY	0.46	0/510	0.75	0/677
25	CY	0.47	0/510	0.74	0/677
25	EY	0.49	0/510	0.81	0/677
25	GY	0.55	0/510	0.75	0/677
26	AZ	0.54	0/453	0.84	1/605 (0.2%)
26	CZ	0.48	0/453	0.80	1/605 (0.2%)
26	EZ	0.50	0/453	0.75	2/605 (0.3%)
26	GZ	0.57	0/453	0.83	0/605
27	A0	0.54	0/450	0.70	0/599
27	C0	0.48	0/450	0.69	0/599
27	E0	0.49	0/450	0.71	1/599 (0.2%)
27	G0	0.43	0/450	0.64	0/599
28	A1	0.53	0/416	0.74	0/554
28	C1	0.49	0/416	0.73	0/554
28	E1	0.49	0/416	0.70	0/554
28	G1	0.54	0/416	0.78	0/554
29	A2	0.53	0/380	0.70	0/498
29	C2	0.46	0/380	0.77	0/498
29	E2	0.51	0/380	0.69	0/498
29	G2	0.48	0/380	0.65	0/498
30	A3	0.53	0/513	0.75	0/676
30	C3	0.41	0/513	0.63	0/676

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
30	E3	0.54	0/513	0.74	0/676
30	G3	0.49	0/513	0.65	0/676
31	A4	0.59	0/303	0.84	0/397
31	C4	0.48	0/303	0.70	0/397
31	E4	0.56	0/303	0.78	1/397 (0.3%)
31	G4	0.50	0/303	0.78	0/397
32	A5	0.74	0/1131	1.32	26/1524 (1.7%)
32	C5	0.70	0/1131	1.31	26/1524 (1.7%)
32	E5	0.69	0/1115	1.33	24/1502 (1.6%)
33	A6	0.59	0/227	0.65	0/304
34	BB	0.49	0/1735	0.71	0/2338
34	DB	0.51	0/1735	0.72	0/2338
34	FB	0.50	0/1735	0.76	0/2338
34	HB	0.56	0/1735	0.73	0/2338
35	BA	0.65	3/36834 (0.0%)	1.14	96/57462 (0.2%)
35	DA	0.60	0/36834	1.06	47/57462 (0.1%)
35	FA	0.62	1/36834 (0.0%)	1.11	98/57462 (0.2%)
35	HA	0.72	2/36834 (0.0%)	1.11	74/57462 (0.1%)
36	BC	0.45	0/1651	0.69	0/2225
36	DC	0.43	0/1651	0.66	0/2225
36	FC	0.46	0/1651	0.70	0/2225
36	HC	0.57	0/1651	0.73	1/2225 (0.0%)
37	BD	0.53	0/1665	0.79	0/2227
37	DD	0.51	0/1665	0.73	0/2227
37	FD	0.52	0/1665	0.69	0/2227
37	HD	0.52	0/1665	0.73	0/2227
38	BE	0.49	0/1118	0.76	0/1504
38	DE	0.46	0/1118	0.71	0/1504
38	FE	0.47	0/1118	0.69	0/1504
38	HE	0.48	0/1118	0.68	0/1504
39	BF	0.50	0/851	0.70	0/1150
39	DF	0.54	0/835	0.75	0/1128
39	FF	0.47	0/835	0.72	0/1128
39	HF	0.56	0/835	0.73	0/1128
40	BG	0.49	0/1195	0.67	0/1602
40	DG	0.52	0/1195	0.69	0/1602
40	FG	0.48	0/1195	0.69	0/1602
40	HG	0.60	0/1195	0.74	1/1602 (0.1%)
41	BH	0.48	0/989	0.65	0/1326
41	DH	0.48	0/989	0.63	0/1326
41	FH	0.44	0/989	0.62	0/1326
41	HH	0.54	0/989	0.77	1/1326 (0.1%)
42	BI	0.54	0/1034	0.81	0/1375

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
42	DI	0.52	0/1034	0.70	0/1375
42	FI	0.54	0/1034	0.77	0/1375
42	HI	0.57	0/1034	0.79	2/1375 (0.1%)
43	BJ	0.54	0/796	0.80	0/1077
43	DJ	0.55	0/796	0.73	0/1077
43	FJ	0.51	0/796	0.74	0/1077
43	HJ	0.59	0/796	0.80	0/1077
44	BK	0.50	0/893	0.74	0/1205
44	DK	0.51	0/893	0.67	0/1205
44	FK	0.50	0/893	0.75	1/1205 (0.1%)
44	HK	0.63	0/893	0.79	0/1205
45	BL	0.54	0/969	0.82	0/1300
45	DL	0.51	0/969	0.79	0/1300
45	FL	0.47	0/969	0.78	0/1300
45	HL	0.47	0/969	0.77	0/1300
46	BM	0.48	0/892	0.70	0/1193
46	DM	0.51	0/892	0.71	0/1193
46	FM	0.42	0/892	0.71	0/1193
46	HM	0.66	0/892	0.80	0/1193
47	BN	0.48	0/785	0.78	0/1043
47	DN	0.47	0/785	0.72	0/1043
47	FN	0.50	0/785	0.80	0/1043
47	HN	0.53	0/785	0.73	0/1043
48	BO	0.44	0/722	0.66	0/964
48	DO	0.44	0/722	0.67	0/964
48	FO	0.42	0/722	0.63	0/964
48	HO	0.56	0/722	0.69	0/964
49	BP	0.48	0/659	0.74	0/884
49	DP	0.45	0/659	0.69	0/884
49	FP	0.48	0/659	0.68	0/884
49	HP	0.46	0/659	0.65	0/884
50	BQ	0.46	0/657	0.73	0/881
50	DQ	0.49	0/657	0.82	2/881 (0.2%)
50	FQ	0.47	0/657	0.68	0/881
50	HQ	0.53	0/657	0.78	0/881
51	BR	0.45	0/462	0.62	0/621
51	DR	0.50	0/462	0.67	0/621
51	FR	0.46	0/462	0.62	0/621
51	HR	0.58	0/462	0.74	1/621 (0.2%)
52	BS	0.47	0/652	0.81	0/877
52	DS	0.50	0/652	0.72	0/877
52	FS	0.46	0/652	0.71	0/877
52	HS	0.67	0/652	0.85	1/877 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
53	BT	0.47	0/671	0.60	0/888
53	DT	0.49	0/671	0.64	0/888
53	FT	0.45	0/671	0.64	0/888
53	HT	0.43	0/671	0.66	0/888
54	BU	0.66	0/430	0.84	0/570
54	DU	0.73	0/430	0.83	0/570
54	FU	0.73	1/430 (0.2%)	0.88	0/570
54	HU	0.68	0/430	0.73	0/570
55	BV	0.46	0/5444	0.67	2/7367 (0.0%)
55	DV	0.45	0/5439	0.65	0/7360
55	FV	0.46	0/5439	0.65	1/7360 (0.0%)
55	HV	0.48	0/5439	0.65	0/7360
56	BW	2.29	1/11 (9.1%)	1.55	0/13
56	DW	2.28	1/11 (9.1%)	1.54	0/13
56	FW	2.37	1/11 (9.1%)	1.57	0/13
56	HW	2.38	1/11 (9.1%)	1.80	0/13
All	All	0.64	55/636829 (0.0%)	1.05	1375/948879 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	AC	0	1
2	GC	0	1
4	AD	0	1
4	CD	0	2
4	ED	0	1
4	GD	0	1
10	AJ	0	1
10	GJ	0	1
11	AK	0	1
32	A5	0	1
39	BF	0	1
39	FF	0	1
42	DI	0	1
45	BL	0	1
45	DL	0	1
45	HL	0	1
53	DT	0	1
55	BV	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
55	DV	0	1
55	FV	0	1
55	HV	0	1
All	All	0	22

The worst 5 of 55 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	HA	753	A	N7-C5	8.68	1.44	1.39
3	EA	528	A	N9-C4	-8.47	1.32	1.37
3	AA	984	A	N9-C4	-8.47	1.32	1.37
35	BA	1362	A	N7-C5	7.96	1.44	1.39
3	AA	528	A	N9-C4	-6.66	1.33	1.37

The worst 5 of 1375 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AA	1073	A	N1-C6-N6	-20.05	106.57	118.60
3	EA	1936	A	N1-C6-N6	15.79	128.07	118.60
3	AA	1073	A	C5-C6-N6	14.08	134.96	123.70
3	AA	2053	G	N1-C6-O6	13.88	128.23	119.90
3	EA	1936	A	C5-C6-N6	-13.76	112.69	123.70

There are no chirality outliers.

5 of 22 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
32	A5	130	PRO	Peptide
2	AC	233	GLY	Peptide
4	AD	9	VAL	Peptide
10	AJ	110	PRO	Peptide
11	AK	71	ARG	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AB	2529	0	1281	20	0
1	CB	2529	0	1281	30	0
1	EB	2529	0	1281	33	0
1	GB	2529	0	1281	59	0
2	AC	2082	0	2157	52	0
2	CC	2082	0	2157	66	0
2	EC	2082	0	2157	65	0
2	GC	2082	0	2157	68	0
3	AA	61274	0	30819	778	0
3	CA	61274	0	30819	819	0
3	EA	61274	0	30819	734	0
3	GA	61274	0	30817	1239	2
4	AD	1565	0	1616	53	0
4	CD	1565	0	1616	49	0
4	ED	1565	0	1616	49	0
4	GD	1565	0	1616	48	0
5	AE	1552	0	1619	36	0
5	CE	1552	0	1619	44	0
5	EE	1552	0	1619	34	0
5	GE	1552	0	1619	72	0
6	AF	1410	0	1447	41	0
6	CF	1410	0	1447	39	0
6	EF	1410	0	1447	48	0
6	GF	1410	0	1447	57	0
7	AG	1323	0	1374	39	0
7	CG	1323	0	1374	50	0
7	EG	1323	0	1374	43	0
7	GG	1323	0	1374	56	0
8	AH	384	0	405	14	0
8	CH	384	0	405	20	0
8	EH	384	0	405	9	0
8	GH	384	0	405	7	0
9	AI	1032	0	1088	52	0
9	CI	1032	0	1088	38	0
9	EI	1032	0	1088	45	0
9	GI	1032	0	1088	64	0
10	AJ	1129	0	1162	53	0
10	CJ	1129	0	1162	54	0
10	EJ	1129	0	1162	49	0
10	GJ	1129	0	1162	53	0
11	AK	938	0	1012	40	0
11	CK	938	0	1012	38	0
11	EK	938	0	1012	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	GK	938	0	1012	24	0
12	AL	1045	0	1117	35	0
12	CL	1045	0	1116	36	0
12	EL	1045	0	1117	34	0
12	GL	1045	0	1117	52	0
13	AM	1074	0	1157	26	0
13	CM	1074	0	1157	32	0
13	EM	1074	0	1157	23	0
13	GM	1074	0	1157	26	0
14	AN	960	0	1000	30	0
14	CN	960	0	1000	34	0
14	EN	960	0	1000	24	0
14	GN	960	0	1000	23	0
15	AO	892	0	923	18	0
15	CO	892	0	923	27	0
15	EO	892	0	923	18	0
15	GO	892	0	923	32	0
16	AP	917	0	965	44	0
16	CP	917	0	965	41	0
16	EP	917	0	965	44	0
16	GP	917	0	965	36	0
17	AQ	947	0	1022	52	0
17	CQ	947	0	1022	50	0
17	EQ	947	0	1022	44	0
17	GQ	947	0	1022	56	0
18	AR	816	0	839	35	0
18	CR	816	0	839	36	0
18	ER	816	0	839	34	0
18	GR	816	0	839	46	0
19	AS	857	0	922	29	0
19	CS	857	0	922	18	0
19	ES	857	0	922	20	0
19	GS	857	0	922	29	0
20	AT	738	0	807	35	0
20	CT	738	0	807	26	0
20	ET	738	0	807	33	0
20	GT	738	0	807	29	0
21	AU	779	0	834	27	0
21	CU	779	0	834	12	0
21	EU	779	0	834	23	0
21	GU	779	0	834	29	0
22	AV	753	0	780	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	CV	753	0	780	17	0
22	EV	753	0	780	10	0
22	GV	753	0	780	13	0
23	AW	596	0	610	77	0
23	CW	596	0	610	62	0
23	EW	596	0	610	74	0
23	GW	596	0	610	60	0
24	AX	625	0	655	17	0
24	CX	625	0	655	14	0
24	EX	625	0	655	21	0
24	GX	625	0	655	18	0
25	AY	509	0	543	13	0
25	CY	509	0	543	9	0
25	EY	509	0	543	16	0
25	GY	509	0	543	11	0
26	AZ	449	0	491	16	0
26	CZ	449	0	491	21	0
26	EZ	449	0	491	10	0
26	GZ	449	0	491	27	0
27	A0	444	0	461	19	0
27	C0	444	0	461	17	0
27	E0	444	0	461	12	0
27	G0	444	0	461	8	0
28	A1	409	0	440	15	0
28	C1	409	0	440	11	0
28	E1	409	0	440	15	0
28	G1	409	0	440	17	0
29	A2	377	0	418	5	0
29	C2	377	0	418	11	0
29	E2	377	0	418	9	0
29	G2	377	0	418	17	0
30	A3	504	0	574	10	0
30	C3	504	0	574	7	0
30	E3	504	0	574	15	0
30	G3	504	0	574	27	0
31	A4	302	0	340	15	0
31	C4	302	0	340	12	0
31	E4	302	0	340	8	0
31	G4	302	0	340	12	0
32	A5	1117	0	1155	122	0
32	C5	1117	0	1155	136	0
32	E5	1101	0	1140	128	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	A6	227	0	237	7	0
34	BB	1704	0	1732	54	0
34	DB	1704	0	1732	62	0
34	FB	1704	0	1732	74	0
34	HB	1704	0	1732	58	0
35	BA	32895	0	16553	336	0
35	DA	32895	0	16553	472	0
35	FA	32895	0	16553	401	1
35	HA	32895	0	16552	581	0
36	BC	1624	0	1696	33	0
36	DC	1624	0	1696	41	0
36	FC	1624	0	1696	44	0
36	HC	1624	0	1696	35	0
37	BD	1643	0	1707	69	0
37	DD	1643	0	1707	63	0
37	FD	1643	0	1707	63	0
37	HD	1643	0	1707	73	0
38	BE	1105	0	1148	45	0
38	DE	1105	0	1148	35	0
38	FE	1105	0	1148	36	0
38	HE	1105	0	1148	36	0
39	BF	832	0	824	23	0
39	DF	817	0	808	36	0
39	FF	817	0	808	21	0
39	HF	817	0	808	36	0
40	BG	1181	0	1238	22	0
40	DG	1181	0	1238	30	0
40	FG	1181	0	1238	18	0
40	HG	1181	0	1238	50	0
41	BH	979	0	1031	28	0
41	DH	979	0	1031	25	0
41	FH	979	0	1031	28	0
41	HH	979	0	1031	33	0
42	BI	1022	0	1070	46	0
42	DI	1022	0	1070	39	0
42	FI	1022	0	1070	43	0
42	HI	1022	0	1070	38	0
43	BJ	786	0	828	23	0
43	DJ	786	0	828	28	0
43	FJ	786	0	828	18	1
43	HJ	786	0	828	29	0
44	BK	877	0	887	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	DK	877	0	887	40	0
44	FK	877	0	887	40	0
44	HK	877	0	887	57	0
45	BL	955	0	1016	36	0
45	DL	955	0	1016	37	0
45	FL	955	0	1016	33	0
45	HL	955	0	1016	41	0
46	BM	883	0	941	20	0
46	DM	883	0	941	33	0
46	FM	883	0	941	33	0
46	HM	883	0	941	39	0
47	BN	774	0	824	25	0
47	DN	774	0	824	31	0
47	FN	774	0	824	27	0
47	HN	774	0	824	28	0
48	BO	714	0	734	8	0
48	DO	714	0	734	13	0
48	FO	714	0	734	12	0
48	HO	714	0	734	18	0
49	BP	649	0	666	13	0
49	DP	649	0	666	17	0
49	FP	649	0	666	15	0
49	HP	649	0	666	12	0
50	BQ	648	0	691	11	0
50	DQ	648	0	691	33	0
50	FQ	648	0	691	23	0
50	HQ	648	0	691	28	0
51	BR	455	0	478	10	0
51	DR	455	0	478	9	0
51	FR	455	0	478	4	0
51	HR	455	0	478	24	0
52	BS	637	0	665	18	0
52	DS	637	0	665	14	0
52	FS	637	0	665	29	0
52	HS	637	0	665	32	0
53	BT	665	0	714	11	0
53	DT	665	0	714	23	0
53	FT	665	0	714	15	0
53	HT	665	0	714	13	0
54	BU	425	0	449	30	0
54	DU	425	0	449	17	0
54	FU	425	0	449	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	HU	425	0	449	27	0
55	BV	5345	0	5311	117	0
55	DV	5340	0	5306	132	0
55	FV	5340	0	5306	103	0
55	HV	5340	0	5307	116	0
56	BW	48	0	41	5	0
56	DW	48	0	41	5	0
56	FW	48	0	41	3	0
56	HW	48	0	40	6	0
57	A4	1	0	0	0	0
57	AA	136	0	0	0	0
57	AB	4	0	0	0	0
57	AC	1	0	0	0	0
57	AE	1	0	0	0	0
57	BA	40	0	0	0	0
57	BE	1	0	0	0	0
57	BN	1	0	0	0	0
57	BU	1	0	0	0	0
57	BV	1	0	0	0	0
57	C4	1	0	0	0	0
57	CA	136	0	0	0	0
57	CB	4	0	0	0	0
57	CE	1	0	0	0	0
57	CN	1	0	0	0	0
57	DA	43	0	0	0	0
57	DV	1	0	0	0	0
57	EA	137	0	0	0	0
57	EB	4	0	0	0	0
57	ED	1	0	0	0	0
57	EE	1	0	0	0	0
57	FA	39	0	0	0	0
57	FE	1	0	0	0	0
57	FN	2	0	0	0	0
57	FU	1	0	0	0	0
57	FV	1	0	0	0	0
57	GA	136	0	0	0	0
57	GB	4	0	0	0	0
57	GC	2	0	0	0	0
57	GL	1	0	0	0	0
57	HA	41	0	0	0	0
57	HE	1	0	0	0	0
57	HK	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	HV	1	0	0	0	0
58	A4	1	0	0	0	0
58	C4	1	0	0	0	0
58	E4	1	0	0	0	0
58	G4	1	0	0	0	0
59	BV	32	0	14	1	0
59	DV	32	0	14	2	0
59	FV	32	0	14	2	0
59	HV	32	0	14	1	0
60	A0	2	0	0	0	0
60	A2	1	0	0	0	0
60	A3	1	0	0	0	0
60	A4	1	0	0	0	0
60	AA	614	0	0	102	0
60	AB	18	0	0	1	0
60	AC	6	0	0	1	0
60	AD	4	0	0	0	0
60	AE	1	0	0	0	0
60	AF	1	0	0	0	0
60	AJ	1	0	0	0	0
60	AL	5	0	0	1	0
60	AN	2	0	0	0	0
60	AP	1	0	0	0	0
60	AQ	2	0	0	0	0
60	AS	1	0	0	0	0
60	BA	202	0	0	31	0
60	BL	1	0	0	0	0
60	BN	2	0	0	0	0
60	BT	2	0	0	0	0
60	BV	1	0	0	1	0
60	C0	1	0	0	0	0
60	C2	1	0	0	0	0
60	C3	1	0	0	0	0
60	C4	2	0	0	0	0
60	CA	607	0	0	84	0
60	CB	21	0	0	2	0
60	CC	8	0	0	0	0
60	CD	3	0	0	0	0
60	CE	1	0	0	0	0
60	CJ	2	0	0	1	0
60	CL	5	0	0	0	0
60	CN	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	CQ	1	0	0	1	0
60	CS	2	0	0	1	0
60	CT	2	0	0	1	0
60	CU	1	0	0	0	0
60	DA	186	0	0	27	0
60	DC	2	0	0	0	0
60	DD	1	0	0	0	0
60	DE	1	0	0	0	0
60	DG	1	0	0	0	0
60	DK	1	0	0	0	0
60	DL	2	0	0	0	0
60	DN	8	0	0	3	0
60	DQ	1	0	0	0	0
60	DT	4	0	0	1	0
60	DU	1	0	0	0	0
60	DV	1	0	0	0	0
60	E0	1	0	0	0	0
60	E2	1	0	0	0	0
60	E3	2	0	0	0	0
60	E4	2	0	0	0	0
60	EA	610	0	0	105	0
60	EB	18	0	0	3	0
60	EC	9	0	0	1	0
60	ED	3	0	0	0	0
60	EE	2	0	0	1	0
60	EL	4	0	0	0	0
60	EN	3	0	0	0	0
60	ER	1	0	0	0	0
60	ET	2	0	0	0	0
60	EV	2	0	0	0	0
60	FA	197	0	0	24	0
60	FC	1	0	0	0	0
60	FE	2	0	0	0	0
60	FN	3	0	0	0	0
60	FT	4	0	0	0	0
60	FU	1	0	0	0	0
60	FV	1	0	0	0	0
60	G2	2	0	0	0	0
60	G3	1	0	0	0	0
60	G4	1	0	0	0	0
60	GA	606	0	0	136	0
60	GB	19	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	GC	10	0	0	0	0
60	GD	3	0	0	0	0
60	GE	2	0	0	1	0
60	GJ	1	0	0	0	0
60	GL	4	0	0	1	0
60	GN	4	0	0	0	0
60	GQ	1	0	0	0	0
60	GR	2	0	0	1	0
60	GS	2	0	0	0	0
60	GU	1	0	0	0	0
60	GV	1	0	0	0	0
60	HA	193	0	0	31	0
60	HD	3	0	0	2	0
60	HE	3	0	0	0	0
60	HN	7	0	0	3	0
60	HQ	1	0	0	0	0
60	HT	1	0	0	0	0
60	HV	1	0	0	0	0
All	All	592086	0	404164	11056	2

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 12.

The worst 5 of 11056 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:C5:24:SER:CB	32:C5:116:GLU:HG2	1.46	1.44
32:C5:24:SER:O	32:C5:116:GLU:HB3	1.41	1.16
32:C5:24:SER:HB2	32:C5:116:GLU:CG	1.76	1.14
32:E5:24:SER:HB2	32:E5:116:GLU:HG2	1.27	1.14
3:AA:912:C:OP1	13:AM:8:LYS:NZ	1.79	1.12

All (2) 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)
35:FA:1029:U:O3'	3:GA:1508:A:N6[1_565]	2.04	0.16
43:FJ:85:ASP:OD1	3:GA:1722:A:O2'[1_565]	2.16	0.04

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AC	269/273 (98%)	211 (78%)	43 (16%)	15 (6%)	2	6
2	CC	269/273 (98%)	211 (78%)	42 (16%)	16 (6%)	2	6
2	EC	269/273 (98%)	212 (79%)	44 (16%)	13 (5%)	2	10
2	GC	269/273 (98%)	210 (78%)	42 (16%)	17 (6%)	1	4
4	AD	207/209 (99%)	163 (79%)	30 (14%)	14 (7%)	1	4
4	CD	207/209 (99%)	166 (80%)	27 (13%)	14 (7%)	1	4
4	ED	207/209 (99%)	165 (80%)	29 (14%)	13 (6%)	1	4
4	GD	207/209 (99%)	161 (78%)	32 (16%)	14 (7%)	1	4
5	AE	199/201 (99%)	162 (81%)	27 (14%)	10 (5%)	2	8
5	CE	199/201 (99%)	159 (80%)	27 (14%)	13 (6%)	1	4
5	EE	199/201 (99%)	164 (82%)	24 (12%)	11 (6%)	2	7
5	GE	199/201 (99%)	159 (80%)	30 (15%)	10 (5%)	2	8
6	AF	175/179 (98%)	141 (81%)	30 (17%)	4 (2%)	7	27
6	CF	175/179 (98%)	145 (83%)	25 (14%)	5 (3%)	5	21
6	EF	175/179 (98%)	140 (80%)	26 (15%)	9 (5%)	2	8
6	GF	175/179 (98%)	140 (80%)	26 (15%)	9 (5%)	2	8
7	AG	174/177 (98%)	127 (73%)	30 (17%)	17 (10%)	1	1
7	CG	174/177 (98%)	131 (75%)	28 (16%)	15 (9%)	1	2
7	EG	174/177 (98%)	125 (72%)	35 (20%)	14 (8%)	1	2
7	GG	174/177 (98%)	126 (72%)	30 (17%)	18 (10%)	0	1
8	AH	48/50 (96%)	29 (60%)	14 (29%)	5 (10%)	0	1
8	CH	48/50 (96%)	31 (65%)	12 (25%)	5 (10%)	0	1
8	EH	48/50 (96%)	31 (65%)	12 (25%)	5 (10%)	0	1
8	GH	48/50 (96%)	30 (62%)	15 (31%)	3 (6%)	1	4
9	AI	139/142 (98%)	97 (70%)	33 (24%)	9 (6%)	1	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	CI	139/142 (98%)	95 (68%)	38 (27%)	6 (4%)	3	12
9	EI	139/142 (98%)	97 (70%)	38 (27%)	4 (3%)	5	21
9	GI	139/142 (98%)	95 (68%)	34 (24%)	10 (7%)	1	3
10	AJ	140/142 (99%)	113 (81%)	18 (13%)	9 (6%)	1	4
10	CJ	140/142 (99%)	112 (80%)	20 (14%)	8 (6%)	2	6
10	EJ	140/142 (99%)	114 (81%)	17 (12%)	9 (6%)	1	4
10	GJ	140/142 (99%)	113 (81%)	19 (14%)	8 (6%)	2	6
11	AK	120/123 (98%)	96 (80%)	14 (12%)	10 (8%)	1	2
11	CK	120/123 (98%)	93 (78%)	21 (18%)	6 (5%)	2	8
11	EK	120/123 (98%)	92 (77%)	21 (18%)	7 (6%)	2	6
11	GK	120/123 (98%)	92 (77%)	20 (17%)	8 (7%)	1	4
12	AL	141/144 (98%)	104 (74%)	32 (23%)	5 (4%)	4	17
12	CL	141/144 (98%)	103 (73%)	33 (23%)	5 (4%)	4	17
12	EL	141/144 (98%)	108 (77%)	26 (18%)	7 (5%)	2	8
12	GL	141/144 (98%)	103 (73%)	32 (23%)	6 (4%)	3	12
13	AM	134/136 (98%)	107 (80%)	16 (12%)	11 (8%)	1	2
13	CM	134/136 (98%)	110 (82%)	16 (12%)	8 (6%)	2	5
13	EM	134/136 (98%)	106 (79%)	18 (13%)	10 (8%)	1	3
13	GM	134/136 (98%)	109 (81%)	17 (13%)	8 (6%)	2	5
14	AN	118/127 (93%)	101 (86%)	16 (14%)	1 (1%)	22	57
14	CN	118/127 (93%)	103 (87%)	14 (12%)	1 (1%)	22	57
14	EN	118/127 (93%)	100 (85%)	17 (14%)	1 (1%)	22	57
14	GN	118/127 (93%)	98 (83%)	19 (16%)	1 (1%)	22	57
15	AO	114/117 (97%)	95 (83%)	18 (16%)	1 (1%)	20	54
15	CO	114/117 (97%)	95 (83%)	15 (13%)	4 (4%)	4	17
15	EO	114/117 (97%)	95 (83%)	18 (16%)	1 (1%)	20	54
15	GO	114/117 (97%)	95 (83%)	15 (13%)	4 (4%)	4	17
16	AP	112/115 (97%)	86 (77%)	17 (15%)	9 (8%)	1	2
16	CP	112/115 (97%)	87 (78%)	16 (14%)	9 (8%)	1	2
16	EP	112/115 (97%)	84 (75%)	16 (14%)	12 (11%)	0	1
16	GP	112/115 (97%)	85 (76%)	19 (17%)	8 (7%)	1	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	AQ	115/118 (98%)	99 (86%)	12 (10%)	4 (4%)	4	17
17	CQ	115/118 (98%)	99 (86%)	12 (10%)	4 (4%)	4	17
17	EQ	115/118 (98%)	99 (86%)	12 (10%)	4 (4%)	4	17
17	GQ	115/118 (98%)	99 (86%)	14 (12%)	2 (2%)	11	36
18	AR	101/103 (98%)	83 (82%)	15 (15%)	3 (3%)	5	20
18	CR	101/103 (98%)	83 (82%)	15 (15%)	3 (3%)	5	20
18	ER	101/103 (98%)	83 (82%)	15 (15%)	3 (3%)	5	20
18	GR	101/103 (98%)	83 (82%)	13 (13%)	5 (5%)	2	8
19	AS	108/110 (98%)	94 (87%)	9 (8%)	5 (5%)	3	11
19	CS	108/110 (98%)	95 (88%)	9 (8%)	4 (4%)	4	16
19	ES	108/110 (98%)	92 (85%)	10 (9%)	6 (6%)	2	6
19	GS	108/110 (98%)	91 (84%)	11 (10%)	6 (6%)	2	6
20	AT	91/100 (91%)	57 (63%)	24 (26%)	10 (11%)	0	1
20	CT	91/100 (91%)	55 (60%)	25 (28%)	11 (12%)	0	1
20	ET	91/100 (91%)	56 (62%)	26 (29%)	9 (10%)	1	1
20	GT	91/100 (91%)	58 (64%)	23 (25%)	10 (11%)	0	1
21	AU	100/104 (96%)	74 (74%)	16 (16%)	10 (10%)	1	1
21	CU	100/104 (96%)	75 (75%)	17 (17%)	8 (8%)	1	2
21	EU	100/104 (96%)	74 (74%)	15 (15%)	11 (11%)	0	1
21	GU	100/104 (96%)	76 (76%)	14 (14%)	10 (10%)	1	1
22	AV	92/94 (98%)	81 (88%)	11 (12%)	0	100	100
22	CV	92/94 (98%)	80 (87%)	11 (12%)	1 (1%)	17	48
22	EV	92/94 (98%)	80 (87%)	12 (13%)	0	100	100
22	GV	92/94 (98%)	78 (85%)	13 (14%)	1 (1%)	17	48
23	AW	77/85 (91%)	39 (51%)	22 (29%)	16 (21%)	0	0
23	CW	77/85 (91%)	41 (53%)	17 (22%)	19 (25%)	0	0
23	EW	77/85 (91%)	41 (53%)	21 (27%)	15 (20%)	0	0
23	GW	77/85 (91%)	40 (52%)	21 (27%)	16 (21%)	0	0
24	AX	75/78 (96%)	64 (85%)	8 (11%)	3 (4%)	3	14
24	CX	75/78 (96%)	63 (84%)	10 (13%)	2 (3%)	6	23
24	EX	75/78 (96%)	63 (84%)	9 (12%)	3 (4%)	3	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	GX	75/78 (96%)	63 (84%)	9 (12%)	3 (4%)	3	14
25	AY	61/63 (97%)	39 (64%)	18 (30%)	4 (7%)	1	4
25	CY	61/63 (97%)	42 (69%)	15 (25%)	4 (7%)	1	4
25	EY	61/63 (97%)	40 (66%)	17 (28%)	4 (7%)	1	4
25	GY	61/63 (97%)	39 (64%)	20 (33%)	2 (3%)	4	18
26	AZ	56/59 (95%)	46 (82%)	8 (14%)	2 (4%)	4	17
26	CZ	56/59 (95%)	46 (82%)	8 (14%)	2 (4%)	4	17
26	EZ	56/59 (95%)	46 (82%)	8 (14%)	2 (4%)	4	17
26	GZ	56/59 (95%)	44 (79%)	10 (18%)	2 (4%)	4	17
27	A0	54/57 (95%)	43 (80%)	7 (13%)	4 (7%)	1	3
27	C0	54/57 (95%)	45 (83%)	3 (6%)	6 (11%)	0	1
27	E0	54/57 (95%)	44 (82%)	6 (11%)	4 (7%)	1	3
27	G0	54/57 (95%)	46 (85%)	4 (7%)	4 (7%)	1	3
28	A1	48/55 (87%)	42 (88%)	3 (6%)	3 (6%)	1	4
28	C1	48/55 (87%)	42 (88%)	4 (8%)	2 (4%)	3	12
28	E1	48/55 (87%)	42 (88%)	4 (8%)	2 (4%)	3	12
28	G1	48/55 (87%)	42 (88%)	3 (6%)	3 (6%)	1	4
29	A2	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
29	C2	44/46 (96%)	41 (93%)	2 (4%)	1 (2%)	7	27
29	E2	44/46 (96%)	40 (91%)	4 (9%)	0	100	100
29	G2	44/46 (96%)	40 (91%)	3 (7%)	1 (2%)	7	27
30	A3	62/65 (95%)	53 (86%)	7 (11%)	2 (3%)	5	19
30	C3	62/65 (95%)	54 (87%)	6 (10%)	2 (3%)	5	19
30	E3	62/65 (95%)	56 (90%)	4 (6%)	2 (3%)	5	19
30	G3	62/65 (95%)	54 (87%)	6 (10%)	2 (3%)	5	19
31	A4	36/38 (95%)	29 (81%)	4 (11%)	3 (8%)	1	2
31	C4	36/38 (95%)	29 (81%)	4 (11%)	3 (8%)	1	2
31	E4	36/38 (95%)	29 (81%)	4 (11%)	3 (8%)	1	2
31	G4	36/38 (95%)	30 (83%)	2 (6%)	4 (11%)	0	1
32	A5	146/165 (88%)	77 (53%)	40 (27%)	29 (20%)	0	0
32	C5	146/165 (88%)	78 (53%)	45 (31%)	23 (16%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	E5	143/165 (87%)	79 (55%)	41 (29%)	23 (16%)	0	0
33	A6	28/121 (23%)	20 (71%)	7 (25%)	1 (4%)	4	17
34	BB	216/241 (90%)	151 (70%)	51 (24%)	14 (6%)	1	4
34	DB	216/241 (90%)	157 (73%)	47 (22%)	12 (6%)	2	6
34	FB	216/241 (90%)	153 (71%)	51 (24%)	12 (6%)	2	6
34	HB	216/241 (90%)	153 (71%)	51 (24%)	12 (6%)	2	6
36	BC	204/233 (88%)	181 (89%)	18 (9%)	5 (2%)	6	25
36	DC	204/233 (88%)	179 (88%)	20 (10%)	5 (2%)	6	25
36	FC	204/233 (88%)	180 (88%)	18 (9%)	6 (3%)	5	21
36	HC	204/233 (88%)	181 (89%)	17 (8%)	6 (3%)	5	21
37	BD	203/206 (98%)	162 (80%)	30 (15%)	11 (5%)	2	7
37	DD	203/206 (98%)	162 (80%)	29 (14%)	12 (6%)	2	6
37	FD	203/206 (98%)	163 (80%)	29 (14%)	11 (5%)	2	7
37	HD	203/206 (98%)	165 (81%)	26 (13%)	12 (6%)	2	6
38	BE	148/167 (89%)	123 (83%)	18 (12%)	7 (5%)	3	10
38	DE	148/167 (89%)	125 (84%)	18 (12%)	5 (3%)	4	18
38	FE	148/167 (89%)	122 (82%)	20 (14%)	6 (4%)	3	13
38	HE	148/167 (89%)	121 (82%)	20 (14%)	7 (5%)	3	10
39	BF	100/135 (74%)	79 (79%)	15 (15%)	6 (6%)	2	5
39	DF	98/135 (73%)	80 (82%)	13 (13%)	5 (5%)	2	8
39	FF	98/135 (73%)	81 (83%)	11 (11%)	6 (6%)	2	5
39	HF	98/135 (73%)	76 (78%)	18 (18%)	4 (4%)	3	13
40	BG	149/179 (83%)	128 (86%)	20 (13%)	1 (1%)	25	60
40	DG	149/179 (83%)	125 (84%)	22 (15%)	2 (1%)	14	43
40	FG	149/179 (83%)	127 (85%)	21 (14%)	1 (1%)	25	60
40	HG	149/179 (83%)	127 (85%)	20 (13%)	2 (1%)	14	43
41	BH	127/130 (98%)	114 (90%)	12 (9%)	1 (1%)	22	57
41	DH	127/130 (98%)	113 (89%)	12 (9%)	2 (2%)	11	37
41	FH	127/130 (98%)	112 (88%)	13 (10%)	2 (2%)	11	37
41	HH	127/130 (98%)	112 (88%)	13 (10%)	2 (2%)	11	37
42	BI	125/130 (96%)	105 (84%)	14 (11%)	6 (5%)	2	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	DI	125/130 (96%)	102 (82%)	22 (18%)	1 (1%)	22	57
42	FI	125/130 (96%)	106 (85%)	13 (10%)	6 (5%)	2	10
42	HI	125/130 (96%)	103 (82%)	19 (15%)	3 (2%)	7	27
43	BJ	96/103 (93%)	69 (72%)	20 (21%)	7 (7%)	1	3
43	DJ	96/103 (93%)	71 (74%)	19 (20%)	6 (6%)	1	4
43	FJ	96/103 (93%)	69 (72%)	21 (22%)	6 (6%)	1	4
43	HJ	96/103 (93%)	68 (71%)	19 (20%)	9 (9%)	1	1
44	BK	115/129 (89%)	97 (84%)	12 (10%)	6 (5%)	2	8
44	DK	115/129 (89%)	92 (80%)	19 (16%)	4 (4%)	4	17
44	FK	115/129 (89%)	96 (84%)	13 (11%)	6 (5%)	2	8
44	HK	115/129 (89%)	91 (79%)	15 (13%)	9 (8%)	1	3
45	BL	121/124 (98%)	101 (84%)	16 (13%)	4 (3%)	4	18
45	DL	121/124 (98%)	98 (81%)	20 (16%)	3 (2%)	6	25
45	FL	121/124 (98%)	100 (83%)	14 (12%)	7 (6%)	2	6
45	HL	121/124 (98%)	101 (84%)	15 (12%)	5 (4%)	3	13
46	BM	112/118 (95%)	98 (88%)	8 (7%)	6 (5%)	2	7
46	DM	112/118 (95%)	96 (86%)	11 (10%)	5 (4%)	3	11
46	FM	112/118 (95%)	99 (88%)	7 (6%)	6 (5%)	2	7
46	HM	112/118 (95%)	92 (82%)	12 (11%)	8 (7%)	1	3
47	BN	92/101 (91%)	73 (79%)	13 (14%)	6 (6%)	1	4
47	DN	92/101 (91%)	71 (77%)	19 (21%)	2 (2%)	8	29
47	FN	92/101 (91%)	71 (77%)	17 (18%)	4 (4%)	3	12
47	HN	92/101 (91%)	70 (76%)	18 (20%)	4 (4%)	3	12
48	BO	86/89 (97%)	75 (87%)	9 (10%)	2 (2%)	7	27
48	DO	86/89 (97%)	75 (87%)	11 (13%)	0	100	100
48	FO	86/89 (97%)	75 (87%)	11 (13%)	0	100	100
48	HO	86/89 (97%)	72 (84%)	11 (13%)	3 (4%)	4	17
49	BP	80/82 (98%)	60 (75%)	17 (21%)	3 (4%)	4	15
49	DP	80/82 (98%)	60 (75%)	15 (19%)	5 (6%)	1	4
49	FP	80/82 (98%)	62 (78%)	15 (19%)	3 (4%)	4	15
49	HP	80/82 (98%)	56 (70%)	21 (26%)	3 (4%)	4	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	BQ	78/84 (93%)	59 (76%)	15 (19%)	4 (5%)	2	8
50	DQ	78/84 (93%)	58 (74%)	14 (18%)	6 (8%)	1	3
50	FQ	78/84 (93%)	58 (74%)	17 (22%)	3 (4%)	4	15
50	HQ	78/84 (93%)	58 (74%)	13 (17%)	7 (9%)	1	2
51	BR	53/75 (71%)	47 (89%)	6 (11%)	0	100	100
51	DR	53/75 (71%)	46 (87%)	7 (13%)	0	100	100
51	FR	53/75 (71%)	48 (91%)	5 (9%)	0	100	100
51	HR	53/75 (71%)	49 (92%)	4 (8%)	0	100	100
52	BS	77/92 (84%)	65 (84%)	11 (14%)	1 (1%)	14	43
52	DS	77/92 (84%)	66 (86%)	11 (14%)	0	100	100
52	FS	77/92 (84%)	64 (83%)	11 (14%)	2 (3%)	6	24
52	HS	77/92 (84%)	66 (86%)	9 (12%)	2 (3%)	6	24
53	BT	83/87 (95%)	74 (89%)	7 (8%)	2 (2%)	7	27
53	DT	83/87 (95%)	74 (89%)	6 (7%)	3 (4%)	4	17
53	FT	83/87 (95%)	75 (90%)	6 (7%)	2 (2%)	7	27
53	HT	83/87 (95%)	73 (88%)	8 (10%)	2 (2%)	7	27
54	BU	49/71 (69%)	26 (53%)	20 (41%)	3 (6%)	2	5
54	DU	49/71 (69%)	25 (51%)	20 (41%)	4 (8%)	1	2
54	FU	49/71 (69%)	24 (49%)	21 (43%)	4 (8%)	1	2
54	HU	49/71 (69%)	29 (59%)	18 (37%)	2 (4%)	3	13
55	BV	686/704 (97%)	559 (82%)	92 (13%)	35 (5%)	2	8
55	DV	685/704 (97%)	559 (82%)	93 (14%)	33 (5%)	2	10
55	FV	685/704 (97%)	564 (82%)	89 (13%)	32 (5%)	3	10
55	HV	685/704 (97%)	562 (82%)	88 (13%)	35 (5%)	2	8
56	BW	2/6 (33%)	0	0	2 (100%)	0	0
56	DW	2/6 (33%)	0	1 (50%)	1 (50%)	0	0
56	FW	2/6 (33%)	2 (100%)	0	0	100	100
56	HW	2/6 (33%)	1 (50%)	0	1 (50%)	0	0
All	All	25302/27000 (94%)	20075 (79%)	3885 (15%)	1342 (5%)	2	7

5 of 1342 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AC	70	LYS
2	AC	104	LEU
2	AC	121	ALA
2	AC	140	VAL
4	AD	43	ASP

### 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	
2	AC	216/218 (99%)	202 (94%)	14 (6%)	20	49
2	CC	216/218 (99%)	197 (91%)	19 (9%)	12	34
2	EC	216/218 (99%)	194 (90%)	22 (10%)	8	26
2	GC	216/218 (99%)	203 (94%)	13 (6%)	22	54
4	AD	164/164 (100%)	151 (92%)	13 (8%)	14	39
4	CD	164/164 (100%)	152 (93%)	12 (7%)	16	43
4	ED	164/164 (100%)	152 (93%)	12 (7%)	16	43
4	GD	164/164 (100%)	151 (92%)	13 (8%)	14	39
5	AE	165/165 (100%)	146 (88%)	19 (12%)	6	20
5	CE	165/165 (100%)	157 (95%)	8 (5%)	30	64
5	EE	165/165 (100%)	153 (93%)	12 (7%)	16	43
5	GE	165/165 (100%)	152 (92%)	13 (8%)	14	39
6	AF	148/150 (99%)	138 (93%)	10 (7%)	18	47
6	CF	148/150 (99%)	140 (95%)	8 (5%)	26	59
6	EF	148/150 (99%)	133 (90%)	15 (10%)	9	27
6	GF	148/150 (99%)	146 (99%)	2 (1%)	71	91
7	AG	137/138 (99%)	122 (89%)	15 (11%)	7	22
7	CG	137/138 (99%)	125 (91%)	12 (9%)	12	34
7	EG	137/138 (99%)	119 (87%)	18 (13%)	5	14
7	GG	137/138 (99%)	128 (93%)	9 (7%)	19	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	AH	40/40 (100%)	39 (98%)	1 (2%)	53	83
8	CH	40/40 (100%)	38 (95%)	2 (5%)	28	62
8	EH	40/40 (100%)	37 (92%)	3 (8%)	16	42
8	GH	40/40 (100%)	39 (98%)	1 (2%)	53	83
9	AI	109/110 (99%)	105 (96%)	4 (4%)	39	74
9	CI	109/110 (99%)	106 (97%)	3 (3%)	49	82
9	EI	109/110 (99%)	106 (97%)	3 (3%)	49	82
9	GI	109/110 (99%)	107 (98%)	2 (2%)	64	89
10	AJ	116/116 (100%)	100 (86%)	16 (14%)	4	12
10	CJ	116/116 (100%)	101 (87%)	15 (13%)	5	15
10	EJ	116/116 (100%)	97 (84%)	19 (16%)	2	8
10	GJ	116/116 (100%)	104 (90%)	12 (10%)	8	25
11	AK	103/104 (99%)	92 (89%)	11 (11%)	8	23
11	CK	103/104 (99%)	87 (84%)	16 (16%)	3	9
11	EK	103/104 (99%)	87 (84%)	16 (16%)	3	9
11	GK	103/104 (99%)	90 (87%)	13 (13%)	5	15
12	AL	102/103 (99%)	95 (93%)	7 (7%)	18	46
12	CL	102/103 (99%)	94 (92%)	8 (8%)	15	39
12	EL	102/103 (99%)	96 (94%)	6 (6%)	23	55
12	GL	102/103 (99%)	96 (94%)	6 (6%)	23	55
13	AM	109/109 (100%)	93 (85%)	16 (15%)	3	11
13	CM	109/109 (100%)	98 (90%)	11 (10%)	9	27
13	EM	109/109 (100%)	100 (92%)	9 (8%)	13	36
13	GM	109/109 (100%)	103 (94%)	6 (6%)	25	58
14	AN	100/103 (97%)	93 (93%)	7 (7%)	18	45
14	CN	100/103 (97%)	96 (96%)	4 (4%)	36	71
14	EN	100/103 (97%)	96 (96%)	4 (4%)	36	71
14	GN	100/103 (97%)	93 (93%)	7 (7%)	18	45
15	AO	86/87 (99%)	78 (91%)	8 (9%)	10	31
15	CO	86/87 (99%)	80 (93%)	6 (7%)	18	45
15	EO	86/87 (99%)	81 (94%)	5 (6%)	23	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	GO	86/87 (99%)	81 (94%)	5 (6%)	23	56
16	AP	99/100 (99%)	91 (92%)	8 (8%)	14	38
16	CP	99/100 (99%)	90 (91%)	9 (9%)	11	32
16	EP	99/100 (99%)	88 (89%)	11 (11%)	7	21
16	GP	99/100 (99%)	90 (91%)	9 (9%)	11	32
17	AQ	89/90 (99%)	81 (91%)	8 (9%)	11	33
17	CQ	89/90 (99%)	84 (94%)	5 (6%)	25	57
17	EQ	89/90 (99%)	83 (93%)	6 (7%)	19	48
17	GQ	89/90 (99%)	83 (93%)	6 (7%)	19	48
18	AR	84/84 (100%)	78 (93%)	6 (7%)	17	44
18	CR	84/84 (100%)	79 (94%)	5 (6%)	22	54
18	ER	84/84 (100%)	76 (90%)	8 (10%)	10	29
18	GR	84/84 (100%)	79 (94%)	5 (6%)	22	54
19	AS	93/93 (100%)	84 (90%)	9 (10%)	9	29
19	CS	93/93 (100%)	86 (92%)	7 (8%)	16	42
19	ES	93/93 (100%)	84 (90%)	9 (10%)	9	29
19	GS	93/93 (100%)	88 (95%)	5 (5%)	26	59
20	AT	80/84 (95%)	77 (96%)	3 (4%)	38	73
20	CT	80/84 (95%)	75 (94%)	5 (6%)	21	51
20	ET	80/84 (95%)	74 (92%)	6 (8%)	16	42
20	GT	80/84 (95%)	77 (96%)	3 (4%)	38	73
21	AU	83/85 (98%)	76 (92%)	7 (8%)	13	36
21	CU	83/85 (98%)	80 (96%)	3 (4%)	40	75
21	EU	83/85 (98%)	78 (94%)	5 (6%)	22	54
21	GU	83/85 (98%)	79 (95%)	4 (5%)	30	64
22	AV	78/78 (100%)	75 (96%)	3 (4%)	38	73
22	CV	78/78 (100%)	73 (94%)	5 (6%)	20	50
22	EV	78/78 (100%)	75 (96%)	3 (4%)	38	73
22	GV	78/78 (100%)	77 (99%)	1 (1%)	73	93
23	AW	59/63 (94%)	53 (90%)	6 (10%)	8	26
23	CW	59/63 (94%)	55 (93%)	4 (7%)	18	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	EW	59/63 (94%)	49 (83%)	10 (17%)	2	7
23	GW	59/63 (94%)	57 (97%)	2 (3%)	42	76
24	AX	67/68 (98%)	61 (91%)	6 (9%)	11	33
24	CX	67/68 (98%)	60 (90%)	7 (10%)	8	25
24	EX	67/68 (98%)	57 (85%)	10 (15%)	3	10
24	GX	67/68 (98%)	63 (94%)	4 (6%)	22	54
25	AY	55/55 (100%)	52 (94%)	3 (6%)	25	58
25	CY	55/55 (100%)	51 (93%)	4 (7%)	16	43
25	EY	55/55 (100%)	50 (91%)	5 (9%)	11	32
25	GY	55/55 (100%)	52 (94%)	3 (6%)	25	58
26	AZ	48/49 (98%)	40 (83%)	8 (17%)	2	7
26	CZ	48/49 (98%)	39 (81%)	9 (19%)	2	5
26	EZ	48/49 (98%)	41 (85%)	7 (15%)	3	11
26	GZ	48/49 (98%)	46 (96%)	2 (4%)	34	69
27	A0	47/48 (98%)	46 (98%)	1 (2%)	59	86
27	C0	47/48 (98%)	47 (100%)	0	100	100
27	E0	47/48 (98%)	46 (98%)	1 (2%)	59	86
27	G0	47/48 (98%)	45 (96%)	2 (4%)	33	68
28	A1	45/49 (92%)	42 (93%)	3 (7%)	19	48
28	C1	45/49 (92%)	42 (93%)	3 (7%)	19	48
28	E1	45/49 (92%)	42 (93%)	3 (7%)	19	48
28	G1	45/49 (92%)	43 (96%)	2 (4%)	33	67
29	A2	38/38 (100%)	35 (92%)	3 (8%)	14	39
29	C2	38/38 (100%)	34 (90%)	4 (10%)	8	24
29	E2	38/38 (100%)	36 (95%)	2 (5%)	26	60
29	G2	38/38 (100%)	35 (92%)	3 (8%)	14	39
30	A3	51/52 (98%)	46 (90%)	5 (10%)	9	28
30	C3	51/52 (98%)	49 (96%)	2 (4%)	37	72
30	E3	51/52 (98%)	47 (92%)	4 (8%)	15	39
30	G3	51/52 (98%)	48 (94%)	3 (6%)	23	55
31	A4	34/34 (100%)	31 (91%)	3 (9%)	12	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	C4	34/34 (100%)	32 (94%)	2 (6%)	23	55
31	E4	34/34 (100%)	32 (94%)	2 (6%)	23	55
31	G4	34/34 (100%)	33 (97%)	1 (3%)	48	81
32	A5	112/123 (91%)	93 (83%)	19 (17%)	2	7
32	C5	112/123 (91%)	95 (85%)	17 (15%)	3	10
32	E5	111/123 (90%)	93 (84%)	18 (16%)	3	8
33	A6	26/85 (31%)	22 (85%)	4 (15%)	3	10
34	BB	180/199 (90%)	170 (94%)	10 (6%)	25	57
34	DB	180/199 (90%)	170 (94%)	10 (6%)	25	57
34	FB	180/199 (90%)	171 (95%)	9 (5%)	28	62
34	HB	180/199 (90%)	174 (97%)	6 (3%)	43	77
36	BC	170/190 (90%)	156 (92%)	14 (8%)	13	37
36	DC	170/190 (90%)	162 (95%)	8 (5%)	30	65
36	FC	170/190 (90%)	158 (93%)	12 (7%)	17	44
36	HC	170/190 (90%)	163 (96%)	7 (4%)	35	70
37	BD	172/173 (99%)	165 (96%)	7 (4%)	35	70
37	DD	172/173 (99%)	163 (95%)	9 (5%)	27	61
37	FD	172/173 (99%)	165 (96%)	7 (4%)	35	70
37	HD	172/173 (99%)	167 (97%)	5 (3%)	48	81
38	BE	113/126 (90%)	108 (96%)	5 (4%)	33	67
38	DE	113/126 (90%)	109 (96%)	4 (4%)	41	75
38	FE	113/126 (90%)	107 (95%)	6 (5%)	26	60
38	HE	113/126 (90%)	105 (93%)	8 (7%)	17	44
39	BF	89/116 (77%)	82 (92%)	7 (8%)	14	39
39	DF	87/116 (75%)	86 (99%)	1 (1%)	78	94
39	FF	87/116 (75%)	82 (94%)	5 (6%)	24	56
39	HF	87/116 (75%)	85 (98%)	2 (2%)	56	85
40	BG	124/147 (84%)	115 (93%)	9 (7%)	16	43
40	DG	124/147 (84%)	123 (99%)	1 (1%)	85	96
40	FG	124/147 (84%)	122 (98%)	2 (2%)	68	90
40	HG	124/147 (84%)	124 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	BH	104/105 (99%)	96 (92%)	8 (8%)	15	40
41	DH	104/105 (99%)	97 (93%)	7 (7%)	19	48
41	FH	104/105 (99%)	99 (95%)	5 (5%)	30	64
41	HH	104/105 (99%)	97 (93%)	7 (7%)	19	48
42	BI	105/107 (98%)	96 (91%)	9 (9%)	12	35
42	DI	105/107 (98%)	101 (96%)	4 (4%)	38	73
42	FI	105/107 (98%)	96 (91%)	9 (9%)	12	35
42	HI	105/107 (98%)	102 (97%)	3 (3%)	48	81
43	BJ	86/90 (96%)	83 (96%)	3 (4%)	41	75
43	DJ	86/90 (96%)	82 (95%)	4 (5%)	30	65
43	FJ	86/90 (96%)	83 (96%)	3 (4%)	41	75
43	HJ	86/90 (96%)	81 (94%)	5 (6%)	23	56
44	BK	90/99 (91%)	85 (94%)	5 (6%)	25	57
44	DK	90/99 (91%)	87 (97%)	3 (3%)	43	77
44	FK	90/99 (91%)	81 (90%)	9 (10%)	9	27
44	HK	90/99 (91%)	83 (92%)	7 (8%)	15	39
45	BL	103/104 (99%)	96 (93%)	7 (7%)	18	47
45	DL	103/104 (99%)	96 (93%)	7 (7%)	18	47
45	FL	103/104 (99%)	96 (93%)	7 (7%)	18	47
45	HL	103/104 (99%)	99 (96%)	4 (4%)	37	72
46	BM	92/96 (96%)	88 (96%)	4 (4%)	33	68
46	DM	92/96 (96%)	92 (100%)	0	100	100
46	FM	92/96 (96%)	91 (99%)	1 (1%)	78	94
46	HM	92/96 (96%)	91 (99%)	1 (1%)	78	94
47	BN	79/84 (94%)	75 (95%)	4 (5%)	28	62
47	DN	79/84 (94%)	78 (99%)	1 (1%)	73	93
47	FN	79/84 (94%)	76 (96%)	3 (4%)	38	73
47	HN	79/84 (94%)	79 (100%)	0	100	100
48	BO	76/77 (99%)	72 (95%)	4 (5%)	26	60
48	DO	76/77 (99%)	74 (97%)	2 (3%)	51	83
48	FO	76/77 (99%)	71 (93%)	5 (7%)	19	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	HO	76/77 (99%)	74 (97%)	2 (3%)	51	83
49	BP	65/65 (100%)	61 (94%)	4 (6%)	21	52
49	DP	65/65 (100%)	62 (95%)	3 (5%)	31	65
49	FP	65/65 (100%)	64 (98%)	1 (2%)	70	91
49	HP	65/65 (100%)	63 (97%)	2 (3%)	45	79
50	BQ	74/78 (95%)	66 (89%)	8 (11%)	7	23
50	DQ	74/78 (95%)	71 (96%)	3 (4%)	35	70
50	FQ	74/78 (95%)	72 (97%)	2 (3%)	50	82
50	HQ	74/78 (95%)	68 (92%)	6 (8%)	14	38
51	BR	48/65 (74%)	47 (98%)	1 (2%)	59	86
51	DR	48/65 (74%)	48 (100%)	0	100	100
51	FR	48/65 (74%)	48 (100%)	0	100	100
51	HR	48/65 (74%)	48 (100%)	0	100	100
52	BS	70/79 (89%)	64 (91%)	6 (9%)	12	35
52	DS	70/79 (89%)	67 (96%)	3 (4%)	33	68
52	FS	70/79 (89%)	67 (96%)	3 (4%)	33	68
52	HS	70/79 (89%)	69 (99%)	1 (1%)	71	91
53	BT	65/66 (98%)	60 (92%)	5 (8%)	15	40
53	DT	65/66 (98%)	58 (89%)	7 (11%)	7	23
53	FT	65/66 (98%)	58 (89%)	7 (11%)	7	23
53	HT	65/66 (98%)	57 (88%)	8 (12%)	5	16
54	BU	44/61 (72%)	36 (82%)	8 (18%)	2	6
54	DU	44/61 (72%)	42 (96%)	2 (4%)	32	66
54	FU	44/61 (72%)	39 (89%)	5 (11%)	7	20
54	HU	44/61 (72%)	43 (98%)	1 (2%)	56	85
55	BV	568/578 (98%)	521 (92%)	47 (8%)	13	36
55	DV	568/578 (98%)	527 (93%)	41 (7%)	17	43
55	FV	568/578 (98%)	528 (93%)	40 (7%)	18	45
55	HV	568/578 (98%)	535 (94%)	33 (6%)	23	56
56	BW	2/2 (100%)	1 (50%)	1 (50%)	0	0
56	DW	2/2 (100%)	1 (50%)	1 (50%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
56	FW	2/2 (100%)	1 (50%)	1 (50%)	<b>0</b> <b>0</b>
56	HW	2/2 (100%)	0	2 (100%)	<b>0</b> <b>0</b>
All	All	21011/21990 (96%)	19590 (93%)	1421 (7%)	<b>18</b> 47

5 of 1421 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
34	DB	71	THR
5	EE	44	ARG
34	HB	90	PHE
37	DD	171	LEU
55	DV	77	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 99 such sidechains are listed below:

Mol	Chain	Res	Type
55	DV	465	HIS
38	FE	82	GLN
43	HJ	56	HIS
4	ED	49	GLN
18	ER	66	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AB	117/120 (97%)	17 (14%)	0
1	CB	117/120 (97%)	19 (16%)	0
1	EB	117/120 (97%)	18 (15%)	0
1	GB	117/120 (97%)	20 (17%)	0
3	AA	2850/2904 (98%)	455 (15%)	0
3	CA	2850/2904 (98%)	457 (16%)	0
3	EA	2850/2904 (98%)	452 (15%)	0
3	GA	2850/2904 (98%)	459 (16%)	0
35	BA	1532/1542 (99%)	264 (17%)	0
35	DA	1532/1542 (99%)	264 (17%)	0
35	FA	1532/1542 (99%)	263 (17%)	0
35	HA	1532/1542 (99%)	268 (17%)	0
All	All	17996/18264 (98%)	2956 (16%)	0

5 of 2956 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AB	3	C
1	AB	15	A
1	AB	16	G
1	AB	21	G
1	AB	30	C

There are no RNA pucker outliers to report.

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

16 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	$\# Z  > 2$
56	KBE	BW	1	56	8,8,9	1.34	1 (12%)	7,8,10	1.26	1 (14%)
56	DPP	BW	2	56	4,5,6	1.00	0	1,5,7	2.90	1 (100%)
56	UAL	BW	5	56	8,8,9	3.14	5 (62%)	4,9,11	4.42	1 (25%)
56	5OH	BW	6	56	8,12,13	1.62	2 (25%)	5,16,18	2.71	3 (60%)
56	KBE	DW	1	56	8,8,9	1.09	1 (12%)	7,8,10	1.41	2 (28%)
56	DPP	DW	2	56	4,5,6	0.97	0	1,5,7	2.03	1 (100%)
56	UAL	DW	5	56	8,8,9	3.21	5 (62%)	4,9,11	4.27	1 (25%)
56	5OH	DW	6	56	8,12,13	1.61	2 (25%)	5,16,18	1.78	2 (40%)
56	KBE	FW	1	56	8,8,9	1.07	1 (12%)	7,8,10	1.06	0
56	DPP	FW	2	56	4,5,6	0.92	0	1,5,7	2.51	1 (100%)
56	UAL	FW	5	56	8,8,9	3.17	5 (62%)	4,9,11	5.08	1 (25%)
56	5OH	FW	6	56	8,12,13	1.78	2 (25%)	5,16,18	1.72	2 (40%)
56	KBE	HW	1	56	8,8,9	1.08	1 (12%)	7,8,10	1.08	1 (14%)
56	DPP	HW	2	56	4,5,6	1.18	0	1,5,7	2.62	1 (100%)
56	UAL	HW	5	56	8,8,9	3.67	5 (62%)	4,9,11	4.58	2 (50%)
56	5OH	HW	6	56	8,12,13	1.84	3 (37%)	5,16,18	1.87	2 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	KBE	BW	1	56	-	0/7/7/8	0/0/0/0
56	DPP	BW	2	56	-	0/2/4/6	0/0/0/0
56	UAL	BW	5	56	-	0/3/7/9	0/0/0/0
56	5OH	BW	6	56	-	0/2/18/20	0/1/1/1
56	KBE	DW	1	56	-	0/7/7/8	0/0/0/0
56	DPP	DW	2	56	-	0/2/4/6	0/0/0/0
56	UAL	DW	5	56	-	1/3/7/9	0/0/0/0
56	5OH	DW	6	56	-	0/2/18/20	0/1/1/1
56	KBE	FW	1	56	-	0/7/7/8	0/0/0/0
56	DPP	FW	2	56	-	0/2/4/6	0/0/0/0
56	UAL	FW	5	56	-	0/3/7/9	0/0/0/0
56	5OH	FW	6	56	-	0/2/18/20	0/1/1/1
56	KBE	HW	1	56	-	0/7/7/8	0/0/0/0
56	DPP	HW	2	56	-	0/2/4/6	0/0/0/0
56	UAL	HW	5	56	-	0/3/7/9	0/0/0/0
56	5OH	HW	6	56	-	0/2/18/20	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	FW	6	5OH	CR-CB	-3.17	1.47	1.53
56	BW	1	KBE	CB-N	-2.82	1.39	1.47
56	HW	1	KBE	CB-N	-2.55	1.40	1.47
56	BW	6	5OH	CR-CB	-2.53	1.48	1.53
56	FW	1	KBE	CB-N	-2.36	1.40	1.47

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	FW	5	UAL	O-C-CA	-10.00	112.69	125.47
56	BW	5	UAL	O-C-CA	-8.70	114.35	125.47
56	HW	5	UAL	O-C-CA	-8.63	114.45	125.47
56	DW	5	UAL	O-C-CA	-8.14	115.06	125.47
56	BW	6	5OH	O-C-CA	-4.24	115.26	125.15

There are no chirality outliers.

All (1) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
56	DW	5	UAL	CA-CB-N1-C1

There are no ring outliers.

12 monomers are involved in 15 short contacts:

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 756 ligands modelled in this entry, 752 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	$\# Z  > 2$
59	GCP	BV	801	57	25,34,34	2.83	9 (36%)	28,54,54	1.61	3 (10%)
59	GCP	DV	801	57	25,34,34	2.90	9 (36%)	28,54,54	1.65	4 (14%)
59	GCP	FV	801	57	25,34,34	2.72	8 (32%)	28,54,54	1.42	3 (10%)
59	GCP	HV	801	57	25,34,34	2.72	8 (32%)	28,54,54	1.40	6 (21%)

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
59	GCP	BV	801	57	-	0/18/38/38	0/3/3/3
59	GCP	DV	801	57	-	0/18/38/38	0/3/3/3
59	GCP	FV	801	57	-	0/18/38/38	0/3/3/3
59	GCP	HV	801	57	-	0/18/38/38	0/3/3/3

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	DV	801	GCP	C4-N9	-8.30	1.36	1.47
59	DV	801	GCP	C5-C6	-7.67	1.39	1.53
59	HV	801	GCP	C4-N9	-7.63	1.37	1.47
59	BV	801	GCP	C4-N9	-7.58	1.37	1.47
59	BV	801	GCP	C5-C6	-7.50	1.39	1.53

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	BV	801	GCP	PA-O3A-PB	-5.90	113.39	132.39
59	DV	801	GCP	PA-O3A-PB	-5.29	115.35	132.39
59	FV	801	GCP	PA-O3A-PB	-5.11	115.94	132.39
59	DV	801	GCP	C4'-O4'-C1'	-3.91	100.76	109.47
59	HV	801	GCP	C4'-O4'-C1'	-3.73	101.14	109.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

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

## 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	AB	118/120 (98%)	-0.52	0 100 100	7, 25, 37, 49	0
1	CB	118/120 (98%)	-0.70	0 100 100	19, 41, 55, 61	0
1	EB	118/120 (98%)	-0.43	0 100 100	6, 27, 41, 51	0
1	GB	118/120 (98%)	-0.01	1 (0%) 86 85	34, 57, 66, 70	0
2	AC	271/273 (99%)	-0.01	4 (1%) 74 72	2, 14, 26, 50	0
2	CC	271/273 (99%)	0.32	12 (4%) 35 30	14, 33, 45, 54	0
2	EC	271/273 (99%)	0.03	2 (0%) 87 86	3, 17, 30, 42	0
2	GC	271/273 (99%)	0.35	20 (7%) 15 11	12, 29, 43, 52	0
3	AA	2854/2904 (98%)	-0.08	51 (1%) 69 66	2, 14, 50, 79	0
3	CA	2854/2904 (98%)	-0.25	39 (1%) 75 74	8, 29, 57, 78	0
3	EA	2854/2904 (98%)	-0.09	48 (1%) 70 68	2, 16, 52, 83	0
3	GA	2854/2904 (98%)	-0.09	59 (2%) 64 60	10, 42, 64, 76	0
4	AD	209/209 (100%)	0.02	4 (1%) 67 64	2, 15, 35, 57	0
4	CD	209/209 (100%)	0.17	5 (2%) 59 55	5, 23, 42, 56	0
4	ED	209/209 (100%)	0.02	2 (0%) 82 81	2, 20, 40, 52	0
4	GD	209/209 (100%)	0.20	8 (3%) 41 35	10, 30, 46, 55	0
5	AE	201/201 (100%)	0.05	0 100 100	3, 19, 40, 51	0
5	CE	201/201 (100%)	0.38	18 (8%) 10 7	9, 34, 47, 57	0
5	EE	201/201 (100%)	0.10	3 (1%) 74 72	2, 21, 43, 57	0
5	GE	201/201 (100%)	1.27	53 (26%) 1 0	25, 51, 61, 68	0
6	AF	177/179 (98%)	0.39	9 (5%) 29 24	19, 33, 50, 60	0
6	CF	177/179 (98%)	0.98	39 (22%) 1 0	31, 47, 56, 62	0
6	EF	177/179 (98%)	0.59	20 (11%) 6 4	16, 34, 49, 58	0
6	GF	177/179 (98%)	3.10	105 (59%) 0 0	47, 59, 67, 72	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
7	AG	176/177 (99%)	0.30	11 (6%) 21 16	9, 25, 46, 59	0
7	CG	176/177 (99%)	0.50	16 (9%) 10 7	18, 36, 51, 61	0
7	EG	176/177 (99%)	0.30	12 (6%) 18 13	16, 31, 44, 55	0
7	GG	176/177 (99%)	1.03	35 (19%) 1 1	26, 43, 54, 65	0
8	AH	50/50 (100%)	0.88	11 (22%) 1 0	16, 41, 55, 57	0
8	CH	50/50 (100%)	3.69	38 (76%) 0 0	46, 57, 64, 68	0
8	EH	50/50 (100%)	1.17	11 (22%) 1 0	14, 38, 56, 62	0
8	GH	50/50 (100%)	2.27	25 (50%) 0 0	39, 52, 61, 64	0
9	AI	141/142 (99%)	2.48	64 (45%) 0 0	31, 53, 66, 78	0
9	CI	141/142 (99%)	2.16	69 (48%) 0 0	36, 54, 63, 72	0
9	EI	141/142 (99%)	2.23	65 (46%) 0 0	32, 54, 66, 76	0
9	GI	141/142 (99%)	3.98	111 (78%) 0 0	42, 59, 69, 80	0
10	AJ	142/142 (100%)	0.03	1 (0%) 87 86	4, 11, 29, 39	0
10	CJ	142/142 (100%)	0.21	3 (2%) 64 60	8, 24, 37, 54	0
10	EJ	142/142 (100%)	0.19	4 (2%) 53 48	5, 14, 28, 43	0
10	GJ	142/142 (100%)	0.35	6 (4%) 37 32	21, 36, 47, 55	0
11	AK	122/123 (99%)	0.12	1 (0%) 86 85	4, 10, 25, 50	0
11	CK	122/123 (99%)	0.07	2 (1%) 72 70	9, 18, 35, 42	0
11	EK	122/123 (99%)	0.18	4 (3%) 47 40	7, 18, 34, 47	0
11	GK	122/123 (99%)	0.65	9 (7%) 15 11	12, 24, 39, 53	0
12	AL	143/144 (99%)	0.16	4 (2%) 53 48	2, 18, 34, 39	0
12	CL	143/144 (99%)	0.52	14 (9%) 8 6	11, 31, 46, 54	0
12	EL	143/144 (99%)	0.25	5 (3%) 44 38	2, 18, 37, 49	0
12	GL	143/144 (99%)	1.76	61 (42%) 0 0	29, 46, 59, 65	0
13	AM	136/136 (100%)	0.16	2 (1%) 74 72	2, 9, 25, 48	0
13	CM	136/136 (100%)	0.34	5 (3%) 42 37	10, 21, 36, 52	0
13	EM	136/136 (100%)	0.14	2 (1%) 74 72	4, 13, 29, 43	0
13	GM	136/136 (100%)	1.45	37 (27%) 1 0	28, 44, 56, 60	0
14	AN	120/127 (94%)	0.17	2 (1%) 70 68	5, 13, 25, 56	0
14	CN	120/127 (94%)	0.21	1 (0%) 86 85	13, 24, 35, 56	0
14	EN	120/127 (94%)	0.19	2 (1%) 70 68	9, 19, 31, 59	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
14	GN	120/127 (94%)	0.24	4 (3%) 47 40	16, 28, 37, 58	0
15	AO	116/117 (99%)	0.04	2 (1%) 70 68	12, 24, 37, 46	0
15	CO	116/117 (99%)	0.56	10 (8%) 11 8	29, 40, 53, 59	0
15	EO	116/117 (99%)	0.32	5 (4%) 36 31	14, 27, 40, 44	0
15	GO	116/117 (99%)	1.75	44 (37%) 0 0	39, 52, 58, 65	0
16	AP	114/115 (99%)	0.04	2 (1%) 69 66	5, 19, 36, 44	0
16	CP	114/115 (99%)	0.17	2 (1%) 69 66	11, 25, 41, 54	0
16	EP	114/115 (99%)	0.01	1 (0%) 84 83	14, 26, 41, 60	0
16	GP	114/115 (99%)	0.13	4 (3%) 44 38	13, 27, 42, 51	0
17	AQ	117/118 (99%)	0.11	3 (2%) 56 51	3, 10, 26, 53	0
17	CQ	117/118 (99%)	0.16	3 (2%) 56 51	9, 23, 35, 54	0
17	EQ	117/118 (99%)	0.15	3 (2%) 56 51	2, 12, 27, 52	0
17	GQ	117/118 (99%)	0.93	19 (16%) 2 1	24, 41, 53, 58	0
18	AR	103/103 (100%)	0.01	2 (1%) 67 64	2, 18, 34, 47	0
18	CR	103/103 (100%)	0.28	4 (3%) 40 35	12, 31, 45, 55	0
18	ER	103/103 (100%)	0.27	5 (4%) 30 26	3, 23, 42, 49	0
18	GR	103/103 (100%)	1.50	33 (32%) 0 0	30, 47, 56, 64	0
19	AS	110/110 (100%)	0.19	2 (1%) 69 66	3, 12, 32, 54	0
19	CS	110/110 (100%)	0.41	5 (4%) 34 29	13, 22, 40, 47	0
19	ES	110/110 (100%)	0.30	3 (2%) 55 50	5, 14, 36, 51	0
19	GS	110/110 (100%)	0.99	21 (19%) 1 1	20, 39, 50, 55	0
20	AT	93/100 (93%)	0.62	10 (10%) 6 4	7, 24, 51, 55	0
20	CT	93/100 (93%)	0.99	16 (17%) 2 1	22, 36, 52, 56	0
20	ET	93/100 (93%)	0.86	14 (15%) 3 2	13, 26, 50, 58	0
20	GT	93/100 (93%)	1.78	39 (41%) 0 0	26, 45, 57, 64	0
21	AU	102/104 (98%)	0.55	6 (5%) 23 18	9, 22, 41, 62	0
21	CU	102/104 (98%)	1.32	28 (27%) 1 0	25, 36, 52, 65	0
21	EU	102/104 (98%)	0.58	10 (9%) 8 6	14, 30, 44, 59	0
21	GU	102/104 (98%)	2.69	63 (61%) 0 0	35, 53, 61, 68	0
22	AV	94/94 (100%)	-0.24	0 100 100	8, 23, 40, 46	0
22	CV	94/94 (100%)	-0.15	0 100 100	22, 31, 44, 52	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
22	EV	94/94 (100%)	-0.09	2 (2%) 64 60	12, 23, 40, 48	0
22	GV	94/94 (100%)	0.86	17 (18%) 1 1	36, 49, 59, 61	0
23	AW	79/85 (92%)	0.75	13 (16%) 2 1	8, 19, 41, 49	0
23	CW	79/85 (92%)	0.88	12 (15%) 2 1	18, 32, 48, 60	0
23	EW	79/85 (92%)	0.73	10 (12%) 4 3	6, 20, 38, 51	0
23	GW	79/85 (92%)	2.39	40 (50%) 0 0	35, 49, 59, 71	0
24	AX	77/78 (98%)	0.35	2 (2%) 56 51	7, 17, 37, 41	0
24	CX	77/78 (98%)	1.19	19 (24%) 1 0	22, 37, 49, 54	0
24	EX	77/78 (98%)	0.43	0 100 100	5, 15, 36, 37	0
24	GX	77/78 (98%)	1.26	22 (28%) 1 0	26, 44, 53, 58	0
25	AY	63/63 (100%)	0.52	7 (11%) 6 4	16, 34, 48, 52	0
25	CY	63/63 (100%)	1.06	13 (20%) 1 1	30, 43, 55, 62	0
25	EY	63/63 (100%)	0.88	13 (20%) 1 1	18, 33, 45, 56	0
25	GY	63/63 (100%)	2.50	36 (57%) 0 0	44, 51, 58, 60	0
26	AZ	58/59 (98%)	0.56	1 (1%) 70 68	4, 13, 39, 51	0
26	CZ	58/59 (98%)	0.67	3 (5%) 28 23	11, 26, 46, 59	0
26	EZ	58/59 (98%)	0.29	2 (3%) 46 39	3, 15, 37, 47	0
26	GZ	58/59 (98%)	1.85	24 (41%) 0 0	25, 48, 58, 63	0
27	A0	56/57 (98%)	0.43	4 (7%) 17 12	3, 19, 42, 51	0
27	C0	56/57 (98%)	0.27	2 (3%) 43 37	10, 27, 44, 55	0
27	E0	56/57 (98%)	0.31	3 (5%) 26 22	3, 22, 40, 47	0
27	G0	56/57 (98%)	0.61	6 (10%) 7 5	18, 35, 49, 57	0
28	A1	50/55 (90%)	0.66	5 (10%) 8 6	13, 24, 37, 43	0
28	C1	50/55 (90%)	1.61	14 (28%) 1 0	25, 39, 50, 51	0
28	E1	50/55 (90%)	0.68	4 (8%) 13 10	12, 22, 36, 43	0
28	G1	50/55 (90%)	2.69	27 (54%) 0 0	38, 50, 60, 65	0
29	A2	46/46 (100%)	0.09	2 (4%) 36 31	4, 8, 18, 44	0
29	C2	46/46 (100%)	0.47	2 (4%) 36 31	17, 24, 34, 43	0
29	E2	46/46 (100%)	0.06	0 100 100	5, 11, 21, 36	0
29	G2	46/46 (100%)	1.02	6 (13%) 4 3	20, 36, 43, 54	0
30	A3	64/65 (98%)	0.17	0 100 100	3, 10, 18, 30	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
30	C3	64/65 (98%)	0.66	6 (9%) 9 6	15, 28, 36, 39	0
30	E3	64/65 (98%)	0.30	1 (1%) 72 70	4, 9, 19, 31	0
30	G3	64/65 (98%)	1.63	18 (28%) 1 0	32, 43, 52, 60	0
31	A4	38/38 (100%)	0.17	0 100 100	5, 11, 25, 27	0
31	C4	38/38 (100%)	0.31	0 100 100	14, 23, 37, 39	0
31	E4	38/38 (100%)	0.09	0 100 100	7, 16, 27, 30	0
31	G4	38/38 (100%)	0.70	3 (7%) 13 10	24, 37, 50, 53	0
32	A5	148/165 (89%)	1.81	53 (35%) 0 0	30, 49, 61, 72	0
32	C5	148/165 (89%)	2.49	71 (47%) 0 0	37, 54, 64, 72	0
32	E5	145/165 (87%)	3.15	92 (63%) 0 0	36, 53, 62, 67	0
33	A6	30/121 (24%)	3.13	15 (50%) 0 0	47, 53, 62, 65	0
34	BB	218/241 (90%)	0.75	29 (13%) 4 2	24, 41, 56, 66	0
34	DB	218/241 (90%)	1.76	85 (38%) 0 0	35, 52, 61, 69	0
34	FB	218/241 (90%)	0.72	32 (14%) 3 2	25, 43, 56, 66	0
34	HB	218/241 (90%)	2.14	101 (46%) 0 0	42, 56, 66, 71	0
35	BA	1533/1542 (99%)	-0.25	15 (0%) 82 81	7, 21, 52, 78	0
35	DA	1533/1542 (99%)	-0.24	23 (1%) 74 72	13, 42, 64, 78	0
35	FA	1533/1542 (99%)	-0.19	23 (1%) 74 72	9, 31, 57, 75	0
35	HA	1533/1542 (99%)	0.36	146 (9%) 9 6	20, 52, 71, 78	0
36	BC	206/233 (88%)	-0.07	0 100 100	8, 26, 39, 57	0
36	DC	206/233 (88%)	0.60	19 (9%) 10 6	30, 45, 52, 59	0
36	FC	206/233 (88%)	0.25	4 (1%) 67 64	15, 30, 44, 57	0
36	HC	206/233 (88%)	2.15	99 (48%) 0 0	36, 52, 61, 67	0
37	BD	205/206 (99%)	0.34	13 (6%) 21 16	12, 28, 44, 51	0
37	DD	205/206 (99%)	0.38	15 (7%) 16 11	14, 30, 47, 55	0
37	FD	205/206 (99%)	1.48	60 (29%) 1 0	29, 45, 56, 68	0
37	HD	205/206 (99%)	0.99	41 (20%) 1 1	32, 45, 56, 65	0
38	BE	150/167 (89%)	0.05	4 (2%) 55 50	11, 26, 45, 63	0
38	DE	150/167 (89%)	0.09	3 (2%) 65 62	24, 38, 51, 60	0
38	FE	150/167 (89%)	0.27	11 (7%) 16 11	16, 35, 49, 64	0
38	HE	150/167 (89%)	1.21	43 (28%) 1 0	34, 49, 56, 59	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
39	BF	102/135 (75%)	-0.01	1 (0%) 82 81	15, 30, 42, 51	0
39	DF	100/135 (74%)	1.55	32 (32%) 0 0	42, 52, 59, 63	0
39	FF	100/135 (74%)	0.23	4 (4%) 39 34	13, 32, 44, 49	0
39	HF	100/135 (74%)	2.39	51 (51%) 0 0	46, 56, 65, 69	0
40	BG	151/179 (84%)	0.29	10 (6%) 19 14	10, 27, 46, 60	0
40	DG	151/179 (84%)	1.84	62 (41%) 0 0	41, 54, 61, 67	0
40	FG	151/179 (84%)	0.71	18 (11%) 5 3	15, 32, 50, 59	0
40	HG	151/179 (84%)	3.31	93 (61%) 0 0	46, 58, 66, 69	0
41	BH	129/130 (99%)	0.15	2 (1%) 72 70	15, 26, 40, 58	0
41	DH	129/130 (99%)	0.78	21 (16%) 2 1	27, 43, 55, 61	0
41	FH	129/130 (99%)	0.29	6 (4%) 32 28	19, 35, 47, 55	0
41	HH	129/130 (99%)	1.84	51 (39%) 0 0	36, 50, 58, 64	0
42	BI	127/130 (97%)	0.44	7 (5%) 26 21	8, 25, 47, 58	0
42	DI	127/130 (97%)	2.30	61 (48%) 0 0	41, 55, 62, 68	0
42	FI	127/130 (97%)	0.35	8 (6%) 21 16	9, 27, 50, 56	0
42	HI	127/130 (97%)	2.45	68 (53%) 0 0	46, 57, 65, 68	0
43	BJ	98/103 (95%)	0.72	11 (11%) 6 4	9, 35, 56, 61	0
43	DJ	98/103 (95%)	1.62	35 (35%) 0 0	38, 52, 60, 68	0
43	FJ	98/103 (95%)	0.90	16 (16%) 2 1	16, 31, 53, 59	0
43	HJ	98/103 (95%)	2.67	63 (64%) 0 0	40, 54, 63, 66	0
44	BK	117/129 (90%)	0.21	7 (5%) 23 17	14, 26, 40, 52	0
44	DK	117/129 (90%)	1.29	32 (27%) 1 0	38, 52, 60, 62	0
44	FK	117/129 (90%)	-0.05	4 (3%) 46 39	13, 24, 36, 41	0
44	HK	117/129 (90%)	2.81	72 (61%) 0 0	45, 58, 68, 73	0
45	BL	123/124 (99%)	0.05	2 (1%) 72 70	5, 12, 29, 52	0
45	DL	123/124 (99%)	0.21	6 (4%) 30 26	12, 24, 40, 49	0
45	FL	123/124 (99%)	0.17	3 (2%) 59 55	11, 26, 43, 51	0
45	HL	123/124 (99%)	0.96	22 (17%) 2 1	24, 41, 53, 63	0
46	BM	114/118 (96%)	-0.02	2 (1%) 69 66	11, 30, 51, 54	0
46	DM	114/118 (96%)	1.35	30 (26%) 1 0	39, 53, 62, 66	0
46	FM	114/118 (96%)	0.34	11 (9%) 9 6	17, 36, 52, 59	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
46	HM	114/118 (96%)	4.31	88 (77%) 0 0	48, 60, 68, 77	0
47	BN	96/101 (95%)	0.29	4 (4%) 37 32	10, 22, 46, 57	0
47	DN	96/101 (95%)	0.68	12 (12%) 4 3	31, 45, 55, 62	0
47	FN	96/101 (95%)	0.49	7 (7%) 16 11	19, 29, 50, 64	0
47	HN	96/101 (95%)	2.32	46 (47%) 0 0	41, 56, 66, 71	0
48	BO	88/89 (98%)	0.03	0 100 100	12, 27, 40, 42	0
48	DO	88/89 (98%)	0.96	18 (20%) 1 1	36, 46, 55, 59	0
48	FO	88/89 (98%)	0.46	7 (7%) 13 10	16, 31, 44, 51	0
48	HO	88/89 (98%)	1.15	22 (25%) 1 0	37, 49, 58, 63	0
49	BP	82/82 (100%)	0.55	5 (6%) 22 17	13, 21, 46, 63	0
49	DP	82/82 (100%)	0.84	10 (12%) 5 3	16, 27, 48, 59	0
49	FP	82/82 (100%)	1.25	19 (23%) 1 0	24, 35, 54, 70	0
49	HP	82/82 (100%)	0.97	17 (20%) 1 1	25, 37, 49, 59	0
50	BQ	80/84 (95%)	0.34	3 (3%) 41 35	14, 26, 39, 48	0
50	DQ	80/84 (95%)	0.62	7 (8%) 11 7	26, 37, 45, 48	0
50	FQ	80/84 (95%)	0.58	6 (7%) 15 11	18, 36, 50, 55	0
50	HQ	80/84 (95%)	1.19	18 (22%) 1 0	35, 44, 55, 62	0
51	BR	55/75 (73%)	0.32	2 (3%) 43 37	16, 26, 39, 48	0
51	DR	55/75 (73%)	2.03	21 (38%) 0 0	43, 52, 60, 62	0
51	FR	55/75 (73%)	0.30	2 (3%) 43 37	18, 26, 37, 45	0
51	HR	55/75 (73%)	3.32	38 (69%) 0 0	43, 54, 61, 63	0
52	BS	79/92 (85%)	0.24	4 (5%) 29 24	14, 23, 39, 65	0
52	DS	79/92 (85%)	1.43	24 (30%) 0 0	31, 49, 58, 61	0
52	FS	79/92 (85%)	0.27	3 (3%) 41 35	22, 34, 48, 52	0
52	HS	79/92 (85%)	4.41	64 (81%) 0 0	50, 60, 70, 73	0
53	BT	85/87 (97%)	0.46	4 (4%) 32 28	12, 23, 42, 47	0
53	DT	85/87 (97%)	0.51	7 (8%) 12 9	17, 28, 44, 53	0
53	FT	85/87 (97%)	0.74	9 (10%) 7 5	25, 38, 47, 63	0
53	HT	85/87 (97%)	0.92	10 (11%) 5 4	22, 33, 46, 52	0
54	BU	51/71 (71%)	1.00	11 (21%) 1 1	22, 37, 52, 61	0
54	DU	51/71 (71%)	2.21	25 (49%) 0 0	36, 54, 60, 64	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
54	FU	51/71 (71%)	0.79	8 (15%) 2 1	25, 35, 54, 61	0
54	HU	51/71 (71%)	4.14	41 (80%) 0 0	40, 54, 65, 71	0
55	BV	690/704 (98%)	0.02	26 (3%) 41 35	10, 30, 48, 66	0
55	DV	689/704 (97%)	0.25	56 (8%) 13 9	16, 37, 53, 63	0
55	FV	689/704 (97%)	0.58	81 (11%) 5 4	16, 41, 54, 63	0
55	HV	689/704 (97%)	1.14	166 (24%) 1 0	25, 51, 62, 73	0
56	BW	2/6 (33%)	0.14	0 100 100	16, 16, 16, 20	0
56	DW	2/6 (33%)	-0.24	0 100 100	32, 32, 32, 34	0
56	FW	2/6 (33%)	0.75	0 100 100	23, 23, 23, 29	0
56	HW	2/6 (33%)	0.85	1 (50%) 0 0	51, 51, 51, 58	0
All	All	43746/45264 (96%)	0.42	4537 (10%) 7 5	2, 33, 60, 83	0

The worst 5 of 4537 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
46	HM	84	GLY	19.7
26	CZ	1	ALA	18.7
26	AZ	1	ALA	16.4
6	GF	169	LEU	15.6
28	C1	52	LYS	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	KBE	DW	1	9/10	0.83	0.27	-	33,35,41,48	0
56	5OH	BW	6	12/13	0.94	0.14	-	11,17,21,21	0
56	5OH	DW	6	12/13	0.95	0.13	-	22,29,35,37	0
56	5OH	FW	6	12/13	0.96	0.16	-	10,24,29,30	0
56	KBE	FW	1	9/10	0.89	0.42	-	17,21,37,51	0
56	KBE	HW	1	9/10	0.84	0.31	-	27,45,52,55	0
56	KBE	BW	1	9/10	0.93	0.19	-	4,9,22,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	UAL	BW	5	9/10	0.92	0.21	-	16,20,27,32	0
56	DPP	HW	2	6/7	0.82	0.15	-	30,41,49,53	0
56	DPP	BW	2	6/7	0.96	0.18	-	6,12,15,22	0
56	UAL	HW	5	9/10	0.87	0.25	-	36,48,56,60	0
56	DPP	FW	2	6/7	0.98	0.20	-	18,22,27,32	0
56	5OH	HW	6	12/13	0.80	0.27	-	48,54,58,60	0
56	UAL	DW	5	9/10	0.93	0.12	-	17,27,36,48	0
56	UAL	FW	5	9/10	0.93	0.15	-	15,18,29,38	0
56	DPP	DW	2	6/7	0.96	0.12	-	25,37,38,39	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	GA	3131	1/1	0.83	1.13	47.87	43,43,43,43	0
57	MG	AA	3097	1/1	0.70	0.56	28.93	34,34,34,34	0
57	MG	GA	3055	1/1	0.91	0.64	22.04	21,21,21,21	0
57	MG	GA	3021	1/1	0.97	0.67	19.81	20,20,20,20	0
57	MG	EA	3040	1/1	0.97	0.28	16.70	11,11,11,11	0
57	MG	CA	3112	1/1	0.99	0.30	16.06	10,10,10,10	0
57	MG	AA	3078	1/1	0.99	0.34	10.55	13,13,13,13	0
57	MG	AA	3129	1/1	0.98	0.24	10.06	9,9,9,9	0
57	MG	HA	1628	1/1	0.98	0.26	9.28	29,29,29,29	0
57	MG	AA	3111	1/1	0.99	0.25	7.12	3,3,3,3	0
57	MG	GA	3050	1/1	0.96	0.28	6.75	26,26,26,26	0
57	MG	AA	3037	1/1	0.96	0.43	6.71	30,30,30,30	0
57	MG	AA	3100	1/1	0.95	0.29	6.37	1,1,1,1	0
57	MG	GA	3107	1/1	0.99	0.26	5.98	13,13,13,13	0
57	MG	AA	3041	1/1	0.99	0.24	5.97	7,7,7,7	0
57	MG	AA	3135	1/1	0.97	0.37	5.96	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	AA	3047	1/1	0.95	0.21	5.89	12,12,12,12	0
57	MG	EA	3005	1/1	0.99	0.20	5.78	16,16,16,16	0
57	MG	DA	1628	1/1	0.97	0.32	5.64	44,44,44,44	0
57	MG	BA	1616	1/1	0.99	0.27	5.59	3,3,3,3	0
57	MG	AA	3107	1/1	1.00	0.24	5.54	4,4,4,4	0
57	MG	EA	3042	1/1	0.99	0.23	5.39	13,13,13,13	0
57	MG	AA	3095	1/1	0.98	0.26	5.21	4,4,4,4	0
57	MG	CA	3046	1/1	0.99	0.22	5.21	21,21,21,21	0
57	MG	AA	3068	1/1	0.99	0.23	4.91	2,2,2,2	0
57	MG	GA	3100	1/1	0.98	0.29	4.79	12,12,12,12	0
57	MG	AA	3115	1/1	0.99	0.24	4.71	1,1,1,1	0
57	MG	AA	3090	1/1	0.94	0.24	4.62	32,32,32,32	0
57	MG	BA	1627	1/1	0.98	0.22	4.35	19,19,19,19	0
57	MG	GA	3009	1/1	0.95	0.22	4.22	35,35,35,35	0
57	MG	FA	1635	1/1	0.85	0.34	4.11	41,41,41,41	0
57	MG	EA	3123	1/1	0.99	0.23	4.07	3,3,3,3	0
57	MG	FA	1609	1/1	0.99	0.25	4.00	7,7,7,7	0
57	MG	HA	1613	1/1	0.97	0.27	4.00	32,32,32,32	0
57	MG	CA	3131	1/1	0.99	0.27	3.87	11,11,11,11	0
57	MG	EA	3046	1/1	0.97	0.23	3.86	9,9,9,9	0
57	MG	EA	3038	1/1	0.98	0.22	3.85	2,2,2,2	0
57	MG	AA	3026	1/1	0.99	0.22	3.76	4,4,4,4	0
57	MG	CA	3068	1/1	0.98	0.19	3.69	9,9,9,9	0
57	MG	GA	3104	1/1	0.99	0.29	3.62	12,12,12,12	0
57	MG	CA	3040	1/1	0.99	0.21	3.52	11,11,11,11	0
57	MG	FA	1626	1/1	0.98	0.23	3.24	22,22,22,22	0
57	MG	AA	3050	1/1	1.00	0.20	3.21	2,2,2,2	0
57	MG	BA	1607	1/1	0.88	0.27	3.19	34,34,34,34	0
57	MG	AA	3108	1/1	0.99	0.26	3.18	1,1,1,1	0
57	MG	GA	3023	1/1	0.99	0.33	3.17	27,27,27,27	0
57	MG	EA	3103	1/1	0.99	0.26	3.10	0,0,0,0	0
57	MG	AA	3029	1/1	0.99	0.24	3.02	0,0,0,0	0
57	MG	GA	3030	1/1	0.98	0.26	2.96	15,15,15,15	0
57	MG	CA	3109	1/1	0.98	0.24	2.93	7,7,7,7	0
57	MG	AA	3106	1/1	0.99	0.21	2.85	4,4,4,4	0
57	MG	GA	3115	1/1	0.98	0.23	2.80	20,20,20,20	0
57	MG	DA	1642	1/1	1.00	0.21	2.71	4,4,4,4	0
57	MG	CA	3105	1/1	0.99	0.23	2.65	14,14,14,14	0
57	MG	GA	3119	1/1	0.97	0.21	2.60	18,18,18,18	0
57	MG	EA	3025	1/1	0.98	0.23	2.57	1,1,1,1	0
57	MG	EA	3096	1/1	0.99	0.22	2.50	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	FA	1611	1/1	0.98	0.21	2.50	7,7,7,7	0
57	MG	CA	3136	1/1	0.85	0.28	2.42	22,22,22,22	0
57	MG	FA	1613	1/1	1.00	0.20	2.35	6,6,6,6	0
57	MG	EA	3104	1/1	0.99	0.23	2.34	0,0,0,0	0
57	MG	EA	3023	1/1	0.99	0.22	2.33	9,9,9,9	0
57	MG	DV	802	1/1	0.99	0.20	2.27	14,14,14,14	0
57	MG	EA	3100	1/1	0.98	0.22	2.23	1,1,1,1	0
57	MG	CA	3120	1/1	0.99	0.21	2.08	11,11,11,11	0
57	MG	CA	3023	1/1	0.98	0.26	1.81	5,5,5,5	0
57	MG	AA	3060	1/1	0.89	0.27	1.68	34,34,34,34	0
57	MG	FA	1622	1/1	0.98	0.20	1.63	9,9,9,9	0
57	MG	HA	1623	1/1	0.98	0.20	1.58	36,36,36,36	0
57	MG	GA	3049	1/1	1.00	0.22	1.55	12,12,12,12	0
57	MG	EA	3037	1/1	0.99	0.19	1.51	2,2,2,2	0
57	MG	CN	201	1/1	0.97	0.21	1.44	20,20,20,20	0
57	MG	DA	1616	1/1	0.98	0.34	1.42	28,28,28,28	0
57	MG	CA	3110	1/1	0.96	0.18	1.42	23,23,23,23	0
57	MG	CA	3009	1/1	0.99	0.18	1.37	10,10,10,10	0
57	MG	DA	1639	1/1	0.98	0.16	1.36	30,30,30,30	0
57	MG	CA	3024	1/1	0.98	0.20	1.32	6,6,6,6	0
57	MG	AA	3035	1/1	0.98	0.20	1.31	5,5,5,5	0
57	MG	CB	1202	1/1	0.92	0.16	1.29	44,44,44,44	0
57	MG	BA	1638	1/1	1.00	0.18	1.29	13,13,13,13	0
57	MG	CA	3005	1/1	0.99	0.15	1.24	35,35,35,35	0
57	MG	CA	3079	1/1	0.99	0.20	1.24	27,27,27,27	0
57	MG	AA	3094	1/1	1.00	0.19	1.19	16,16,16,16	0
57	MG	BA	1626	1/1	0.98	0.21	1.06	5,5,5,5	0
57	MG	CA	3121	1/1	1.00	0.22	1.05	8,8,8,8	0
57	MG	EA	3053	1/1	0.99	0.20	1.04	1,1,1,1	0
57	MG	CA	3066	1/1	0.98	0.17	0.97	4,4,4,4	0
57	MG	EA	3084	1/1	0.99	0.22	0.94	7,7,7,7	0
57	MG	BA	1605	1/1	0.98	0.16	0.91	28,28,28,28	0
57	MG	BV	802	1/1	0.98	0.20	0.83	22,22,22,22	0
57	MG	DA	1610	1/1	0.98	0.10	0.81	28,28,28,28	0
57	MG	EA	3130	1/1	0.98	0.20	0.63	0,0,0,0	0
57	MG	BA	1640	1/1	0.99	0.22	0.61	11,11,11,11	0
57	MG	BA	1632	1/1	0.99	0.16	0.51	14,14,14,14	0
57	MG	BA	1628	1/1	1.00	0.19	0.50	18,18,18,18	0
57	MG	GA	3109	1/1	0.87	0.16	0.44	35,35,35,35	0
57	MG	EA	3120	1/1	0.99	0.20	0.37	5,5,5,5	0
57	MG	CA	3113	1/1	0.95	0.20	0.33	10,10,10,10	0
57	MG	GA	3022	1/1	0.99	0.17	0.31	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	GA	3040	1/1	0.97	0.16	0.21	15,15,15,15	0
57	MG	CA	3133	1/1	0.99	0.21	0.17	13,13,13,13	0
57	MG	AA	3009	1/1	1.00	0.19	0.15	2,2,2,2	0
57	MG	FV	802	1/1	0.99	0.18	0.15	24,24,24,24	0
57	MG	AA	3130	1/1	0.98	0.20	0.13	3,3,3,3	0
57	MG	DA	1606	1/1	0.98	0.20	0.13	15,15,15,15	0
57	MG	CA	3107	1/1	0.98	0.17	0.13	14,14,14,14	0
57	MG	GA	3108	1/1	0.97	0.18	0.09	38,38,38,38	0
57	MG	GA	3099	1/1	0.97	0.14	0.06	33,33,33,33	0
57	MG	BA	1636	1/1	0.95	0.15	0.03	24,24,24,24	0
57	MG	AA	3114	1/1	0.95	0.20	-0.00	10,10,10,10	0
57	MG	HV	802	1/1	0.99	0.17	-0.04	38,38,38,38	0
57	MG	GA	3047	1/1	0.99	0.13	-0.06	38,38,38,38	0
57	MG	GA	3024	1/1	0.96	0.19	-0.10	14,14,14,14	0
57	MG	CA	3116	1/1	0.98	0.16	-0.10	7,7,7,7	0
57	MG	EA	3133	1/1	1.00	0.21	-0.14	0,0,0,0	0
57	MG	AA	3065	1/1	1.00	0.18	-0.15	11,11,11,11	0
57	MG	HA	1611	1/1	0.88	0.20	-0.15	26,26,26,26	0
57	MG	BA	1613	1/1	0.96	0.17	-0.17	8,8,8,8	0
57	MG	GA	3053	1/1	0.99	0.17	-0.20	6,6,6,6	0
57	MG	FA	1628	1/1	0.99	0.16	-0.22	27,27,27,27	0
59	GCP	FV	801	32/32	0.95	0.16	-0.23	16,28,45,57	0
57	MG	EA	3014	1/1	0.97	0.21	-0.28	1,1,1,1	0
57	MG	GL	201	1/1	0.85	0.30	-0.31	47,47,47,47	0
57	MG	CA	3049	1/1	0.98	0.17	-0.31	7,7,7,7	0
57	MG	GA	3008	1/1	0.93	0.17	-0.32	24,24,24,24	0
57	MG	BA	1619	1/1	0.99	0.17	-0.34	13,13,13,13	0
57	MG	HA	1606	1/1	0.98	0.17	-0.35	29,29,29,29	0
57	MG	HA	1633	1/1	0.99	0.17	-0.38	46,46,46,46	0
59	GCP	DV	801	32/32	0.96	0.14	-0.39	17,28,38,41	0
57	MG	AA	3104	1/1	0.98	0.20	-0.41	2,2,2,2	0
57	MG	HA	1627	1/1	0.96	0.20	-0.42	41,41,41,41	0
57	MG	CA	3069	1/1	0.84	0.12	-0.42	61,61,61,61	0
57	MG	EA	3024	1/1	0.99	0.19	-0.43	2,2,2,2	0
57	MG	EA	3115	1/1	0.98	0.17	-0.43	6,6,6,6	0
57	MG	EA	3112	1/1	0.99	0.17	-0.43	2,2,2,2	0
57	MG	EA	3008	1/1	1.00	0.18	-0.48	1,1,1,1	0
57	MG	EA	3113	1/1	0.99	0.14	-0.49	7,7,7,7	0
57	MG	CA	3028	1/1	1.00	0.18	-0.52	9,9,9,9	0
57	MG	AA	3103	1/1	0.98	0.18	-0.55	0,0,0,0	0
57	MG	HA	1637	1/1	0.92	0.14	-0.56	51,51,51,51	0
57	MG	EA	3034	1/1	0.98	0.17	-0.57	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	EB	1202	1/1	0.98	0.13	-0.60	17,17,17,17	0
57	MG	GA	3078	1/1	0.99	0.12	-0.61	35,35,35,35	0
59	GCP	BV	801	32/32	0.98	0.14	-0.62	9,25,32,35	0
57	MG	GA	3032	1/1	0.94	0.16	-0.65	22,22,22,22	0
57	MG	EA	3108	1/1	0.98	0.20	-0.66	15,15,15,15	0
57	MG	FN	202	1/1	1.00	0.15	-0.80	26,26,26,26	0
57	MG	GA	3113	1/1	0.97	0.13	-0.80	32,32,32,32	0
57	MG	HA	1640	1/1	1.00	0.15	-0.81	18,18,18,18	0
57	MG	HA	1620	1/1	0.94	0.17	-0.83	32,32,32,32	0
57	MG	GA	3012	1/1	0.99	0.16	-0.85	22,22,22,22	0
57	MG	GA	3062	1/1	0.98	0.17	-0.86	19,19,19,19	0
57	MG	EA	3079	1/1	0.99	0.15	-0.88	8,8,8,8	0
57	MG	AA	3073	1/1	0.99	0.18	-0.89	2,2,2,2	0
58	ZN	C4	102	1/1	0.99	0.14	-0.90	41,41,41,41	0
57	MG	GA	3122	1/1	0.99	0.17	-0.93	16,16,16,16	0
57	MG	CA	3008	1/1	0.99	0.16	-0.95	14,14,14,14	0
57	MG	AA	3109	1/1	0.99	0.08	-0.96	20,20,20,20	0
57	MG	AA	3039	1/1	0.99	0.18	-0.97	3,3,3,3	0
57	MG	CA	3003	1/1	0.98	0.13	-0.98	10,10,10,10	0
57	MG	GA	3069	1/1	0.83	0.11	-0.99	70,70,70,70	0
57	MG	GA	3132	1/1	0.98	0.15	-1.00	28,28,28,28	0
57	MG	AA	3002	1/1	0.98	0.15	-1.00	25,25,25,25	0
57	MG	AA	3062	1/1	0.99	0.18	-1.01	4,4,4,4	0
57	MG	DA	1609	1/1	0.98	0.15	-1.01	13,13,13,13	0
59	GCP	HV	801	32/32	0.96	0.12	-1.04	18,36,48,55	0
57	MG	GA	3036	1/1	0.98	0.15	-1.04	38,38,38,38	0
57	MG	GA	3106	1/1	0.98	0.15	-1.05	7,7,7,7	0
57	MG	AA	3132	1/1	0.99	0.17	-1.07	0,0,0,0	0
57	MG	EA	3035	1/1	0.98	0.18	-1.07	12,12,12,12	0
57	MG	CA	3104	1/1	0.99	0.16	-1.10	8,8,8,8	0
57	MG	CA	3071	1/1	0.99	0.17	-1.14	10,10,10,10	0
57	MG	GA	3111	1/1	0.98	0.14	-1.15	35,35,35,35	0
57	MG	DA	1621	1/1	0.98	0.12	-1.16	44,44,44,44	0
58	ZN	A4	102	1/1	0.99	0.13	-1.17	42,42,42,42	0
57	MG	CA	3114	1/1	0.99	0.12	-1.17	26,26,26,26	0
57	MG	CA	3053	1/1	0.98	0.15	-1.18	20,20,20,20	0
57	MG	CE	301	1/1	0.98	0.07	-1.20	19,19,19,19	0
57	MG	ED	301	1/1	0.99	0.16	-1.21	7,7,7,7	0
57	MG	CA	3027	1/1	0.99	0.10	-1.23	10,10,10,10	0
57	MG	DA	1613	1/1	0.99	0.13	-1.24	23,23,23,23	0
57	MG	GA	3064	1/1	0.99	0.12	-1.25	11,11,11,11	0
57	MG	GA	3130	1/1	1.00	0.11	-1.32	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BU	101	1/1	0.98	0.14	-1.36	19,19,19,19	0
57	MG	EA	3022	1/1	0.99	0.17	-1.36	2,2,2,2	0
57	MG	FA	1630	1/1	0.98	0.08	-1.38	44,44,44,44	0
57	MG	HA	1629	1/1	0.91	0.12	-1.38	45,45,45,45	0
58	ZN	G4	101	1/1	0.98	0.07	-1.47	66,66,66,66	0
57	MG	EA	3131	1/1	0.98	0.11	-1.49	3,3,3,3	0
57	MG	GA	3017	1/1	0.96	0.12	-1.50	10,10,10,10	0
57	MG	BA	1604	1/1	0.99	0.07	-1.50	17,17,17,17	0
57	MG	EA	3049	1/1	0.98	0.17	-1.51	8,8,8,8	0
57	MG	BA	1610	1/1	0.98	0.09	-1.52	41,41,41,41	0
57	MG	DA	1607	1/1	0.98	0.14	-1.54	16,16,16,16	0
57	MG	CA	3095	1/1	0.98	0.15	-1.55	14,14,14,14	0
57	MG	EA	3114	1/1	0.96	0.17	-1.55	17,17,17,17	0
57	MG	EA	3002	1/1	0.99	0.14	-1.61	7,7,7,7	0
57	MG	AA	3113	1/1	0.97	0.12	-1.63	8,8,8,8	0
57	MG	GA	3007	1/1	0.92	0.07	-1.65	39,39,39,39	0
57	MG	DA	1633	1/1	0.99	0.08	-1.87	29,29,29,29	0
57	MG	GA	3134	1/1	0.98	0.08	-1.88	28,28,28,28	0
57	MG	FA	1604	1/1	0.96	0.08	-2.06	34,34,34,34	0
57	MG	EA	3095	1/1	0.94	0.13	-2.07	6,6,6,6	0
57	MG	FA	1620	1/1	0.97	0.09	-2.08	41,41,41,41	0
57	MG	FA	1607	1/1	0.99	0.10	-2.09	21,21,21,21	0
57	MG	FA	1631	1/1	0.99	0.10	-2.13	24,24,24,24	0
57	MG	EA	3105	1/1	0.99	0.14	-2.14	5,5,5,5	0
57	MG	CA	3118	1/1	0.98	0.12	-2.14	31,31,31,31	0
57	MG	CA	3073	1/1	0.98	0.13	-2.17	4,4,4,4	0
57	MG	EA	3110	1/1	0.91	0.14	-2.17	12,12,12,12	0
57	MG	GA	3096	1/1	0.99	0.15	-2.23	15,15,15,15	0
57	MG	EA	3107	1/1	1.00	0.15	-2.23	5,5,5,5	0
57	MG	AA	3018	1/1	1.00	0.16	-2.24	2,2,2,2	0
57	MG	AA	3025	1/1	0.97	0.15	-2.25	0,0,0,0	0
57	MG	EA	3065	1/1	0.99	0.14	-2.30	5,5,5,5	0
57	MG	FA	1616	1/1	0.99	0.12	-2.50	18,18,18,18	0
57	MG	DA	1604	1/1	0.96	0.07	-2.51	18,18,18,18	0
57	MG	FA	1638	1/1	0.98	0.12	-2.51	16,16,16,16	0
57	MG	DA	1634	1/1	0.93	0.08	-2.58	34,34,34,34	0
57	MG	AA	3003	1/1	0.99	0.13	-2.59	11,11,11,11	0
57	MG	GA	3128	1/1	0.92	0.10	-2.61	18,18,18,18	0
57	MG	CA	3124	1/1	0.99	0.13	-2.63	26,26,26,26	0
57	MG	AA	3004	1/1	0.99	0.12	-2.72	20,20,20,20	0
57	MG	DA	1630	1/1	0.96	0.11	-2.72	25,25,25,25	0
57	MG	HA	1604	1/1	0.96	0.04	-2.74	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	AA	3012	1/1	0.97	0.21	-2.77	32,32,32,32	0
57	MG	DA	1624	1/1	0.96	0.14	-2.77	18,18,18,18	0
57	MG	CA	3063	1/1	0.99	0.14	-2.85	4,4,4,4	0
57	MG	EA	3106	1/1	0.99	0.13	-2.86	9,9,9,9	0
57	MG	DA	1611	1/1	0.99	0.11	-2.88	35,35,35,35	0
57	MG	AA	3054	1/1	1.00	0.14	-3.01	3,3,3,3	0
57	MG	AA	3024	1/1	0.99	0.15	-3.15	5,5,5,5	0
57	MG	AA	3119	1/1	0.98	0.15	-3.18	0,0,0,0	0
57	MG	EA	3109	1/1	0.96	0.11	-3.22	19,19,19,19	0
57	MG	AA	3082	1/1	0.99	0.07	-3.26	22,22,22,22	0
58	ZN	E4	101	1/1	0.99	0.09	-3.28	59,59,59,59	0
57	MG	EA	3064	1/1	0.99	0.14	-3.32	2,2,2,2	0
57	MG	AB	1202	1/1	0.99	0.08	-3.35	25,25,25,25	0
57	MG	AA	3014	1/1	0.99	0.14	-3.43	2,2,2,2	0
57	MG	GA	3002	1/1	0.98	0.07	-3.61	31,31,31,31	0
57	MG	CA	3012	1/1	0.94	0.13	-3.63	6,6,6,6	0
57	MG	GA	3118	1/1	0.99	0.11	-3.65	39,39,39,39	0
57	MG	GA	3074	1/1	0.99	0.14	-3.75	10,10,10,10	0
57	MG	EA	3111	1/1	0.98	0.13	-3.92	5,5,5,5	0
57	MG	DA	1617	1/1	0.97	0.08	-4.07	39,39,39,39	0
57	MG	CA	3070	1/1	0.99	0.10	-4.10	8,8,8,8	0
57	MG	CA	3058	1/1	1.00	0.14	-4.21	18,18,18,18	0
57	MG	CA	3050	1/1	0.99	0.08	-4.25	14,14,14,14	0
57	MG	AA	3123	1/1	0.99	0.11	-4.26	5,5,5,5	0
57	MG	AA	3131	1/1	0.99	0.10	-4.43	3,3,3,3	0
57	MG	EA	3066	1/1	0.99	0.12	-4.82	1,1,1,1	0
57	MG	AA	3071	1/1	1.00	0.12	-5.33	4,4,4,4	0
57	MG	EA	3128	1/1	0.98	0.18	-5.48	0,0,0,0	0
57	MG	BA	1631	1/1	0.99	0.07	-5.83	16,16,16,16	0
57	MG	GA	3027	1/1	0.99	0.09	-5.97	17,17,17,17	0
57	MG	AA	3128	1/1	1.00	0.15	-6.05	0,0,0,0	0
57	MG	CA	3119	1/1	0.94	0.08	-6.25	34,34,34,34	0
57	MG	AA	3028	1/1	0.99	0.12	-7.11	4,4,4,4	0
57	MG	CA	3013	1/1	0.99	0.07	-7.12	9,9,9,9	0
57	MG	GA	3065	1/1	0.98	0.12	-	20,20,20,20	0
57	MG	FA	1621	1/1	0.97	0.14	-	13,13,13,13	0
57	MG	FA	1614	1/1	0.98	0.20	-	13,13,13,13	0
57	MG	DA	1631	1/1	0.99	0.06	-	13,13,13,13	0
57	MG	GA	3121	1/1	0.96	0.15	-	16,16,16,16	0
57	MG	EA	3006	1/1	0.99	0.11	-	9,9,9,9	0
57	MG	EA	3134	1/1	0.99	0.24	-	7,7,7,7	0
57	MG	FA	1601	1/1	0.98	0.08	-	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	AA	3008	1/1	0.99	0.06	-	19,19,19,19	0
57	MG	GA	3054	1/1	0.98	0.14	-	12,12,12,12	0
57	MG	EA	3082	1/1	0.99	0.12	-	6,6,6,6	0
57	MG	EA	3124	1/1	0.99	0.43	-	4,4,4,4	0
57	MG	CA	3020	1/1	0.99	0.11	-	6,6,6,6	0
57	MG	GA	3083	1/1	0.91	0.12	-	26,26,26,26	0
57	MG	EA	3126	1/1	0.99	0.13	-	6,6,6,6	0
57	MG	GA	3052	1/1	0.98	0.18	-	4,4,4,4	0
57	MG	AA	3093	1/1	0.91	0.31	-	34,34,34,34	0
57	MG	EA	3045	1/1	0.98	0.17	-	9,9,9,9	0
57	MG	GA	3135	1/1	0.84	0.41	-	28,28,28,28	0
57	MG	AA	3101	1/1	0.99	0.16	-	8,8,8,8	0
57	MG	EA	3125	1/1	0.95	0.24	-	18,18,18,18	0
57	MG	AA	3059	1/1	0.99	0.24	-	1,1,1,1	0
57	MG	CA	3123	1/1	0.99	0.24	-	26,26,26,26	0
57	MG	FU	101	1/1	0.95	0.17	-	21,21,21,21	0
57	MG	EA	3102	1/1	0.98	0.08	-	23,23,23,23	0
57	MG	AA	3084	1/1	0.96	0.19	-	2,2,2,2	0
57	MG	BA	1603	1/1	0.97	0.15	-	18,18,18,18	0
57	MG	GA	3127	1/1	0.98	0.13	-	18,18,18,18	0
57	MG	GA	3105	1/1	0.98	0.17	-	16,16,16,16	0
57	MG	AA	3030	1/1	0.99	0.09	-	1,1,1,1	0
57	MG	GB	1203	1/1	0.98	0.07	-	23,23,23,23	0
57	MG	GA	3014	1/1	0.99	0.07	-	15,15,15,15	0
57	MG	GA	3043	1/1	0.99	0.09	-	20,20,20,20	0
57	MG	GA	3026	1/1	0.98	0.16	-	31,31,31,31	0
57	MG	FA	1625	1/1	0.98	0.15	-	21,21,21,21	0
57	MG	FA	1605	1/1	0.99	0.09	-	30,30,30,30	0
57	MG	AA	3074	1/1	0.99	0.18	-	5,5,5,5	0
57	MG	GA	3094	1/1	0.99	0.06	-	14,14,14,14	0
57	MG	GA	3077	1/1	0.97	0.12	-	55,55,55,55	0
57	MG	HA	1609	1/1	0.91	0.20	-	23,23,23,23	0
57	MG	A4	101	1/1	0.98	0.12	-	20,20,20,20	0
57	MG	BA	1612	1/1	0.99	0.18	-	3,3,3,3	0
57	MG	CA	3117	1/1	0.99	0.12	-	7,7,7,7	0
57	MG	CA	3075	1/1	0.99	0.25	-	11,11,11,11	0
57	MG	AA	3064	1/1	0.99	0.12	-	3,3,3,3	0
57	MG	HA	1608	1/1	0.94	0.43	-	47,47,47,47	0
57	MG	CA	3128	1/1	1.00	0.16	-	17,17,17,17	0
57	MG	CA	3088	1/1	0.96	0.28	-	23,23,23,23	0
57	MG	CA	3134	1/1	0.98	0.20	-	21,21,21,21	0
57	MG	AA	3089	1/1	0.99	0.09	-	4,4,4,4	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	GA	3010	1/1	0.98	0.32	-	16,16,16,16	0
57	MG	CA	3025	1/1	0.94	0.14	-	24,24,24,24	0
57	MG	EA	3020	1/1	1.00	0.15	-	7,7,7,7	0
57	MG	BA	1602	1/1	0.88	0.23	-	38,38,38,38	0
57	MG	EA	3121	1/1	0.97	0.30	-	5,5,5,5	0
57	MG	GA	3124	1/1	0.94	0.20	-	36,36,36,36	0
57	MG	EA	3122	1/1	0.97	0.28	-	4,4,4,4	0
57	MG	CA	3044	1/1	0.95	0.08	-	28,28,28,28	0
57	MG	GA	3045	1/1	0.99	0.20	-	17,17,17,17	0
57	MG	FA	1637	1/1	0.97	0.09	-	29,29,29,29	0
57	MG	GA	3004	1/1	0.95	0.39	-	25,25,25,25	0
57	MG	CB	1203	1/1	0.99	0.10	-	12,12,12,12	0
57	MG	GA	3082	1/1	0.98	0.09	-	38,38,38,38	0
57	MG	CA	3122	1/1	1.00	0.20	-	5,5,5,5	0
57	MG	AA	3022	1/1	1.00	0.11	-	2,2,2,2	0
57	MG	EA	3099	1/1	0.99	0.16	-	3,3,3,3	0
57	MG	EA	3068	1/1	1.00	0.20	-	2,2,2,2	0
57	MG	BA	1615	1/1	0.91	0.30	-	25,25,25,25	0
57	MG	HA	1607	1/1	0.98	0.07	-	33,33,33,33	0
57	MG	CA	3026	1/1	0.98	0.15	-	14,14,14,14	0
57	MG	FA	1606	1/1	0.95	0.16	-	15,15,15,15	0
57	MG	EA	3091	1/1	0.95	0.27	-	40,40,40,40	0
57	MG	FA	1629	1/1	0.99	0.12	-	30,30,30,30	0
57	MG	GA	3011	1/1	0.88	0.11	-	46,46,46,46	0
57	MG	EA	3041	1/1	0.98	0.18	-	3,3,3,3	0
57	MG	CA	3074	1/1	0.98	0.16	-	13,13,13,13	0
57	MG	GA	3029	1/1	0.99	0.08	-	16,16,16,16	0
57	MG	BA	1601	1/1	0.98	0.10	-	23,23,23,23	0
57	MG	EA	3058	1/1	0.99	0.14	-	5,5,5,5	0
57	MG	CA	3065	1/1	0.99	0.17	-	11,11,11,11	0
57	MG	EA	3118	1/1	0.93	0.12	-	17,17,17,17	0
57	MG	HA	1624	1/1	0.88	0.11	-	38,38,38,38	0
57	MG	CA	3089	1/1	0.99	0.19	-	14,14,14,14	0
57	MG	DA	1623	1/1	0.97	0.17	-	42,42,42,42	0
57	MG	GA	3016	1/1	0.98	0.12	-	12,12,12,12	0
57	MG	CA	3041	1/1	0.99	0.08	-	12,12,12,12	0
57	MG	EA	3007	1/1	0.98	0.08	-	12,12,12,12	0
57	MG	GA	3028	1/1	0.96	0.17	-	12,12,12,12	0
57	MG	BA	1621	1/1	1.00	0.09	-	11,11,11,11	0
57	MG	EA	3012	1/1	1.00	0.20	-	2,2,2,2	0
57	MG	EA	3059	1/1	1.00	0.17	-	10,10,10,10	0
57	MG	FA	1619	1/1	0.99	0.12	-	7,7,7,7	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	EA	3132	1/1	0.96	0.14	-	21,21,21,21	0
57	MG	BA	1609	1/1	0.99	0.12	-	7,7,7,7	0
57	MG	HA	1632	1/1	0.97	0.10	-	31,31,31,31	0
57	MG	EA	3013	1/1	1.00	0.13	-	1,1,1,1	0
57	MG	EA	3019	1/1	0.96	0.13	-	10,10,10,10	0
57	MG	HA	1631	1/1	0.96	0.17	-	31,31,31,31	0
57	MG	EA	3021	1/1	0.99	0.16	-	11,11,11,11	0
57	MG	CA	3032	1/1	0.99	0.17	-	8,8,8,8	0
57	MG	DA	1619	1/1	0.99	0.18	-	34,34,34,34	0
57	MG	AB	1201	1/1	0.99	0.08	-	34,34,34,34	0
57	MG	AA	3083	1/1	0.94	0.26	-	18,18,18,18	0
57	MG	GA	3080	1/1	0.90	0.21	-	36,36,36,36	0
57	MG	FN	201	1/1	0.96	0.24	-	14,14,14,14	0
57	MG	CA	3087	1/1	0.99	0.14	-	23,23,23,23	0
57	MG	AA	3105	1/1	0.99	0.15	-	2,2,2,2	0
57	MG	AA	3045	1/1	0.97	0.21	-	8,8,8,8	0
57	MG	EB	1203	1/1	0.99	0.17	-	0,0,0,0	0
57	MG	CA	3093	1/1	0.97	0.11	-	40,40,40,40	0
57	MG	AA	3118	1/1	0.97	0.07	-	14,14,14,14	0
57	MG	EA	3061	1/1	0.99	0.17	-	5,5,5,5	0
57	MG	CA	3061	1/1	0.98	0.10	-	4,4,4,4	0
57	MG	CA	3057	1/1	1.00	0.11	-	7,7,7,7	0
57	MG	DA	1622	1/1	0.99	0.14	-	13,13,13,13	0
57	MG	GA	3037	1/1	0.99	0.32	-	18,18,18,18	0
57	MG	CA	3001	1/1	1.00	0.09	-	16,16,16,16	0
57	MG	AA	3086	1/1	0.99	0.08	-	14,14,14,14	0
57	MG	CA	3084	1/1	0.99	0.22	-	20,20,20,20	0
57	MG	EA	3016	1/1	0.99	0.23	-	0,0,0,0	0
57	MG	CA	3031	1/1	0.99	0.15	-	7,7,7,7	0
57	MG	CA	3022	1/1	0.99	0.12	-	17,17,17,17	0
57	MG	AA	3136	1/1	0.97	0.34	-	11,11,11,11	0
57	MG	GA	3116	1/1	0.92	0.31	-	22,22,22,22	0
57	MG	GA	3042	1/1	1.00	0.14	-	20,20,20,20	0
57	MG	GA	3097	1/1	0.99	0.28	-	10,10,10,10	0
57	MG	EA	3076	1/1	0.97	0.13	-	6,6,6,6	0
57	MG	EA	3003	1/1	0.99	0.19	-	9,9,9,9	0
57	MG	CA	3126	1/1	0.99	0.14	-	22,22,22,22	0
57	MG	FE	201	1/1	0.98	0.12	-	35,35,35,35	0
57	MG	HA	1612	1/1	0.97	0.28	-	20,20,20,20	0
57	MG	EA	3043	1/1	1.00	0.17	-	8,8,8,8	0
57	MG	EA	3031	1/1	1.00	0.16	-	1,1,1,1	0
57	MG	GA	3087	1/1	0.98	0.12	-	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	EA	3036	1/1	0.98	0.13	-	12,12,12,12	0
57	MG	HA	1616	1/1	0.96	0.38	-	40,40,40,40	0
57	MG	AA	3031	1/1	0.99	0.20	-	5,5,5,5	0
57	MG	BA	1639	1/1	0.98	0.26	-	12,12,12,12	0
57	MG	AA	3076	1/1	0.98	0.14	-	13,13,13,13	0
57	MG	FA	1634	1/1	0.99	0.18	-	13,13,13,13	0
57	MG	AA	3121	1/1	0.99	0.22	-	3,3,3,3	0
57	MG	HA	1625	1/1	0.94	0.32	-	44,44,44,44	0
57	MG	CA	3052	1/1	1.00	0.14	-	4,4,4,4	0
57	MG	AA	3006	1/1	0.88	0.15	-	32,32,32,32	0
57	MG	AA	3056	1/1	1.00	0.13	-	11,11,11,11	0
57	MG	GA	3041	1/1	0.99	0.12	-	10,10,10,10	0
57	MG	GA	3051	1/1	0.96	0.25	-	20,20,20,20	0
57	MG	CA	3125	1/1	1.00	0.23	-	11,11,11,11	0
57	MG	GA	3092	1/1	0.98	0.17	-	16,16,16,16	0
57	MG	CA	3132	1/1	0.98	0.10	-	9,9,9,9	0
57	MG	EA	3069	1/1	0.95	0.09	-	25,25,25,25	0
57	MG	AE	301	1/1	0.95	0.30	-	21,21,21,21	0
57	MG	HA	1615	1/1	0.89	0.17	-	36,36,36,36	0
57	MG	AA	3046	1/1	0.98	0.29	-	13,13,13,13	0
57	MG	BA	1611	1/1	0.99	0.12	-	7,7,7,7	0
57	MG	CA	3115	1/1	0.87	0.23	-	51,51,51,51	0
57	MG	AA	3077	1/1	0.99	0.11	-	16,16,16,16	0
57	MG	BA	1630	1/1	0.99	0.16	-	26,26,26,26	0
57	MG	EA	3070	1/1	0.93	0.60	-	23,23,23,23	0
57	MG	CA	3056	1/1	0.88	0.72	-	27,27,27,27	0
57	MG	EA	3050	1/1	0.91	0.19	-	23,23,23,23	0
57	MG	BA	1633	1/1	0.98	0.10	-	20,20,20,20	0
57	MG	FA	1632	1/1	0.99	0.13	-	24,24,24,24	0
57	MG	GA	3076	1/1	0.91	0.27	-	34,34,34,34	0
57	MG	EA	3052	1/1	0.97	0.17	-	12,12,12,12	0
57	MG	GA	3114	1/1	0.92	0.31	-	27,27,27,27	0
57	MG	DA	1635	1/1	0.94	0.08	-	37,37,37,37	0
57	MG	EA	3073	1/1	0.99	0.15	-	0,0,0,0	0
57	MG	GA	3071	1/1	0.99	0.16	-	16,16,16,16	0
57	MG	HA	1617	1/1	0.89	0.14	-	49,49,49,49	0
57	MG	AA	3102	1/1	0.99	0.11	-	10,10,10,10	0
57	MG	FA	1608	1/1	0.99	0.23	-	13,13,13,13	0
57	MG	EA	3030	1/1	0.99	0.28	-	7,7,7,7	0
57	MG	HA	1602	1/1	0.95	0.16	-	26,26,26,26	0
57	MG	AA	3088	1/1	0.98	0.18	-	4,4,4,4	0
57	MG	EA	3081	1/1	0.99	0.20	-	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	FA	1610	1/1	0.97	0.25	-	33,33,33,33	0
57	MG	CA	3037	1/1	0.99	0.27	-	6,6,6,6	0
57	MG	AA	3017	1/1	1.00	0.11	-	0,0,0,0	0
57	MG	DA	1638	1/1	0.98	0.09	-	25,25,25,25	0
57	MG	GA	3058	1/1	0.99	0.13	-	24,24,24,24	0
57	MG	EA	3028	1/1	0.98	0.17	-	7,7,7,7	0
57	MG	CA	3098	1/1	0.97	0.15	-	29,29,29,29	0
57	MG	FA	1617	1/1	0.97	0.12	-	40,40,40,40	0
57	MG	HA	1621	1/1	0.99	0.14	-	7,7,7,7	0
57	MG	GA	3075	1/1	0.98	0.18	-	16,16,16,16	0
57	MG	AA	3079	1/1	0.99	0.11	-	4,4,4,4	0
57	MG	AA	3011	1/1	1.00	0.25	-	6,6,6,6	0
57	MG	BA	1620	1/1	0.93	0.12	-	15,15,15,15	0
57	MG	AA	3066	1/1	1.00	0.21	-	0,0,0,0	0
57	MG	BN	201	1/1	0.98	0.20	-	13,13,13,13	0
57	MG	AA	3058	1/1	0.99	0.14	-	9,9,9,9	0
57	MG	CA	3007	1/1	0.98	0.15	-	35,35,35,35	0
57	MG	EA	3117	1/1	0.97	0.09	-	15,15,15,15	0
57	MG	EA	3071	1/1	0.99	0.17	-	0,0,0,0	0
57	MG	BA	1618	1/1	0.99	0.17	-	1,1,1,1	0
57	MG	GC	301	1/1	0.98	0.24	-	26,26,26,26	0
57	MG	CA	3082	1/1	0.98	0.16	-	14,14,14,14	0
57	MG	EA	3063	1/1	0.99	0.14	-	2,2,2,2	0
57	MG	DA	1629	1/1	0.90	0.53	-	43,43,43,43	0
57	MG	CA	3019	1/1	0.98	0.14	-	27,27,27,27	0
57	MG	GA	3006	1/1	0.94	0.12	-	29,29,29,29	0
57	MG	HA	1626	1/1	0.74	0.27	-	32,32,32,32	0
57	MG	EA	3055	1/1	0.89	0.56	-	30,30,30,30	0
57	MG	EA	3078	1/1	0.98	0.10	-	20,20,20,20	0
57	MG	CA	3060	1/1	0.99	0.12	-	7,7,7,7	0
57	MG	EA	3129	1/1	0.99	0.21	-	2,2,2,2	0
57	MG	GA	3066	1/1	0.99	0.16	-	12,12,12,12	0
57	MG	EA	3075	1/1	1.00	0.21	-	11,11,11,11	0
57	MG	CA	3083	1/1	0.99	0.04	-	32,32,32,32	0
57	MG	AA	3040	1/1	1.00	0.25	-	1,1,1,1	0
57	MG	EA	3090	1/1	0.99	0.07	-	11,11,11,11	0
57	MG	CA	3072	1/1	0.99	0.14	-	14,14,14,14	0
57	MG	HK	201	1/1	0.81	0.24	-	28,28,28,28	0
57	MG	EA	3116	1/1	0.99	0.16	-	6,6,6,6	0
57	MG	EB	1201	1/1	0.97	0.10	-	30,30,30,30	0
57	MG	CA	3043	1/1	0.99	0.16	-	4,4,4,4	0
57	MG	HA	1639	1/1	0.96	0.14	-	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	EA	3093	1/1	0.98	0.13	-	11,11,11,11	0
57	MG	GA	3112	1/1	0.99	0.20	-	13,13,13,13	0
57	MG	GA	3085	1/1	0.99	0.17	-	10,10,10,10	0
57	MG	GA	3073	1/1	0.99	0.17	-	10,10,10,10	0
57	MG	AA	3049	1/1	0.99	0.19	-	17,17,17,17	0
57	MG	BA	1637	1/1	0.94	0.34	-	15,15,15,15	0
57	MG	CA	3011	1/1	0.90	0.22	-	31,31,31,31	0
57	MG	CA	3051	1/1	0.99	0.32	-	6,6,6,6	0
57	MG	EA	3086	1/1	1.00	0.19	-	8,8,8,8	0
57	MG	CA	3034	1/1	0.98	0.14	-	13,13,13,13	0
57	MG	FA	1623	1/1	0.99	0.16	-	6,6,6,6	0
57	MG	AA	3033	1/1	0.99	0.19	-	1,1,1,1	0
57	MG	EA	3032	1/1	1.00	0.17	-	1,1,1,1	0
57	MG	HA	1601	1/1	0.94	0.06	-	27,27,27,27	0
57	MG	GA	3056	1/1	1.00	0.06	-	13,13,13,13	0
57	MG	GA	3091	1/1	0.98	0.06	-	28,28,28,28	0
57	MG	GA	3003	1/1	0.98	0.10	-	26,26,26,26	0
57	MG	HA	1634	1/1	0.96	0.10	-	35,35,35,35	0
57	MG	AA	3126	1/1	0.99	0.13	-	2,2,2,2	0
57	MG	EA	3127	1/1	0.99	0.15	-	11,11,11,11	0
57	MG	AA	3133	1/1	0.99	0.18	-	10,10,10,10	0
57	MG	AA	3007	1/1	0.97	0.10	-	19,19,19,19	0
57	MG	AA	3099	1/1	0.99	0.14	-	13,13,13,13	0
57	MG	DA	1615	1/1	0.99	0.20	-	45,45,45,45	0
57	MG	EA	3027	1/1	1.00	0.17	-	4,4,4,4	0
57	MG	BE	201	1/1	0.81	0.15	-	31,31,31,31	0
57	MG	AA	3001	1/1	0.95	0.72	-	20,20,20,20	0
57	MG	EA	3060	1/1	0.99	0.20	-	2,2,2,2	0
57	MG	DA	1602	1/1	0.97	0.08	-	28,28,28,28	0
57	MG	AA	3052	1/1	0.98	0.16	-	3,3,3,3	0
57	MG	AA	3019	1/1	0.98	0.14	-	15,15,15,15	0
57	MG	AA	3127	1/1	0.99	0.13	-	10,10,10,10	0
57	MG	GA	3067	1/1	0.99	0.27	-	29,29,29,29	0
57	MG	GA	3103	1/1	0.99	0.22	-	12,12,12,12	0
57	MG	DA	1612	1/1	0.97	0.14	-	33,33,33,33	0
57	MG	EA	3051	1/1	0.98	0.27	-	6,6,6,6	0
57	MG	FA	1633	1/1	0.98	0.15	-	24,24,24,24	0
57	MG	EA	3101	1/1	0.98	0.14	-	7,7,7,7	0
57	MG	EA	3067	1/1	0.99	0.21	-	3,3,3,3	0
57	MG	GA	3133	1/1	0.91	0.42	-	15,15,15,15	0
57	MG	CA	3106	1/1	0.99	0.26	-	12,12,12,12	0
57	MG	AA	3069	1/1	0.86	0.13	-	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	EA	3039	1/1	0.93	0.19	-	15,15,15,15	0
57	MG	AA	3016	1/1	0.95	0.17	-	11,11,11,11	0
57	MG	DA	1608	1/1	0.96	0.22	-	30,30,30,30	0
57	MG	CA	3077	1/1	0.90	0.63	-	37,37,37,37	0
57	MG	DA	1625	1/1	0.98	0.14	-	29,29,29,29	0
57	MG	EA	3083	1/1	0.59	0.43	-	35,35,35,35	0
57	MG	CA	3091	1/1	0.94	0.44	-	38,38,38,38	0
57	MG	BA	1625	1/1	0.96	0.17	-	23,23,23,23	0
57	MG	FA	1624	1/1	0.98	0.20	-	27,27,27,27	0
57	MG	CA	3067	1/1	1.00	0.20	-	6,6,6,6	0
57	MG	CA	3054	1/1	0.99	0.09	-	14,14,14,14	0
57	MG	BA	1608	1/1	0.99	0.23	-	11,11,11,11	0
57	MG	EA	3089	1/1	0.99	0.14	-	6,6,6,6	0
57	MG	HA	1622	1/1	0.97	0.21	-	30,30,30,30	0
57	MG	GA	3129	1/1	0.94	0.28	-	29,29,29,29	0
57	MG	GA	3120	1/1	0.97	0.20	-	19,19,19,19	0
57	MG	CA	3035	1/1	1.00	0.13	-	7,7,7,7	0
57	MG	EA	3062	1/1	0.99	0.16	-	4,4,4,4	0
57	MG	AA	3112	1/1	0.98	0.25	-	0,0,0,0	0
57	MG	EA	3085	1/1	0.99	0.26	-	11,11,11,11	0
57	MG	GA	3015	1/1	0.95	0.22	-	27,27,27,27	0
57	MG	AA	3032	1/1	0.99	0.17	-	0,0,0,0	0
57	MG	CA	3004	1/1	0.99	0.09	-	24,24,24,24	0
57	MG	CA	3103	1/1	0.98	0.11	-	17,17,17,17	0
57	MG	GA	3095	1/1	0.85	0.42	-	43,43,43,43	0
57	MG	AA	3042	1/1	0.98	0.20	-	8,8,8,8	0
57	MG	CA	3101	1/1	1.00	0.18	-	5,5,5,5	0
57	MG	AA	3027	1/1	0.99	0.17	-	15,15,15,15	0
57	MG	GA	3072	1/1	0.99	0.08	-	24,24,24,24	0
57	MG	AA	3124	1/1	0.97	0.25	-	4,4,4,4	0
57	MG	EA	3080	1/1	0.98	0.20	-	15,15,15,15	0
57	MG	GB	1201	1/1	0.82	0.26	-	62,62,62,62	0
57	MG	DA	1626	1/1	0.92	0.15	-	44,44,44,44	0
57	MG	GA	3098	1/1	1.00	0.15	-	15,15,15,15	0
57	MG	BA	1614	1/1	0.99	0.11	-	7,7,7,7	0
57	MG	CA	3097	1/1	0.99	0.13	-	3,3,3,3	0
57	MG	GA	3019	1/1	1.00	0.15	-	6,6,6,6	0
57	MG	FA	1636	1/1	0.71	0.24	-	35,35,35,35	0
57	MG	DA	1620	1/1	1.00	0.04	-	12,12,12,12	0
57	MG	AA	3070	1/1	0.98	0.27	-	6,6,6,6	0
57	MG	BA	1617	1/1	0.99	0.06	-	21,21,21,21	0
57	MG	CA	3100	1/1	0.99	0.07	-	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	GA	3070	1/1	0.94	0.14	-	22,22,22,22	0
57	MG	GA	3048	1/1	0.99	0.16	-	15,15,15,15	0
57	MG	EA	3056	1/1	0.98	0.13	-	13,13,13,13	0
57	MG	GA	3001	1/1	0.99	0.06	-	31,31,31,31	0
57	MG	CA	3036	1/1	0.98	0.12	-	28,28,28,28	0
57	MG	GA	3126	1/1	0.98	0.07	-	35,35,35,35	0
57	MG	GA	3039	1/1	0.98	0.25	-	28,28,28,28	0
57	MG	CA	3078	1/1	0.96	0.08	-	34,34,34,34	0
57	MG	AA	3075	1/1	0.98	0.11	-	15,15,15,15	0
57	MG	AA	3134	1/1	0.96	0.24	-	21,21,21,21	0
57	MG	FA	1603	1/1	0.92	0.14	-	20,20,20,20	0
57	MG	AA	3043	1/1	0.99	0.15	-	5,5,5,5	0
57	MG	CA	3059	1/1	0.98	0.18	-	10,10,10,10	0
57	MG	AA	3072	1/1	0.99	0.17	-	5,5,5,5	0
57	MG	CB	1204	1/1	0.97	0.05	-	15,15,15,15	0
57	MG	GA	3018	1/1	0.96	0.05	-	21,21,21,21	0
57	MG	FA	1639	1/1	0.99	0.16	-	20,20,20,20	0
57	MG	GA	3034	1/1	0.99	0.09	-	36,36,36,36	0
57	MG	GA	3123	1/1	0.98	0.20	-	44,44,44,44	0
57	MG	HA	1618	1/1	0.92	0.16	-	35,35,35,35	0
57	MG	CA	3029	1/1	0.99	0.15	-	19,19,19,19	0
57	MG	CA	3081	1/1	0.99	0.24	-	6,6,6,6	0
57	MG	GA	3136	1/1	0.95	0.22	-	27,27,27,27	0
57	MG	CA	3135	1/1	0.94	0.36	-	8,8,8,8	0
57	MG	CA	3085	1/1	0.95	0.16	-	5,5,5,5	0
57	MG	GA	3093	1/1	0.99	0.11	-	21,21,21,21	0
57	MG	CA	3039	1/1	0.99	0.25	-	4,4,4,4	0
57	MG	GA	3033	1/1	0.97	0.28	-	30,30,30,30	0
57	MG	EA	3017	1/1	0.99	0.15	-	8,8,8,8	0
57	MG	AA	3005	1/1	0.97	0.13	-	16,16,16,16	0
57	MG	GA	3063	1/1	0.98	0.14	-	27,27,27,27	0
57	MG	EB	1204	1/1	0.99	0.12	-	8,8,8,8	0
57	MG	DA	1640	1/1	0.98	0.06	-	24,24,24,24	0
57	MG	AA	3092	1/1	0.94	0.10	-	14,14,14,14	0
57	MG	DA	1643	1/1	0.94	0.22	-	32,32,32,32	0
57	MG	EA	3015	1/1	0.87	0.55	-	2,2,2,2	0
57	MG	AA	3038	1/1	0.98	0.26	-	3,3,3,3	0
57	MG	GA	3057	1/1	0.92	0.14	-	28,28,28,28	0
57	MG	HA	1603	1/1	0.99	0.08	-	25,25,25,25	0
57	MG	EA	3077	1/1	0.99	0.09	-	18,18,18,18	0
57	MG	EA	3029	1/1	1.00	0.25	-	2,2,2,2	0
57	MG	DA	1603	1/1	0.95	0.13	-	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	FA	1618	1/1	0.96	0.27	-	21,21,21,21	0
57	MG	AA	3080	1/1	0.99	0.22	-	0,0,0,0	0
57	MG	GA	3090	1/1	0.94	0.10	-	27,27,27,27	0
57	MG	CA	3062	1/1	0.99	0.16	-	15,15,15,15	0
57	MG	GA	3060	1/1	0.98	0.15	-	18,18,18,18	0
57	MG	DA	1637	1/1	0.98	0.12	-	25,25,25,25	0
57	MG	HA	1605	1/1	0.98	0.15	-	40,40,40,40	0
57	MG	BA	1624	1/1	0.99	0.21	-	9,9,9,9	0
57	MG	EA	3057	1/1	0.97	0.07	-	18,18,18,18	0
57	MG	HA	1619	1/1	0.91	0.10	-	19,19,19,19	0
57	MG	CA	3092	1/1	0.93	0.27	-	58,58,58,58	0
57	MG	AA	3021	1/1	0.99	0.20	-	6,6,6,6	0
57	MG	AB	1204	1/1	0.99	0.06	-	18,18,18,18	0
57	MG	EA	3088	1/1	0.96	0.35	-	19,19,19,19	0
57	MG	CA	3108	1/1	1.00	0.21	-	11,11,11,11	0
57	MG	DA	1632	1/1	0.98	0.09	-	22,22,22,22	0
57	MG	CA	3010	1/1	0.96	0.28	-	8,8,8,8	0
57	MG	HA	1641	1/1	0.93	0.19	-	30,30,30,30	0
57	MG	CA	3094	1/1	0.92	0.43	-	37,37,37,37	0
57	MG	AA	3048	1/1	0.99	0.08	-	16,16,16,16	0
57	MG	EA	3033	1/1	0.97	0.26	-	0,0,0,0	0
57	MG	EA	3010	1/1	1.00	0.16	-	6,6,6,6	0
57	MG	CA	3017	1/1	1.00	0.18	-	7,7,7,7	0
57	MG	GA	3086	1/1	0.95	0.13	-	24,24,24,24	0
57	MG	GA	3046	1/1	0.99	0.12	-	35,35,35,35	0
57	MG	CA	3002	1/1	0.97	0.16	-	38,38,38,38	0
57	MG	AA	3051	1/1	0.99	0.10	-	9,9,9,9	0
57	MG	GA	3110	1/1	0.92	0.21	-	11,11,11,11	0
57	MG	CA	3064	1/1	0.99	0.16	-	6,6,6,6	0
57	MG	GA	3079	1/1	0.72	0.80	-	52,52,52,52	0
57	MG	EA	3092	1/1	0.97	0.13	-	22,22,22,22	0
57	MG	AA	3013	1/1	0.99	0.18	-	0,0,0,0	0
57	MG	EA	3011	1/1	0.91	0.88	-	24,24,24,24	0
57	MG	AA	3110	1/1	0.98	0.20	-	9,9,9,9	0
57	MG	CA	3111	1/1	0.96	0.15	-	18,18,18,18	0
57	MG	CA	3047	1/1	0.99	0.10	-	23,23,23,23	0
57	MG	EA	3074	1/1	0.98	0.19	-	11,11,11,11	0
57	MG	AA	3036	1/1	1.00	0.18	-	2,2,2,2	0
57	MG	BA	1622	1/1	0.99	0.16	-	17,17,17,17	0
57	MG	AA	3015	1/1	0.99	0.27	-	0,0,0,0	0
57	MG	CA	3076	1/1	0.98	0.13	-	16,16,16,16	0
57	MG	AA	3010	1/1	0.99	0.18	-	8,8,8,8	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	HA	1610	1/1	0.98	0.07	-	31,31,31,31	0
57	MG	AA	3081	1/1	0.99	0.11	-	1,1,1,1	0
57	MG	DA	1627	1/1	0.99	0.14	-	23,23,23,23	0
57	MG	CA	3006	1/1	0.94	0.08	-	30,30,30,30	0
57	MG	GA	3025	1/1	0.94	0.17	-	25,25,25,25	0
57	MG	CA	3048	1/1	0.99	0.17	-	17,17,17,17	0
57	MG	AA	3087	1/1	0.97	0.15	-	19,19,19,19	0
57	MG	EA	3047	1/1	0.99	0.08	-	25,25,25,25	0
57	MG	CA	3127	1/1	0.99	0.17	-	3,3,3,3	0
57	MG	CA	3090	1/1	0.97	0.21	-	19,19,19,19	0
57	MG	CA	3102	1/1	0.99	0.24	-	9,9,9,9	0
57	MG	EE	301	1/1	0.98	0.09	-	19,19,19,19	0
57	MG	GA	3125	1/1	1.00	0.12	-	10,10,10,10	0
57	MG	AC	301	1/1	0.99	0.14	-	3,3,3,3	0
57	MG	AA	3091	1/1	0.99	0.08	-	33,33,33,33	0
57	MG	CA	3055	1/1	0.96	0.19	-	19,19,19,19	0
57	MG	C4	101	1/1	0.97	0.09	-	17,17,17,17	0
57	MG	GA	3068	1/1	0.94	0.40	-	30,30,30,30	0
57	MG	GA	3061	1/1	0.98	0.11	-	20,20,20,20	0
57	MG	EA	3009	1/1	0.98	0.25	-	2,2,2,2	0
57	MG	DA	1618	1/1	0.97	0.04	-	37,37,37,37	0
57	MG	EA	3135	1/1	0.98	0.14	-	25,25,25,25	0
57	MG	HA	1614	1/1	0.94	0.17	-	49,49,49,49	0
57	MG	CA	3086	1/1	0.99	0.17	-	15,15,15,15	0
57	MG	GA	3038	1/1	0.98	0.17	-	21,21,21,21	0
57	MG	AA	3096	1/1	1.00	0.15	-	0,0,0,0	0
57	MG	GA	3013	1/1	0.98	0.08	-	18,18,18,18	0
57	MG	CA	3129	1/1	0.99	0.12	-	9,9,9,9	0
57	MG	CA	3080	1/1	0.97	0.17	-	20,20,20,20	0
57	MG	CA	3015	1/1	0.94	0.12	-	25,25,25,25	0
57	MG	AA	3098	1/1	0.99	0.21	-	0,0,0,0	0
57	MG	GA	3020	1/1	0.99	0.19	-	3,3,3,3	0
57	MG	AA	3034	1/1	0.99	0.21	-	4,4,4,4	0
57	MG	EA	3044	1/1	0.99	0.10	-	15,15,15,15	0
57	MG	AB	1203	1/1	0.98	0.16	-	0,0,0,0	0
57	MG	CA	3042	1/1	0.98	0.08	-	16,16,16,16	0
57	MG	FA	1615	1/1	0.99	0.12	-	16,16,16,16	0
57	MG	AA	3057	1/1	0.99	0.09	-	25,25,25,25	0
57	MG	CA	3038	1/1	0.99	0.20	-	9,9,9,9	0
57	MG	GA	3081	1/1	0.99	0.19	-	14,14,14,14	0
57	MG	GA	3089	1/1	0.99	0.20	-	8,8,8,8	0
57	MG	FA	1602	1/1	0.98	0.12	-	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	EA	3098	1/1	0.99	0.17	-	4,4,4,4	0
57	MG	HE	201	1/1	0.90	0.34	-	55,55,55,55	0
57	MG	GA	3117	1/1	0.97	0.13	-	10,10,10,10	0
57	MG	AA	3116	1/1	0.99	0.14	-	0,0,0,0	0
57	MG	GA	3044	1/1	0.98	0.06	-	21,21,21,21	0
57	MG	HA	1635	1/1	0.98	0.11	-	28,28,28,28	0
57	MG	DA	1641	1/1	0.99	0.11	-	28,28,28,28	0
57	MG	AA	3044	1/1	0.98	0.10	-	4,4,4,4	0
57	MG	HA	1636	1/1	0.99	0.13	-	28,28,28,28	0
57	MG	HA	1630	1/1	0.99	0.23	-	32,32,32,32	0
57	MG	AA	3053	1/1	1.00	0.17	-	4,4,4,4	0
57	MG	BA	1634	1/1	0.99	0.10	-	13,13,13,13	0
57	MG	CA	3030	1/1	0.99	0.16	-	39,39,39,39	0
57	MG	GA	3031	1/1	0.98	0.10	-	15,15,15,15	0
57	MG	AA	3122	1/1	0.99	0.16	-	6,6,6,6	0
57	MG	DA	1601	1/1	0.97	0.12	-	26,26,26,26	0
57	MG	CA	3096	1/1	0.98	0.21	-	16,16,16,16	0
57	MG	CA	3033	1/1	0.99	0.17	-	6,6,6,6	0
57	MG	AA	3063	1/1	1.00	0.19	-	0,0,0,0	0
57	MG	AA	3085	1/1	1.00	0.14	-	7,7,7,7	0
57	MG	AA	3125	1/1	0.99	0.22	-	8,8,8,8	0
57	MG	GB	1202	1/1	0.93	0.14	-	64,64,64,64	0
57	MG	CA	3021	1/1	0.98	0.11	-	5,5,5,5	0
57	MG	EA	3072	1/1	1.00	0.15	-	2,2,2,2	0
57	MG	DA	1636	1/1	0.95	0.77	-	34,34,34,34	0
57	MG	GA	3101	1/1	0.96	0.14	-	13,13,13,13	0
57	MG	GA	3059	1/1	0.96	0.12	-	25,25,25,25	0
57	MG	FA	1627	1/1	0.49	0.53	-	53,53,53,53	0
57	MG	GA	3005	1/1	0.83	0.11	-	42,42,42,42	0
57	MG	GB	1204	1/1	0.97	0.04	-	37,37,37,37	0
57	MG	BA	1629	1/1	0.98	0.15	-	15,15,15,15	0
57	MG	AA	3120	1/1	0.98	0.24	-	9,9,9,9	0
57	MG	GA	3088	1/1	0.90	0.67	-	37,37,37,37	0
57	MG	GA	3035	1/1	0.92	0.14	-	24,24,24,24	0
57	MG	EA	3136	1/1	0.86	0.37	-	15,15,15,15	0
57	MG	AA	3117	1/1	0.99	0.10	-	11,11,11,11	0
57	MG	EA	3048	1/1	0.99	0.22	-	25,25,25,25	0
57	MG	GA	3084	1/1	0.97	0.40	-	30,30,30,30	0
57	MG	DA	1605	1/1	0.99	0.15	-	18,18,18,18	0
57	MG	BA	1606	1/1	0.99	0.18	-	14,14,14,14	0
57	MG	DA	1614	1/1	0.85	0.25	-	46,46,46,46	0
57	MG	BA	1623	1/1	0.99	0.10	-	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	EA	3119	1/1	0.98	0.23	-	1,1,1,1	0
57	MG	EA	3097	1/1	0.94	0.21	-	19,19,19,19	0
57	MG	CA	3014	1/1	1.00	0.27	-	13,13,13,13	0
57	MG	EA	3137	1/1	0.98	0.32	-	11,11,11,11	0
57	MG	EA	3094	1/1	0.93	0.12	-	33,33,33,33	0
57	MG	AA	3023	1/1	1.00	0.08	-	0,0,0,0	0
57	MG	CB	1201	1/1	0.93	0.19	-	28,28,28,28	0
57	MG	GA	3102	1/1	0.99	0.14	-	19,19,19,19	0
57	MG	AA	3061	1/1	0.98	0.28	-	5,5,5,5	0
57	MG	EA	3001	1/1	0.97	0.18	-	11,11,11,11	0
57	MG	CA	3099	1/1	0.99	0.18	-	5,5,5,5	0
57	MG	EA	3018	1/1	0.99	0.19	-	9,9,9,9	0
57	MG	EA	3026	1/1	0.99	0.18	-	0,0,0,0	0
57	MG	EA	3054	1/1	0.99	0.12	-	2,2,2,2	0
57	MG	AA	3067	1/1	0.99	0.17	-	2,2,2,2	0
57	MG	GC	302	1/1	0.98	0.07	-	22,22,22,22	0
57	MG	CA	3045	1/1	0.98	0.20	-	5,5,5,5	0
57	MG	EA	3004	1/1	0.98	0.13	-	12,12,12,12	0
57	MG	CA	3016	1/1	0.97	0.18	-	11,11,11,11	0
57	MG	AA	3055	1/1	0.99	0.16	-	0,0,0,0	0
57	MG	BA	1635	1/1	0.98	0.14	-	29,29,29,29	0
57	MG	CA	3018	1/1	0.99	0.08	-	30,30,30,30	0
57	MG	AA	3020	1/1	0.99	0.09	-	9,9,9,9	0
57	MG	CA	3130	1/1	0.99	0.16	-	21,21,21,21	0
57	MG	EA	3087	1/1	0.98	0.10	-	21,21,21,21	0
57	MG	HA	1638	1/1	0.99	0.04	-	28,28,28,28	0
57	MG	FA	1612	1/1	0.99	0.30	-	4,4,4,4	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.