



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 22, 2025 – 11:37 AM EDT

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

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.21  
EDS : **FAILED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.41.4

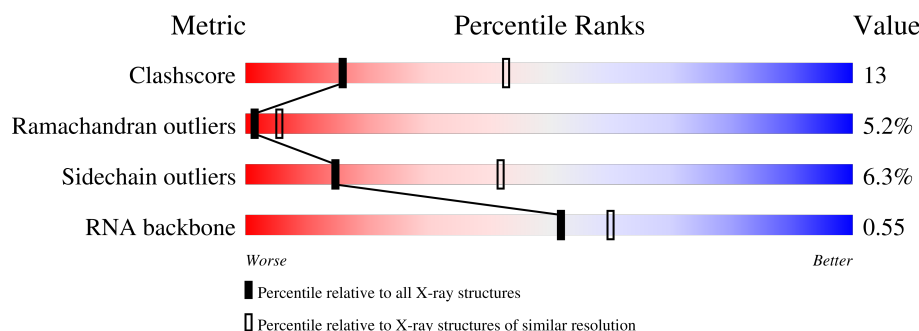
# 1 Overall quality at a glance

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))
Clashscore	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)
RNA backbone	3690	1039 (3.10-2.70)


























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

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	AA	2904	
1	CA	2904	
1	EA	2904	
1	GA	2904	
2	AB	120	
2	CB	120	





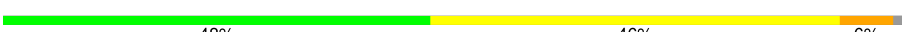







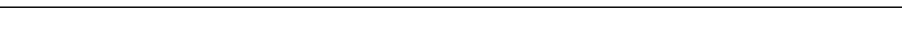

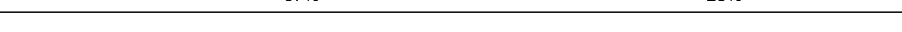

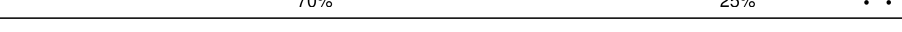








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Mol	Chain	Length	Quality of chain
2	EB	120	
2	GB	120	
3	AC	273	
3	CC	273	
3	EC	273	
3	GC	273	
4	AD	209	
4	CD	209	
4	ED	209	
4	GD	209	
5	AE	201	
5	CE	201	
5	EE	201	
5	GE	201	
6	AF	179	
6	CF	179	
6	EF	179	
6	GF	179	
7	AG	177	
7	CG	177	
7	EG	177	
7	GG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


























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Mol	Chain	Length	Quality of chain
8	GH	50	 58% 40% .
9	AI	142	 46% 51% ..
9	CI	142	 50% 44% 5% .
9	EI	142	 61% 35% ..
9	GI	142	 48% 46% 6% .
10	AJ	142	 60% 30% 9% .
10	CJ	142	 58% 31% 11% .
10	EJ	142	 53% 33% 11% .
10	GJ	142	 58% 32% 9% .
11	AK	123	 51% 39% 8% ..
11	CK	123	 47% 44% 7% ..
11	EK	123	 54% 37% 9% .
11	GK	123	 50% 42% 7% .
12	AL	144	 67% 28% ..
12	CL	144	 63% 32% ..
12	EL	144	 70% 25% ..
12	GL	144	 57% 38% ..
13	AM	136	 61% 31% 6% .
13	CM	136	 63% 32% 5% .
13	EM	136	 66% 27% 6% .
13	GM	136	 71% 26% .
14	AN	127	 62% 30% .. 6%
14	CN	127	 60% 28% 6% . 6%
14	EN	127	 62% 30% . 6%
14	GN	127	 56% 36% . 6%








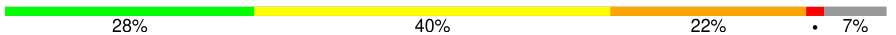
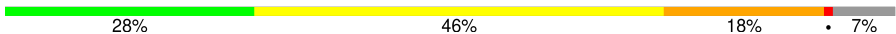
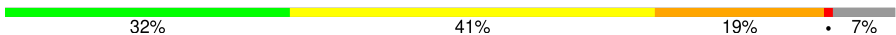
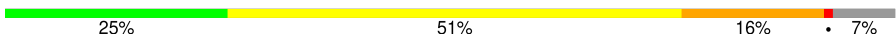














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Mol	Chain	Length	Quality of chain
15	AO	117	
15	CO	117	
15	EO	117	
15	GO	117	
16	AP	115	
16	CP	115	
16	EP	115	
16	GP	115	
17	AQ	118	
17	CQ	118	
17	EQ	118	
17	GQ	118	
18	AR	103	
18	CR	103	
18	ER	103	
18	GR	103	
19	AS	110	
19	CS	110	
19	ES	110	
19	GS	110	
20	AT	100	
20	CT	100	
20	ET	100	
20	GT	100	
21	AU	104	


























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Mol	Chain	Length	Quality of chain
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	
27	A0	57	
27	C0	57	

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Mol	Chain	Length	Quality of chain
27	E0	57	
27	G0	57	
28	A1	55	
28	C1	55	
28	E1	55	
28	G1	55	
29	A2	46	
29	C2	46	
29	E2	46	
29	G2	46	
30	A3	65	
30	C3	65	
30	E3	65	
30	G3	65	
31	A4	38	
31	C4	38	
31	E4	38	
31	G4	38	
32	A5	165	
32	E5	165	
33	BA	1542	
33	DA	1542	
33	FA	1542	
33	HA	1542	
34	BB	241	

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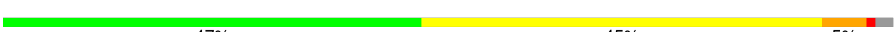






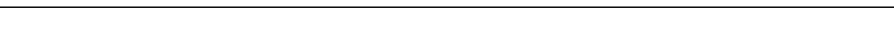

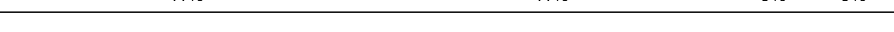

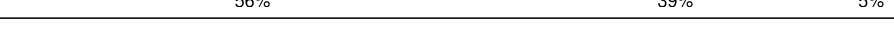








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Mol	Chain	Length	Quality of chain
34	DB	241	
34	FB	241	
34	HB	241	
35	BC	233	
35	DC	233	
35	FC	233	
35	HC	233	
36	BD	206	
36	DD	206	
36	FD	206	
36	HD	206	
37	BE	167	
37	DE	167	
37	FE	167	
37	HE	167	
38	BF	135	
38	DF	135	
38	FF	135	
38	HF	135	
39	BG	179	
39	DG	179	
39	FG	179	
39	HG	179	
40	BH	130	
40	DH	130	

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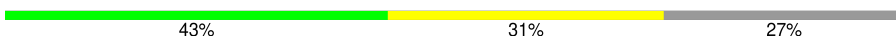













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Mol	Chain	Length	Quality of chain
40	FH	130	
40	HH	130	
41	BI	130	
41	DI	130	
41	FI	130	
41	HI	130	
42	BJ	103	
42	DJ	103	
42	FJ	103	
42	HJ	103	
43	BK	129	
43	DK	129	
43	FK	129	
43	HK	129	
44	BL	124	
44	DL	124	
44	FL	124	
44	HL	124	
45	BM	118	
45	DM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

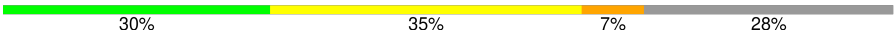

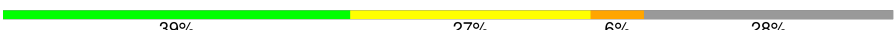
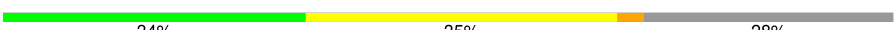






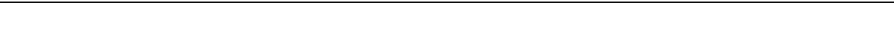
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Mol	Chain	Length	Quality of chain
46	HN	101	
47	BO	89	
47	DO	89	
47	FO	89	
47	HO	89	
48	BP	82	
48	DP	82	
48	FP	82	
48	HP	82	
49	BQ	84	
49	DQ	84	
49	FQ	84	
49	HQ	84	
50	BR	75	
50	DR	75	
50	FR	75	
50	HR	75	
51	BS	92	
51	DS	92	
51	FS	92	
51	HS	92	
52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

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Mol	Chain	Length	Quality of chain
53	BU	71	
53	DU	71	
53	FU	71	
53	HU	71	
54	BV	704	
54	DV	704	
54	FV	704	
54	HV	704	
55	BW	6	
55	DW	6	
55	FW	6	

## 2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 590573 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S rRNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 54 is a protein called elongation factor G.

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

- Molecule 55 is a protein called Viomycin.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AA	130	Total	Mg	0	0
			130	130		
56	AB	4	Total	Mg	0	0
			4	4		
56	AC	3	Total	Mg	0	0
			3	3		
56	AD	1	Total	Mg	0	0
			1	1		
56	AE	1	Total	Mg	0	0
			1	1		
56	AT	1	Total	Mg	0	0
			1	1		
56	A3	1	Total	Mg	0	0
			1	1		

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

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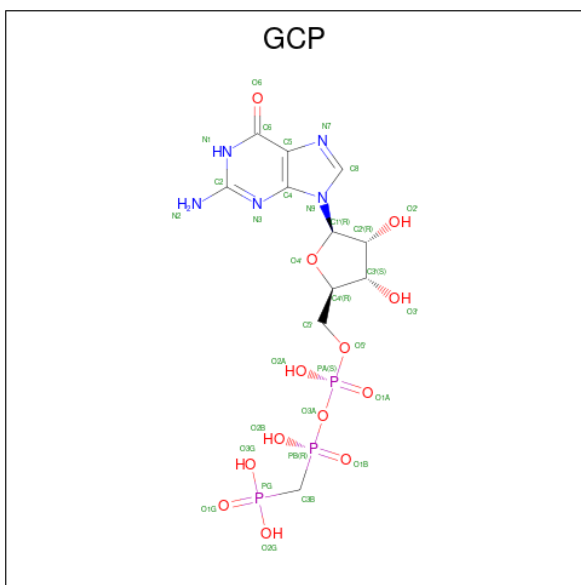
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	FV	1	Total 1	Mg 1	0	0
56	GA	134	Total 134	Mg 134	0	0
56	GB	4	Total 4	Mg 4	0	0
56	GC	1	Total 1	Mg 1	0	0
56	GL	1	Total 1	Mg 1	0	0
56	GS	1	Total 1	Mg 1	0	0
56	HA	40	Total 40	Mg 40	0	0
56	HC	1	Total 1	Mg 1	0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

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

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

- Molecule 58 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: C<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
58	BV	1	Total 32	C 11	N 5	O 13	P 3	0	0
58	DV	1	Total 32	C 11	N 5	O 13	P 3	0	0
58	FV	1	Total 32	C 11	N 5	O 13	P 3	0	0
58	HV	1	Total 32	C 11	N 5	O 13	P 3	0	0

- Molecule 59 is water.

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

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

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

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

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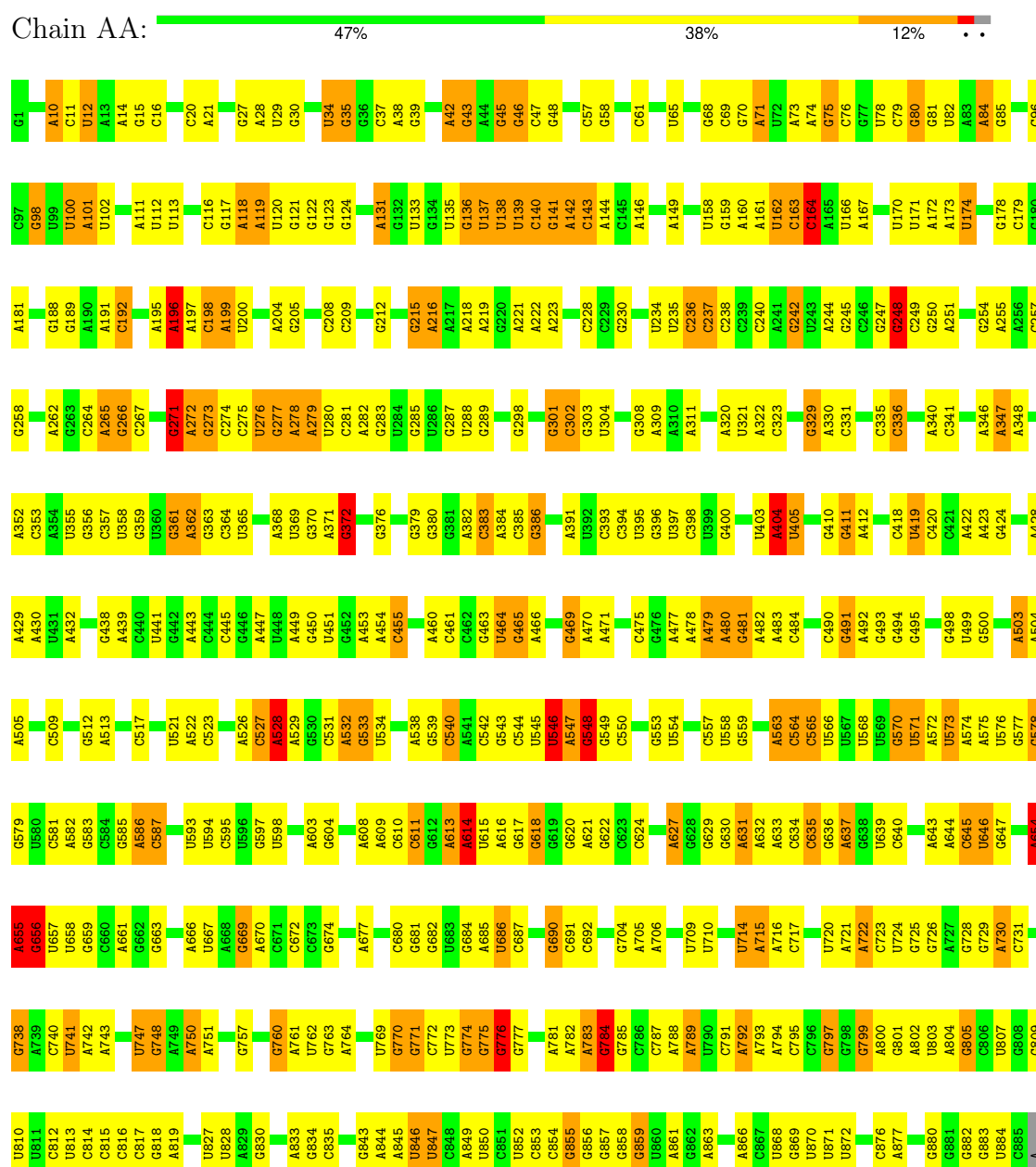
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	GD	4	Total 4	O 4	0	0
59	GE	2	Total 2	O 2	0	0
59	GL	4	Total 4	O 4	0	0
59	GN	3	Total 3	O 3	0	0
59	GQ	1	Total 1	O 1	0	0
59	GR	2	Total 2	O 2	0	0
59	GS	1	Total 1	O 1	0	0
59	GT	1	Total 1	O 1	0	0
59	GU	2	Total 2	O 2	0	0
59	GV	1	Total 1	O 1	0	0
59	G2	2	Total 2	O 2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

### 3 Residue-property plots

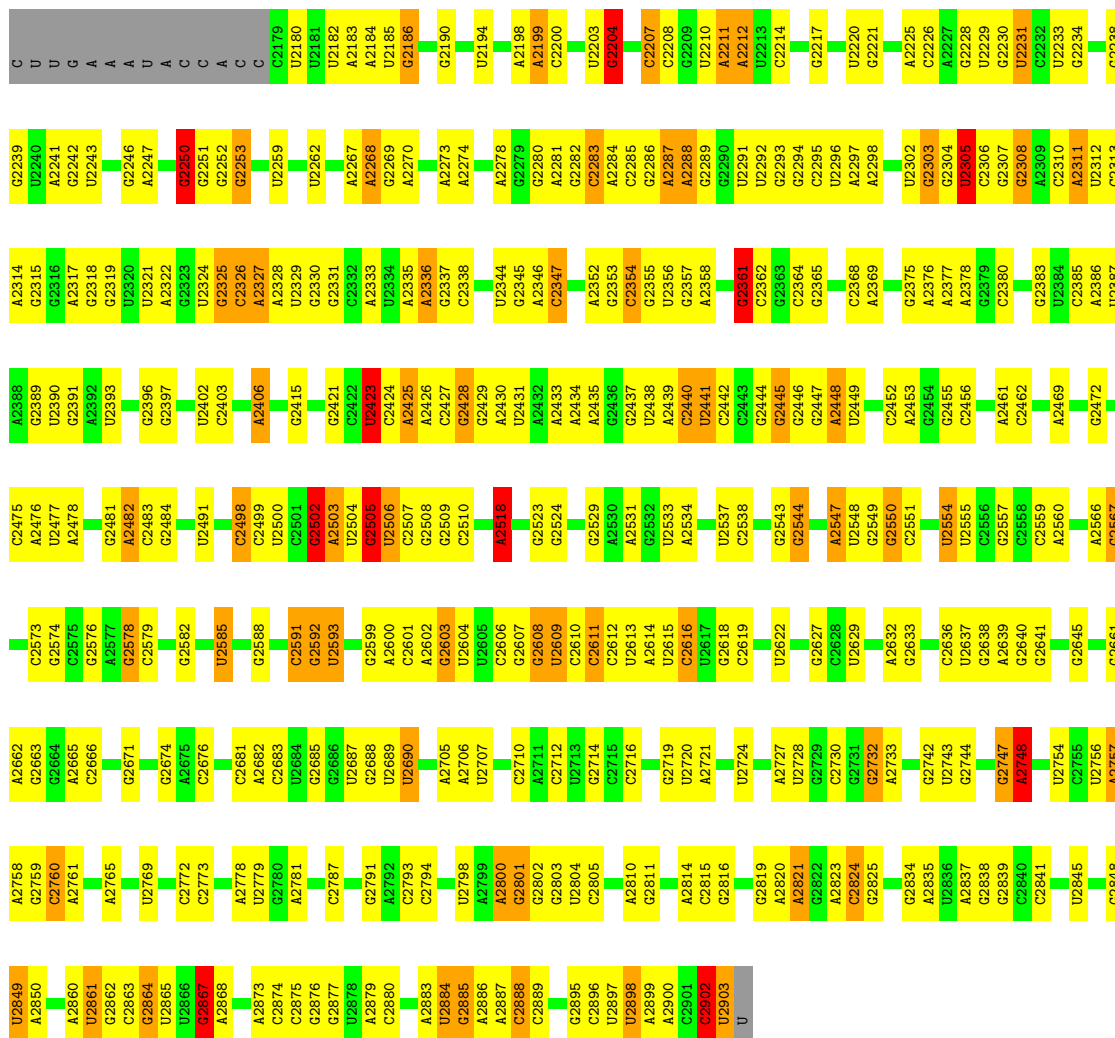
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS failed to run properly.

#### • Molecule 1: 23S rRNA

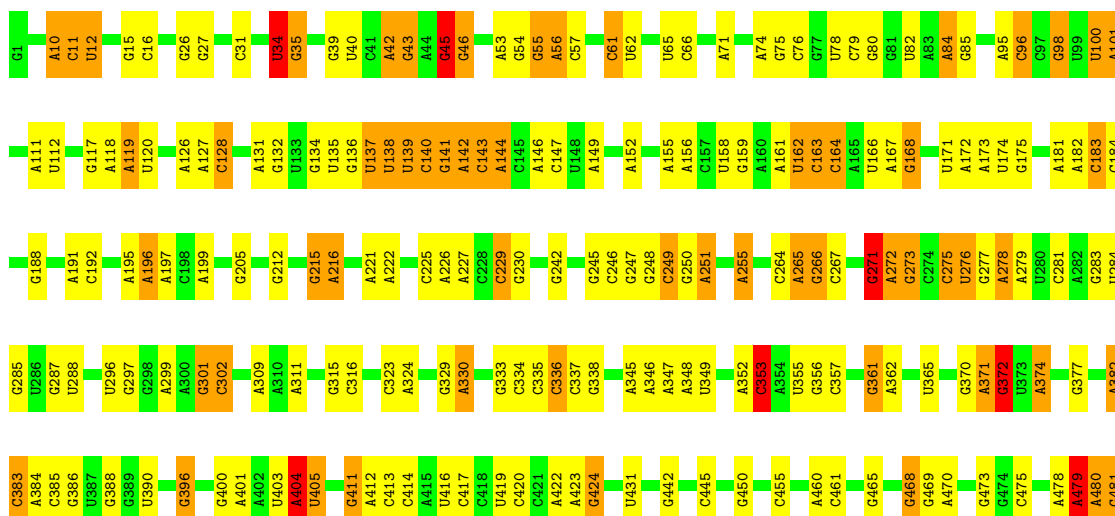


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G2107	C2023	A1916	A1802	C1726	G1645	A1548	U1474	U1390	A1301	U1231	G1138	G1062	A983	C
U2109	G2024	C1924	A1806	C1727	C1646	A1551	G1476	U1395	C1305	U1232	G1139	C1063	A984	C
G2110	C2025	U1927	G1807	U1728	U1647	A1555	A1477	U1396	C1306	C1233	U1141	C1064	C985	G
U	G2026	A1928	A1808	C1730	G1648	G1556	G1478	U1397	A1307	U1234	A1142	U1065	C989	A892
G	G2027	A1929	A1809	G1731	G1649	C1556	C1480	U1398	A1309	U1235	C1146	U1066	A990	C993
U	A2030	G1929	G1811	C1732	A1650	G1565	U1481	U1400	G1307	U1236	U1150	A1067	A896	A896
A	A2031	G1930	U1812	G1733	A1652	C1566	U1482	U1401	A1307	U1237	C1150	A1069	C897	C897
G	A2032	G1935	G1813	U1734	G1653	C1567	U1483	U1402	A1307	A1237	A1151	G1071	C995	C995
A	A2033	A1936	G1814	U1735	A1654	G1567	G1483	A1403	A1307	U1238	U1170	G1072	A996	A996
U	G2038	A1937	A1815	U1736	G1655	G1568	U1484	A1404	G1316	U1239	G1161	A1070	A910	A910
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G	C2047	U1944	U1819	C1741	A1665	U1578	C1493	G1410	A1322	A1246	C1167	C1076	G916	G916
G	G	G1945	U1820	U1742	G1666	U1578	A1494	U1411	A1327	A1247	G1168	A1077	A917	A917
G	C2050	U1955	G1823	G1743	G1667	G1581	A1495	U1412	A1328	U1248	A1169	C1079	A918	A918
A	A2051	U1956	G1824	A1744	A1668	G1582	A1496	U1413	U1329	U1249	A1170	A1080	A919	A919
G	A2052	U1957	A1825	A1745	A1669	A1583	U1497	U1414	U1330	C1250	A1181	U1081	A920	A920
C	G2053	C1957	G1826	U1746	C1670	A1584	G1500	G1416	C1330	C1251	U1182	U1082	C921	C921
U	A2054	C1958	G1827	U1747	U1671	U1584	G1501	C1417	G1331	G1252	U1175	U1083	C922	C922
U	C2055	C1958	C1828	U1748	U1672	A1585	A1504	A1419	G1332	A1253	A1176	A1084	G923	G923
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G	A2058	C1967	C1831	A1751	C1675	A1591	A1508	G1422	G1338	C1257	U1179	A1088	U932	U932
A	G2059	U1968	C1832	G1752	A1676	C1592	G1509	G1423	U1339	C1258	U1180	A1089	U933	U933
G	A2060	A1969	C1833	U1753	A1677	A1593	G1510	G1424	U1340	C1259	U1181	A1090	A933	A933
G	G2061	U1970	U1841	A1754	U1678	U1594	C1512	A1427	G1341	A1260	G1182	A1091	U934	U934
A	A2062	U1971	C1842	U1755	G1684	C1595	U1513	C1428	G1342	C1261	U1183	U1092	C935	C935
U	C2063	G1972	G1843	C1760	C1685	C1595	G1514	G1429	G1343	A1262	U1184	U1093	G1022	G1022
U	C2064	U1973	A1847	C1761	C1686	G1601	A1515	G1430	U1344	U1263	G1185	U1094	G1023	G1023
U	G2065	G1974	A1848	U1762	G1687	U1602	G1516	G1431	C1350	A1264	G1186	U1097	G1024	A941
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U	U2074	U1984	A1856	U1775	G1696	A1610	G1524	U1442	A1365	A1272	C1196	G1110	A1032	G954
U	U2075	U1985	A1857	U1776	A1705	A1611	A1525	U1443	G1366	U1273	G1197	A1111	U1033	U958
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U	U2120	U2030	A1902	U1821	G1750	G1657	U1570	G1489	A1415	G1323	G1252	C1165	G1090	
U	U2121	U2031	A1903	U1822	G1751	G1658	U1571	G1490	A1416	G1324	G1253	C1166	G1091	
U	U2122	U2032												

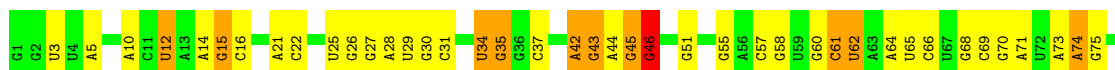
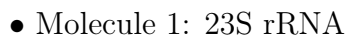


● Molecule 1: 23S rRNA

Chain CA: 52% 33% 11%



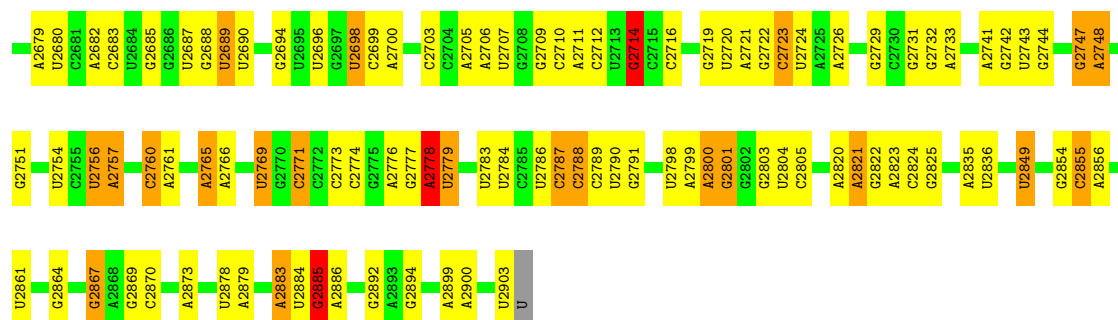




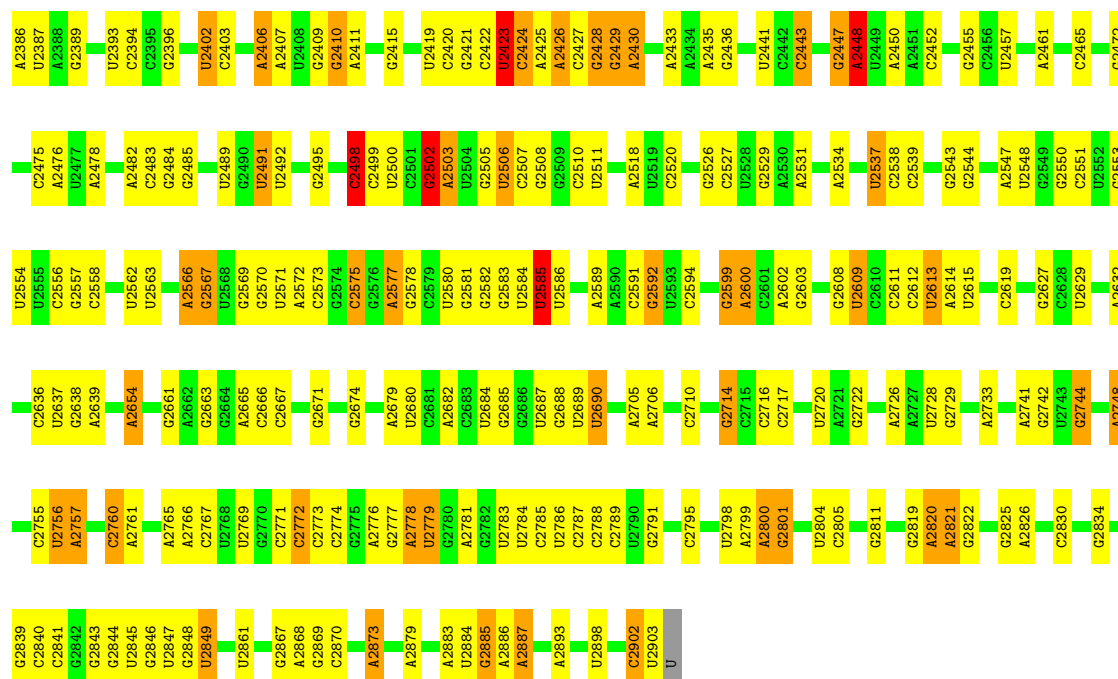
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G1251	U1083	C1170	U1084	C1007	U931	U847	U779	G674	C435	G520	C435	C341	G260	U172	G80
A1253	A1085	G1171	A1085	G1011	U931	C848	G780	A677	C436	G526	A436	A346	G264	U173	U82
A1254	A1086	G1172	A1086	U1012	A933	A849	A781	G578	A526	G527	A437	A347	C264	U174	A83
U1255	G1087	U1173	G1087	C1013	U934	A849	A783	C579	A528	A529	A443	A348	A265		A84
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G1257	A1089	U1175	A1089	U1019	A936	G857	G785	G681	A531	G531	U451	C353	C268	G178	G86
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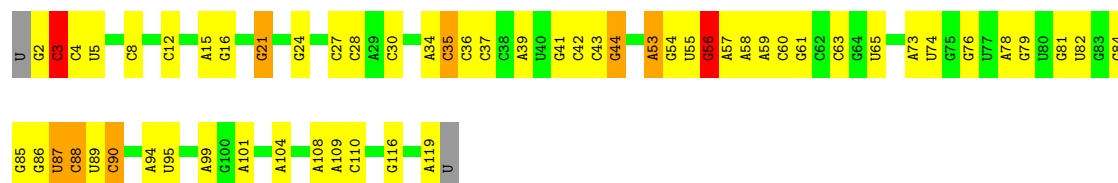


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A2316	G2232	A2154	A2094	A2013	A1901	U1808	U1725	A1610	U1493	U1406	G1310	G1236	C1140	G1063
A2317	G2233	U2155	C2095	A2016	C1902	A1808	G1726	C1611	C1493	U1406	G1311	A1237	U1141	U1064
U2321	U2233	G2156	U2096	U2016	G1906	G1811	U1729	A1614	A1503	G1410	U1311	G1238	A1142	C1064
A2322	G2234	G2157	A2097	U2017	G1906	U1812	C1730	C1615	A1504	U1411	U1312	G1239	G1149	U1066
G2323	G2238	A	U2098	G2018	A1913	G1813	G1731	A1616	A1504	U1412	U1313	A1244	G1150	U1067
U2324	G2239	C	U2099	A2019	C1914	A1814	C1732	C1617	C1507	A1413	G1317	A1247	A1151	A1067
G2325	G2239	C	A2100	A2020	C1914	G1815	U1735	A1618	C1508	G1416	A1321	G1248	G1154	A1069
C2326	G2243	C	A2101	C2021	U1915	A1816	U1736	A1619	A1509	G1422	A1322	U1249	G1157	A1070
A2327	U2243	G	G2102	U2022	U1916	C1816	U1737	G1620	G1510	A1427	A1323	G1250	G1160	C1072
U2328	G2246	C	C2103	C2023	U1917	G1817	G1738	G1621	G1511	A1419	A1327	G1251	G1161	A1073
G2331	A2247	C	U2104	G2024	C1924	U1820	G1739	G1622	G1512	A1420	U1328	G1252	G1162	G1074
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U2334	G2250	U	U2106	U2026	U1926	U1825	A1745	A1628	G1514	G1422	U1328	A1254	G1164	U1076
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C2347	A2273	C	U	U2039	U1940	G1835	A1762	A1654	G1537	C1437	A1347	A1265	U1174	A1086
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U2360	G2285	U2187	G	A2058	G1972	A1859	U1782	A1675	G1568	C1451	A1368	G1279	U1188	A1098
G2361	C2286	U2188	C	U2059	C1983	G1863	A1783	A1676	A1569	G1452	G1368	G1280	G1196	A1103
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G2365	G2290	U2194	U	U2063	C1987	U1867	U1789	U1683	U1578	G1459	U1379	A1285	G1202	A1111
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G2367	G2292	A2199	G	U2068	C1990	U1870	A1791	G1685	C1582	G1471	G1382	C1289	A1204	G1126
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C2370	G2298	U2204	U	C2071	U1993	A1873	C1795	G1687	C1585				G1207	
A2381	A2298	G2204	U	A2072	U1993	A1873	C1795	G1687	C1585					
G2382	G2304	A2205	C	C2073	U1993	A1873	C1795	G1687	C1585					
G2383	U2305	U2210	G	U2075	U1993	A1873	C1795	G1687	C1585					
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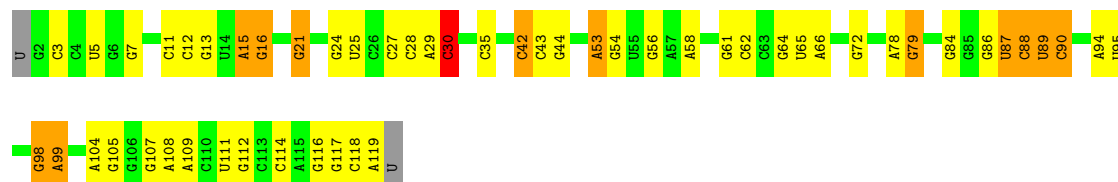
• Molecule 2: 5S rRNA

Chain AB: 51% 40% 6% ..



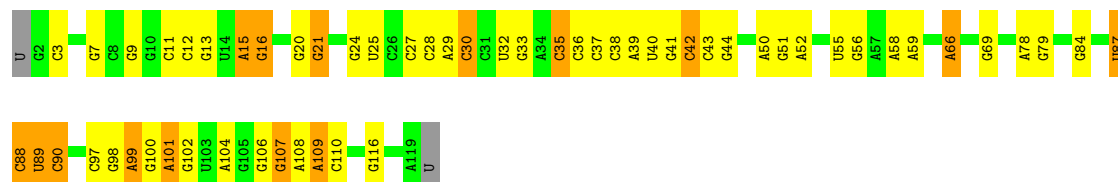
• Molecule 2: 5S rRNA

Chain CB: 54% 33% 10% ..



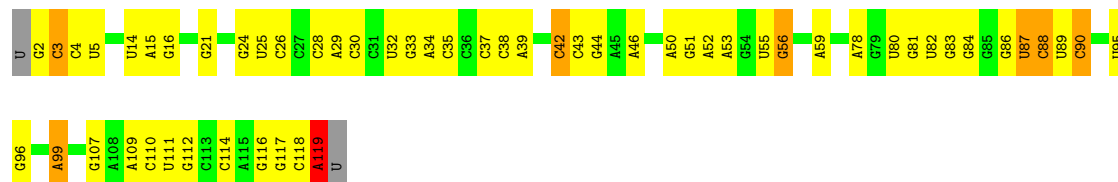
• Molecule 2: 5S rRNA

Chain EB: 51% 35% 12% .



- Molecule 2: 5S rRNA

Chain GB:  52% 40% 6% ..



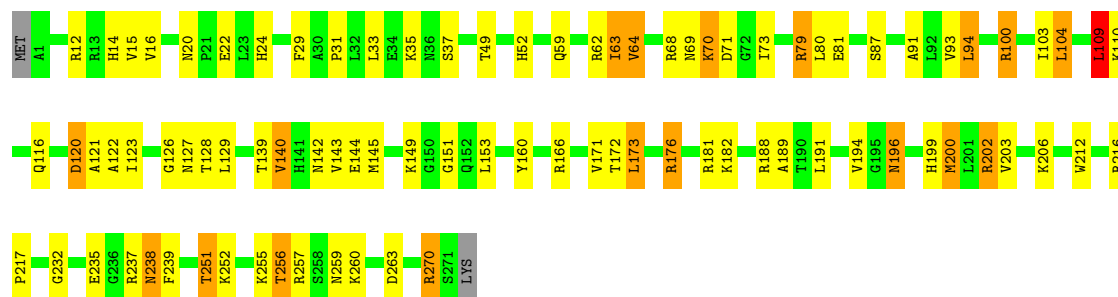
- Molecule 3: 50S ribosomal protein L2

Chain AC:  68% 28% ...



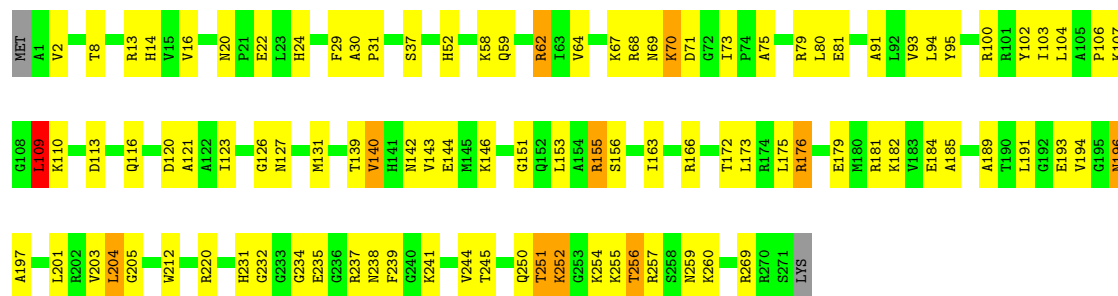
- Molecule 3: 50S ribosomal protein L2

Chain CC:  67% 25% 7% .

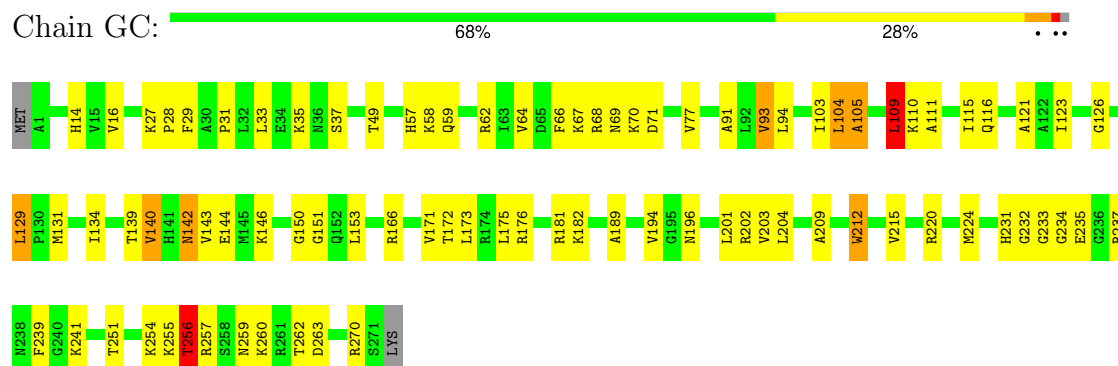


- Molecule 3: 50S ribosomal protein L2

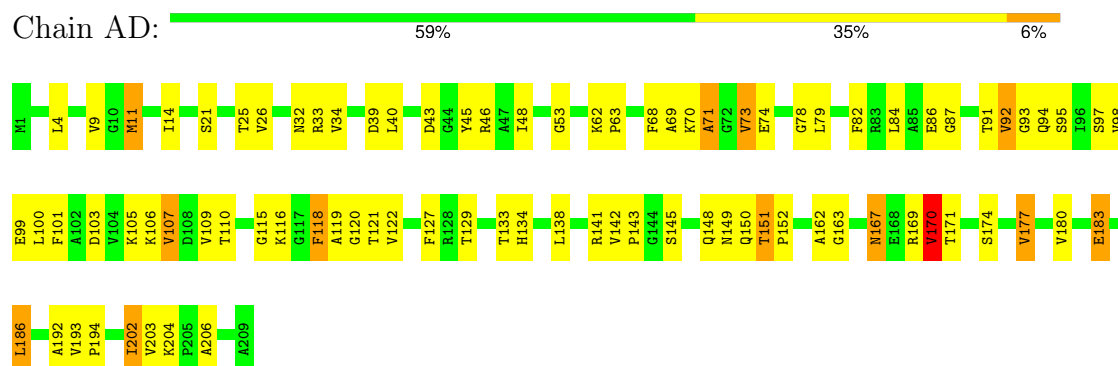
Chain EC:  63% 33% ..



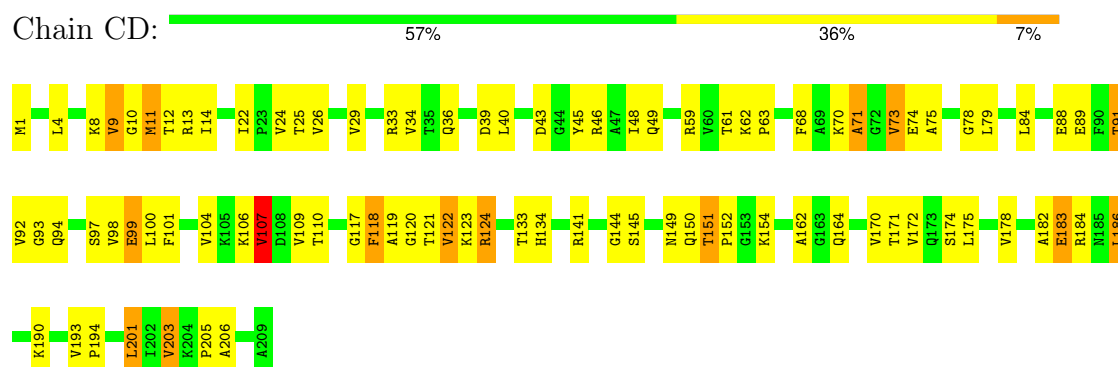
- Molecule 3: 50S ribosomal protein L2



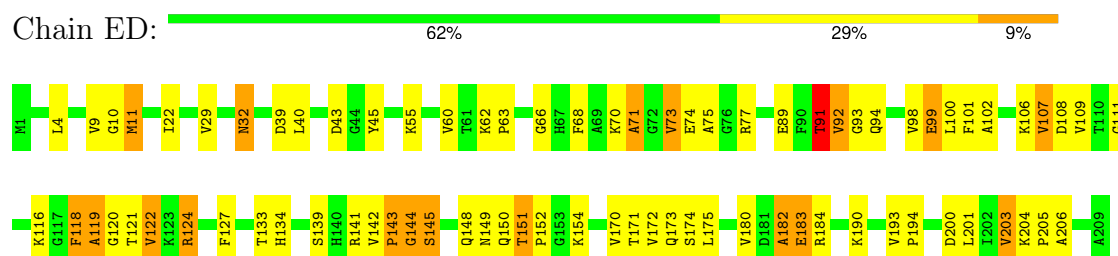
- Molecule 4: 50S ribosomal protein L3



- Molecule 4: 50S ribosomal protein L3

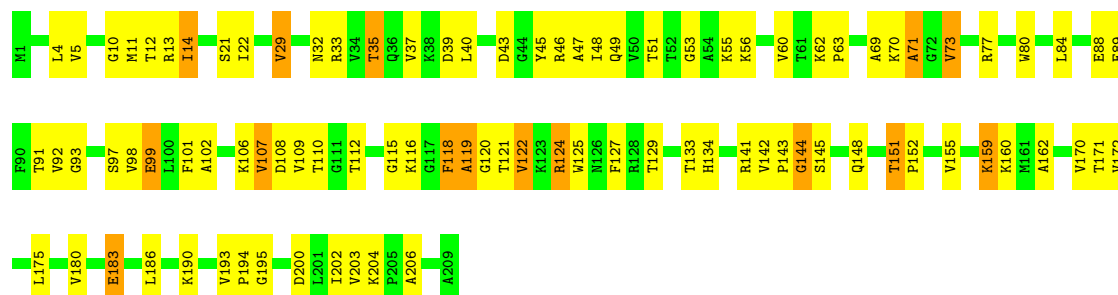


- Molecule 4: 50S ribosomal protein L3



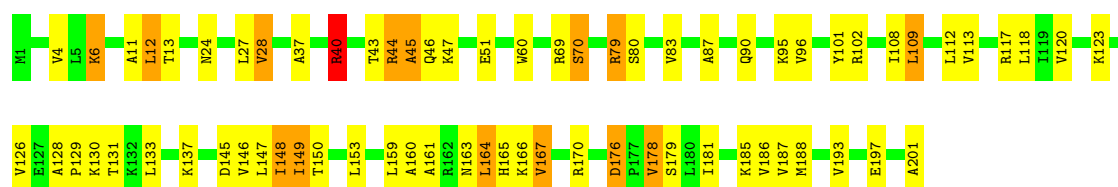
- Molecule 4: 50S ribosomal protein L3

Chain GD:  56% 37% 7%



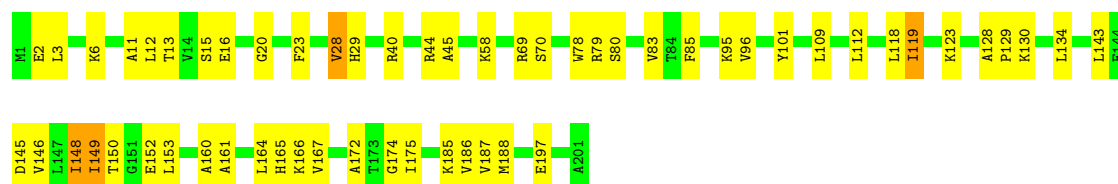
- Molecule 5: 50S ribosomal protein L4

Chain AE:  65% 27% 7%



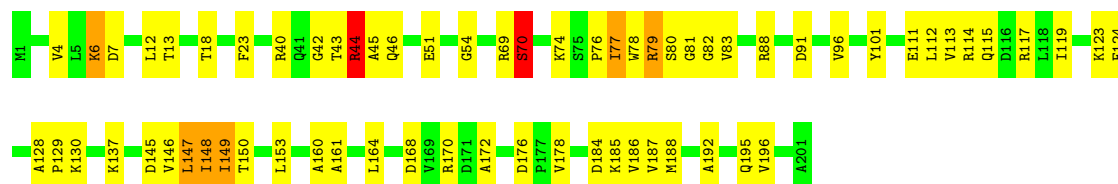
- Molecule 5: 50S ribosomal protein L4

Chain CE:  72% 26% 2%



- Molecule 5: 50S ribosomal protein L4

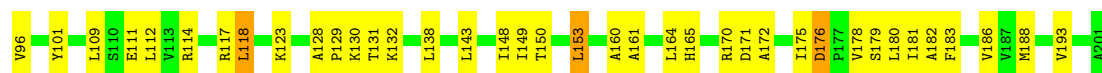
Chain EE:  67% 29% 4%



- Molecule 5: 50S ribosomal protein L4

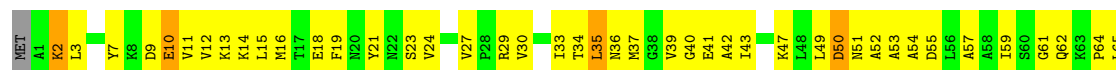
Chain GE:  62% 34% 4%





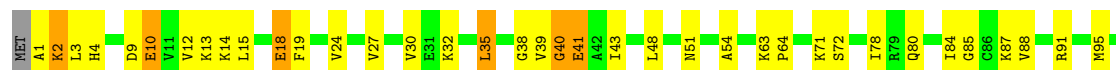
- Molecule 6: 50S ribosomal protein L5

Chain AF: 40% 53% 6% .



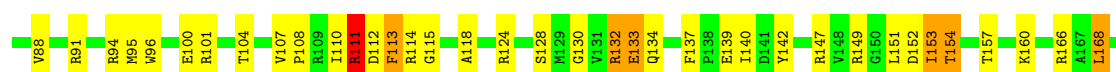
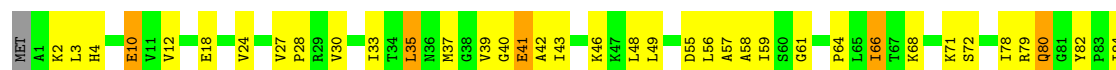
- Molecule 6: 50S ribosomal protein L5

Chain CF: 61% 32% 6% .



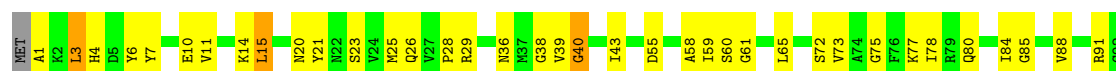
- Molecule 6: 50S ribosomal protein L5

Chain EF: 55% 36% 7% ..



- Molecule 6: 50S ribosomal protein L5

Chain GF: 52% 43% . .

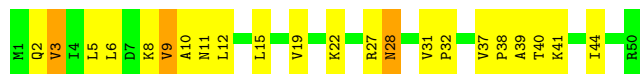






- Molecule 8: 50S ribosomal protein L9

Chain CH:  56% 38% 6%



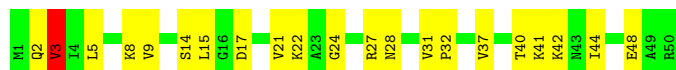
- Molecule 8: 50S ribosomal protein L9

Chain EH:  62% 32% 6%



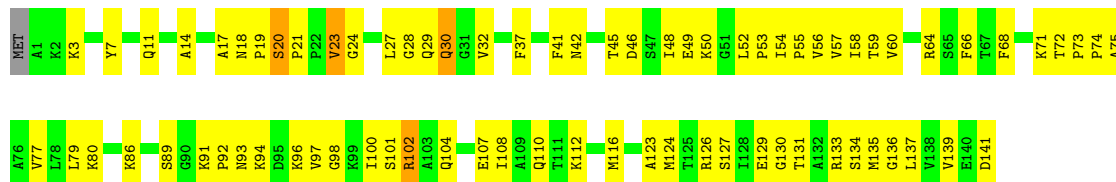
- Molecule 8: 50S ribosomal protein L9

Chain GH:  58% 40% 2%



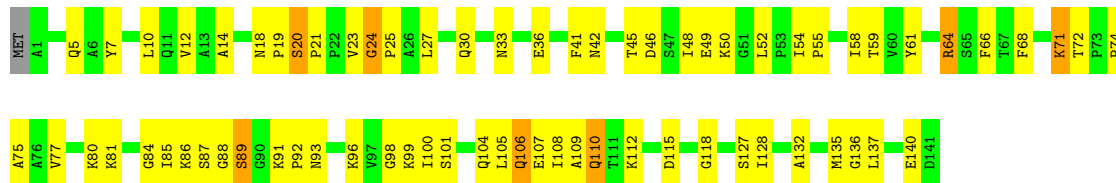
- Molecule 9: 50S ribosomal protein L11

Chain AI:  46% 51% 3%



- Molecule 9: 50S ribosomal protein L11

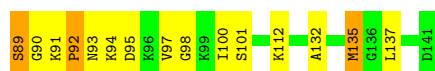
Chain CI:  50% 44% 6%



- Molecule 9: 50S ribosomal protein L11

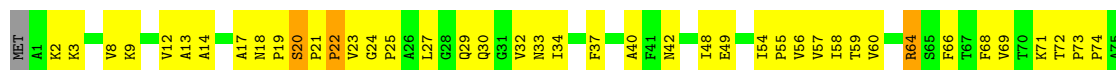
Chain EI:  61% 35% 4%





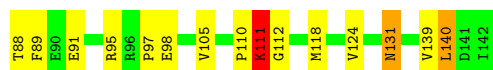
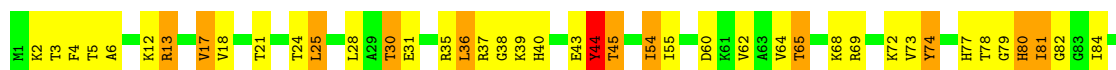
- Molecule 9: 50S ribosomal protein L11

Chain GI: 48% 46% 6% .



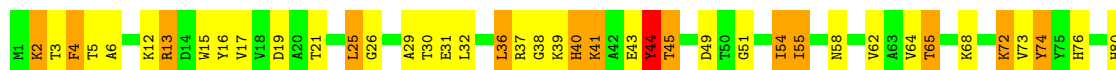
- Molecule 10: 50S ribosomal protein L13

Chain AJ: 60% 30% 9% .



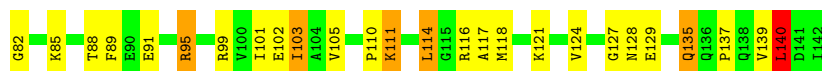
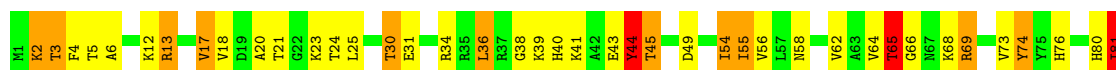
- Molecule 10: 50S ribosomal protein L13

Chain CJ: 58% 31% 11% .



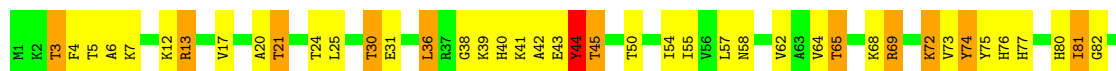
- Molecule 10: 50S ribosomal protein L13

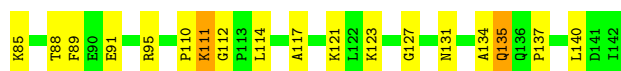
Chain EJ: 53% 33% 11% .



- Molecule 10: 50S ribosomal protein L13

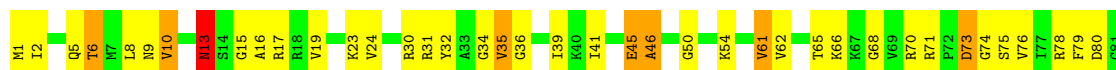
Chain GJ: 58% 32% 9% .





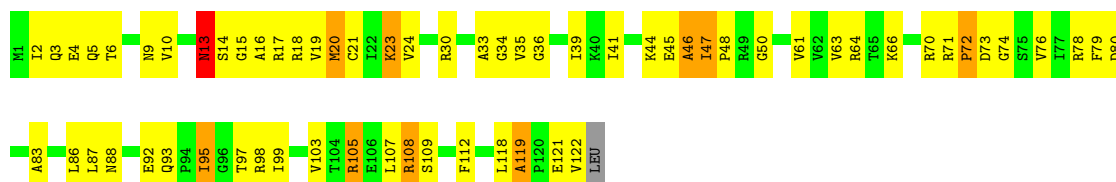
- Molecule 11: 50S ribosomal protein L14

Chain AK: 51% 39% 8% ..



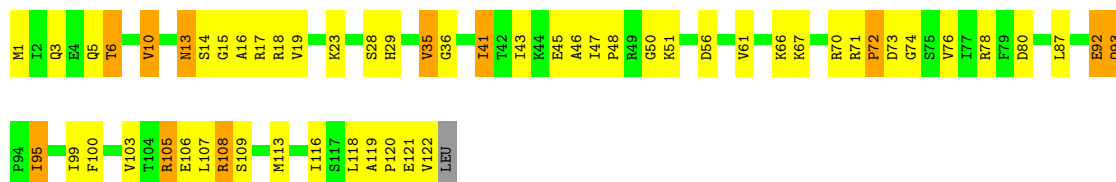
- Molecule 11: 50S ribosomal protein L14

Chain CK: 47% 44% 7% ..



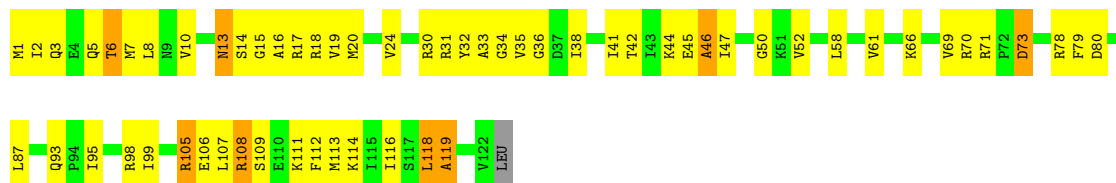
- Molecule 11: 50S ribosomal protein L14

Chain EK: 54% 37% 9% .



- Molecule 11: 50S ribosomal protein L14

Chain GK: 50% 42% 7% .



- Molecule 12: 50S ribosomal protein L15

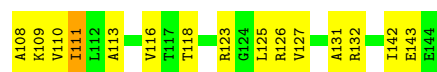
Chain AL: 67% 28% ..





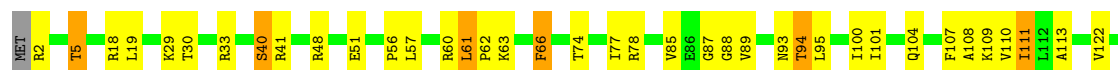
- Molecule 12: 50S ribosomal protein L15

Chain CL: 63% 32% ..



- Molecule 12: 50S ribosomal protein L15

Chain EL: 70% 25% ..



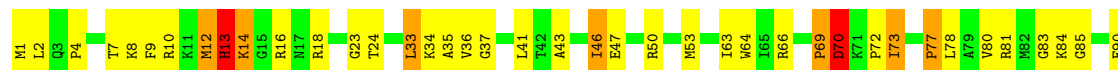
- Molecule 12: 50S ribosomal protein L15

Chain GL: 57% 38% ..



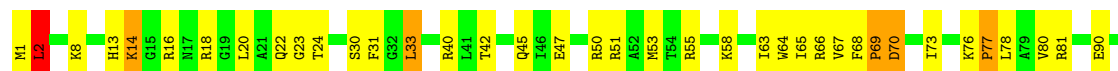
- Molecule 13: 50S ribosomal protein L16

Chain AM: 61% 31% 6% .



- Molecule 13: 50S ribosomal protein L16

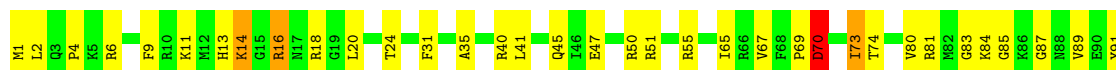
Chain CM: 63% 32% 5% .





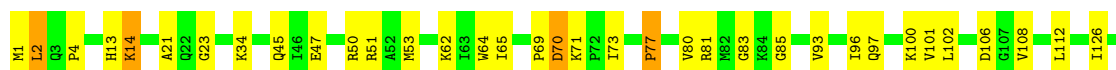
- Molecule 13: 50S ribosomal protein L16

Chain EM: 66% 27% 6% •



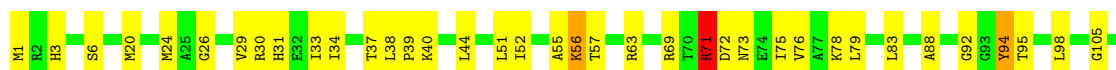
- Molecule 13: 50S ribosomal protein L16

Chain GM: 71% 26% •



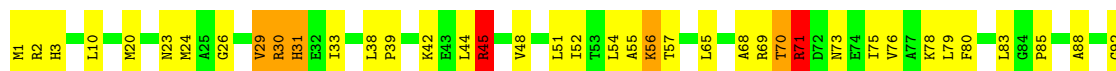
- Molecule 14: 50S ribosomal protein L17

Chain AN: 62% 30% • • 6%



- Molecule 14: 50S ribosomal protein L17

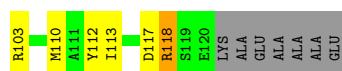
Chain CN: 60% 28% 6% • 6%



- Molecule 14: 50S ribosomal protein L17

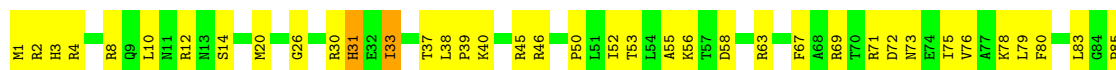
Chain EN: 62% 30% • 6%





- Molecule 14: 50S ribosomal protein L17

Chain GN: 56% 36% 6%



- Molecule 15: 50S ribosomal protein L18

Chain AO: 59% 37% 4%



- Molecule 15: 50S ribosomal protein L18

Chain CO: 69% 26% 5%



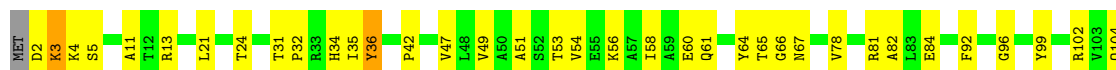
- Molecule 15: 50S ribosomal protein L18

Chain EO: 72% 24% 4%

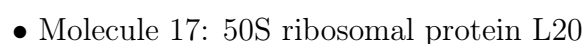
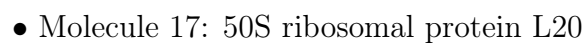
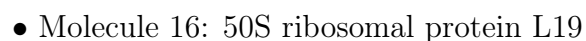
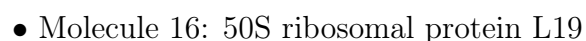
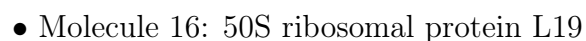


- Molecule 15: 50S ribosomal protein L18

Chain GO: 66% 32% 2%

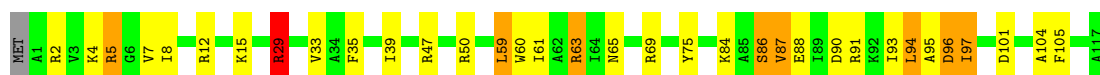


- Molecule 16: 50S ribosomal protein L19



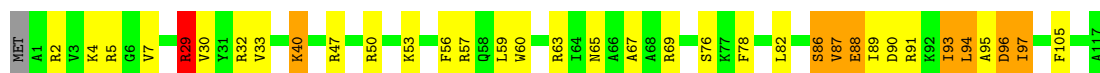


Chain CQ:  70% 21% 7% ..



- Molecule 17: 50S ribosomal protein L20

Chain EQ:  69% 22% 7% ..



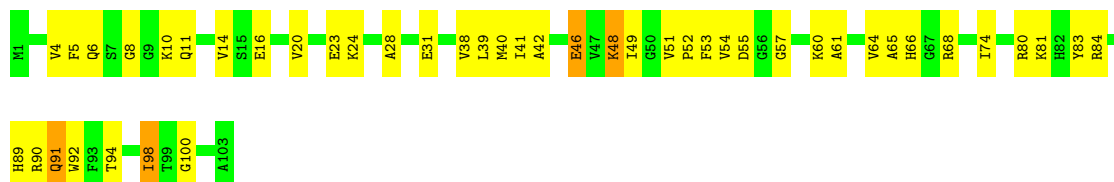
- Molecule 17: 50S ribosomal protein L20

Chain GQ:  67% 28% . .



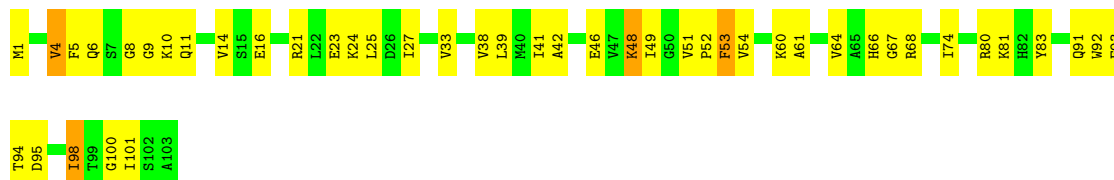
- Molecule 18: 50S ribosomal protein L21

Chain AR:  56% 40% .



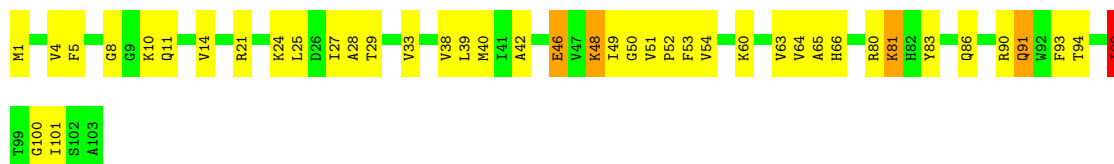
- Molecule 18: 50S ribosomal protein L21

Chain CR:  56% 40% .



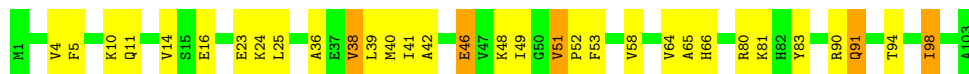
- Molecule 18: 50S ribosomal protein L21

Chain ER:  59% 36% . .



- Molecule 18: 50S ribosomal protein L21

Chain GR: 



- Molecule 19: 50S ribosomal protein L22

Chain AS: 



- Molecule 19: 50S ribosomal protein L22

Chain CS: 



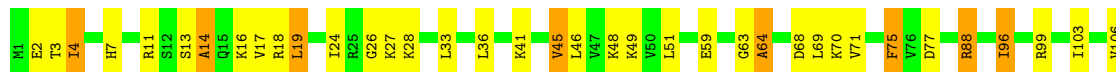
- Molecule 19: 50S ribosomal protein L22

Chain ES: 



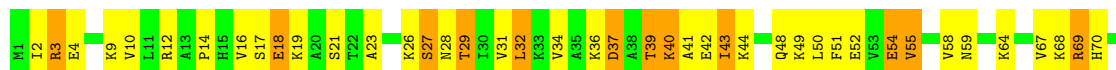
- Molecule 19: 50S ribosomal protein L22

Chain GS: 



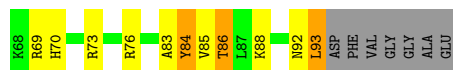
- Molecule 20: 50S ribosomal protein L23

Chain AT: 

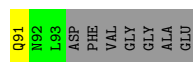
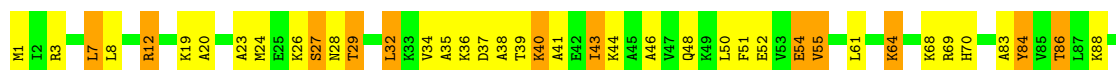




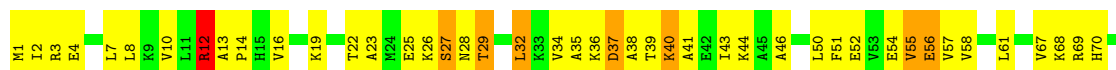
- Molecule 20: 50S ribosomal protein L23



- Molecule 20: 50S ribosomal protein L23



- Molecule 20: 50S ribosomal protein L23



- Molecule 21: 50S ribosomal protein L24

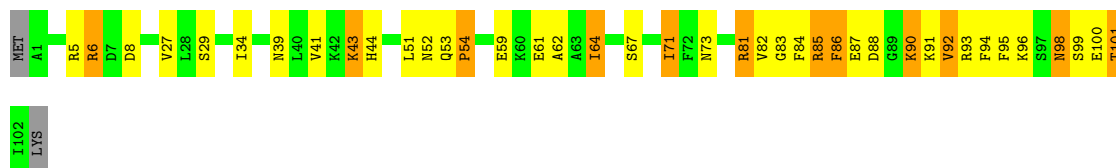


- Molecule 21: 50S ribosomal protein L24



- Molecule 21: 50S ribosomal protein L24

Chain EU: 




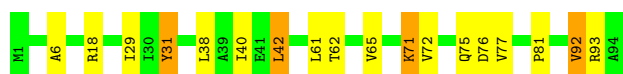
- Molecule 21: 50S ribosomal protein L24

Chain GU: 



- Molecule 22: 50S ribosomal protein L25

Chain AV: 



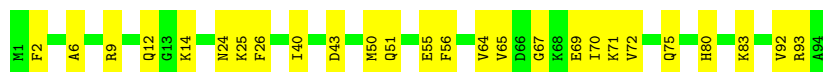
- Molecule 22: 50S ribosomal protein L25

Chain CV: 



- Molecule 22: 50S ribosomal protein L25

Chain EV: 



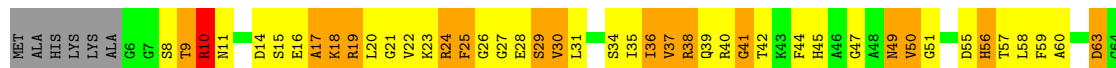
- Molecule 22: 50S ribosomal protein L25

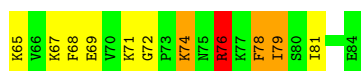
Chain GV: 



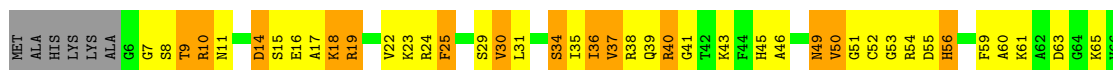
- Molecule 23: 50S ribosomal protein L27

Chain AW: 

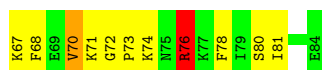
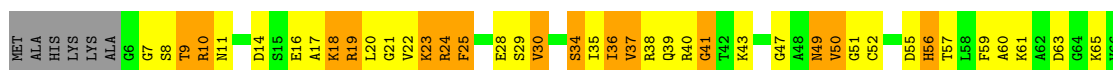




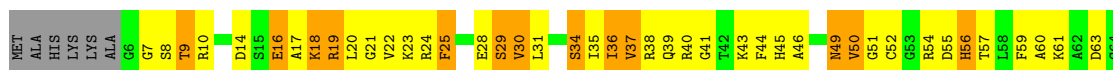
- Molecule 23: 50S ribosomal protein L27



- Molecule 23: 50S ribosomal protein L27



- Molecule 23: 50S ribosomal protein L27



- Molecule 24: 50S ribosomal protein L28

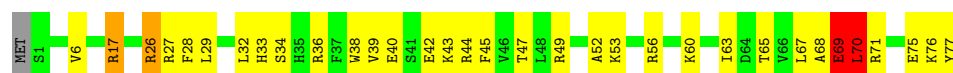


- Molecule 24: 50S ribosomal protein L28



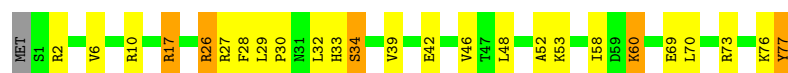
- Molecule 24: 50S ribosomal protein L28

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: 



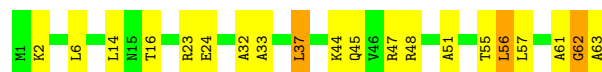
- Molecule 25: 50S ribosomal protein L29

Chain EY: 




- Molecule 25: 50S ribosomal protein L29

Chain GY: 



- Molecule 26: 50S ribosomal protein L30

Chain AZ: 



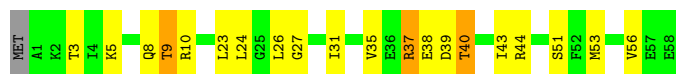
- Molecule 26: 50S ribosomal protein L30

Chain CZ:  69% 25% ..



- Molecule 26: 50S ribosomal protein L30

Chain EZ:  64% 29% 5% ..



- Molecule 26: 50S ribosomal protein L30

Chain GZ:  66% 22% 10% ..



- Molecule 27: 50S ribosomal protein L32

Chain A0:  67% 30% ..




- Molecule 27: 50S ribosomal protein L32

Chain C0:  70% 26% ..



- Molecule 27: 50S ribosomal protein L32

Chain E0:  75% 21% ..



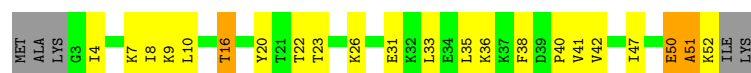
- Molecule 27: 50S ribosomal protein L32

Chain G0:  67% 28% ..



- Molecule 28: 50S ribosomal protein L33

Chain A1: 



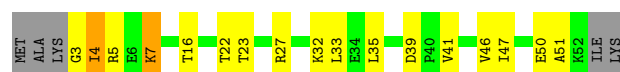
- Molecule 28: 50S ribosomal protein L33

Chain C1: 



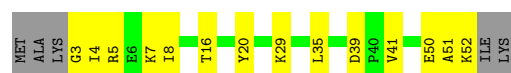
- Molecule 28: 50S ribosomal protein L33

Chain E1: 



- Molecule 28: 50S ribosomal protein L33

Chain G1: 



- Molecule 29: 50S ribosomal protein L34

Chain A2: 



- Molecule 29: 50S ribosomal protein L34

Chain C2: 



- Molecule 29: 50S ribosomal protein L34

Chain E2: 



- Molecule 29: 50S ribosomal protein L34



Chain G2:  67% 28% .




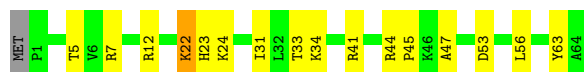
- Molecule 30: 50S ribosomal protein L35

Chain A3:  66% 29% ..



- Molecule 30: 50S ribosomal protein L35

Chain C3:  74% 23% ..



- Molecule 30: 50S ribosomal protein L35

Chain E3:  69% 23% 6% .



- Molecule 30: 50S ribosomal protein L35

Chain G3:  63% 31% 5% .



- Molecule 31: 50S ribosomal protein L36

Chain A4:  61% 32% 8%



- Molecule 31: 50S ribosomal protein L36

Chain C4:  55% 39% 5%



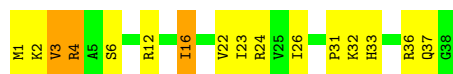
- Molecule 31: 50S ribosomal protein L36

Chain E4: 



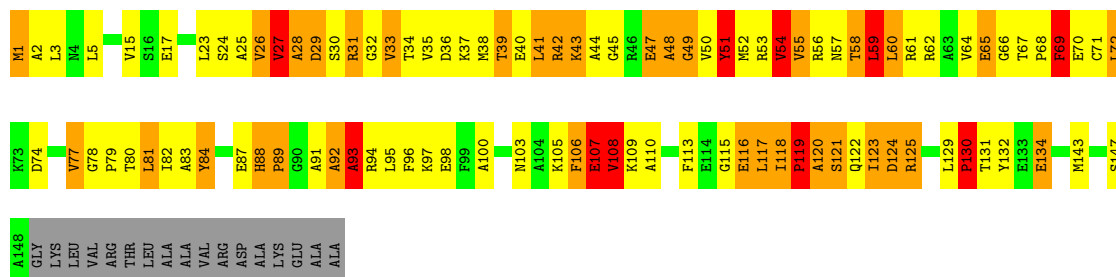
- Molecule 31: 50S ribosomal protein L36

Chain G4: 



- Molecule 32: 50S ribosomal protein L10

Chain A5: 



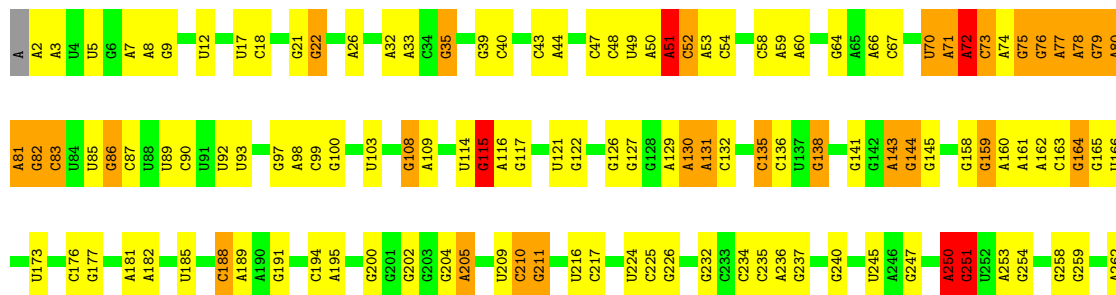
- Molecule 32: 50S ribosomal protein L10

Chain E5: 



- Molecule 33: 16S rRNA

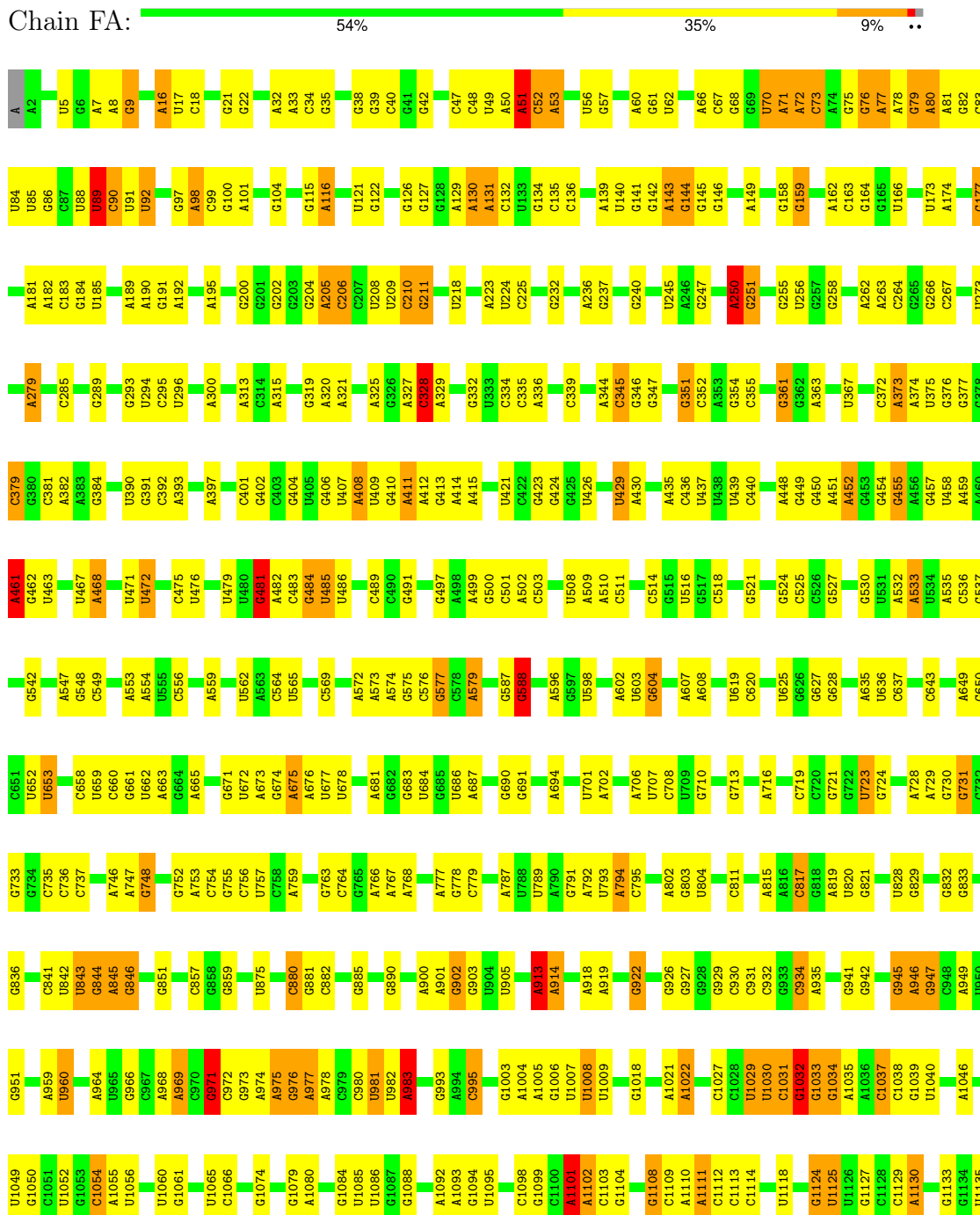
Chain BA: 

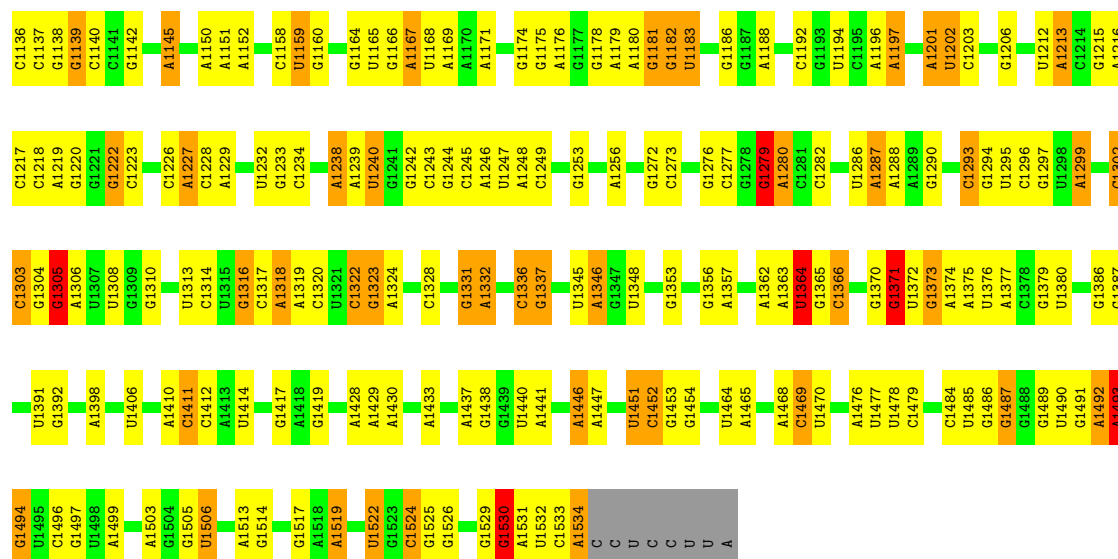


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U1476	A1289	G1198	C1113	U1023	A831	A749	C679	U593	U512	A436	G354	C264
C1479	G1290	A1201	C1114	G1024	G833	G750	C680	C513	C514	U437	G362	G265
A1480	U1291	U1202	U1115	U1025	G833	U751	A681	A596	G515	U438	G362	C267
G1481	G1292	U1202	U1116	G1026	C841	G752	G682	U597			U365	
A1483	C1293	U1212	A1117	C1028	U842	C754	U684	G598			A366	U273
	U1295	A1213	U1118	U1029	U843	G755	G685	A600	C518	A448	U367	
G1487	C1296	A1216	C1119	U1030	U844	C756	G686	G601	C519	G449	U368	G276
G1488	G1297	A1217	G1124	C1031	A845	U757	G687	A602	A520	G450	G369	
G1489	U1298	C1218	A1125	G1032	C846	C758	G688	A603	G521	A451		
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G1491				G1034	C848	G763	G690	U605	A523	G453	C372	G281
A1492	C1302		A1130	A1035	G858	C764	G691	A608	G527	G454	A373	G282
A1493	C1303		A1131	A1036	G859	A767	U697			A456	A374	U283
G1494	G1304	U1223	C1132	C1037	G860	A768		C613	G530	G457	U375	C284
	G1305	A1224	G1133	C1038	C861	G769	G700	U619	U532	U458	G377	C285
	A1306	C1226	G1134	G1041	G865	G770	U701	C618	A533	A459		G289
	G1309	A1227	U1135	A1042	C866	G771	A702	U620	A461	A460		G292
			C1136		U870	G776	A704	G639	G462	A462	C381	
			C1137	U1049	U871	G777	A705	U641	C536	A463	A382	G299
			G1138	G1050	A975	A777	G705	A622	G537	U464	G384	A300
			G1139	G1051	G976	G778	A706	G626	G538	U465		G301
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				C1054	U981	A784	U709	A629	A547	A468	C382	C308
				G1058	U982	A785	G711	A630	G548	A393	A393	A309
				C1059	A983	G786		G639	C549	G394	G396	G310
				U1060	C881	A787	G714	A640		U473		
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					G893	G799	G725		U485	A329		A329
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					G897	G809	G730	G661	A415	A415	C335	C335
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					G899	C811		A665	G417	G417	A337	A337
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					G902	A816	G738	G669	U421	U421	U340	U340
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					G904	G927	U740	G671	G500	G500	A344	A344
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					G906	G929	G742	G673	A502	A502	G346	G346
					G907	G930	A743	G674	G503	G503	G347	G347
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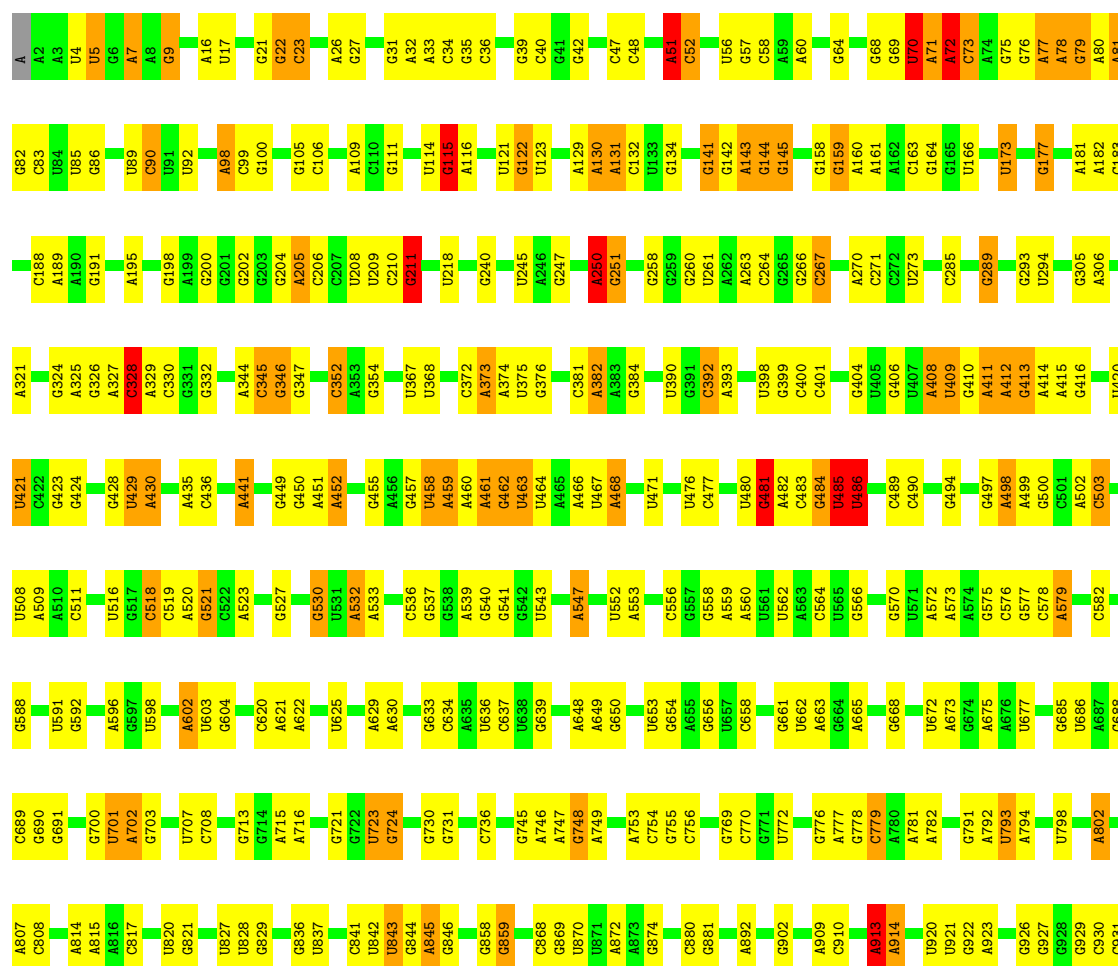
- Molecule 33: 16S rRNA

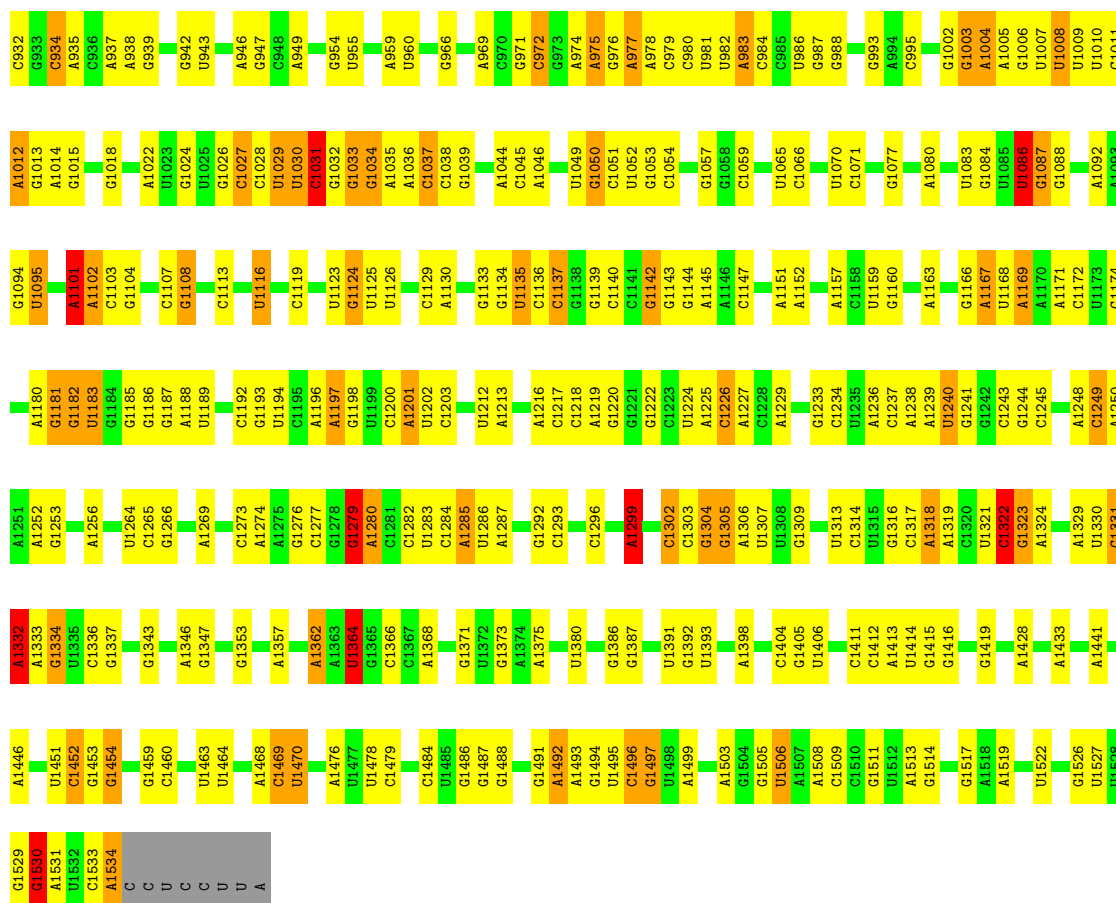




• Molecule 33: 16S rRNA

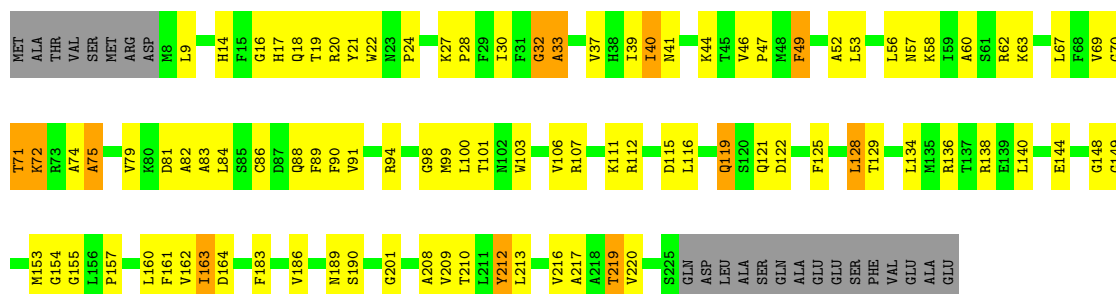
Chain HA: 56% 34% 8% ..





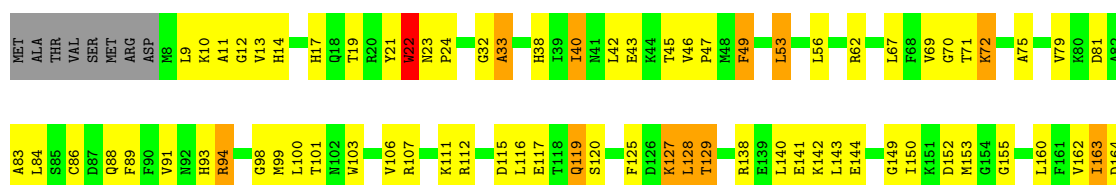
• Molecule 34: 30S ribosomal protein S2

Chain BB: 



• Molecule 34: 30S ribosomal protein S2

Chain DB: 

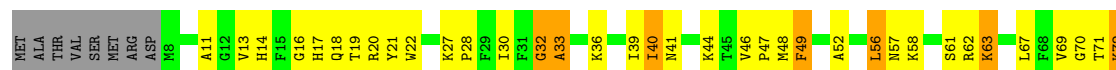




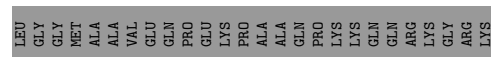
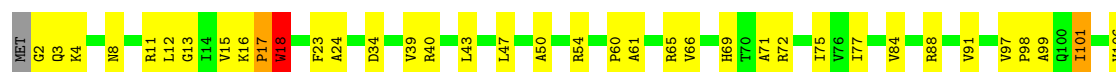
- Molecule 34: 30S ribosomal protein S2



- Molecule 34: 30S ribosomal protein S2



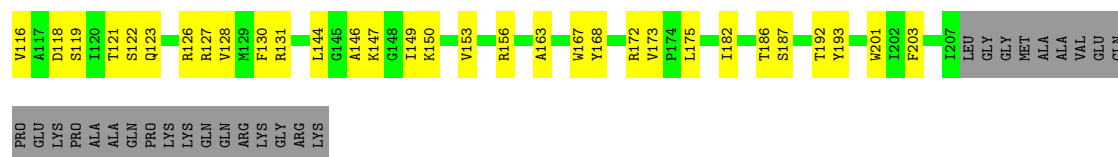
- Molecule 35: 30S ribosomal protein S3



- Molecule 35: 30S ribosomal protein S3

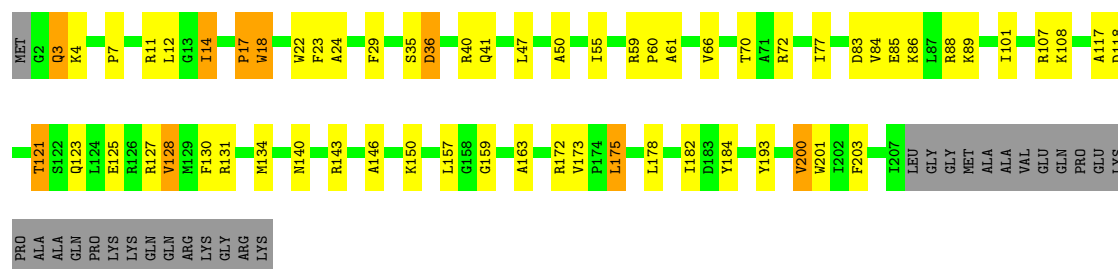






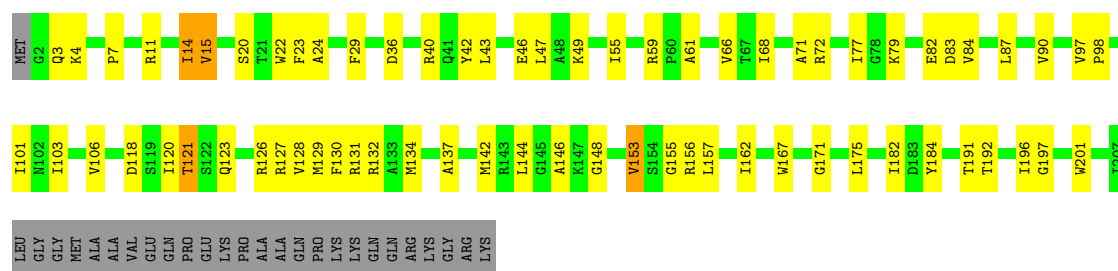
- Molecule 35: 30S ribosomal protein S3

Chain FC: 62% 23% 12%



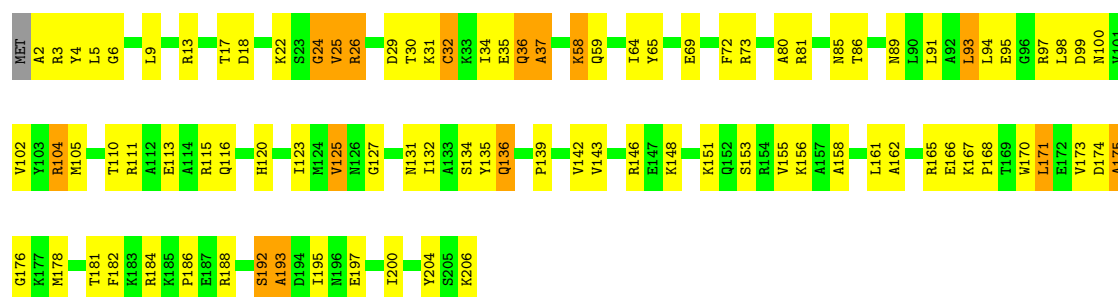
- Molecule 35: 30S ribosomal protein S3

Chain HC: 59% 28% 12%



- Molecule 36: 30S ribosomal protein S4

Chain BD: 54% 38% 7%



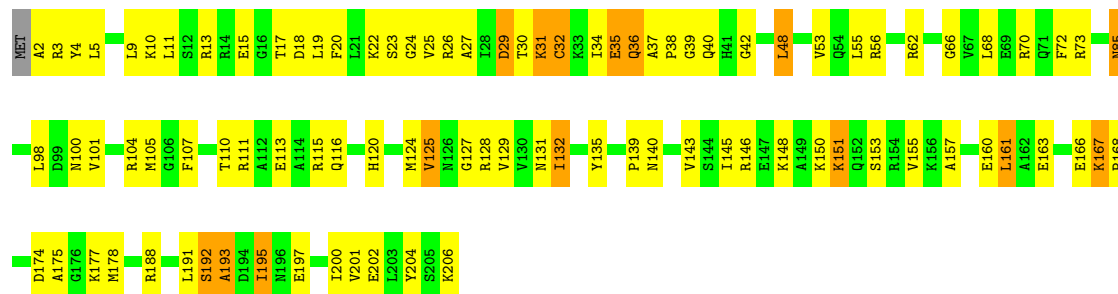
- Molecule 36: 30S ribosomal protein S4

Chain DD: 54% 36% 9%



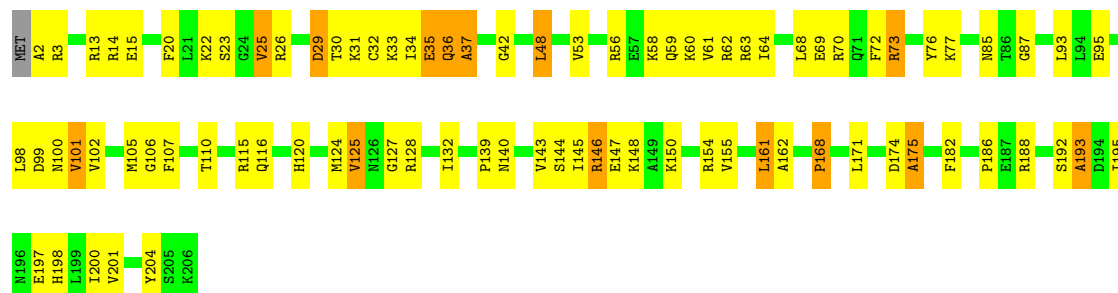
- Molecule 36: 30S ribosomal protein S4

Chain FD: 



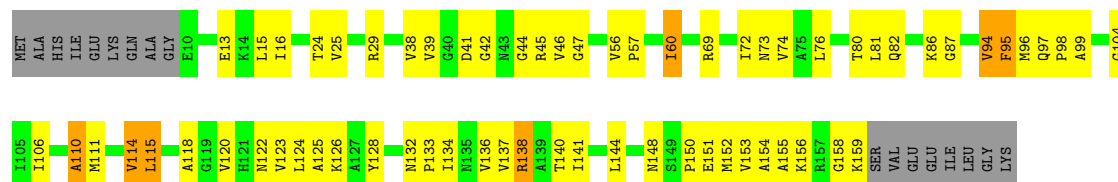
- Molecule 36: 30S ribosomal protein S4

Chain HD: 



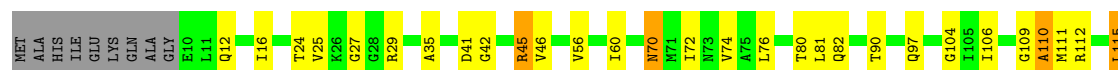
- Molecule 37: 30S ribosomal protein S5

Chain BE:  50% 35% 10%



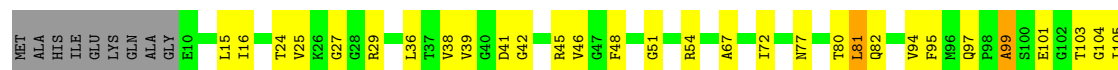
- Molecule 37: 30S ribosomal protein S5

Chain DE: 

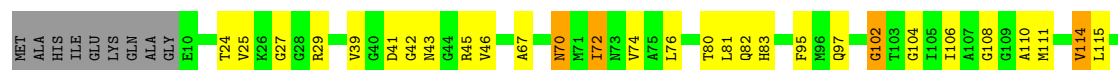




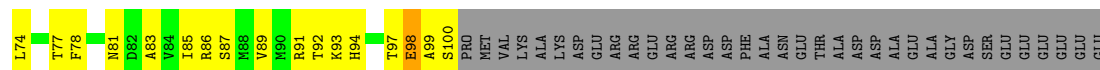
- Molecule 37: 30S ribosomal protein S5



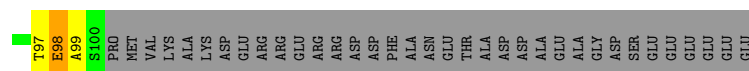
- Molecule 37: 30S ribosomal protein S5



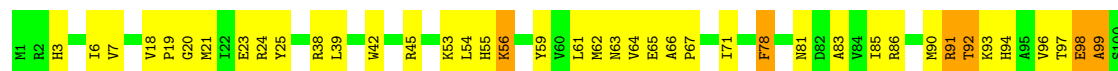
- Molecule 38: 30S ribosomal protein S6



- Molecule 38: 30S ribosomal protein S6



- Molecule 38: 30S ribosomal protein S6



PRO MET VAL LYS LYS LYS ASP ASP ARG ARG ARG ARG ARG ASP ASP PHE PHE ALA ALA ASN GLU THR ALA ASP ASP ASP ALA ALA ALA GLY ASP SER SER GLU GLU GLU GLU GLU

• Molecule 38: 30S ribosomal protein S6

Chain HF: 47% 24% • 26%

H1 H2 H3 H4 H5 H6 H7 V10 H11 Q17 V18 F19 G20 M21 M22 I22 E23 T26 T38 R38 L39 I51 H55 K56 A57 H58 M62 N63 V64 E65 E66 A66 P67 V70 L74 F78 N81 D82 A83 V84 I85 R91 T92 K93 H94 T97 E98 A99 S100 PRO

MET VAL LYS LYS LYS ASP ASP ARG ARG ARG ARG ASP PHE PHE ALA ALA ASN GLU THR ALA ASP ASP ASP ALA ALA ALA GLY ASP SER SER GLU GLU GLU GLU GLU

• Molecule 39: 30S ribosomal protein S7

Chain BG: 62% 22% • 16%

MET P2 P3 R4 R5 V6 V7 D15 F18 L22 K25 F26 V27 N28 Y43 Y44 L50 S57 E58 L59 E60 F61 F62 A65 R70 R79 S77 R78 R79 S83 Q86 V87 P88 V89 R96 W103 D113 L118 N122 A128

E139 D140 V141 H142 M143 M144 A145 A146 A147 N148 A149 A150 F151 A152 HIS TYR ARG TRP LEU SER ARG ARG PHE SER HIS GLN ALA ALA SER SER LYS GLN PRO LEU TYR LEU ASN

• Molecule 39: 30S ribosomal protein S7

Chain DG: 60% 23% • 16%

MET P2 R3 R4 R5 V6 V7 V8 Q9 L13 P14 D15 F18 L22 L29 Y44 L50 A51 S52 S53 S54 S55 F56 S57 E58 L59 E60 F62 R70 E74 R79 S83 P88 R95 R96 W103 E106 K110 D113 R119 N122

S125 D126 A127 A128 V141 A146 E146 A147 K148 K149 A152 HIS TYR ARG TRP LEU SER ARG ARG PHE SER HIS GLN ALA ALA SER SER LYS GLN PRO LEU TYR LEU ASN

• Molecule 39: 30S ribosomal protein S7

Chain FG: 55% 27% • 16%

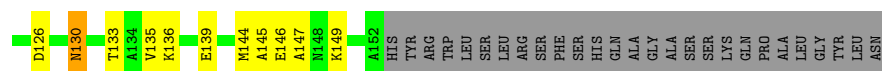
MET P2 R3 R4 R5 V6 Q9 D15 F18 G19 S20 E21 L22 K25 F26 V27 N28 Y43 Y44 L50 R53 S57 S58 L59 E60 A61 F62 L66 E67 R68 V69 R70 R79 G82 V89 E90 R96 N97 M101 R102 W103 W104 V105 E106 A107 A108

R109 K110 R111 G112 D113 M122 E123 L124 S125 D126 M130 G131 T133 D140 V141 H142 M144 A145 E146 A147 H148 K149 A152 HIS TYR ARG TRP LEU SER ARG ARG PHE SER HIS GLN ALA ALA SER SER LYS GLN PRO ALA ALA GLY SER SER LYS GLN PRO ALA ALA GLY TYR LEU ASN

• Molecule 39: 30S ribosomal protein S7

Chain HG: 60% 24% • 16%

MET P2 R3 R4 R5 V6 I12 D15 F18 G19 S20 E21 L23 A46 L47 E48 T49 L50 A51 Q52 R53 S54 G55 K56 S57 E58 A61 E67 V75 S83 T84 Y85 R95 R96 N97 A98 L99 E106 A107 A108 R109 K110 R111 G112 D113 R119 N122

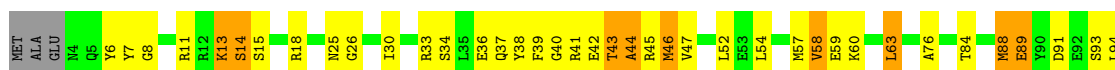




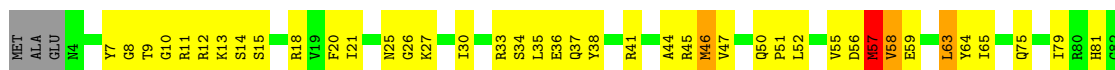
- Molecule 41: 30S ribosomal protein S9



- Molecule 41: 30S ribosomal protein S9



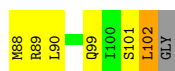
- Molecule 41: 30S ribosomal protein S9



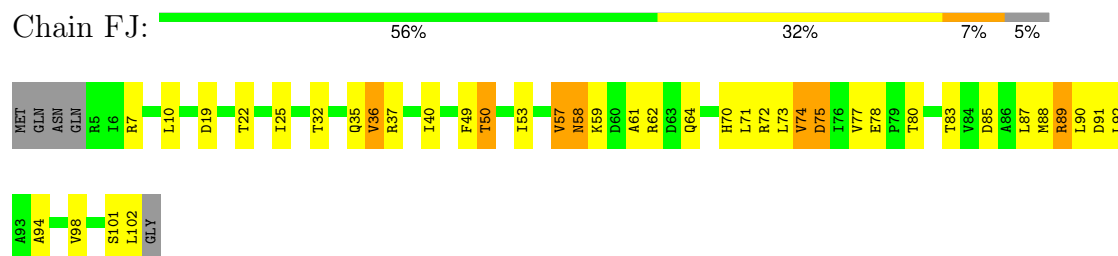
- Molecule 42: 30S ribosomal protein S10



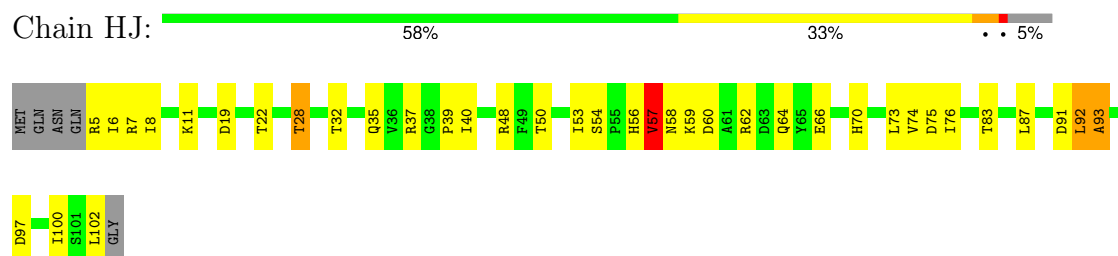
- Molecule 42: 30S ribosomal protein S10



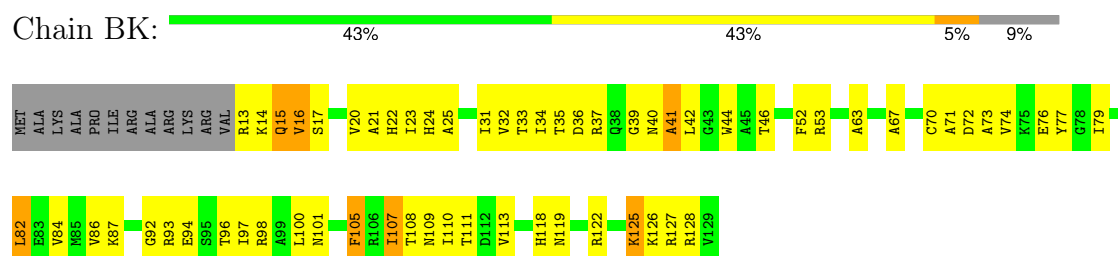
## • Molecule 42: 30S ribosomal protein S10



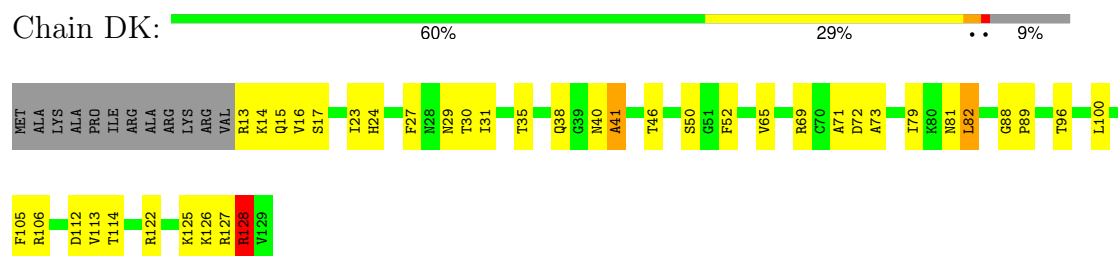
## • Molecule 42: 30S ribosomal protein S10



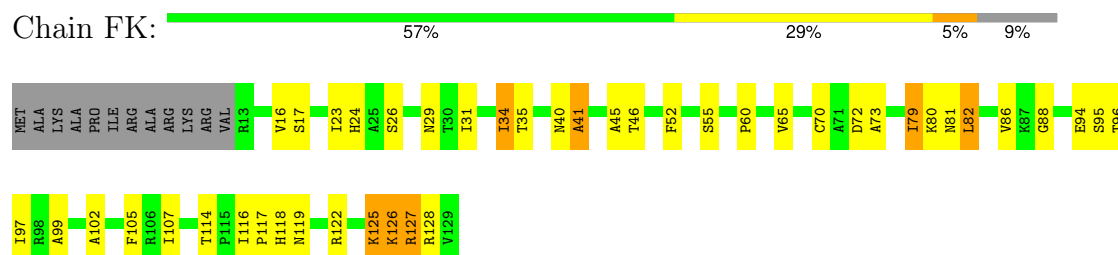
## • Molecule 43: 30S ribosomal protein S11



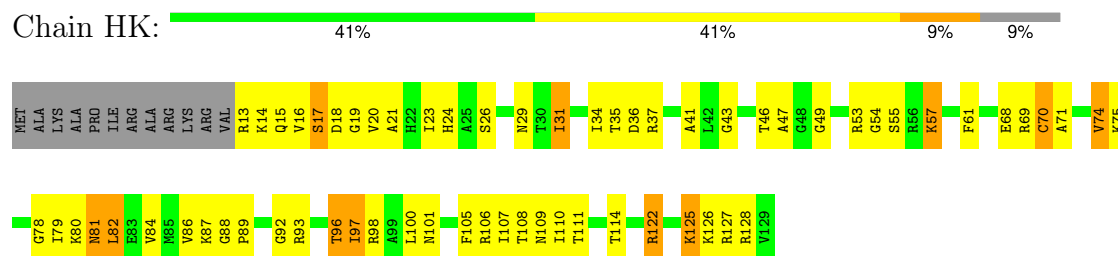
## • Molecule 43: 30S ribosomal protein S11



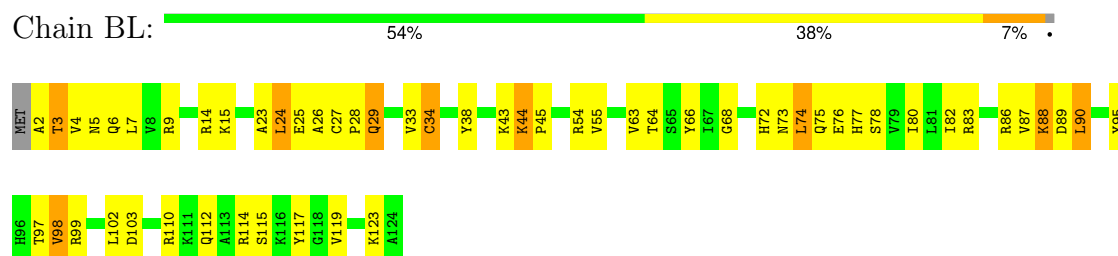
## • Molecule 43: 30S ribosomal protein S11



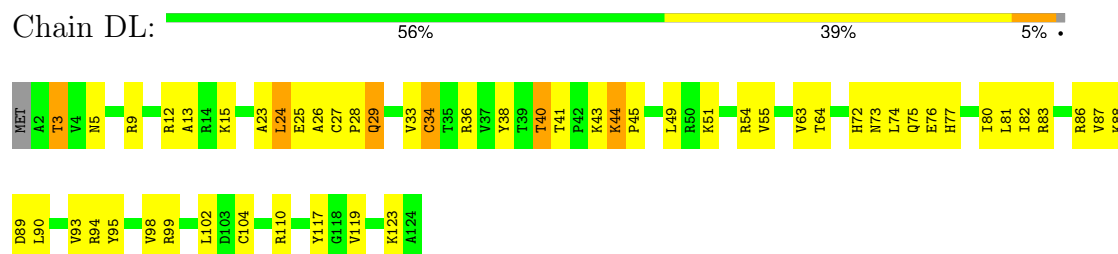
- Molecule 43: 30S ribosomal protein S11



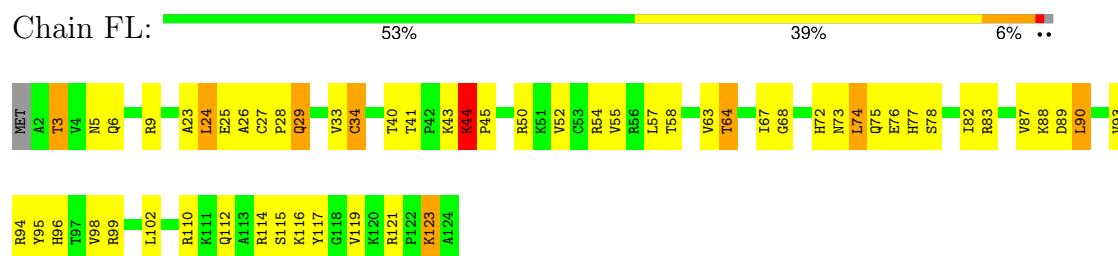
- Molecule 44: 30S ribosomal protein S12



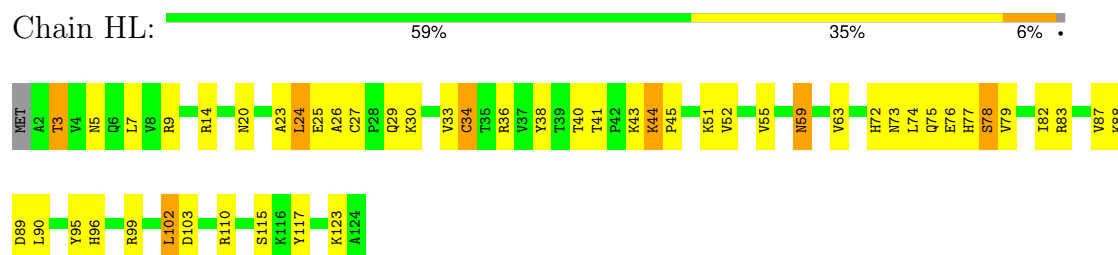
- Molecule 44: 30S ribosomal protein S12



- Molecule 44: 30S ribosomal protein S12

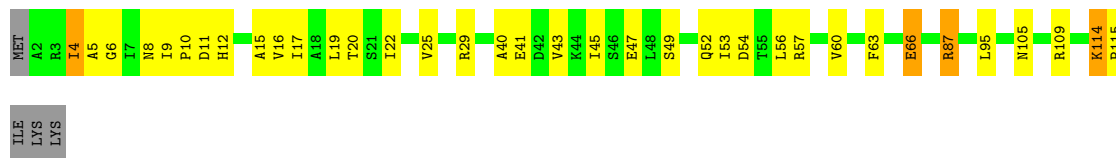


- Molecule 44: 30S ribosomal protein S12





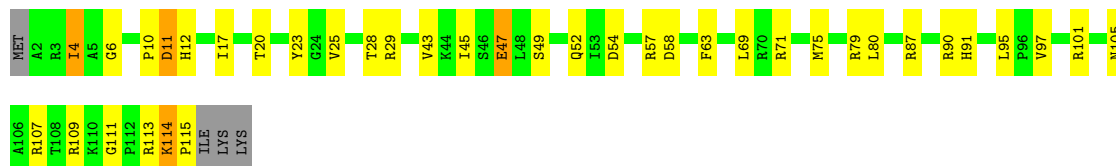
## ● Molecule 45: 30S ribosomal protein S13

Chain BM:  66% 27%

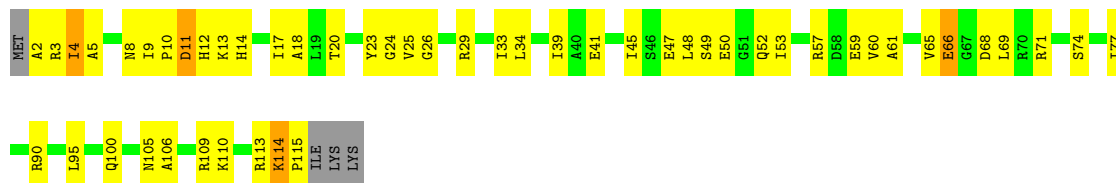
## ● Molecule 45: 30S ribosomal protein S13

Chain DM:  70% 23%

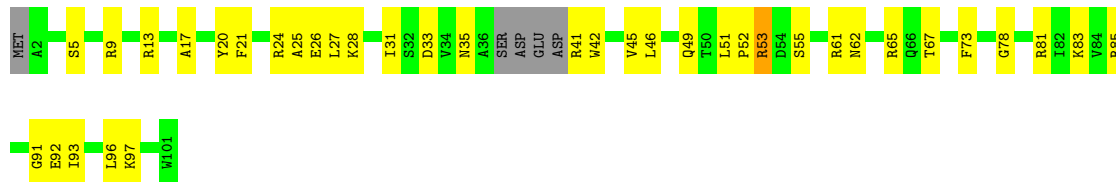
## ● Molecule 45: 30S ribosomal protein S13

Chain FM:  64% 29%

## ● Molecule 45: 30S ribosomal protein S13

Chain HM:  53% 40%

## ● Molecule 46: 30S ribosomal protein S14

Chain BN:  58% 36% 5%

## ● Molecule 46: 30S ribosomal protein S14

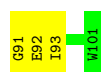
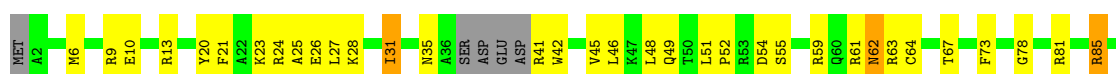
Chain DN:  65% 29% 5%



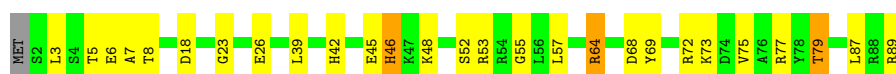
- Molecule 46: 30S ribosomal protein S14



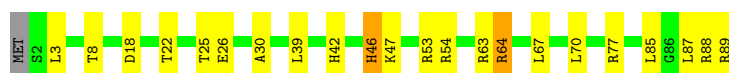
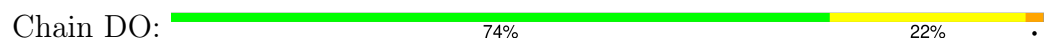
- Molecule 46: 30S ribosomal protein S14



- Molecule 47: 30S ribosomal protein S15



- Molecule 47: 30S ribosomal protein S15



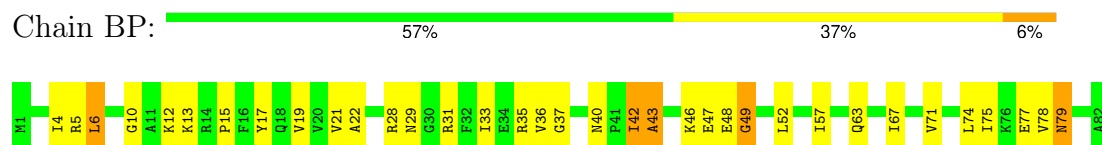
- Molecule 47: 30S ribosomal protein S15



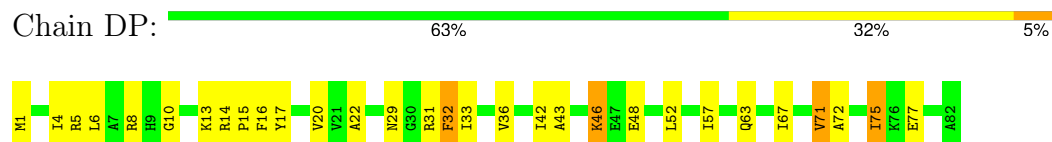
- Molecule 47: 30S ribosomal protein S15



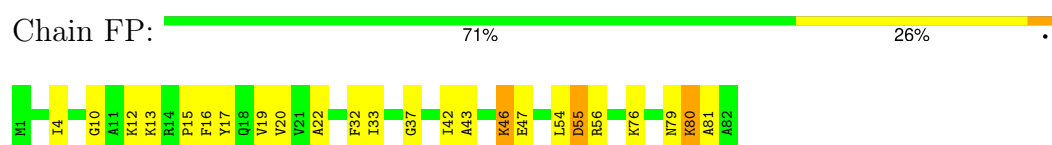
- Molecule 48: 30S ribosomal protein S16



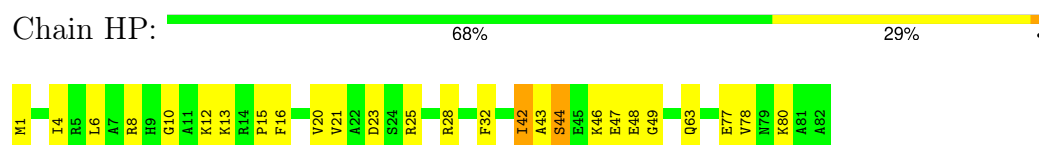
- Molecule 48: 30S ribosomal protein S16



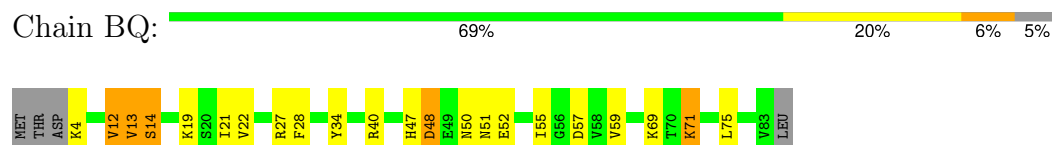
- Molecule 48: 30S ribosomal protein S16



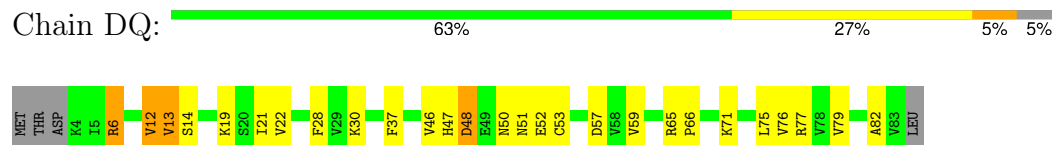
- Molecule 48: 30S ribosomal protein S16



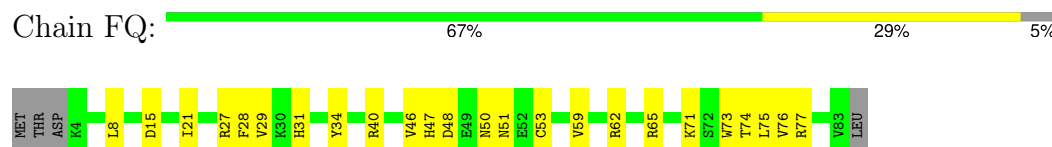
- Molecule 49: 30S ribosomal protein S17



- Molecule 49: 30S ribosomal protein S17



- Molecule 49: 30S ribosomal protein S17



- Molecule 49: 30S ribosomal protein S17

Chain HQ:  60% 31% 5% 5%



- Molecule 50: 30S ribosomal protein S18

Chain BR:  43% 31% 27%



- Molecule 50: 30S ribosomal protein S18

Chain DR:  48% 25% 27%



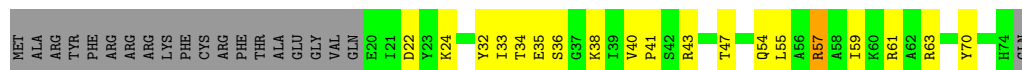
- Molecule 50: 30S ribosomal protein S18

Chain FR:  47% 27% 27%



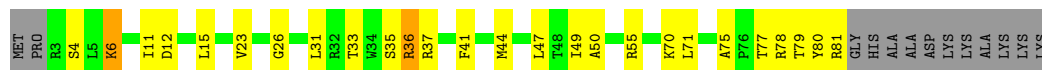
- Molecule 50: 30S ribosomal protein S18

Chain HR:  48% 24% 27%



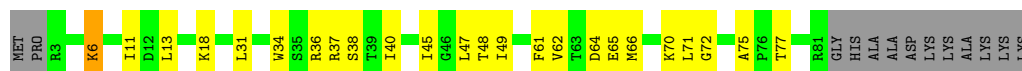
- Molecule 51: 30S ribosomal protein S19

Chain BS:  58% 26% 14%

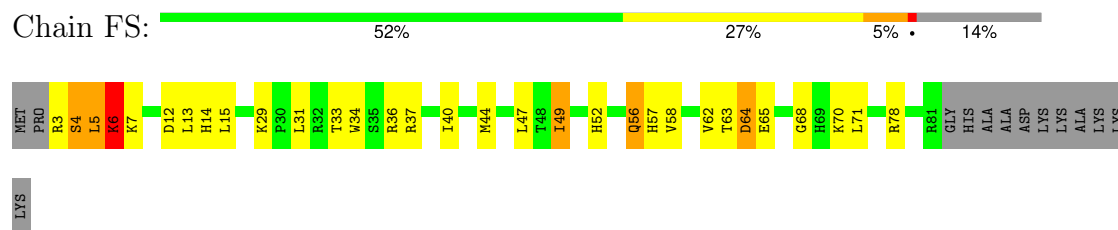


- Molecule 51: 30S ribosomal protein S19

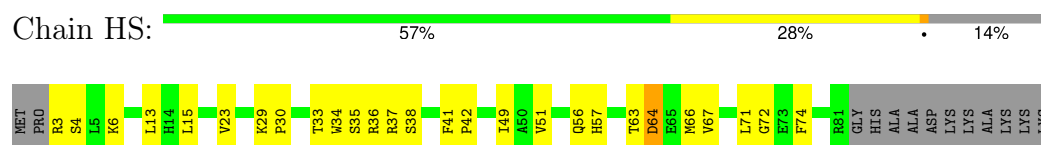
Chain DS:  60% 25% 14%



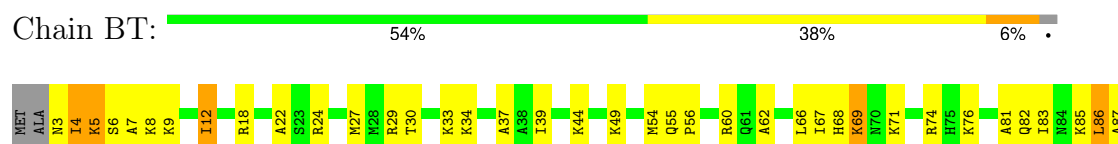
- Molecule 51: 30S ribosomal protein S19



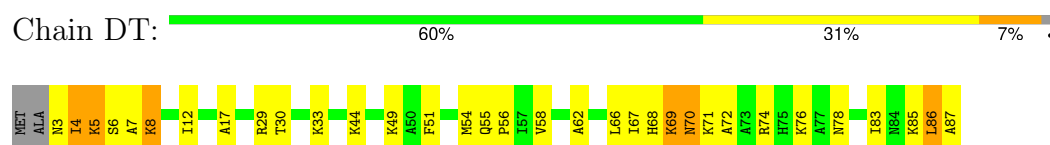
- Molecule 51: 30S ribosomal protein S19



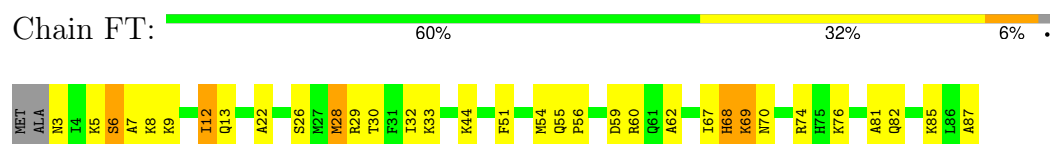
- Molecule 52: 30S ribosomal protein S20



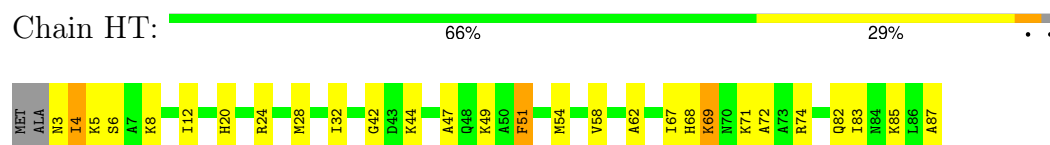
- Molecule 52: 30S ribosomal protein S20



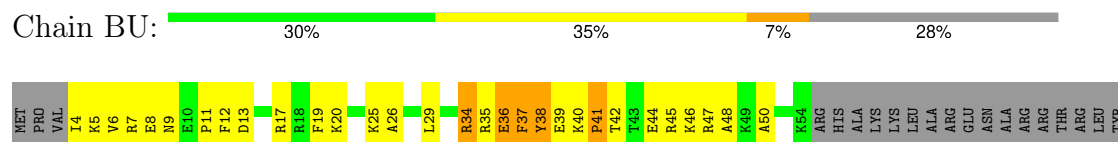
- Molecule 52: 30S ribosomal protein S20



- Molecule 52: 30S ribosomal protein S20

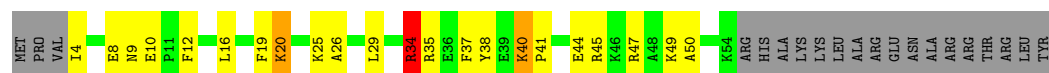


- Molecule 53: 30S ribosomal protein S21



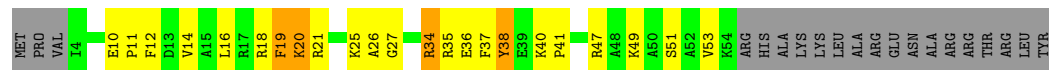
- Molecule 53: 30S ribosomal protein S21

Chain DU:  41% 27% 28%



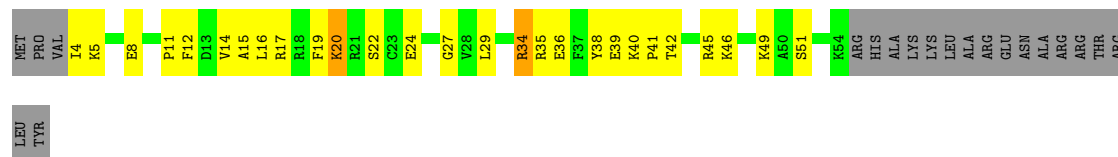
- Molecule 53: 30S ribosomal protein S21

Chain FU:  39% 27% 6% 28%



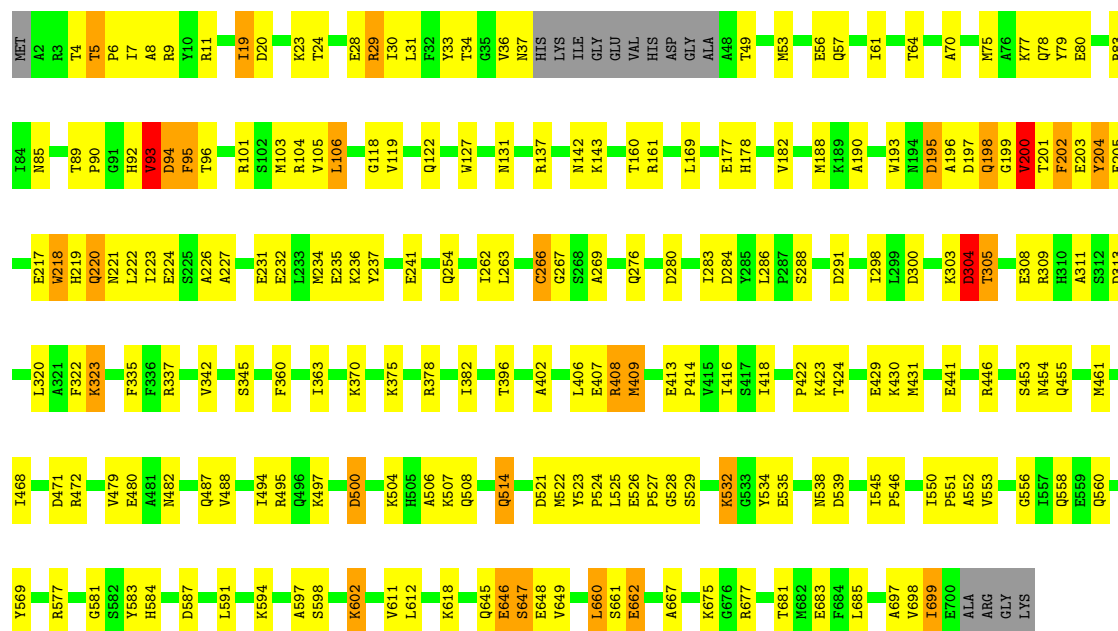
- Molecule 53: 30S ribosomal protein S21

Chain HU:  34% 35% 28%



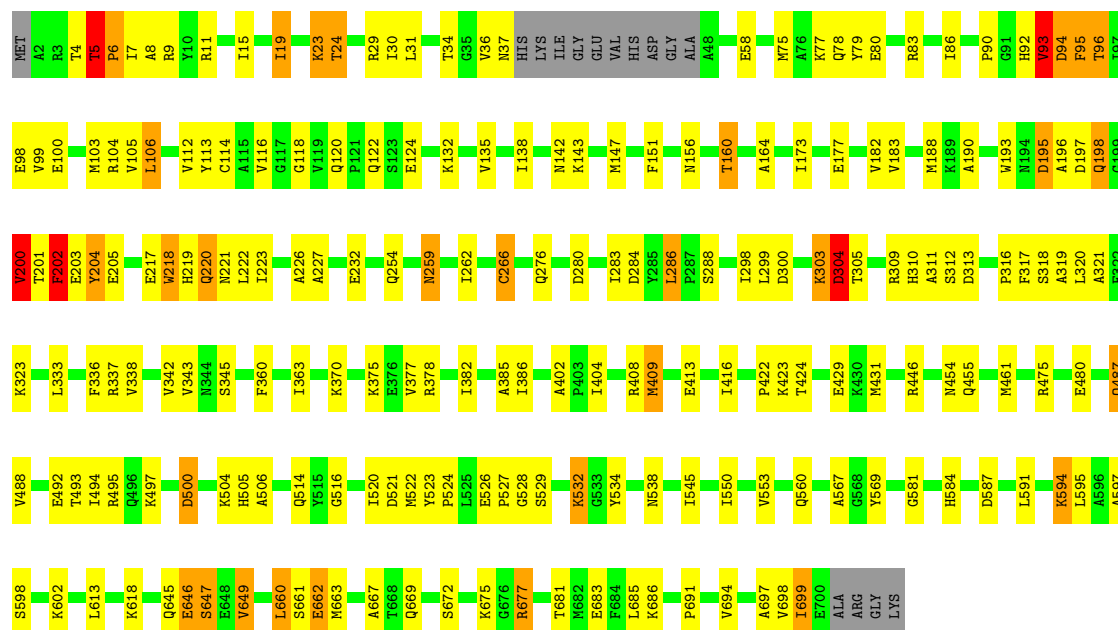
- Molecule 54: elongation factor G

Chain BV:  67% 27%



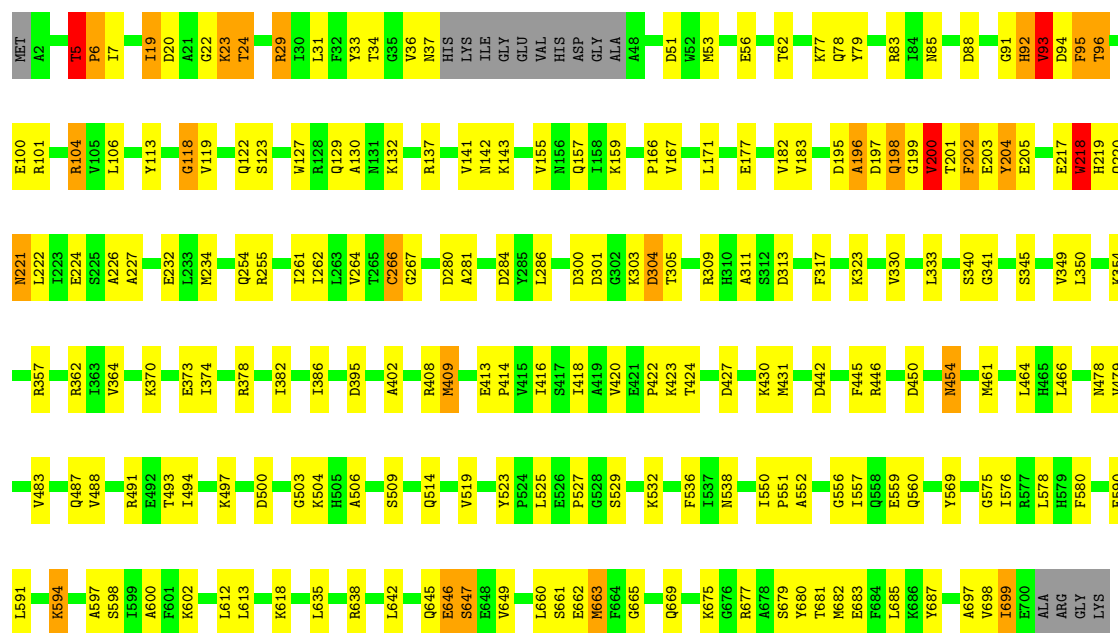
- Molecule 54: elongation factor G

Chain DV:  68% 25%



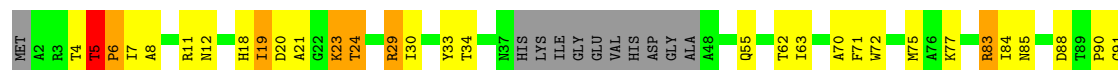
• Molecule 54: elongation factor G

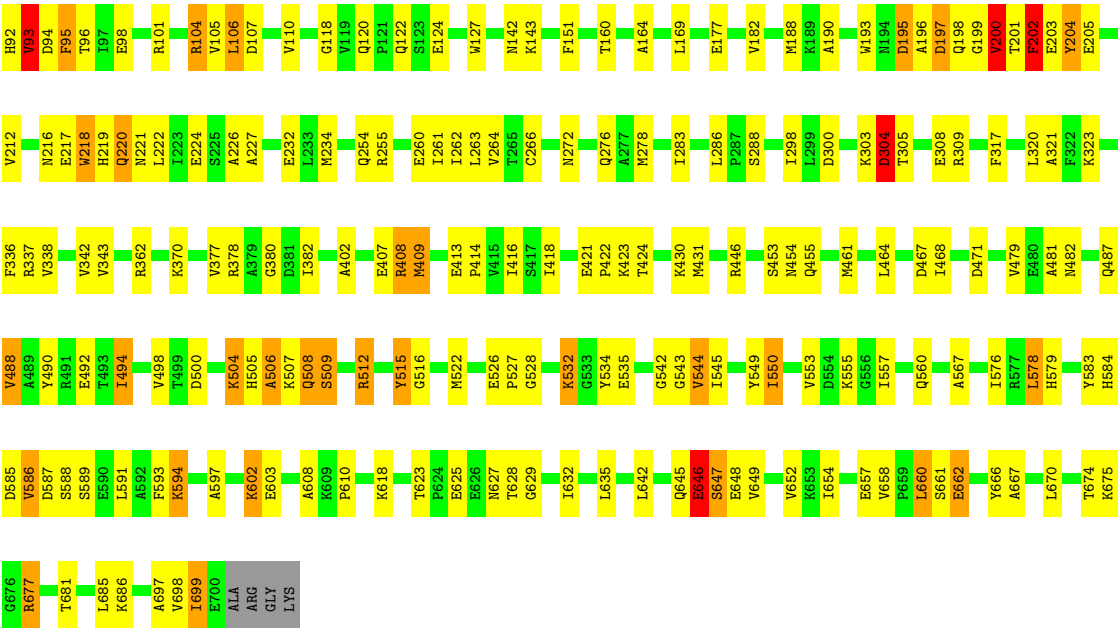
Chain FV: 68% 26% ...



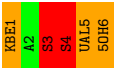
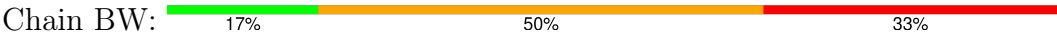
• Molecule 54: elongation factor G

Chain HV: 65% 27% 5% ...

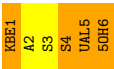




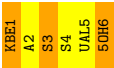
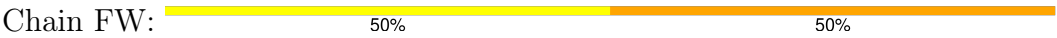
● Molecule 55: Viomycin



● Molecule 55: Viomycin



● Molecule 55: Viomycin





## 4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	361.14Å 360.51Å 429.73Å 90.00° 103.22° 90.00°	Depositor
Resolution (Å)	70.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (70.00-2.90)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.24 (at 2.81Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.215 , 0.267	Depositor
Wilson B-factor (Å <sup>2</sup> )	54.5	Xtriage
Anisotropy	0.324	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	590573	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

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

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are no chirality outliers.

5 of 23 planarity outliers are listed below:

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

## 5.2 Too-close contacts

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

of similar resolution.

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

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	CJ	140/142 (99%)	113 (81%)	19 (14%)	8 (6%)	1	4
10	EJ	140/142 (99%)	113 (81%)	19 (14%)	8 (6%)	1	4
10	GJ	140/142 (99%)	114 (81%)	17 (12%)	9 (6%)	1	3
11	AK	120/123 (98%)	93 (78%)	17 (14%)	10 (8%)	0	2
11	CK	120/123 (98%)	91 (76%)	21 (18%)	8 (7%)	1	3
11	EK	120/123 (98%)	92 (77%)	17 (14%)	11 (9%)	0	1
11	GK	120/123 (98%)	92 (77%)	19 (16%)	9 (8%)	1	2
12	AL	141/144 (98%)	107 (76%)	26 (18%)	8 (6%)	1	4
12	CL	141/144 (98%)	107 (76%)	27 (19%)	7 (5%)	1	6
12	EL	141/144 (98%)	108 (77%)	26 (18%)	7 (5%)	1	6
12	GL	141/144 (98%)	109 (77%)	25 (18%)	7 (5%)	1	6
13	AM	134/136 (98%)	105 (78%)	22 (16%)	7 (5%)	1	5
13	CM	134/136 (98%)	111 (83%)	16 (12%)	7 (5%)	1	5
13	EM	134/136 (98%)	110 (82%)	18 (13%)	6 (4%)	2	8
13	GM	134/136 (98%)	112 (84%)	16 (12%)	6 (4%)	2	8
14	AN	118/127 (93%)	101 (86%)	15 (13%)	2 (2%)	7	27
14	CN	118/127 (93%)	98 (83%)	17 (14%)	3 (2%)	4	18
14	EN	118/127 (93%)	101 (86%)	14 (12%)	3 (2%)	4	18
14	GN	118/127 (93%)	98 (83%)	19 (16%)	1 (1%)	16	45
15	AO	114/117 (97%)	99 (87%)	14 (12%)	1 (1%)	14	43
15	CO	114/117 (97%)	96 (84%)	17 (15%)	1 (1%)	14	43
15	EO	114/117 (97%)	96 (84%)	18 (16%)	0	100	100
15	GO	114/117 (97%)	97 (85%)	13 (11%)	4 (4%)	3	12
16	AP	112/115 (97%)	83 (74%)	22 (20%)	7 (6%)	1	3
16	CP	112/115 (97%)	81 (72%)	22 (20%)	9 (8%)	1	2
16	EP	112/115 (97%)	83 (74%)	22 (20%)	7 (6%)	1	3
16	GP	112/115 (97%)	79 (70%)	21 (19%)	12 (11%)	0	1
17	AQ	115/118 (98%)	101 (88%)	9 (8%)	5 (4%)	2	8
17	CQ	115/118 (98%)	102 (89%)	9 (8%)	4 (4%)	3	12
17	EQ	115/118 (98%)	102 (89%)	8 (7%)	5 (4%)	2	8
17	GQ	115/118 (98%)	103 (90%)	7 (6%)	5 (4%)	2	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	AR	101/103 (98%)	83 (82%)	15 (15%)	3 (3%)	3	15
18	CR	101/103 (98%)	83 (82%)	15 (15%)	3 (3%)	3	15
18	ER	101/103 (98%)	83 (82%)	15 (15%)	3 (3%)	3	15
18	GR	101/103 (98%)	84 (83%)	13 (13%)	4 (4%)	2	10
19	AS	108/110 (98%)	93 (86%)	10 (9%)	5 (5%)	2	8
19	CS	108/110 (98%)	96 (89%)	8 (7%)	4 (4%)	2	11
19	ES	108/110 (98%)	91 (84%)	12 (11%)	5 (5%)	2	8
19	GS	108/110 (98%)	92 (85%)	11 (10%)	5 (5%)	2	8
20	AT	91/100 (91%)	59 (65%)	24 (26%)	8 (9%)	0	1
20	CT	91/100 (91%)	60 (66%)	23 (25%)	8 (9%)	0	1
20	ET	91/100 (91%)	59 (65%)	25 (28%)	7 (8%)	1	2
20	GT	91/100 (91%)	60 (66%)	22 (24%)	9 (10%)	0	1
21	AU	100/104 (96%)	73 (73%)	18 (18%)	9 (9%)	0	1
21	CU	100/104 (96%)	74 (74%)	16 (16%)	10 (10%)	0	1
21	EU	100/104 (96%)	74 (74%)	13 (13%)	13 (13%)	0	0
21	GU	100/104 (96%)	73 (73%)	18 (18%)	9 (9%)	0	1
22	AV	92/94 (98%)	82 (89%)	9 (10%)	1 (1%)	12	37
22	CV	92/94 (98%)	79 (86%)	12 (13%)	1 (1%)	12	37
22	EV	92/94 (98%)	82 (89%)	9 (10%)	1 (1%)	12	37
22	GV	92/94 (98%)	83 (90%)	8 (9%)	1 (1%)	12	37
23	AW	77/85 (91%)	41 (53%)	19 (25%)	17 (22%)	0	0
23	CW	77/85 (91%)	42 (54%)	21 (27%)	14 (18%)	0	0
23	EW	77/85 (91%)	42 (54%)	19 (25%)	16 (21%)	0	0
23	GW	77/85 (91%)	42 (54%)	21 (27%)	14 (18%)	0	0
24	AX	75/78 (96%)	65 (87%)	7 (9%)	3 (4%)	2	10
24	CX	75/78 (96%)	64 (85%)	8 (11%)	3 (4%)	2	10
24	EX	75/78 (96%)	64 (85%)	9 (12%)	2 (3%)	4	17
24	GX	75/78 (96%)	65 (87%)	9 (12%)	1 (1%)	10	33
25	AY	61/63 (97%)	40 (66%)	19 (31%)	2 (3%)	3	13
25	CY	61/63 (97%)	43 (70%)	17 (28%)	1 (2%)	8	28
25	EY	61/63 (97%)	38 (62%)	19 (31%)	4 (7%)	1	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	GY	61/63 (97%)	42 (69%)	17 (28%)	2 (3%)	3	13
26	AZ	56/59 (95%)	49 (88%)	5 (9%)	2 (4%)	3	12
26	CZ	56/59 (95%)	49 (88%)	5 (9%)	2 (4%)	3	12
26	EZ	56/59 (95%)	48 (86%)	6 (11%)	2 (4%)	3	12
26	GZ	56/59 (95%)	49 (88%)	5 (9%)	2 (4%)	3	12
27	A0	54/57 (95%)	45 (83%)	6 (11%)	3 (6%)	1	4
27	C0	54/57 (95%)	45 (83%)	6 (11%)	3 (6%)	1	4
27	E0	54/57 (95%)	45 (83%)	6 (11%)	3 (6%)	1	4
27	G0	54/57 (95%)	45 (83%)	6 (11%)	3 (6%)	1	4
28	A1	48/55 (87%)	40 (83%)	5 (10%)	3 (6%)	1	3
28	C1	48/55 (87%)	40 (83%)	6 (12%)	2 (4%)	2	9
28	E1	48/55 (87%)	42 (88%)	5 (10%)	1 (2%)	5	22
28	G1	48/55 (87%)	41 (85%)	5 (10%)	2 (4%)	2	9
29	A2	44/46 (96%)	39 (89%)	4 (9%)	1 (2%)	5	20
29	C2	44/46 (96%)	39 (89%)	4 (9%)	1 (2%)	5	20
29	E2	44/46 (96%)	39 (89%)	4 (9%)	1 (2%)	5	20
29	G2	44/46 (96%)	39 (89%)	4 (9%)	1 (2%)	5	20
30	A3	62/65 (95%)	56 (90%)	4 (6%)	2 (3%)	3	13
30	C3	62/65 (95%)	56 (90%)	4 (6%)	2 (3%)	3	13
30	E3	62/65 (95%)	55 (89%)	5 (8%)	2 (3%)	3	13
30	G3	62/65 (95%)	56 (90%)	4 (6%)	2 (3%)	3	13
31	A4	36/38 (95%)	31 (86%)	2 (6%)	3 (8%)	0	2
31	C4	36/38 (95%)	31 (86%)	3 (8%)	2 (6%)	1	4
31	E4	36/38 (95%)	31 (86%)	2 (6%)	3 (8%)	0	2
31	G4	36/38 (95%)	30 (83%)	4 (11%)	2 (6%)	1	4
32	A5	146/165 (88%)	80 (55%)	44 (30%)	22 (15%)	0	0
32	E5	142/165 (86%)	80 (56%)	39 (28%)	23 (16%)	0	0
34	BB	216/241 (90%)	147 (68%)	57 (26%)	12 (6%)	1	4
34	DB	216/241 (90%)	145 (67%)	59 (27%)	12 (6%)	1	4
34	FB	216/241 (90%)	146 (68%)	60 (28%)	10 (5%)	2	8
34	HB	216/241 (90%)	149 (69%)	55 (26%)	12 (6%)	1	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	BC	204/233 (88%)	180 (88%)	16 (8%)	8 (4%)	2	10
35	DC	204/233 (88%)	177 (87%)	23 (11%)	4 (2%)	6	23
35	FC	204/233 (88%)	181 (89%)	17 (8%)	6 (3%)	3	15
35	HC	204/233 (88%)	183 (90%)	16 (8%)	5 (2%)	4	18
36	BD	203/206 (98%)	157 (77%)	34 (17%)	12 (6%)	1	4
36	DD	203/206 (98%)	157 (77%)	30 (15%)	16 (8%)	1	2
36	FD	203/206 (98%)	155 (76%)	34 (17%)	14 (7%)	1	2
36	HD	203/206 (98%)	159 (78%)	35 (17%)	9 (4%)	2	8
37	BE	148/167 (89%)	124 (84%)	19 (13%)	5 (3%)	3	13
37	DE	148/167 (89%)	125 (84%)	18 (12%)	5 (3%)	3	13
37	FE	148/167 (89%)	122 (82%)	22 (15%)	4 (3%)	4	17
37	HE	148/167 (89%)	122 (82%)	22 (15%)	4 (3%)	4	17
38	BF	98/135 (73%)	73 (74%)	20 (20%)	5 (5%)	1	6
38	DF	98/135 (73%)	71 (72%)	20 (20%)	7 (7%)	1	2
38	FF	98/135 (73%)	72 (74%)	16 (16%)	10 (10%)	0	1
38	HF	98/135 (73%)	75 (76%)	18 (18%)	5 (5%)	1	6
39	BG	149/179 (83%)	126 (85%)	23 (15%)	0	100	100
39	DG	149/179 (83%)	123 (83%)	25 (17%)	1 (1%)	19	49
39	FG	149/179 (83%)	126 (85%)	23 (15%)	0	100	100
39	HG	149/179 (83%)	122 (82%)	25 (17%)	2 (1%)	10	33
40	BH	127/130 (98%)	108 (85%)	18 (14%)	1 (1%)	16	45
40	DH	127/130 (98%)	110 (87%)	15 (12%)	2 (2%)	8	28
40	FH	127/130 (98%)	113 (89%)	12 (9%)	2 (2%)	8	28
40	HH	127/130 (98%)	111 (87%)	16 (13%)	0	100	100
41	BI	125/130 (96%)	96 (77%)	21 (17%)	8 (6%)	1	3
41	DI	125/130 (96%)	99 (79%)	19 (15%)	7 (6%)	1	4
41	FI	125/130 (96%)	97 (78%)	22 (18%)	6 (5%)	2	7
41	HI	125/130 (96%)	98 (78%)	21 (17%)	6 (5%)	2	7
42	BJ	96/103 (93%)	73 (76%)	16 (17%)	7 (7%)	1	2
42	DJ	96/103 (93%)	72 (75%)	18 (19%)	6 (6%)	1	3
42	FJ	96/103 (93%)	73 (76%)	17 (18%)	6 (6%)	1	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	HJ	96/103 (93%)	73 (76%)	19 (20%)	4 (4%)	2	9
43	BK	115/129 (89%)	92 (80%)	17 (15%)	6 (5%)	1	5
43	DK	115/129 (89%)	90 (78%)	23 (20%)	2 (2%)	7	27
43	FK	115/129 (89%)	92 (80%)	20 (17%)	3 (3%)	4	17
43	HK	115/129 (89%)	87 (76%)	24 (21%)	4 (4%)	3	12
44	BL	121/124 (98%)	95 (78%)	17 (14%)	9 (7%)	1	2
44	DL	121/124 (98%)	95 (78%)	18 (15%)	8 (7%)	1	3
44	FL	121/124 (98%)	96 (79%)	17 (14%)	8 (7%)	1	3
44	HL	121/124 (98%)	97 (80%)	15 (12%)	9 (7%)	1	2
45	BM	112/118 (95%)	98 (88%)	8 (7%)	6 (5%)	1	5
45	DM	112/118 (95%)	99 (88%)	7 (6%)	6 (5%)	1	5
45	FM	112/118 (95%)	98 (88%)	9 (8%)	5 (4%)	2	8
45	HM	112/118 (95%)	91 (81%)	14 (12%)	7 (6%)	1	3
46	BN	92/101 (91%)	71 (77%)	18 (20%)	3 (3%)	3	13
46	DN	92/101 (91%)	71 (77%)	19 (21%)	2 (2%)	5	21
46	FN	92/101 (91%)	69 (75%)	20 (22%)	3 (3%)	3	13
46	HN	92/101 (91%)	70 (76%)	20 (22%)	2 (2%)	5	21
47	BO	86/89 (97%)	72 (84%)	12 (14%)	2 (2%)	5	20
47	DO	86/89 (97%)	73 (85%)	11 (13%)	2 (2%)	5	20
47	FO	86/89 (97%)	72 (84%)	12 (14%)	2 (2%)	5	20
47	HO	86/89 (97%)	70 (81%)	14 (16%)	2 (2%)	5	20
48	BP	80/82 (98%)	60 (75%)	16 (20%)	4 (5%)	1	6
48	DP	80/82 (98%)	62 (78%)	16 (20%)	2 (2%)	4	18
48	FP	80/82 (98%)	65 (81%)	13 (16%)	2 (2%)	4	18
48	HP	80/82 (98%)	61 (76%)	15 (19%)	4 (5%)	1	6
49	BQ	78/84 (93%)	54 (69%)	19 (24%)	5 (6%)	1	3
49	DQ	78/84 (93%)	56 (72%)	16 (20%)	6 (8%)	1	2
49	FQ	78/84 (93%)	57 (73%)	18 (23%)	3 (4%)	2	11
49	HQ	78/84 (93%)	57 (73%)	16 (20%)	5 (6%)	1	3
50	BR	53/75 (71%)	41 (77%)	12 (23%)	0	100	100
50	DR	53/75 (71%)	43 (81%)	10 (19%)	0	100	100

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

5 of 1298 Ramachandran outliers are listed below:

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



### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AC	216/218 (99%)	203 (94%)	13 (6%)	16	44
3	CC	216/218 (99%)	201 (93%)	15 (7%)	13	37
3	EC	216/218 (99%)	200 (93%)	16 (7%)	11	34
3	GC	216/218 (99%)	198 (92%)	18 (8%)	9	28
4	AD	164/164 (100%)	153 (93%)	11 (7%)	13	39
4	CD	164/164 (100%)	156 (95%)	8 (5%)	21	53
4	ED	164/164 (100%)	155 (94%)	9 (6%)	18	48
4	GD	164/164 (100%)	156 (95%)	8 (5%)	21	53
5	AE	165/165 (100%)	154 (93%)	11 (7%)	13	39
5	CE	165/165 (100%)	158 (96%)	7 (4%)	25	59
5	EE	165/165 (100%)	153 (93%)	12 (7%)	11	34
5	GE	165/165 (100%)	160 (97%)	5 (3%)	36	71
6	AF	148/150 (99%)	140 (95%)	8 (5%)	18	49
6	CF	148/150 (99%)	139 (94%)	9 (6%)	15	43
6	EF	148/150 (99%)	138 (93%)	10 (7%)	13	38
6	GF	148/150 (99%)	144 (97%)	4 (3%)	40	73
7	AG	137/138 (99%)	126 (92%)	11 (8%)	10	30
7	CG	137/138 (99%)	126 (92%)	11 (8%)	10	30
7	EG	137/138 (99%)	125 (91%)	12 (9%)	8	26
7	GG	137/138 (99%)	130 (95%)	7 (5%)	20	51
8	AH	40/40 (100%)	38 (95%)	2 (5%)	20	52
8	CH	40/40 (100%)	39 (98%)	1 (2%)	42	75
8	EH	40/40 (100%)	36 (90%)	4 (10%)	6	20
8	GH	40/40 (100%)	36 (90%)	4 (10%)	6	20
9	AI	109/110 (99%)	105 (96%)	4 (4%)	29	64
9	CI	109/110 (99%)	108 (99%)	1 (1%)	75	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	EI	109/110 (99%)	108 (99%)	1 (1%)	75	92
9	GI	109/110 (99%)	108 (99%)	1 (1%)	75	92
10	AJ	116/116 (100%)	97 (84%)	19 (16%)	2	6
10	CJ	116/116 (100%)	102 (88%)	14 (12%)	4	13
10	EJ	116/116 (100%)	96 (83%)	20 (17%)	1	5
10	GJ	116/116 (100%)	103 (89%)	13 (11%)	5	16
11	AK	103/104 (99%)	93 (90%)	10 (10%)	6	22
11	CK	103/104 (99%)	94 (91%)	9 (9%)	8	27
11	EK	103/104 (99%)	95 (92%)	8 (8%)	10	31
11	GK	103/104 (99%)	96 (93%)	7 (7%)	13	38
12	AL	102/103 (99%)	96 (94%)	6 (6%)	16	45
12	CL	102/103 (99%)	96 (94%)	6 (6%)	16	45
12	EL	102/103 (99%)	97 (95%)	5 (5%)	21	53
12	GL	102/103 (99%)	94 (92%)	8 (8%)	10	31
13	AM	109/109 (100%)	94 (86%)	15 (14%)	3	9
13	CM	109/109 (100%)	96 (88%)	13 (12%)	4	13
13	EM	109/109 (100%)	100 (92%)	9 (8%)	9	28
13	GM	109/109 (100%)	102 (94%)	7 (6%)	14	41
14	AN	100/103 (97%)	94 (94%)	6 (6%)	16	44
14	CN	100/103 (97%)	93 (93%)	7 (7%)	12	36
14	EN	100/103 (97%)	98 (98%)	2 (2%)	50	79
14	GN	100/103 (97%)	96 (96%)	4 (4%)	27	61
15	AO	86/87 (99%)	81 (94%)	5 (6%)	17	46
15	CO	86/87 (99%)	80 (93%)	6 (7%)	12	36
15	EO	86/87 (99%)	79 (92%)	7 (8%)	9	29
15	GO	86/87 (99%)	83 (96%)	3 (4%)	31	66
16	AP	99/100 (99%)	85 (86%)	14 (14%)	3	9
16	CP	99/100 (99%)	88 (89%)	11 (11%)	5	16
16	EP	99/100 (99%)	91 (92%)	8 (8%)	9	29
16	GP	99/100 (99%)	88 (89%)	11 (11%)	5	16
17	AQ	89/90 (99%)	83 (93%)	6 (7%)	13	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	CQ	89/90 (99%)	82 (92%)	7 (8%)	10	30
17	EQ	89/90 (99%)	80 (90%)	9 (10%)	6	20
17	GQ	89/90 (99%)	86 (97%)	3 (3%)	32	67
18	AR	84/84 (100%)	79 (94%)	5 (6%)	16	44
18	CR	84/84 (100%)	78 (93%)	6 (7%)	12	36
18	ER	84/84 (100%)	77 (92%)	7 (8%)	9	28
18	GR	84/84 (100%)	80 (95%)	4 (5%)	21	54
19	AS	93/93 (100%)	85 (91%)	8 (9%)	8	27
19	CS	93/93 (100%)	86 (92%)	7 (8%)	11	33
19	ES	93/93 (100%)	84 (90%)	9 (10%)	6	22
19	GS	93/93 (100%)	86 (92%)	7 (8%)	11	33
20	AT	80/84 (95%)	71 (89%)	9 (11%)	4	15
20	CT	80/84 (95%)	77 (96%)	3 (4%)	28	63
20	ET	80/84 (95%)	73 (91%)	7 (9%)	8	26
20	GT	80/84 (95%)	76 (95%)	4 (5%)	20	52
21	AU	83/85 (98%)	79 (95%)	4 (5%)	21	54
21	CU	83/85 (98%)	80 (96%)	3 (4%)	30	65
21	EU	83/85 (98%)	76 (92%)	7 (8%)	9	28
21	GU	83/85 (98%)	80 (96%)	3 (4%)	30	65
22	AV	78/78 (100%)	73 (94%)	5 (6%)	14	41
22	CV	78/78 (100%)	75 (96%)	3 (4%)	28	63
22	EV	78/78 (100%)	76 (97%)	2 (3%)	41	74
22	GV	78/78 (100%)	75 (96%)	3 (4%)	28	63
23	AW	59/63 (94%)	49 (83%)	10 (17%)	1	5
23	CW	59/63 (94%)	51 (86%)	8 (14%)	3	9
23	EW	59/63 (94%)	52 (88%)	7 (12%)	4	13
23	GW	59/63 (94%)	53 (90%)	6 (10%)	6	19
24	AX	67/68 (98%)	61 (91%)	6 (9%)	8	25
24	CX	67/68 (98%)	60 (90%)	7 (10%)	5	18
24	EX	67/68 (98%)	60 (90%)	7 (10%)	5	18
24	GX	67/68 (98%)	61 (91%)	6 (9%)	8	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	AY	55/55 (100%)	49 (89%)	6 (11%)	5	17
25	CY	55/55 (100%)	53 (96%)	2 (4%)	30	65
25	EY	55/55 (100%)	49 (89%)	6 (11%)	5	17
25	GY	55/55 (100%)	51 (93%)	4 (7%)	11	34
26	AZ	48/49 (98%)	44 (92%)	4 (8%)	9	28
26	CZ	48/49 (98%)	43 (90%)	5 (10%)	5	18
26	EZ	48/49 (98%)	44 (92%)	4 (8%)	9	28
26	GZ	48/49 (98%)	43 (90%)	5 (10%)	5	18
27	A0	47/48 (98%)	47 (100%)	0	100	100
27	C0	47/48 (98%)	45 (96%)	2 (4%)	25	57
27	E0	47/48 (98%)	45 (96%)	2 (4%)	25	57
27	G0	47/48 (98%)	47 (100%)	0	100	100
28	A1	45/49 (92%)	42 (93%)	3 (7%)	13	39
28	C1	45/49 (92%)	41 (91%)	4 (9%)	8	26
28	E1	45/49 (92%)	43 (96%)	2 (4%)	24	57
28	G1	45/49 (92%)	44 (98%)	1 (2%)	47	78
29	A2	38/38 (100%)	37 (97%)	1 (3%)	41	74
29	C2	38/38 (100%)	35 (92%)	3 (8%)	10	30
29	E2	38/38 (100%)	33 (87%)	5 (13%)	3	10
29	G2	38/38 (100%)	34 (90%)	4 (10%)	5	18
30	A3	51/52 (98%)	49 (96%)	2 (4%)	27	62
30	C3	51/52 (98%)	50 (98%)	1 (2%)	50	79
30	E3	51/52 (98%)	47 (92%)	4 (8%)	10	31
30	G3	51/52 (98%)	47 (92%)	4 (8%)	10	31
31	A4	34/34 (100%)	32 (94%)	2 (6%)	16	45
31	C4	34/34 (100%)	32 (94%)	2 (6%)	16	45
31	E4	34/34 (100%)	32 (94%)	2 (6%)	16	45
31	G4	34/34 (100%)	31 (91%)	3 (9%)	8	26
32	A5	112/123 (91%)	95 (85%)	17 (15%)	2	7
32	E5	110/123 (89%)	96 (87%)	14 (13%)	3	11
34	BB	180/199 (90%)	171 (95%)	9 (5%)	20	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	DB	180/199 (90%)	171 (95%)	9 (5%)	20	52
34	FB	180/199 (90%)	172 (96%)	8 (4%)	24	57
34	HB	180/199 (90%)	170 (94%)	10 (6%)	17	47
35	BC	170/190 (90%)	167 (98%)	3 (2%)	54	82
35	DC	170/190 (90%)	166 (98%)	4 (2%)	44	76
35	FC	170/190 (90%)	158 (93%)	12 (7%)	12	36
35	HC	170/190 (90%)	164 (96%)	6 (4%)	31	66
36	BD	172/173 (99%)	163 (95%)	9 (5%)	19	50
36	DD	172/173 (99%)	162 (94%)	10 (6%)	17	46
36	FD	172/173 (99%)	162 (94%)	10 (6%)	17	46
36	HD	172/173 (99%)	163 (95%)	9 (5%)	19	50
37	BE	113/126 (90%)	107 (95%)	6 (5%)	19	49
37	DE	113/126 (90%)	110 (97%)	3 (3%)	40	73
37	FE	113/126 (90%)	104 (92%)	9 (8%)	10	30
37	HE	113/126 (90%)	106 (94%)	7 (6%)	15	43
38	BF	87/116 (75%)	83 (95%)	4 (5%)	23	55
38	DF	87/116 (75%)	85 (98%)	2 (2%)	45	77
38	FF	87/116 (75%)	84 (97%)	3 (3%)	32	67
38	HF	87/116 (75%)	85 (98%)	2 (2%)	45	77
39	BG	124/147 (84%)	122 (98%)	2 (2%)	58	84
39	DG	124/147 (84%)	121 (98%)	3 (2%)	44	76
39	FG	124/147 (84%)	120 (97%)	4 (3%)	34	69
39	HG	124/147 (84%)	123 (99%)	1 (1%)	79	93
40	BH	104/105 (99%)	98 (94%)	6 (6%)	17	46
40	DH	104/105 (99%)	97 (93%)	7 (7%)	13	39
40	FH	104/105 (99%)	97 (93%)	7 (7%)	13	39
40	HH	104/105 (99%)	98 (94%)	6 (6%)	17	46
41	BI	105/107 (98%)	96 (91%)	9 (9%)	8	27
41	DI	105/107 (98%)	102 (97%)	3 (3%)	37	72
41	FI	105/107 (98%)	98 (93%)	7 (7%)	13	39
41	HI	105/107 (98%)	99 (94%)	6 (6%)	17	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	BJ	86/90 (96%)	85 (99%)	1 (1%)	67	89
42	DJ	86/90 (96%)	80 (93%)	6 (7%)	12	36
42	FJ	86/90 (96%)	84 (98%)	2 (2%)	45	77
42	HJ	86/90 (96%)	83 (96%)	3 (4%)	31	66
43	BK	90/99 (91%)	87 (97%)	3 (3%)	33	68
43	DK	90/99 (91%)	88 (98%)	2 (2%)	47	78
43	FK	90/99 (91%)	85 (94%)	5 (6%)	17	47
43	HK	90/99 (91%)	82 (91%)	8 (9%)	8	26
44	BL	103/104 (99%)	100 (97%)	3 (3%)	37	72
44	DL	103/104 (99%)	101 (98%)	2 (2%)	52	81
44	FL	103/104 (99%)	97 (94%)	6 (6%)	17	46
44	HL	103/104 (99%)	94 (91%)	9 (9%)	8	27
45	BM	92/96 (96%)	89 (97%)	3 (3%)	33	68
45	DM	92/96 (96%)	92 (100%)	0	100	100
45	FM	92/96 (96%)	92 (100%)	0	100	100
45	HM	92/96 (96%)	92 (100%)	0	100	100
46	BN	79/84 (94%)	79 (100%)	0	100	100
46	DN	79/84 (94%)	78 (99%)	1 (1%)	65	88
46	FN	79/84 (94%)	75 (95%)	4 (5%)	20	51
46	HN	79/84 (94%)	77 (98%)	2 (2%)	42	75
47	BO	76/77 (99%)	72 (95%)	4 (5%)	19	49
47	DO	76/77 (99%)	74 (97%)	2 (3%)	41	74
47	FO	76/77 (99%)	74 (97%)	2 (3%)	41	74
47	HO	76/77 (99%)	74 (97%)	2 (3%)	41	74
48	BP	65/65 (100%)	63 (97%)	2 (3%)	35	70
48	DP	65/65 (100%)	60 (92%)	5 (8%)	10	31
48	FP	65/65 (100%)	64 (98%)	1 (2%)	60	85
48	HP	65/65 (100%)	63 (97%)	2 (3%)	35	70
49	BQ	74/78 (95%)	70 (95%)	4 (5%)	18	49
49	DQ	74/78 (95%)	72 (97%)	2 (3%)	40	73
49	FQ	74/78 (95%)	73 (99%)	1 (1%)	62	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	HQ	74/78 (95%)	69 (93%)	5 (7%)	13	38
50	BR	48/65 (74%)	48 (100%)	0	100	100
50	DR	48/65 (74%)	48 (100%)	0	100	100
50	FR	48/65 (74%)	46 (96%)	2 (4%)	25	59
50	HR	48/65 (74%)	48 (100%)	0	100	100
51	BS	70/79 (89%)	69 (99%)	1 (1%)	62	86
51	DS	70/79 (89%)	67 (96%)	3 (4%)	25	57
51	FS	70/79 (89%)	64 (91%)	6 (9%)	8	27
51	HS	70/79 (89%)	67 (96%)	3 (4%)	25	57
52	BT	65/66 (98%)	60 (92%)	5 (8%)	10	31
52	DT	65/66 (98%)	58 (89%)	7 (11%)	5	17
52	FT	65/66 (98%)	60 (92%)	5 (8%)	10	31
52	HT	65/66 (98%)	60 (92%)	5 (8%)	10	31
53	BU	44/61 (72%)	42 (96%)	2 (4%)	23	56
53	DU	44/61 (72%)	41 (93%)	3 (7%)	13	38
53	FU	44/61 (72%)	41 (93%)	3 (7%)	13	38
53	HU	44/61 (72%)	42 (96%)	2 (4%)	23	56
54	BV	557/578 (96%)	503 (90%)	54 (10%)	6	22
54	DV	557/578 (96%)	508 (91%)	49 (9%)	8	26
54	FV	557/578 (96%)	508 (91%)	49 (9%)	8	26
54	HV	557/578 (96%)	507 (91%)	50 (9%)	8	25
55	BW	2/2 (100%)	1 (50%)	1 (50%)	0	0
55	DW	2/2 (100%)	1 (50%)	1 (50%)	0	0
55	FW	2/2 (100%)	2 (100%)	0	100	100
All	All	20824/21780 (96%)	19507 (94%)	1317 (6%)	15	42

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

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

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

Mol	Chain	Res	Type
54	FV	122	GLN
34	HB	57	ASN
54	FV	310	HIS
4	GD	32	ASN
42	HJ	56	HIS

### 5.3.3 RNA ⓘ

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

5 of 3034 RNA backbone outliers are listed below:

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

5 of 266 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	GA	1509	A
1	GA	1870	C
33	HA	1136	C
1	CA	1535	A
1	CA	1458	U



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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
55	5OH	DW	6	55	7,12,13	1.85	2 (28%)	4,16,18	1.41	1 (25%)
55	UAL	FW	5	55	6,8,9	2.41	3 (50%)	4,9,11	2.80	2 (50%)
55	5OH	BW	6	55	7,12,13	1.66	2 (28%)	4,16,18	1.00	0
55	UAL	DW	5	55	6,8,9	2.69	3 (50%)	4,9,11	4.44	1 (25%)
55	KBE	DW	1	55	8,8,9	0.91	0	6,8,10	1.14	1 (16%)
55	DPP	DW	2	55	4,5,6	0.83	0	1,5,7	0.29	0
55	DPP	BW	2	55	4,5,6	1.07	0	1,5,7	0.71	0
55	KBE	FW	1	55	8,8,9	0.96	0	6,8,10	1.91	1 (16%)
55	5OH	FW	6	55	7,12,13	1.98	2 (28%)	4,16,18	1.25	0
55	UAL	BW	5	55	6,8,9	2.90	3 (50%)	4,9,11	4.66	1 (25%)
55	KBE	BW	1	55	8,8,9	0.90	0	6,8,10	1.09	1 (16%)
55	DPP	FW	2	55	4,5,6	0.83	0	1,5,7	0.01	0

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	KBE	BW	1	55	-	3/7/7/8	-
55	DPP	FW	2	55	-	0/2/4/6	-

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	BW	5	UAL	CB-N1	4.25	1.46	1.35
55	DW	5	UAL	CB-N1	4.07	1.46	1.35
55	BW	5	UAL	C-CA	4.05	1.51	1.45
55	DW	5	UAL	C1-N1	3.84	1.46	1.40
55	FW	5	UAL	CB-N1	3.84	1.45	1.35

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BW	5	UAL	O-C-CA	-9.02	114.08	125.39
55	DW	5	UAL	O-C-CA	-8.62	114.58	125.39
55	FW	5	UAL	O-C-CA	-5.01	119.11	125.39
55	FW	1	KBE	CB-CA-C	4.19	118.93	112.17
55	BW	1	KBE	O-C-CA	-2.37	118.47	125.38

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

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

There are no ring outliers.

10 monomers are involved in 14 short contacts:

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
58	GCP	HV	801	56	27,34,34	2.23	7 (25%)	35,54,54	2.32	7 (20%)
58	GCP	BV	801	56	27,34,34	2.20	7 (25%)	35,54,54	2.79	11 (31%)
58	GCP	DV	801	56	27,34,34	2.23	6 (22%)	35,54,54	2.56	10 (28%)
58	GCP	FV	801	56	27,34,34	1.49	5 (18%)	35,54,54	1.89	8 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	GCP	HV	801	56	-	3/15/38/38	0/3/3/3
58	GCP	BV	801	56	-	3/15/38/38	0/3/3/3
58	GCP	DV	801	56	-	2/15/38/38	0/3/3/3
58	GCP	FV	801	56	-	3/15/38/38	0/3/3/3

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	DV	801	GCP	C2-N2	5.85	1.45	1.33
58	DV	801	GCP	O4'-C1'	5.75	1.48	1.40
58	HV	801	GCP	O4'-C1'	5.70	1.48	1.40
58	HV	801	GCP	C2-N2	5.65	1.45	1.33
58	BV	801	GCP	C2-N2	5.63	1.45	1.33

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	BV	801	GCP	C4'-O4'-C1'	-10.65	100.17	109.92
58	DV	801	GCP	C4'-O4'-C1'	-9.24	101.47	109.92
58	HV	801	GCP	C4'-O4'-C1'	-7.53	103.03	109.92
58	DV	801	GCP	N3-C2-N1	-6.43	119.04	127.21
58	BV	801	GCP	N3-C2-N1	-6.13	119.41	127.21

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	BV	801	GCP	PB-C3B-PG-O1G
58	BV	801	GCP	PB-C3B-PG-O2G
58	BV	801	GCP	PB-C3B-PG-O3G
58	HV	801	GCP	PB-C3B-PG-O1G
58	HV	801	GCP	PB-C3B-PG-O3G

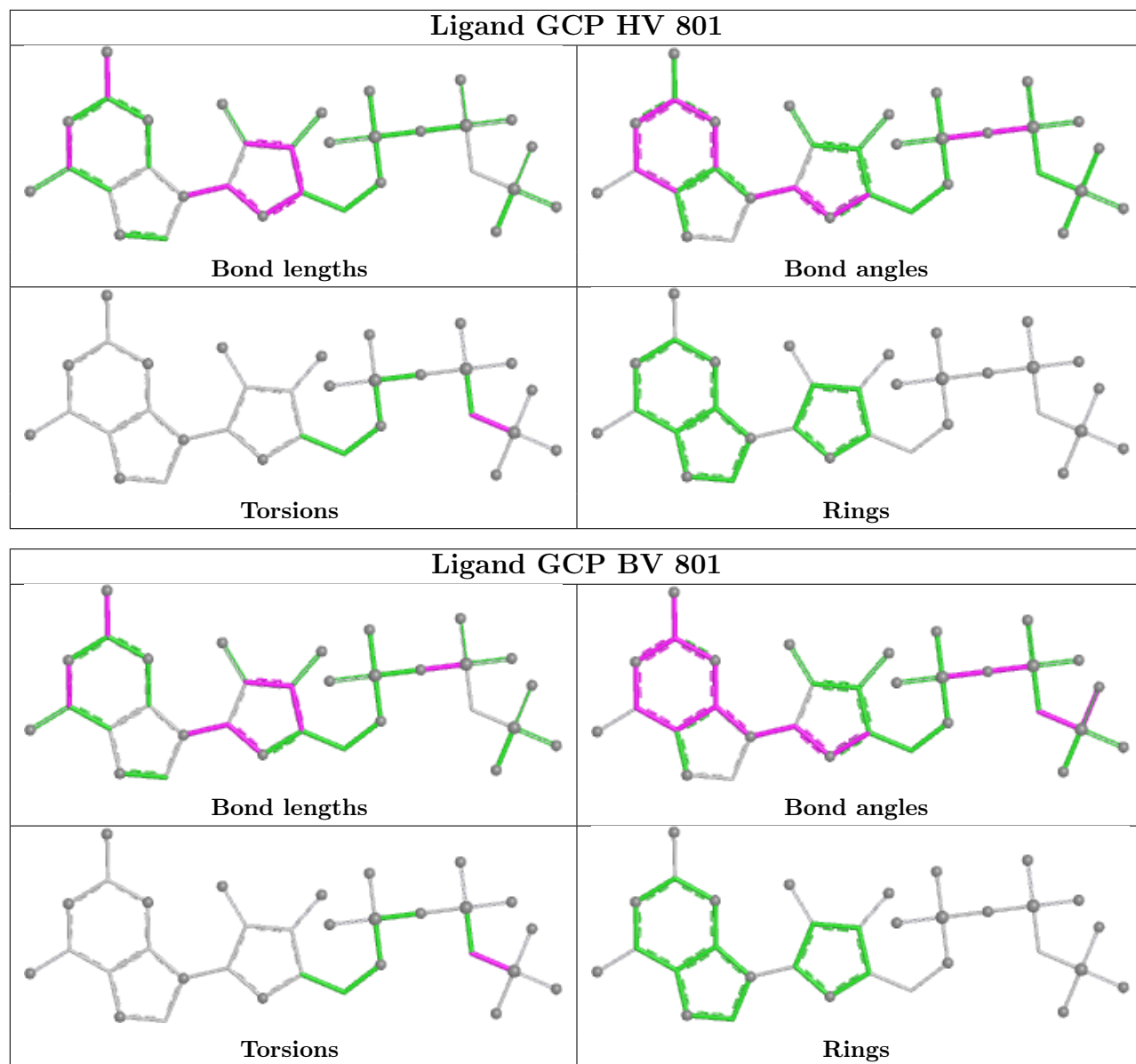
There are no ring outliers.

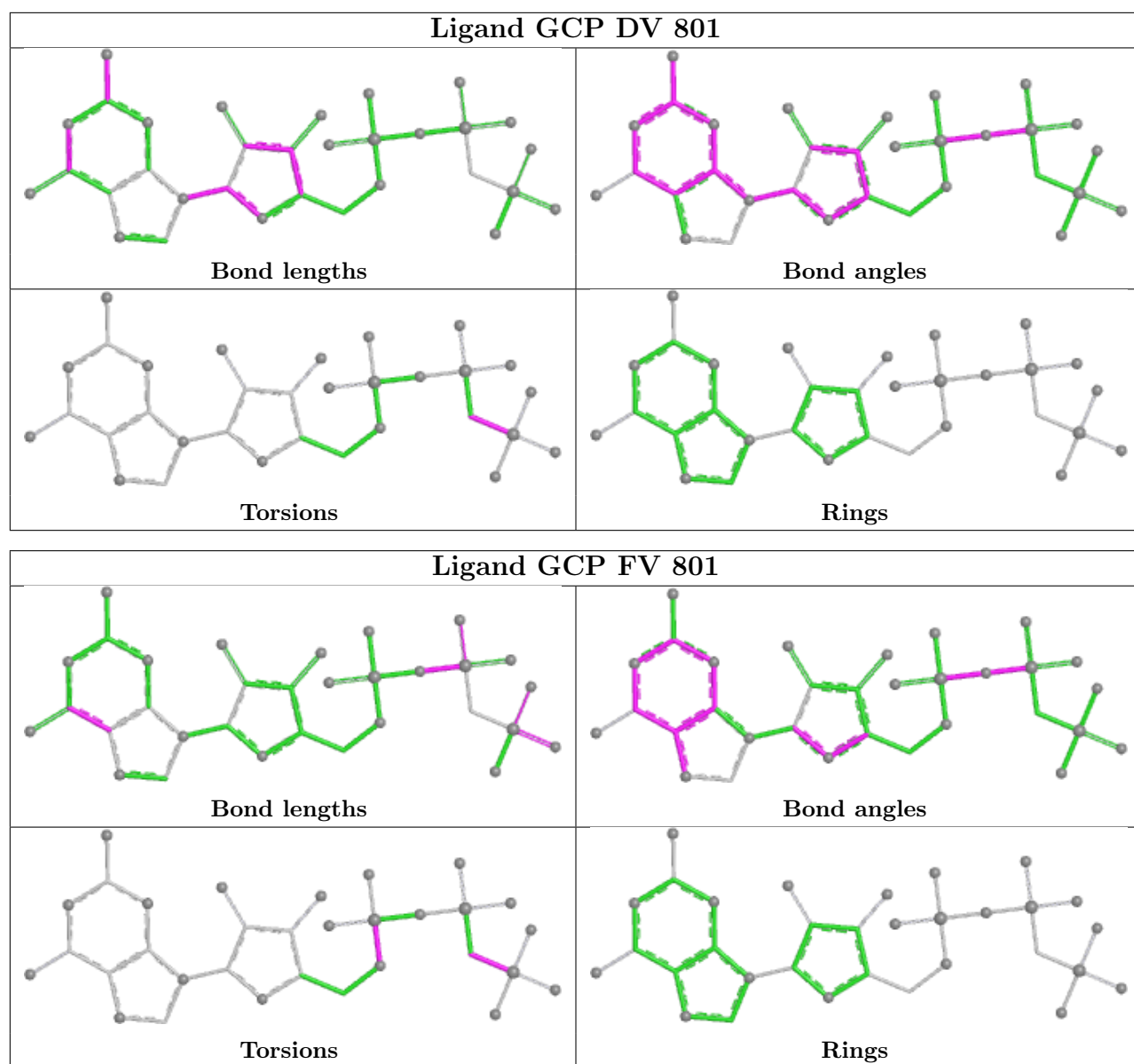
4 monomers are involved in 9 short contacts:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

### 6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

### 6.4 Ligands

EDS failed to run properly - this section is therefore empty.

### 6.5 Other polymers

EDS failed to run properly - this section is therefore empty.