



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 23, 2025 – 06:02 PM EDT

PDB ID : 4V9O  
Title : Control of ribosomal subunit rotation by elongation factor G  
Authors : Pulk, A.; Cate, J.H.D.  
Deposited on : 2013-05-03  
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

<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	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

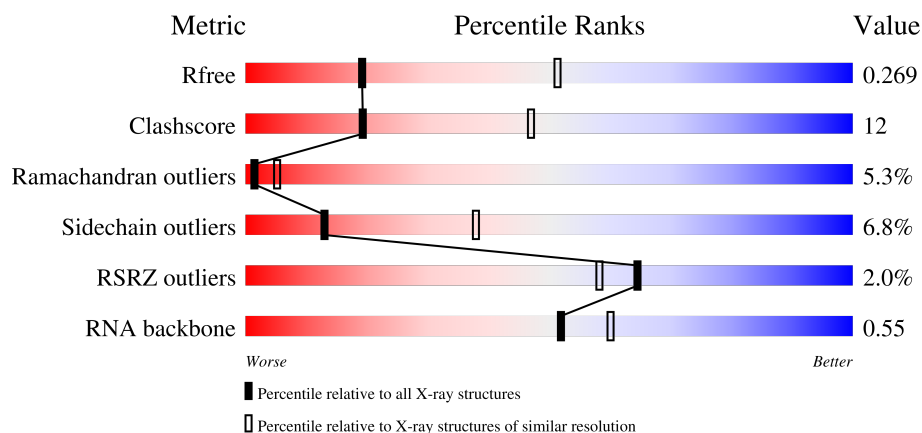
# 1 Overall quality at a glance

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.






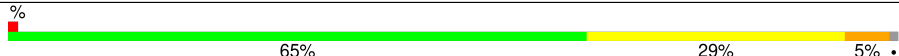
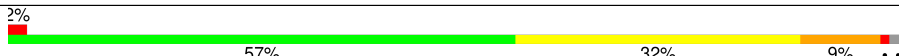
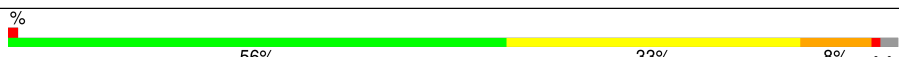
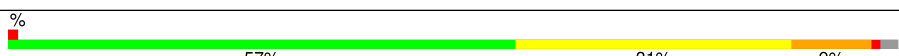

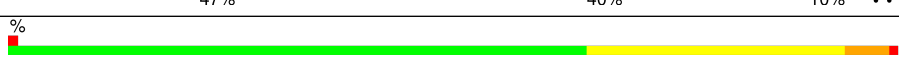

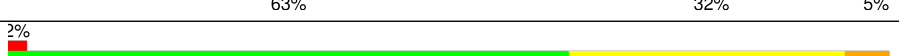
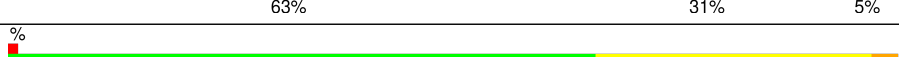

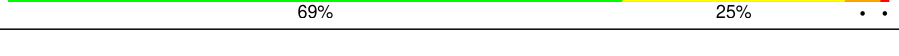
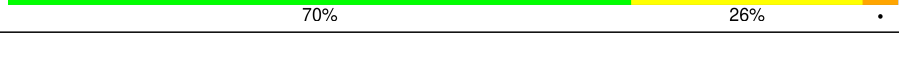




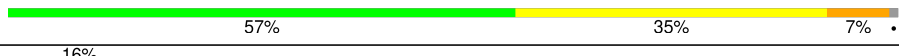

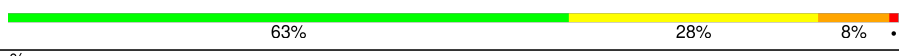



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	2335 (2.90-2.90)
Clashscore	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)
RSRZ outliers	164620	2337 (2.90-2.90)
RNA backbone	3690	1039 (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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AB	120	<div> <div>66%</div> <div>26%</div> <div>7%</div> <div>.</div> </div>
1	CB	120	<div> <div>60%</div> <div>32%</div> <div>7%</div> <div>.</div> </div>
1	EB	120	<div> <div>62%</div> <div>24%</div> <div>9%</div> <div>..</div> </div>
1	GB	120	<div> <div>36%</div> <div>51%</div> <div>10%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
2	AC	273	
2	CC	273	
2	EC	273	
2	GC	273	
3	AA	2904	
3	CA	2904	
3	EA	2904	
3	GA	2904	
4	AD	209	
4	CD	209	
4	ED	209	
4	GD	209	
5	AE	201	
5	CE	201	
5	EE	201	
5	GE	201	
6	AF	179	
6	CF	179	
6	EF	179	
6	GF	179	
7	AG	177	
7	CG	177	
7	EG	177	
7	GG	177	
8	AH	50	

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

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

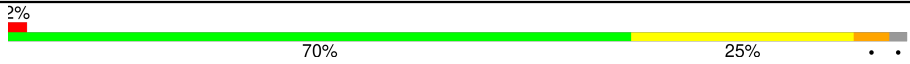
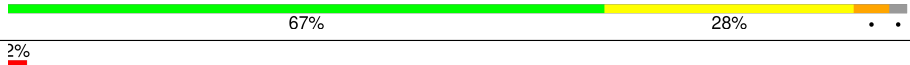
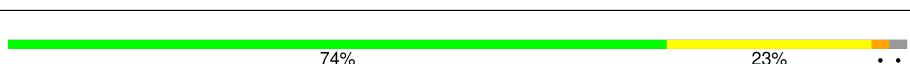
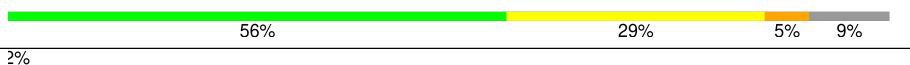
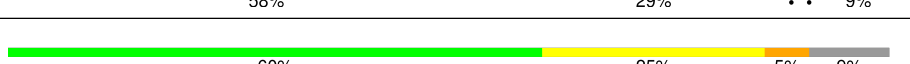




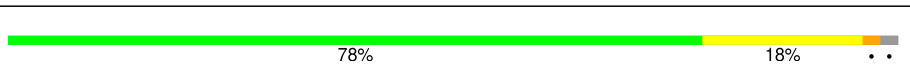

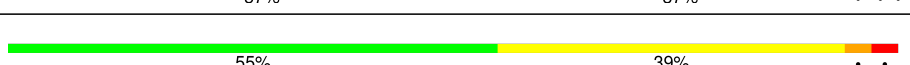


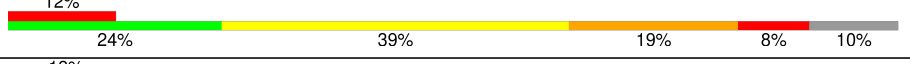
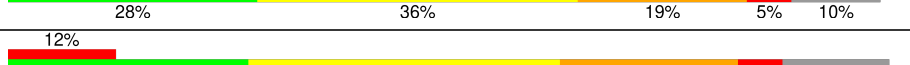




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Mol	Chain	Length	Quality of chain
20	GT	100	
21	AU	104	
21	CU	104	
21	EU	104	
21	GU	104	
22	AV	94	
22	CV	94	
22	EV	94	
22	GV	94	
23	AW	85	
23	CW	85	
23	EW	85	
23	GW	85	
24	AX	78	
24	CX	78	
24	EX	78	
24	GX	78	
25	AY	63	
25	CY	63	
25	EY	63	
25	GY	63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






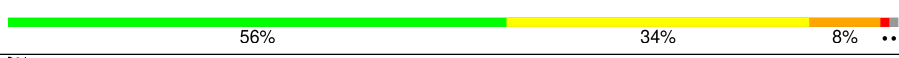

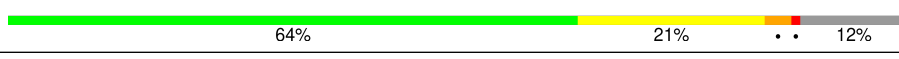
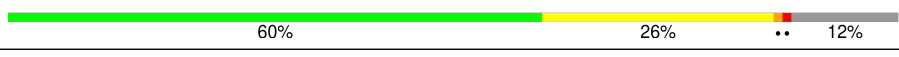


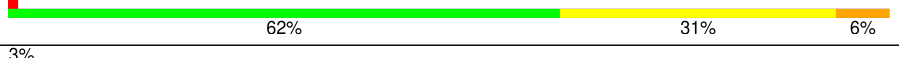







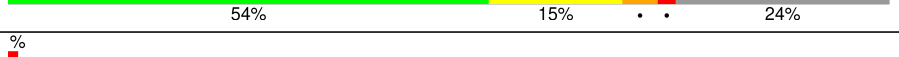
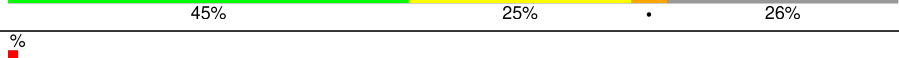
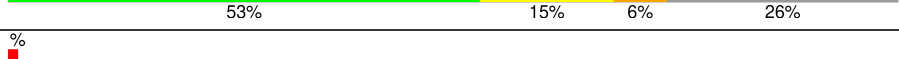

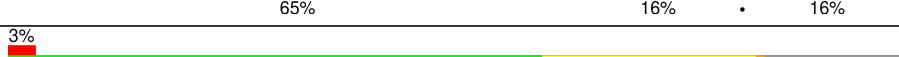

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Mol	Chain	Length	Quality of chain
27	A0	57	
27	C0	57	
27	E0	57	
27	G0	57	
28	A1	55	
28	C1	55	
28	E1	55	
28	G1	55	
29	A2	46	
29	C2	46	
29	E2	46	
29	G2	46	
30	A3	65	
30	C3	65	
30	E3	65	
30	G3	65	
31	A4	38	
31	C4	38	
31	E4	38	
31	G4	38	
32	A5	165	
32	C5	165	
32	E5	165	
33	A6	121	
34	BB	241	

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

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

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

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Mol	Chain	Length	Quality of chain
53	BT	87	
53	DT	87	
53	FT	87	
53	HT	87	
54	BU	71	
54	DU	71	
54	FU	71	
54	HU	71	
55	BV	704	
55	DV	704	
55	FV	704	
55	HV	704	
56	BW	6	
56	DW	6	
56	FW	6	
56	HW	6	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	KBE	BW	1	-	X	-	-

## 2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 592086 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 5S rRNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	A5	148	Total	C	N	O	S	0	0	0
			1117	705	196	209	7			
32	C5	148	Total	C	N	O	S	0	0	0
			1117	705	196	209	7			
32	E5	145	Total	C	N	O	S	0	0	0
			1101	696	193	205	7			

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

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

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

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

- Molecule 35 is a RNA chain called 16S rRNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 55 is a protein called Elongation factor G.

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

- Molecule 56 is a protein called Viomycin.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	AB	4	Total	Mg	0	0
			4	4		
57	AC	1	Total	Mg	0	0
			1	1		
57	AA	136	Total	Mg	0	0
			136	136		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	AE	1	Total 1	Mg 1	0	0
57	A4	1	Total 1	Mg 1	0	0
57	BA	40	Total 40	Mg 40	0	0
57	BE	1	Total 1	Mg 1	0	0
57	BN	1	Total 1	Mg 1	0	0
57	BU	1	Total 1	Mg 1	0	0
57	BV	1	Total 1	Mg 1	0	0
57	CB	4	Total 4	Mg 4	0	0
57	CA	136	Total 136	Mg 136	0	0
57	CE	1	Total 1	Mg 1	0	0
57	CN	1	Total 1	Mg 1	0	0
57	C4	1	Total 1	Mg 1	0	0
57	DA	43	Total 43	Mg 43	0	0
57	DV	1	Total 1	Mg 1	0	0
57	EA	137	Total 137	Mg 137	0	0
57	EB	4	Total 4	Mg 4	0	0
57	ED	1	Total 1	Mg 1	0	0
57	EE	1	Total 1	Mg 1	0	0
57	FA	39	Total 39	Mg 39	0	0
57	FE	1	Total 1	Mg 1	0	0
57	FN	2	Total 2	Mg 2	0	0

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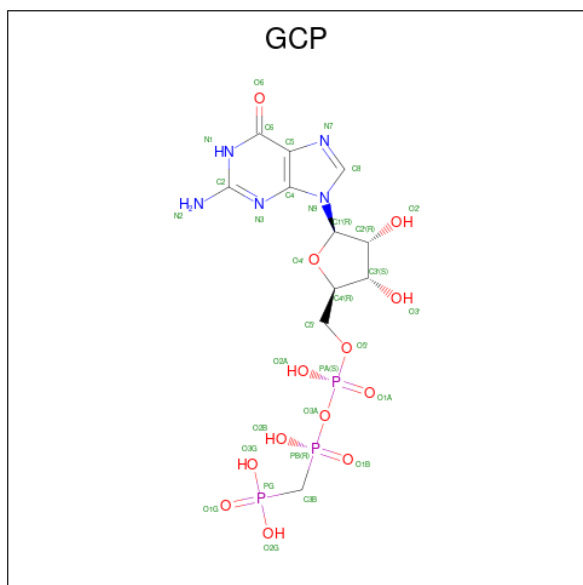
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	FU	1	Total	Mg	0	0
			1	1		
57	FV	1	Total	Mg	0	0
			1	1		
57	GB	4	Total	Mg	0	0
			4	4		
57	GA	136	Total	Mg	0	0
			136	136		
57	GC	2	Total	Mg	0	0
			2	2		
57	GL	1	Total	Mg	0	0
			1	1		
57	HA	41	Total	Mg	0	0
			41	41		
57	HE	1	Total	Mg	0	0
			1	1		
57	HK	1	Total	Mg	0	0
			1	1		
57	HV	1	Total	Mg	0	0
			1	1		

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

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

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



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

- Molecule 60 is water.

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

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

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

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

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

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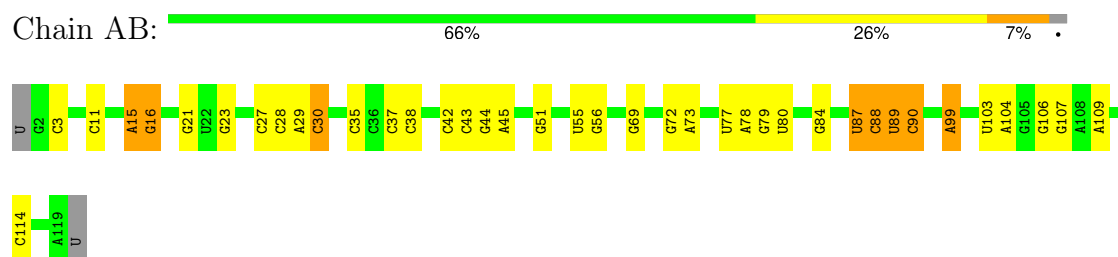
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	HV	1	Total	O	0	0
			1	1		

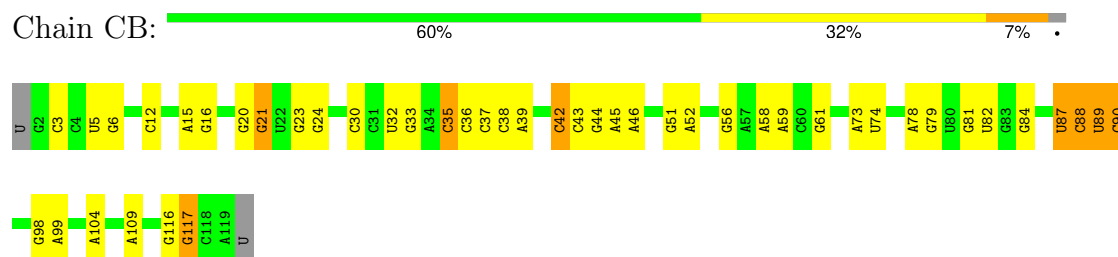
### 3 Residue-property plots [i](#)

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

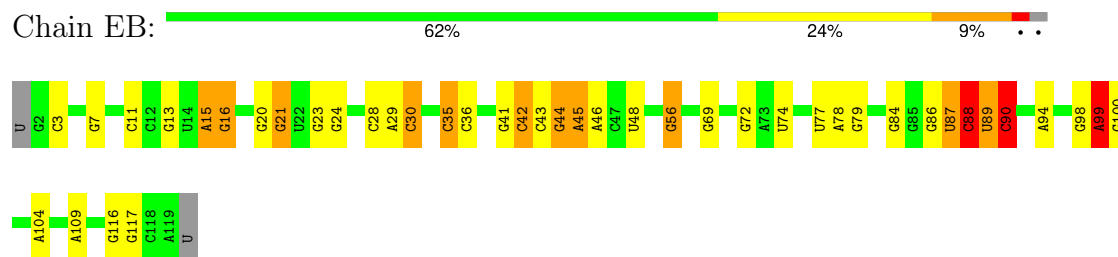
- Molecule 1: 5S rRNA



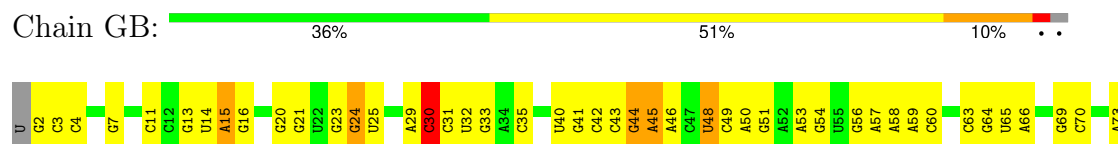
- Molecule 1: 5S rRNA



- Molecule 1: 5S rRNA

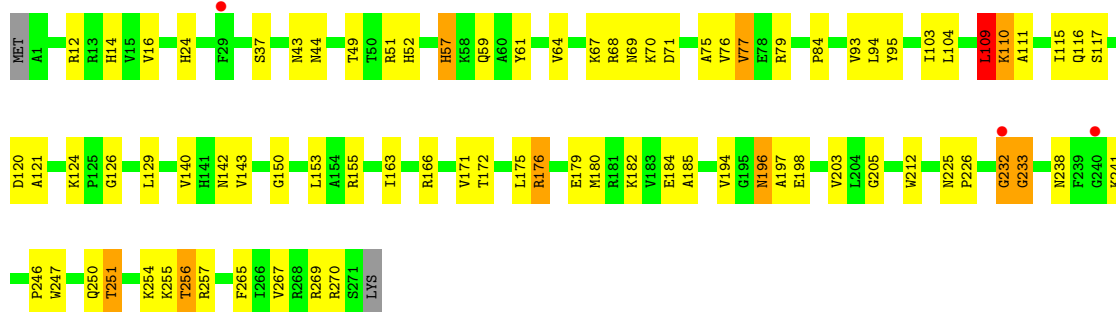


- Molecule 1: 5S rRNA

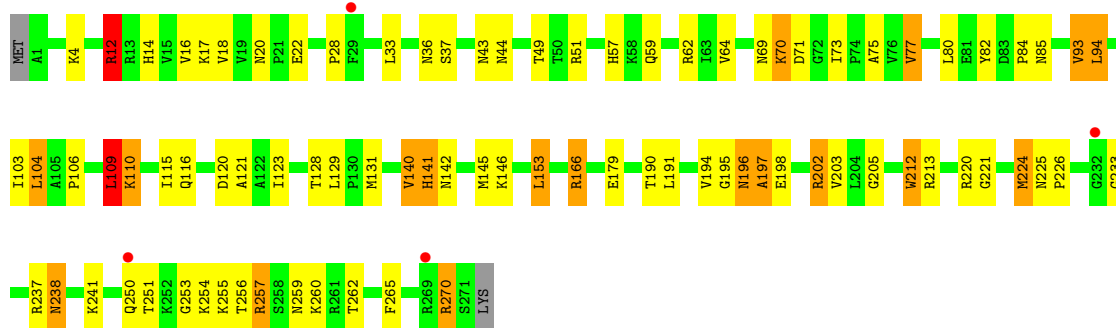




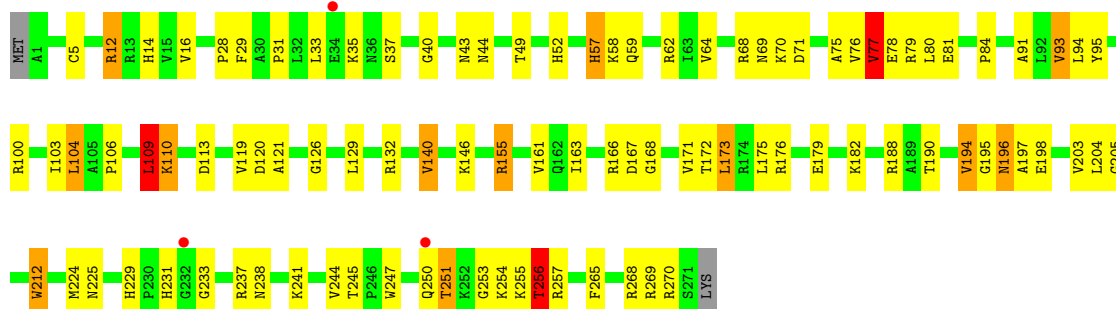
• Molecule 2: 50S ribosomal protein L2



• Molecule 2: 50S ribosomal protein L2

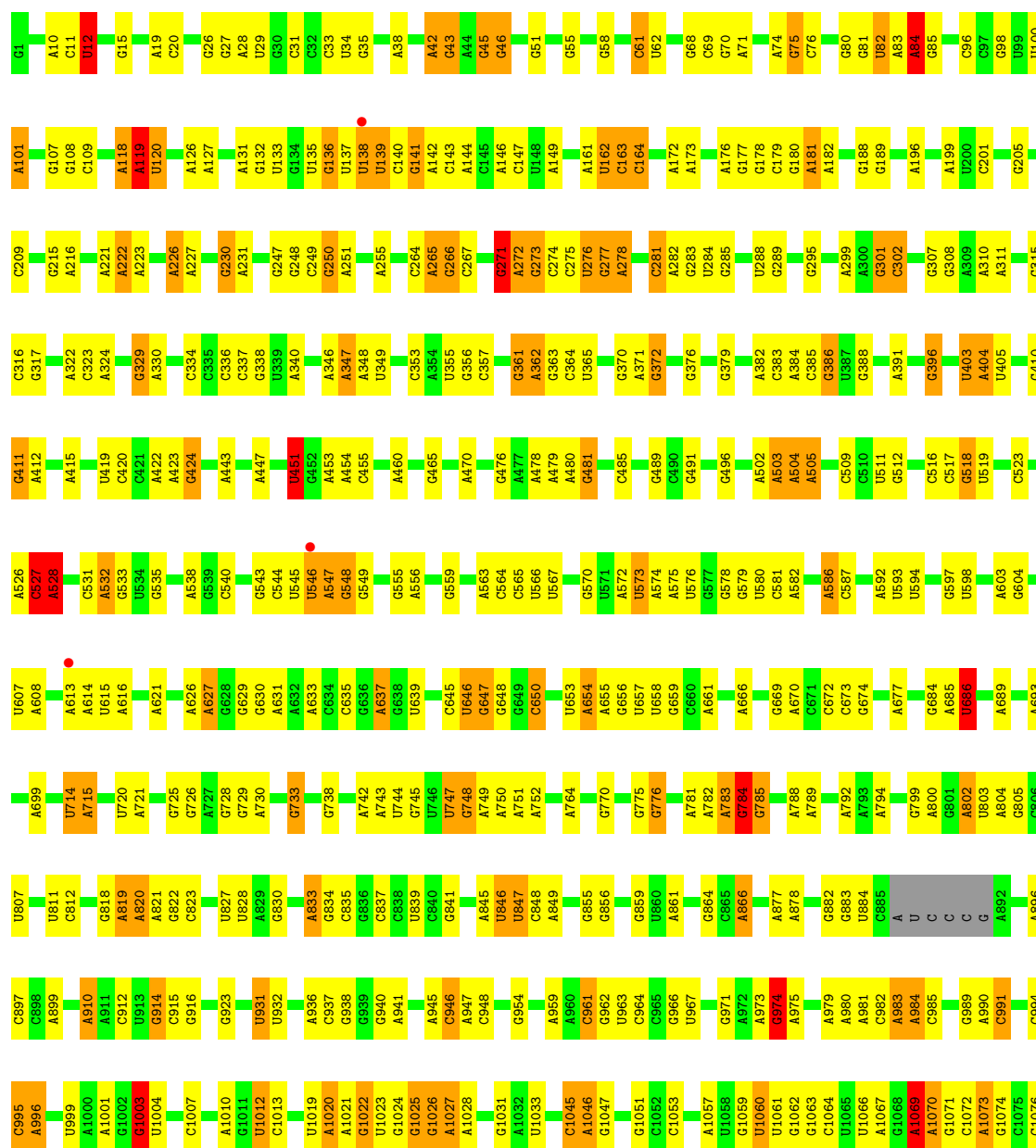


• Molecule 2: 50S ribosomal protein L2

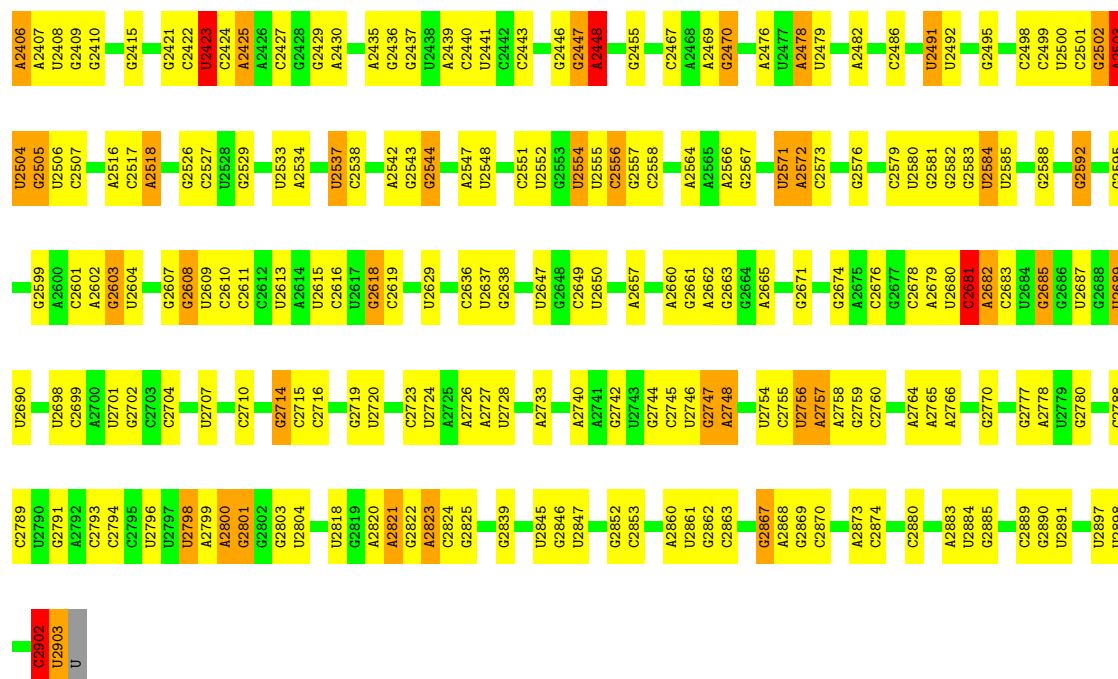


• Molecule 2: 50S ribosomal protein L2

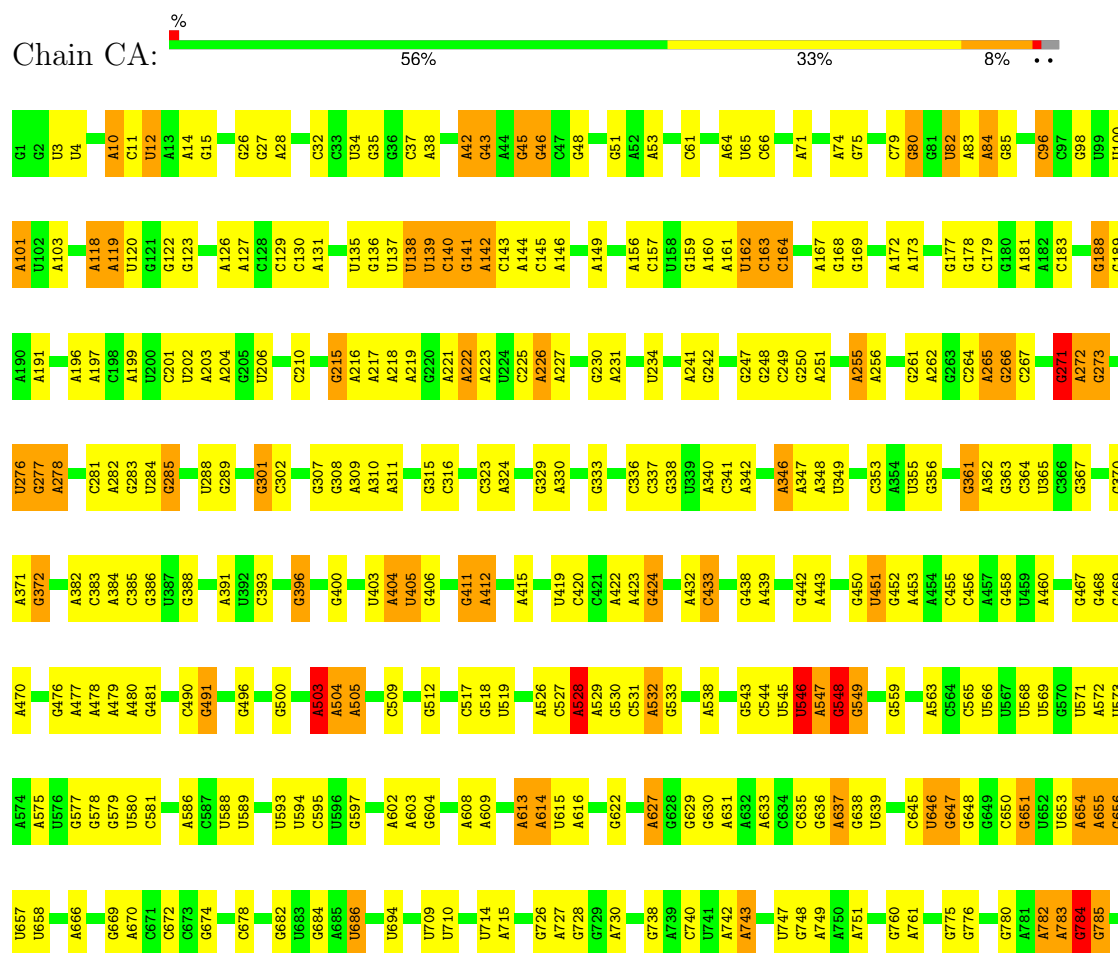








• Molecule 3: 23S rRNA







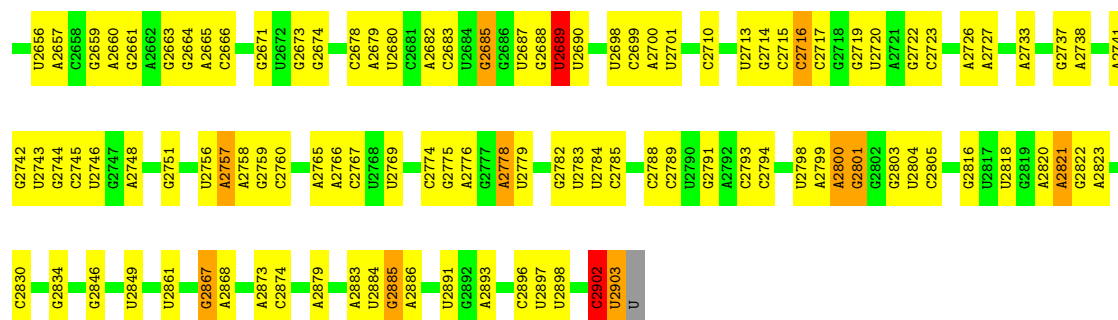


U1898	A1791	A1665	U1559	G1435	U1316	U1322	U1119	C1045	U958	A878	A788	A677	G583	C510
G1906	A1794	G1666	C1564	G1436	G1317	G1223	U1119	A1046	C961	G879	A789	A678	C584	U511
A1913	C1795	A1668	C1565	C1437	U1325	U1224	G1125	G1047	G981	G880	C678	C578	G585	G512
C1914	G1799	A1669	A1566	A1438	A1326	A1226	A1129	U963	U963	G882	C791	C679	A586	C517
A1927	A1800	C1670	G1567	A1439	A1327	C1229	U1130	G1051	U967	U884	U686	U686	C587	G518
A1928	A1801	U1671	G1568	C1446	G1332	G1238	U1131	G1052	C968	C885	G798	G690	U594	A522
G1930	C1806	C1675	U1578	G1450	U1340	A1247	U1132	A1054	G971	A	C691	C691	C595	C523
U1939	G1807	A1677	A1579	C1451	G1341	G1248	A1134	A1057	A972	U	A802	A693	C601	A526
C1934	A1808	A1678	G1452	G1459	C1350	U1249	G1135	U1058	C974	C	A804	U694	A602	C527
G1935	C1582	C1682	G1456	U1468	C1351	G1250	G1136	G1059	A975	C	G805	G695	A603	A528
A1936	A1583	A1583	U1457	U1466	A1352	A1253	G1139	U1061	A892	G808	C698	G704	G605	C531
U1938	U1812	U1584	A1458	U1486	A1353	A1253	C1140	G1062	C893	G809	C692	G701	C611	A532
A1939	G1813	C1694	U1459	U1487	A1354	G1256	A1141	G1063	A896	U810	U702	U702	G612	G533
C1943	A1815	A1700	G1459	U1488	A1355	C1257	A1142	C1064	C897	U811	U703	U703	G613	U534
U1943	G1816	C1594	U1468	U1488	A1356	A1260	A1144	A1067	C898	C812	G704	G704	A614	G536
U1955	U1818	A1596	U1474	U1486	A1357	C1261	C1145	G1068	A899	C816	G726	G726	A615	G537
G1959	G1823	A1603	G1475	U1486	G1360	C1262	G1149	A1069	C901	C817	A730	A730	A616	G538
A1960	G1824	C1605	G1482	U1487	A1364	A1263	C1150	A1070	C902	G818	A715	A715	A617	C540
C1961	C1962	C1606	G1482	U1488	A1365	U1264	A1151	G1071	C991	C819	G725	G725	G618	A541
A1966	U1827	C1607	U1488	U1488	G1368	A1266	C1152	A1073	C994	U826	G726	G726	A621	C542
C1967	G1828	A1608	U1486	U1486	A1372	U1267	G1153	G1075	C995	U827	A730	A730	A622	G543
G1968	C1830	A1609	U1487	U1487	U1372	A1268	C1154	C1076	C996	U828	A730	A730	A626	C544
A1969	C1831	A1610	U1488	U1488	A1376	A1269	A1155	C1077	A996	A626	A731	A731	A627	U545
U1970	C1832	C1732	U1494	U1488	C1377	C1270	A1156	A1078	G914	U832	C732	C732	A627	U546
C1971	G1833	A1614	A1495	U1488	A1378	A1271	G1157	C1079	C998	A833	G733	G733	A547	A547
U1971	C1843	C1615	A1504	U1488	G1380	U1273	C1158	C1080	C916	G834	C737	C737	G630	G548
G1972	A1847	A1618	U1504	U1488	A1383	G1277	G1168	U1082	A917	G835	G738	G738	A631	G549
U1983	A1848	G1619	A1508	U1488	A1384	C1278	C1170	U1083	C921	G836	A739	A739	A632	C550
U1991	A1853	A1626	A1509	U1488	A1385	G1279	C1171	A1084	C922	U839	A741	A741	A633	G551
G1992	A1858	G1627	G1510	U1488	A1386	G1280	C1172	A1085	G923	U843	A742	A742	C634	G555
U1993	A1866	G1628	A1515	U1488	A1387	G1281	U1173	A1086	U929	A844	A743	A743	G635	A556
C1996	C1967	U1629	G1516	U1488	A1394	A1284	A1175	A1087	U930	A845	U747	U747	A637	C557
C1997	G1967	A1630	G1517	U1488	A1395	A1285	U1176	A1088	U931	U846	U748	U748	G638	U558
A1998	G1967	G1631	U1522	U1488	A1396	A1286	C1177	A1090	U932	U847	A749	A749	U639	G559
A2005	G1967	A1634	U1523	U1488	G1407	G1288	G1179	G1091	A936	G855	A750	A750	A644	C560
A2013	A1871	U1647	G1524	U1488	U1415	G1292	U1180	G1092	C937	G856	A751	A751	C645	A563
U2016	A1872	U1648	A1532	U1488	G1416	C1293	G1186	G1093	A941	U857	A752	A752	U646	C564
U2017	G1873	G1649	G1533	U1488	A1419	G1300	G1187	A1094	G942	G858	G759	G759	G647	C565
G2018	A1876	U1650	U1534	U1488	A1420	A1301	U1188	A1095	U1023	G859	U762	U762	G648	U566
A2019	C1877	G1653	C1536	U1488	G1421	A1302	A1189	U1097	G1024	U860	U762	U762	G649	C567
A2020	G1878	U1655	G1537	U1488	G1422	G1303	G1190	A1098	G1025	A861	U762	U762	C650	G570
C2021	G1884	U1656	U1544	U1488	A1427	G1309	U1198	A1103	A945	G864	U762	U762	G651	U571
U2022	A1765	U1657	A1545	U1488	C1428	U1312	A1205	G1106	C946	G865	G775	G775	U652	A572
C2023	A1767	U1658	A1548	U1488	G1429	U1313	A1206	G1107	A947	U870	G776	G776	G653	U573
G2024	C1887	A1664	A1549	U1488	A1430	G1314	G1220	G1110	U1027	U871	U779	U779	A654	A574
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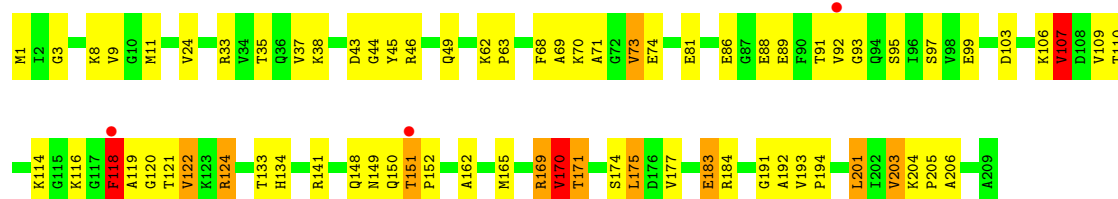




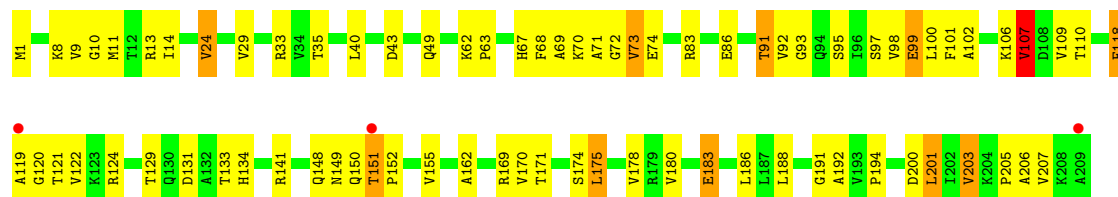
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C2558	U2562	G2481	U2402	C2332	U2259	U2182	U	G2046	G1952	U1851	C1774	A1664	A1545	U1438
A2482	G2483	U2403	U2404	A2333	C2260	A2183	G	C2047	A1952	U1852	U1776	G1665	C1558	A1439
G2484	G2485	A2405	U2406	A2335	C2264	U2186	G	A2051	U1955	A1853	U1777	A1667	A1566	U1440
				A2336	U2266	U2187	A	A2052	U1956	A1854	U1778	A1668	G1567	
G2409		G2340		G2340	A2267	U2188	G	G2053	C1957	A1858	U1780	G1670	G1568	G1448
G2410		G2341		G2341	A2288	G2190	C	A2054	C1958	U1859	U1781	U1671	A1569	G1449
A2411		G2342		G2342	A2273	G2191	U	C2055	G1959	G1860	U1782	G1674	U1570	G1450
G2412		U2343		U2343	A2274	U2194	U	G2056	A1960		A1784		A1571	C1451
G2413		U2344		U2344	G2275	U2195		G2057	C1965	U1864	U1678		G1452	
G2414		G2345		G2345	G2276	C2196			A1966	U1865	A1679		G1455	
G2415		A2346		A2346	G2277	C2197			C1967	A1866	U1680			
G2416		G2347		G2347	A2278	U2198			G1968	G1869	U1681		U1458	
		U2348		U2348	G2279	A2199			A1969	A1870	G1792		G1459	
		G2349		G2349	C2200	C2200			A1970	A1871	G1793		C1462	
		G2350		G2350	G2283				U1971	A1872	U1794		C1463	
		G2351		G2351	A2284				G1972	G1873	C1795			
		A2352		A2352	G2285	G2204			C1965	G1874	U1796			
		G2353		G2353	G2286	A2205			A1966	G1875	G1797		U1594	
		C2354		C2354	A2287	C2207			C1967	G1876	U1798		C1595	
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		A2369		A2369	U2302	G2218			A2007	C1900	U1728		U1486	
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		A2376		A2376	G2307	A2225	A		U2017		A1735		G1619	
		U2377		U2377	G2308	C2226	G		G2018		U1736		G1620	
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		G2384		G2384	G2315	G2235	U		U1915		A1746		G1516	
		G2385		G2385	G2316	G2237	G		U1916		U1747		G1524	
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		G2396		G2396	A2326	G2252	C		A2037		G1763		A1655	
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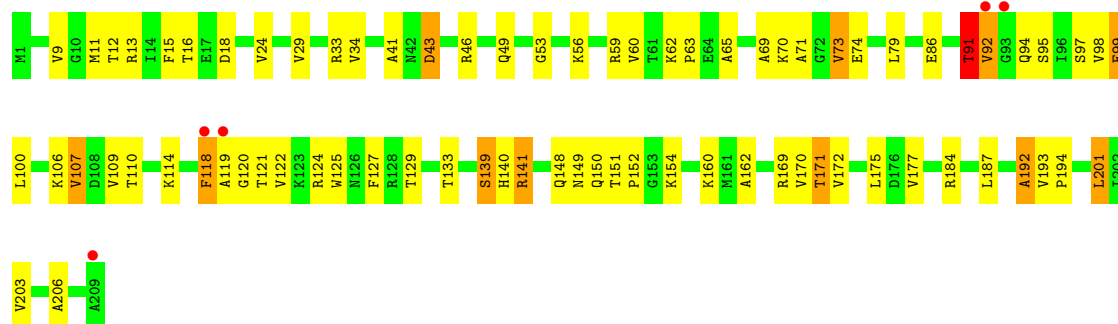
• Molecule 4: 50S ribosomal protein L3



• Molecule 4: 50S ribosomal protein L3

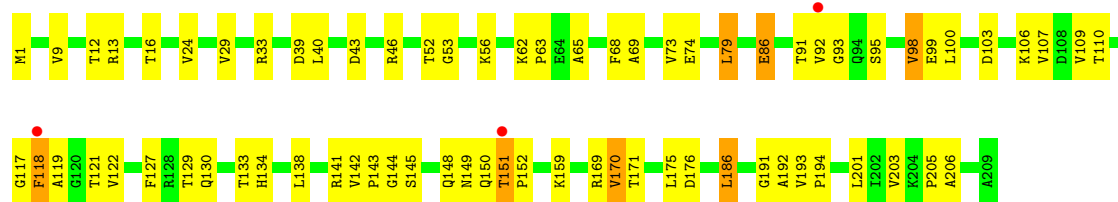


• Molecule 4: 50S ribosomal protein L3

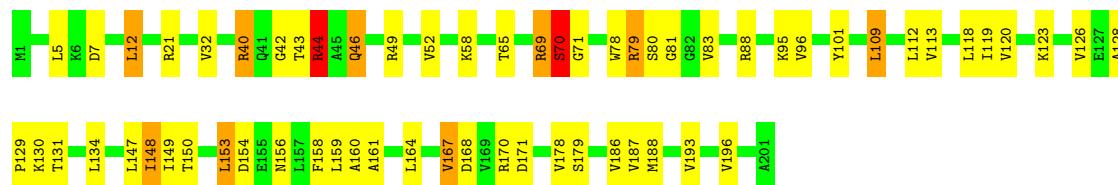


• Molecule 4: 50S ribosomal protein L3

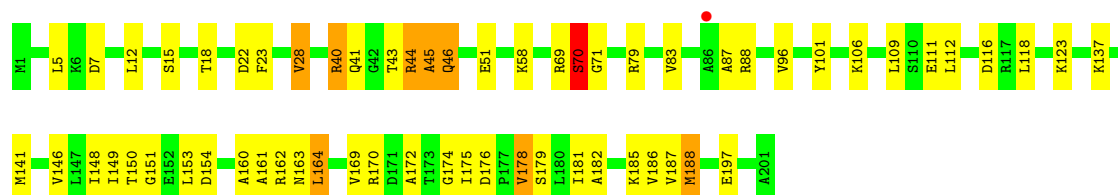




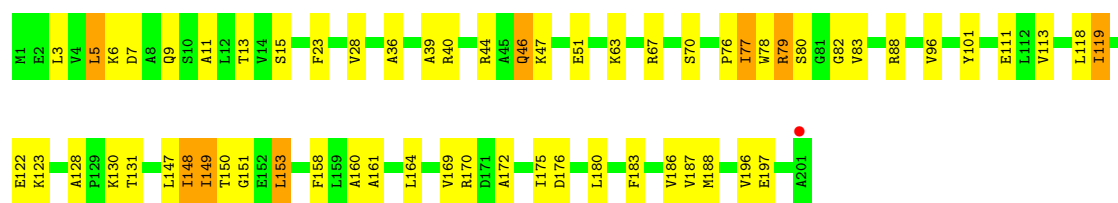
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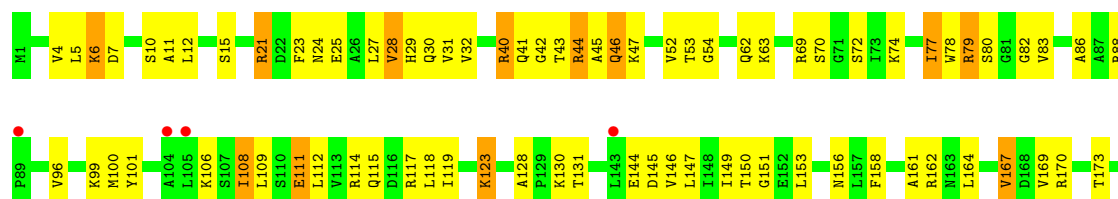
• Molecule 5: 50S ribosomal protein L4



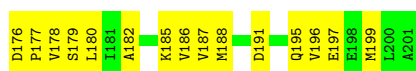
• Molecule 5: 50S ribosomal protein L4



• Molecule 5: 50S ribosomal protein L4

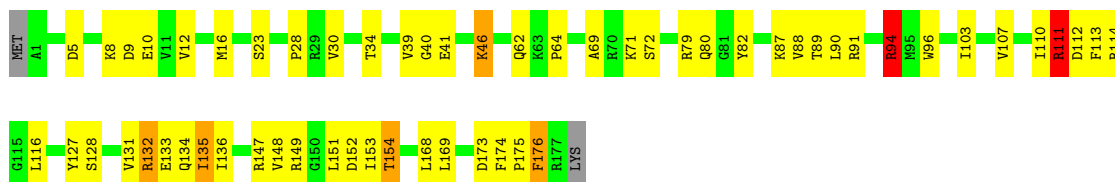






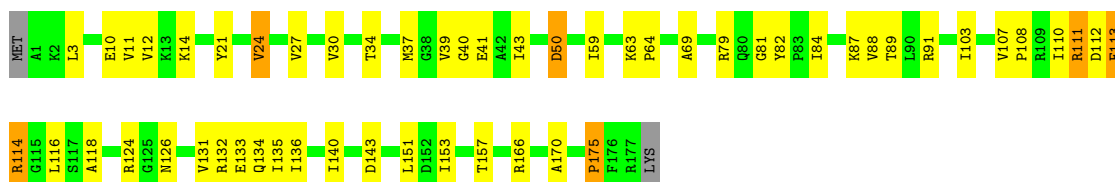
- Molecule 6: 50S ribosomal protein L5

Chain AF: 66% 28% ..



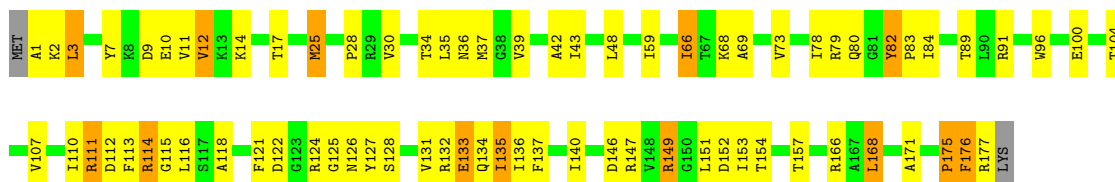
- Molecule 6: 50S ribosomal protein L5

Chain CF: 69% 27% ..



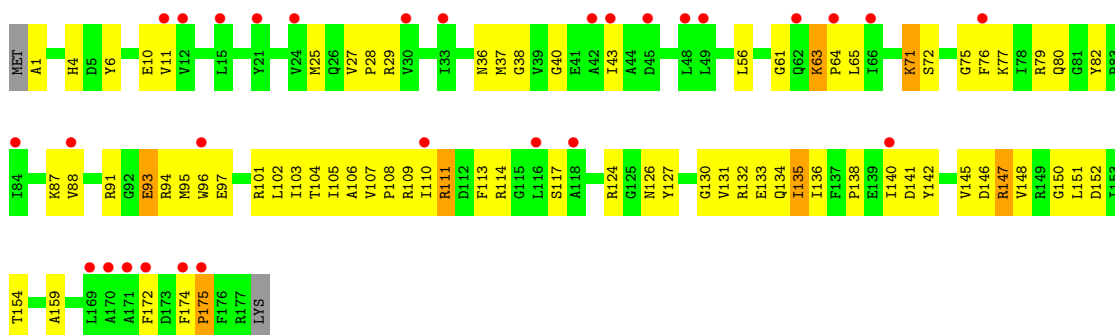
- Molecule 6: 50S ribosomal protein L5

Chain EF: 57% 35% 7% .

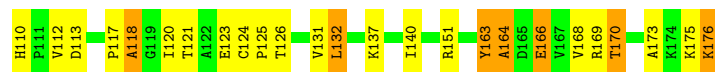
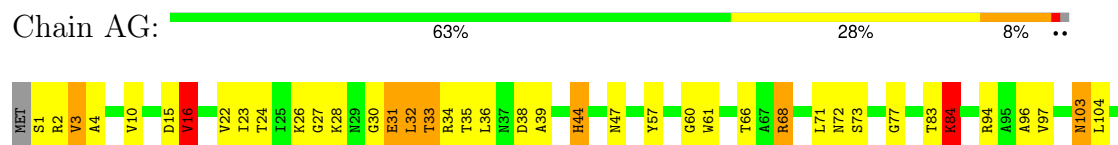


- Molecule 6: 50S ribosomal protein L5

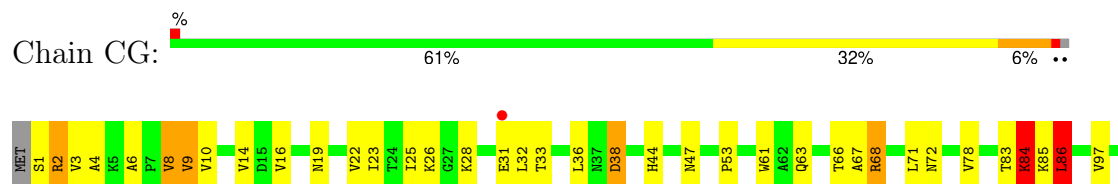
Chain GF: 16% 57% 38% ..



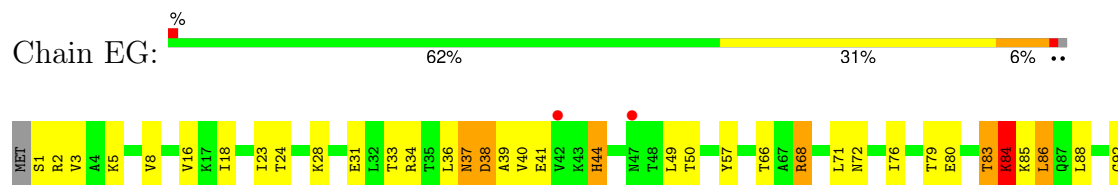
- Molecule 7: 50S ribosomal protein L6



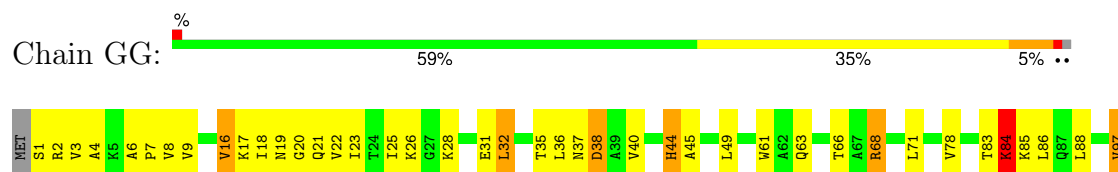
- Molecule 7: 50S ribosomal protein L6



- Molecule 7: 50S ribosomal protein L6



- Molecule 7: 50S ribosomal protein L6



- Molecule 8: 50S ribosomal protein L9



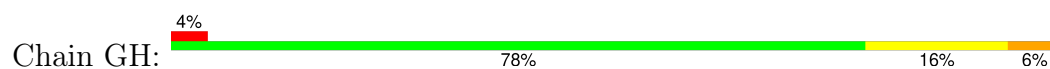
- Molecule 8: 50S ribosomal protein L9



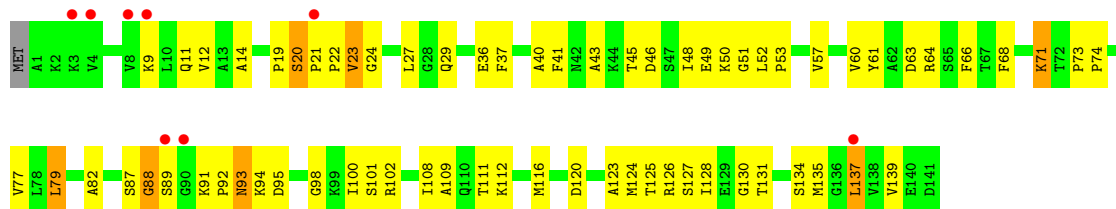
- Molecule 8: 50S ribosomal protein L9



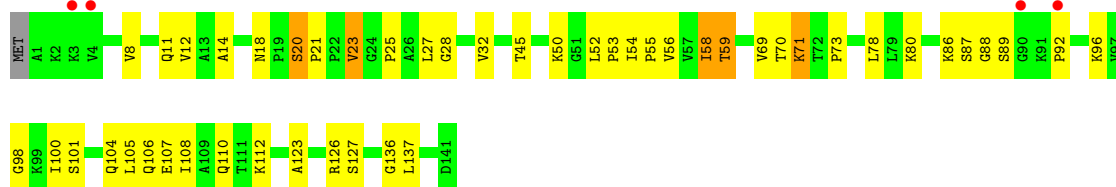
- Molecule 8: 50S ribosomal protein L9



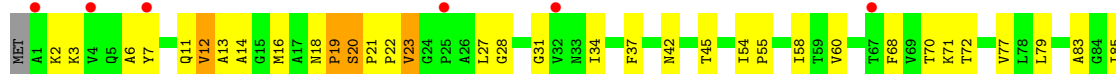
- Molecule 9: 50S ribosomal protein L11



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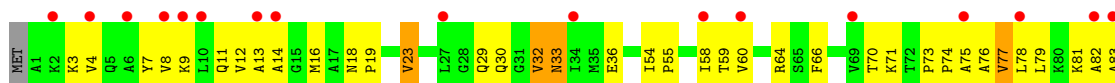


- Molecule 9: 50S ribosomal protein L11

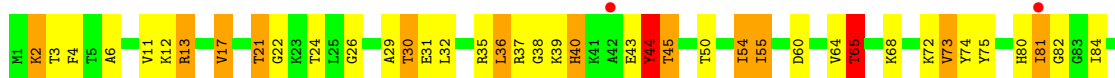




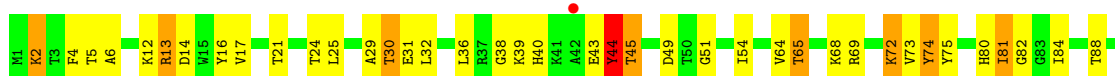
- Molecule 9: 50S ribosomal protein L11



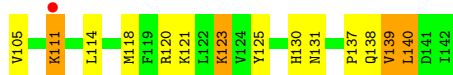
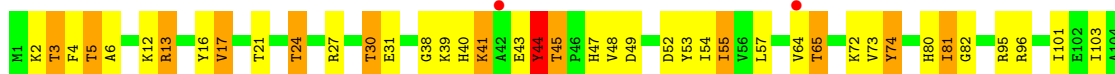
- Molecule 10: 50S ribosomal protein L13



- Molecule 10: 50S ribosomal protein L13

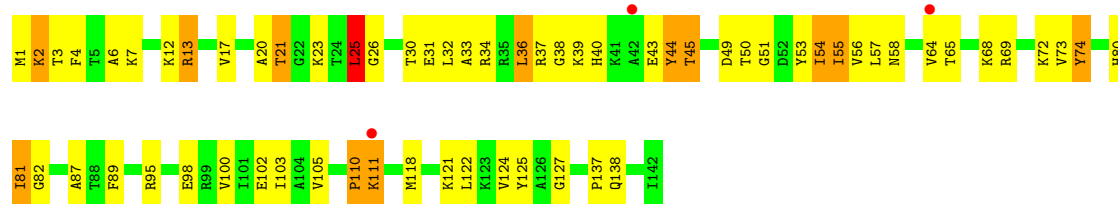


- Molecule 10: 50S ribosomal protein L13

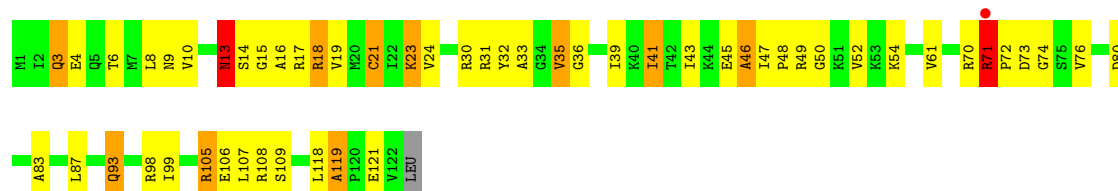


- Molecule 10: 50S ribosomal protein L13

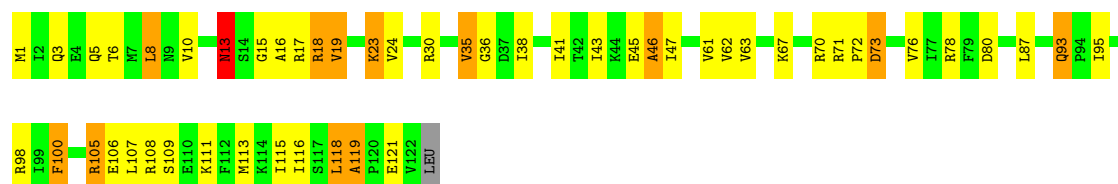




• Molecule 11: 50S ribosomal protein L14



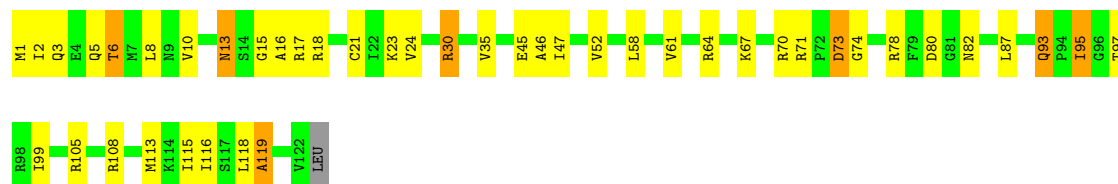
• Molecule 11: 50S ribosomal protein L14



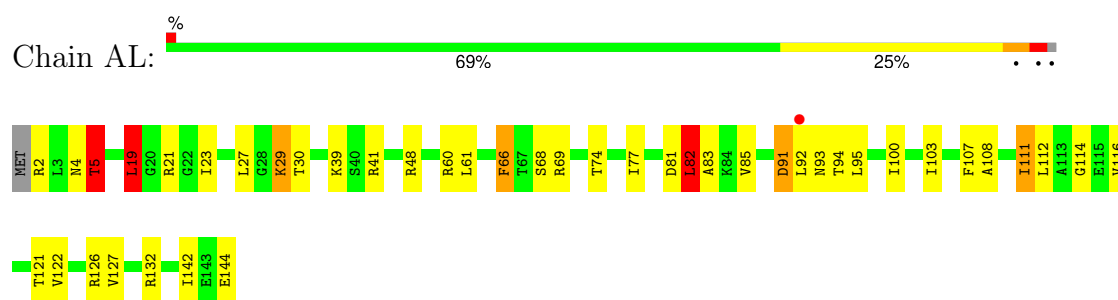
• Molecule 11: 50S ribosomal protein L14



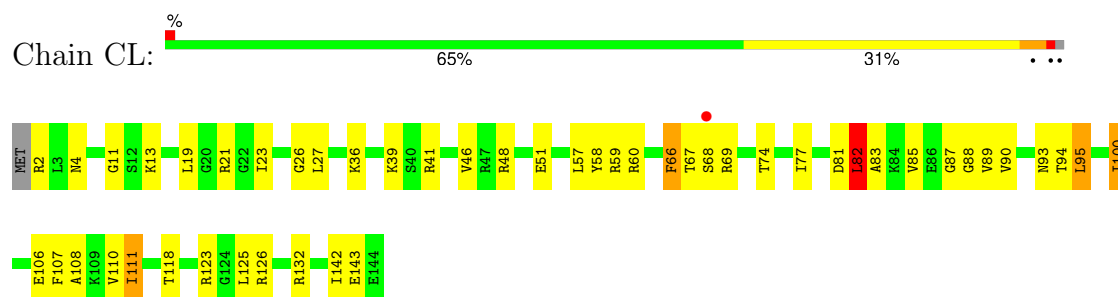
• Molecule 11: 50S ribosomal protein L14



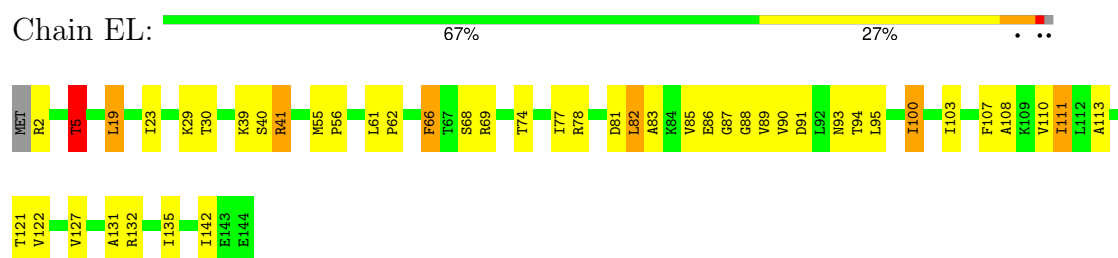
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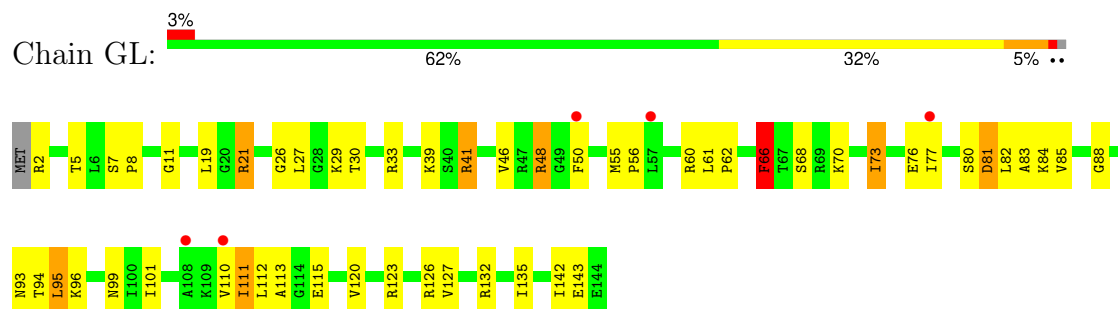
- Molecule 12: 50S ribosomal protein L15



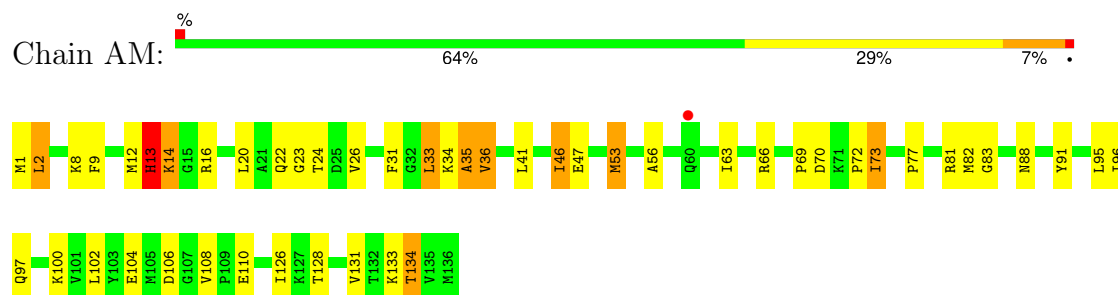
- Molecule 12: 50S ribosomal protein L15



- Molecule 12: 50S ribosomal protein L15

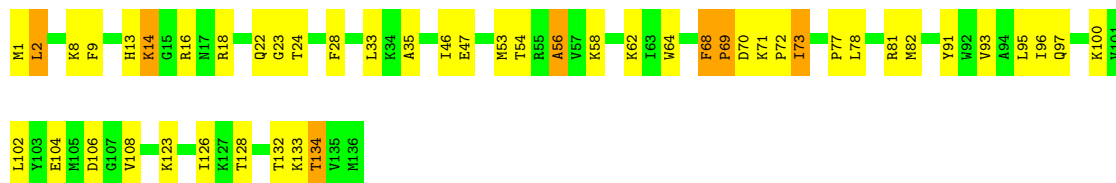


- Molecule 13: 50S ribosomal protein L16



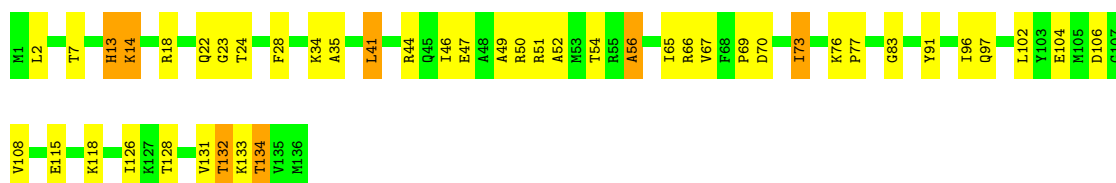
- Molecule 13: 50S ribosomal protein L16

Chain CM: 




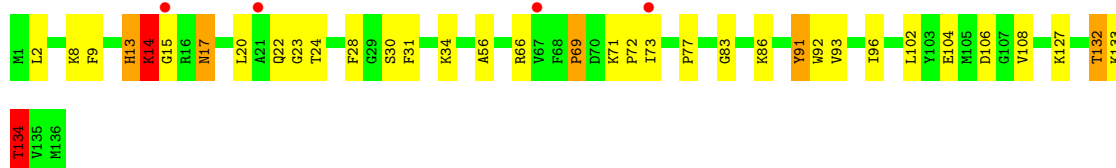
- Molecule 13: 50S ribosomal protein L16

Chain EM: 



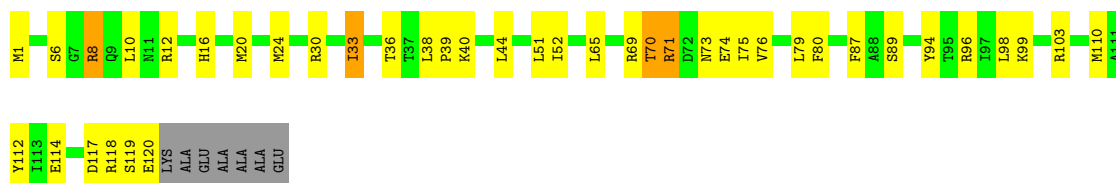
- Molecule 13: 50S ribosomal protein L16

Chain GM: 



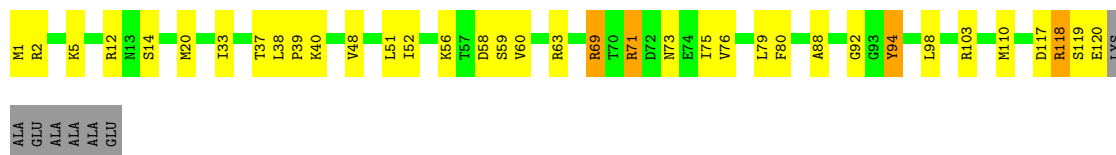
- Molecule 14: 50S ribosomal protein L17

Chain AN: 



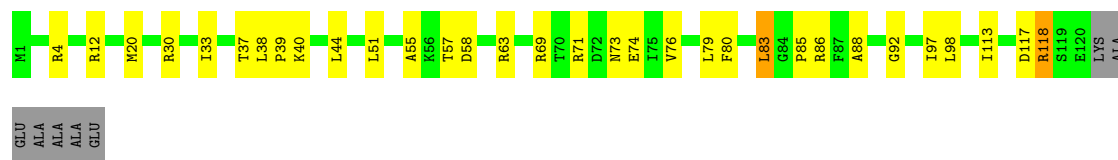
- Molecule 14: 50S ribosomal protein L17

Chain CN: 



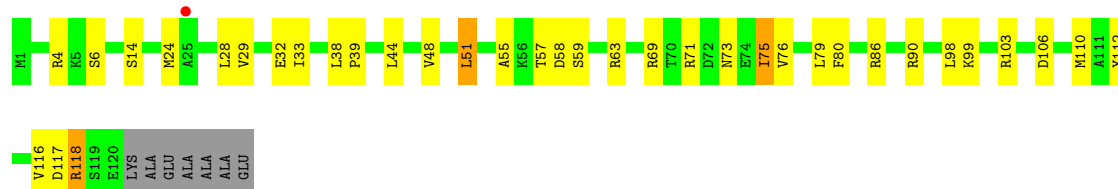
- Molecule 14: 50S ribosomal protein L17

Chain EN:  69% 24% 6%



- Molecule 14: 50S ribosomal protein L17

Chain GN:  66% 26% 6%



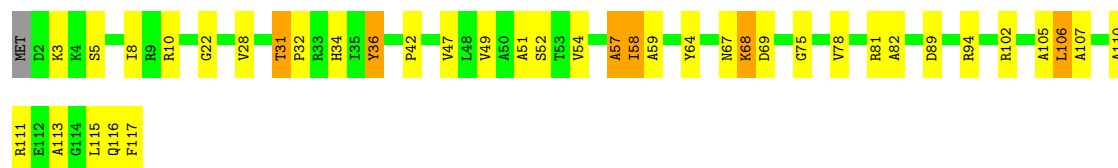
- Molecule 15: 50S ribosomal protein L18

Chain AO:  69% 27% 4%



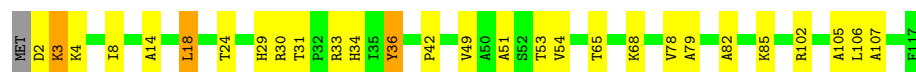
- Molecule 15: 50S ribosomal protein L18

Chain CO:  66% 28% 5%



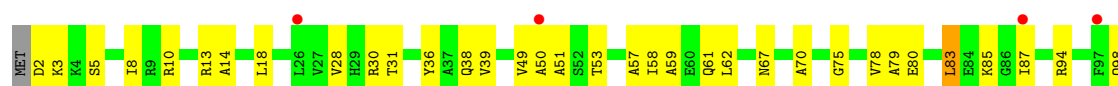
- Molecule 15: 50S ribosomal protein L18

Chain EO:  75% 21% 4%



- Molecule 15: 50S ribosomal protein L18

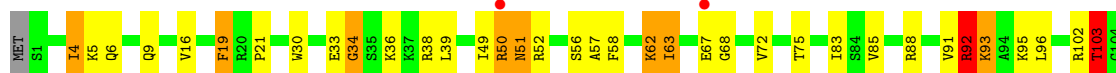
Chain GO:  3% 61% 35% 1%



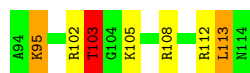




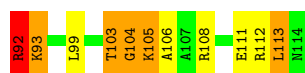
- Molecule 16: 50S ribosomal protein L19



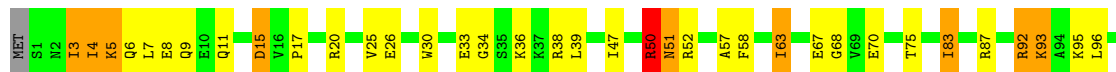
- Molecule 16: 50S ribosomal protein L19



- Molecule 16: 50S ribosomal protein L19

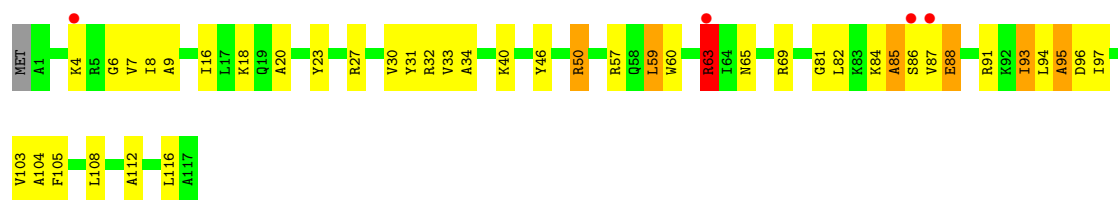


- Molecule 16: 50S ribosomal protein L19

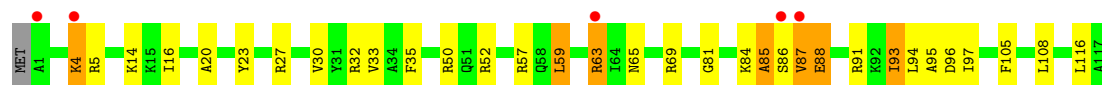
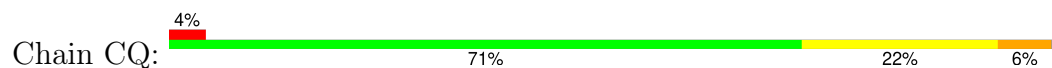


- Molecule 17: 50S ribosomal protein L20

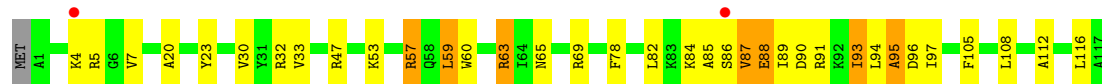




- Molecule 17: 50S ribosomal protein L20



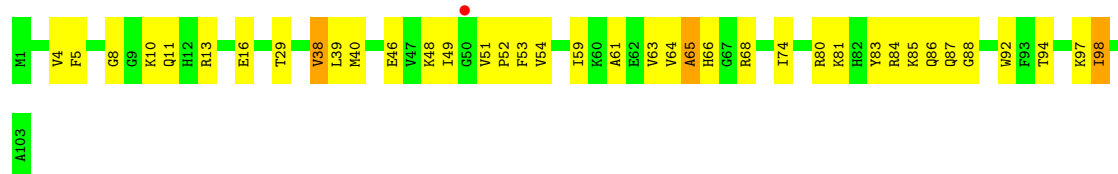
- Molecule 17: 50S ribosomal protein L20



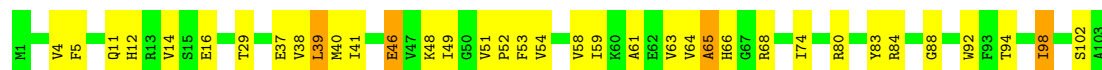
- Molecule 17: 50S ribosomal protein L20



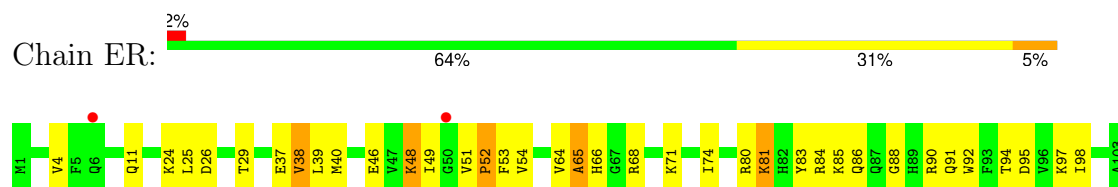
- Molecule 18: 50S ribosomal protein L21



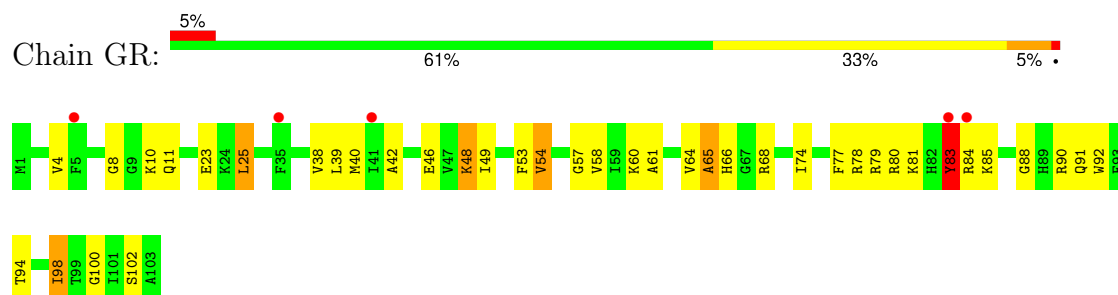
- Molecule 18: 50S ribosomal protein L21



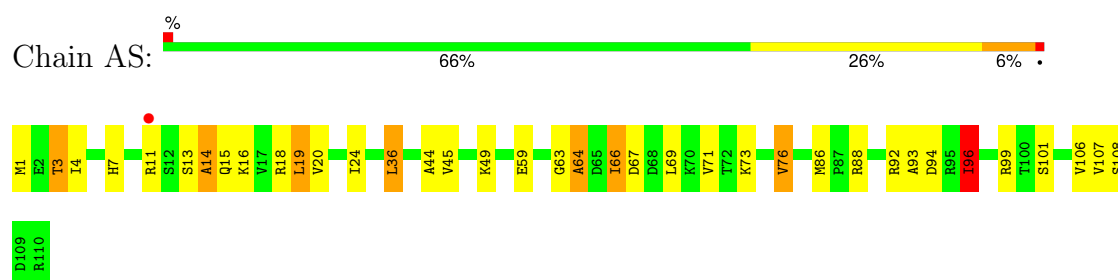
- Molecule 18: 50S ribosomal protein L21



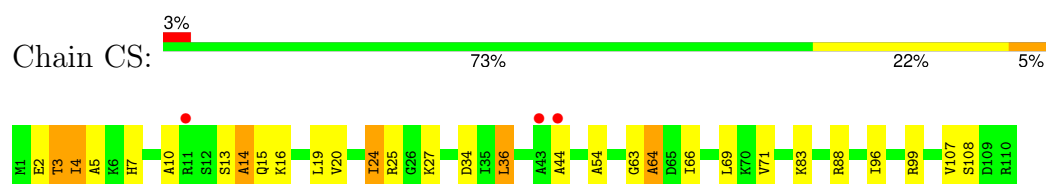
- Molecule 18: 50S ribosomal protein L21



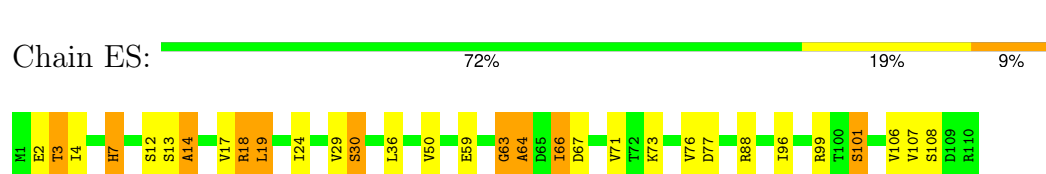
- Molecule 19: 50S ribosomal protein L22



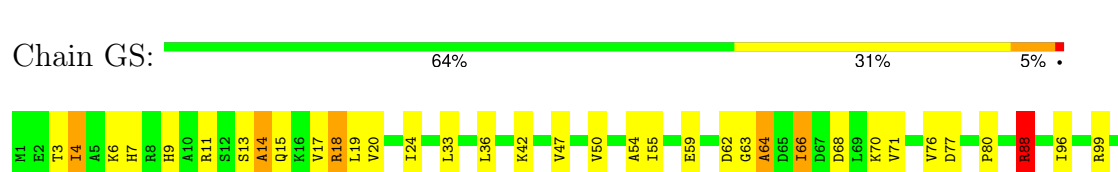
- Molecule 19: 50S ribosomal protein L22

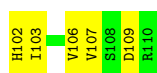


- Molecule 19: 50S ribosomal protein L22

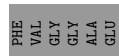
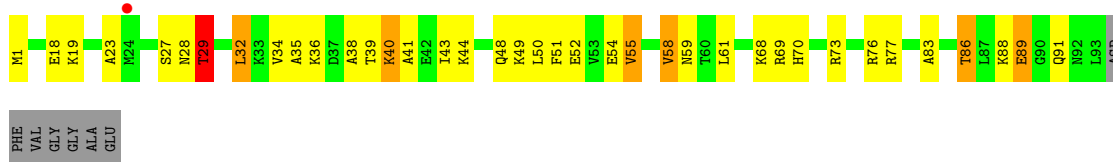


- Molecule 19: 50S ribosomal protein L22

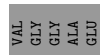
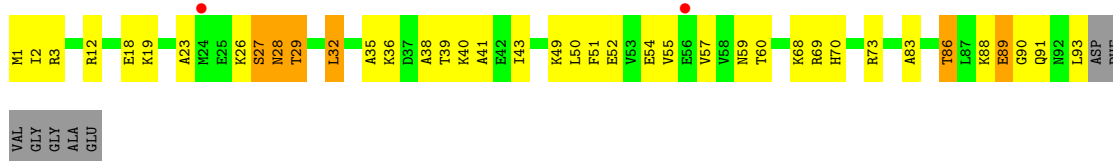




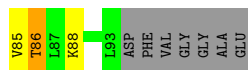
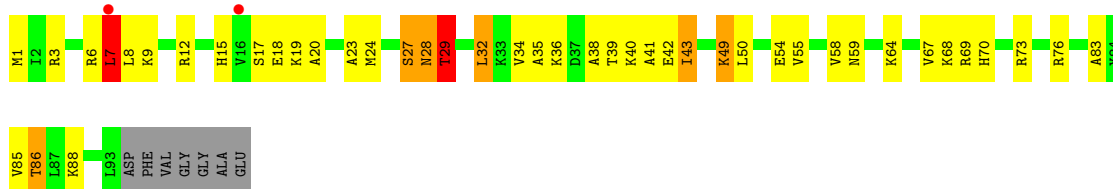
- Molecule 20: 50S ribosomal protein L23



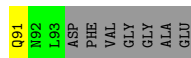
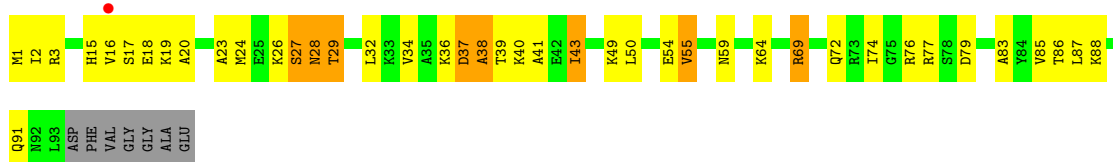
- Molecule 20: 50S ribosomal protein L23



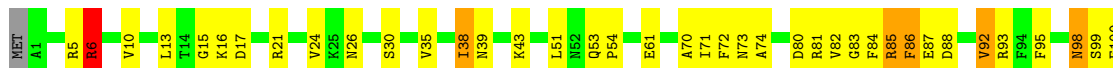
- Molecule 20: 50S ribosomal protein L23



- Molecule 20: 50S ribosomal protein L23

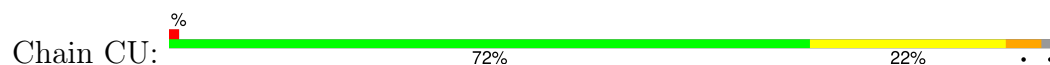


- Molecule 21: 50S ribosomal protein L24

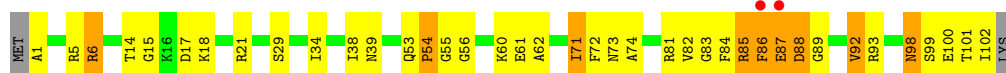




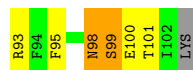
- Molecule 21: 50S ribosomal protein L24



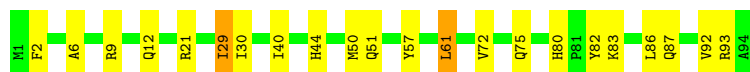
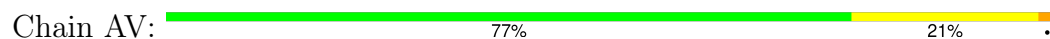
- Molecule 21: 50S ribosomal protein L24



- Molecule 21: 50S ribosomal protein L24



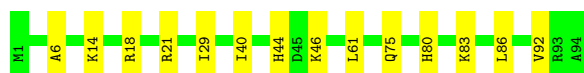
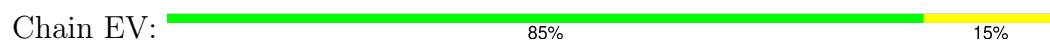
- Molecule 22: 50S ribosomal protein L25



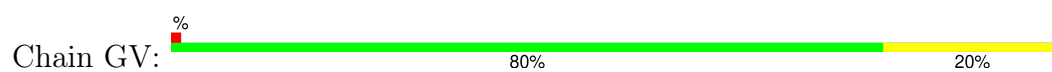
- Molecule 22: 50S ribosomal protein L25



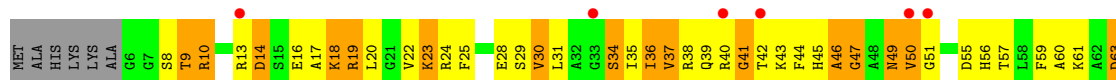
- Molecule 22: 50S ribosomal protein L25



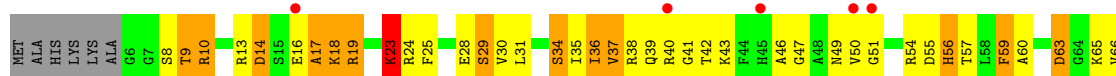
- Molecule 22: 50S ribosomal protein L25



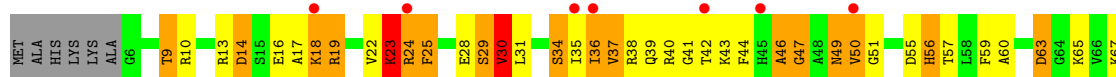
- Molecule 23: 50S ribosomal protein L27



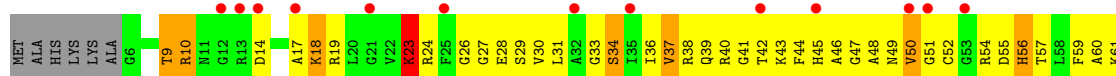
- Molecule 23: 50S ribosomal protein L27



- Molecule 23: 50S ribosomal protein L27



- Molecule 23: 50S ribosomal protein L27



- Molecule 24: 50S ribosomal protein L28

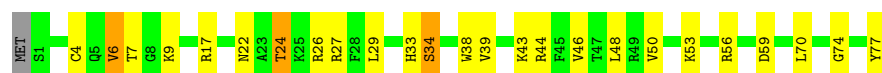


Chain AX:  69% 23% 5% ..



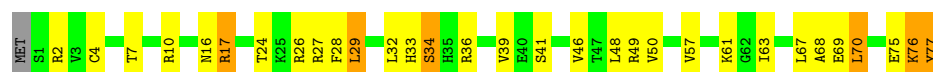
- Molecule 24: 50S ribosomal protein L28

Chain CX:  67% 28% ..



- Molecule 24: 50S ribosomal protein L28

Chain EX:  59% 32% 8% .



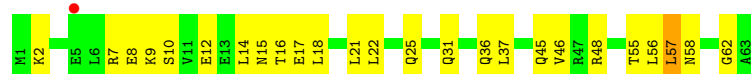
- Molecule 24: 50S ribosomal protein L28

Chain GX:  58% 40% ..




- Molecule 25: 50S ribosomal protein L29

Chain AY:  60% 38% .



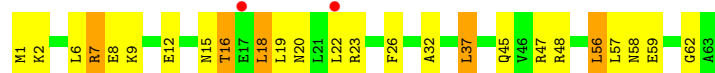
- Molecule 25: 50S ribosomal protein L29

Chain CY:  75% 19% 5% .

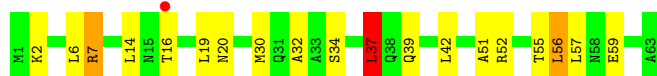
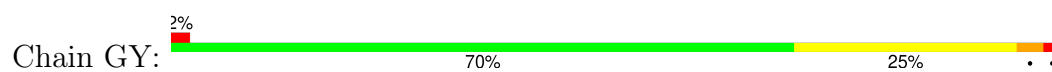


- Molecule 25: 50S ribosomal protein L29

Chain EY:  60% 32% 8%



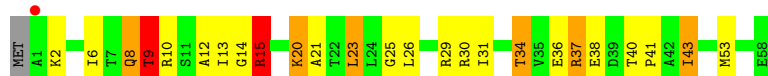
- Molecule 25: 50S ribosomal protein L29



- Molecule 26: 50S ribosomal protein L30



- Molecule 26: 50S ribosomal protein L30



- Molecule 26: 50S ribosomal protein L30



- Molecule 26: 50S ribosomal protein L30



- Molecule 27: 50S ribosomal protein L32

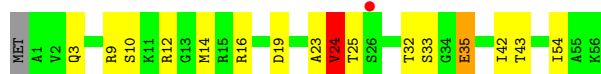


- Molecule 27: 50S ribosomal protein L32

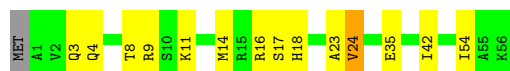


- Molecule 27: 50S ribosomal protein L32





- Molecule 27: 50S ribosomal protein L32



- Molecule 28: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L33



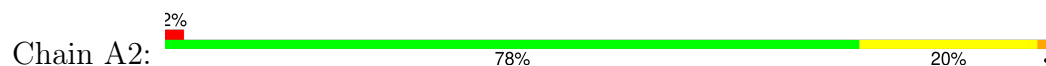
- Molecule 28: 50S ribosomal protein L33



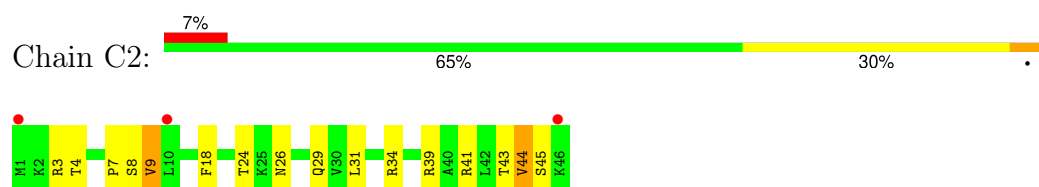
- Molecule 28: 50S ribosomal protein L33



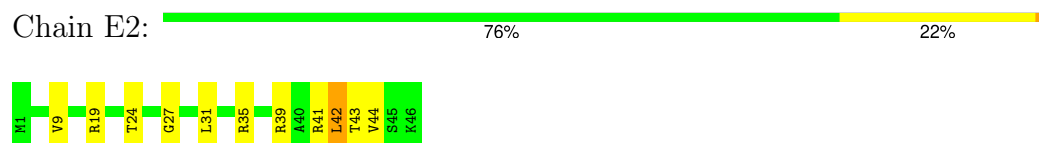
- Molecule 29: 50S ribosomal protein L34



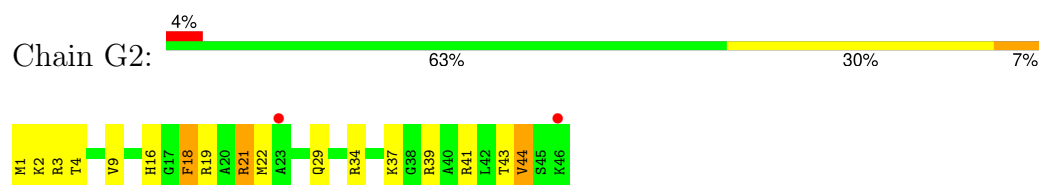
- Molecule 29: 50S ribosomal protein L34



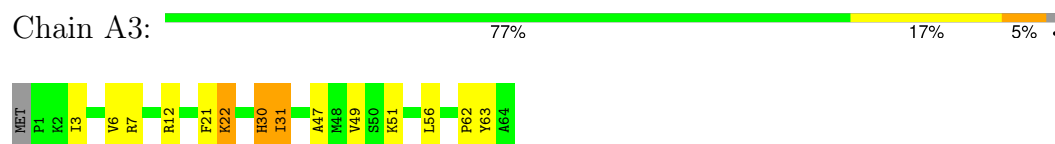
- Molecule 29: 50S ribosomal protein L34



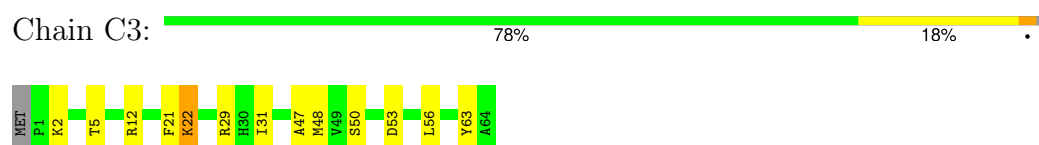
- Molecule 29: 50S ribosomal protein L34



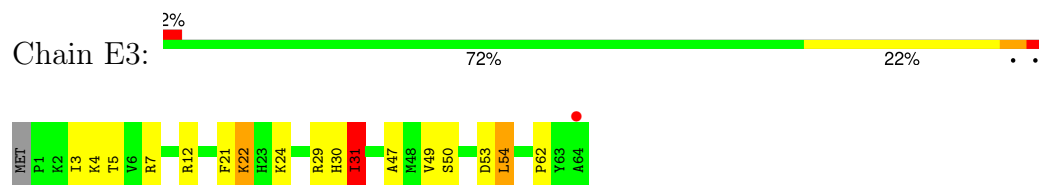
- Molecule 30: 50S ribosomal protein L35



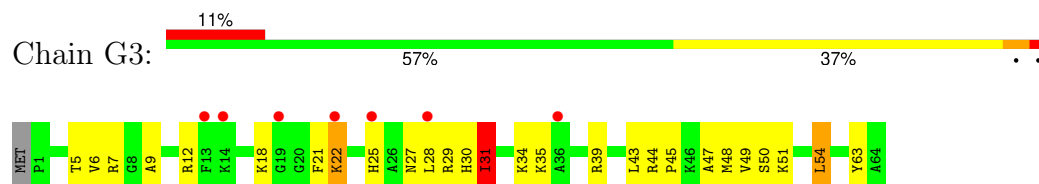
- Molecule 30: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L35



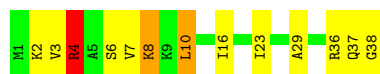
- Molecule 31: 50S ribosomal protein L36

Chain A4:  55% 39% . .



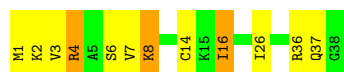
- Molecule 31: 50S ribosomal protein L36

Chain C4:  66% 26% 5% .



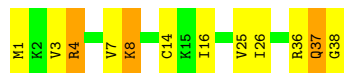
- Molecule 31: 50S ribosomal protein L36

Chain E4:  68% 24% 8%




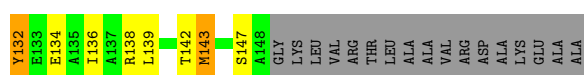
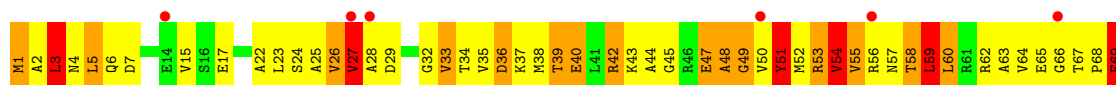
- Molecule 31: 50S ribosomal protein L36

Chain G4:  68% 24% 8%



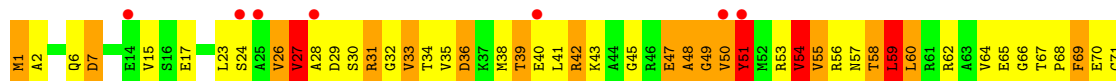
- Molecule 32: 50S ribosomal protein L10

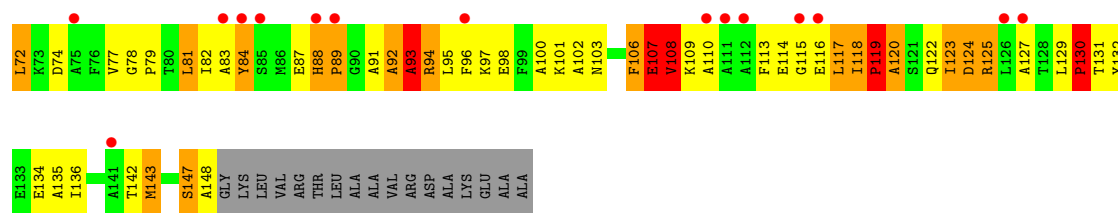
Chain A5:  12% 24% 39% 19% 8% 10%



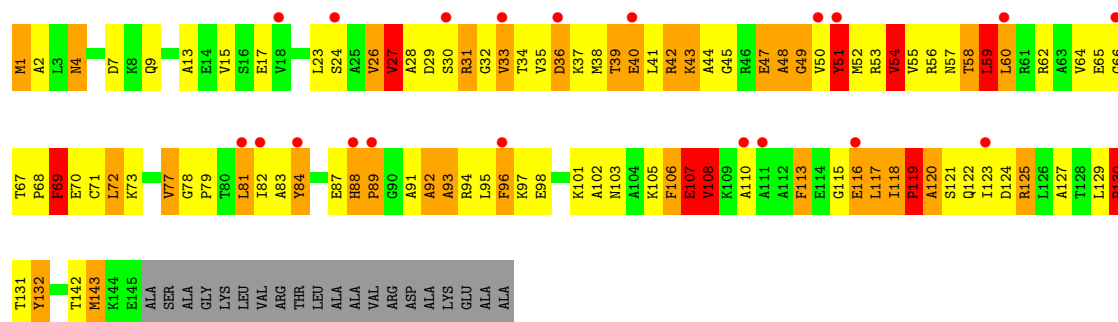
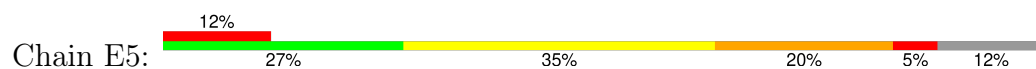
- Molecule 32: 50S ribosomal protein L10

Chain C5:  13% 28% 36% 19% 5% 10%

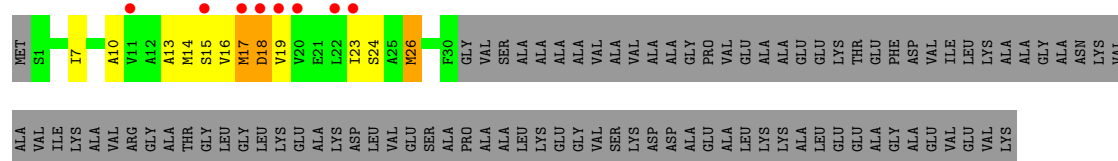




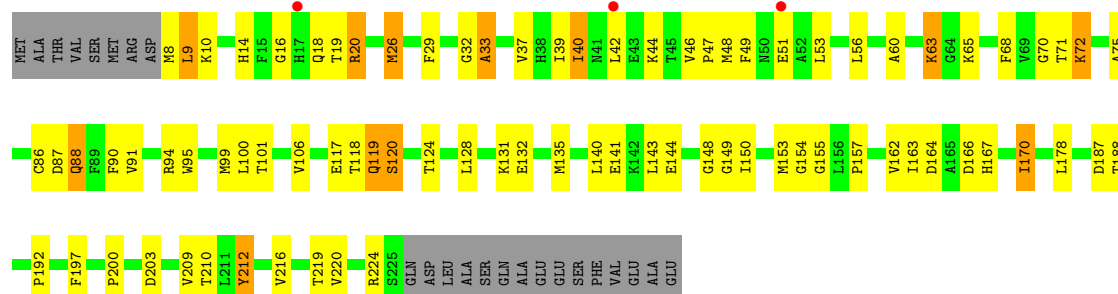
• Molecule 32: 50S ribosomal protein L10



• Molecule 33: 50S ribosomal protein L7/L12

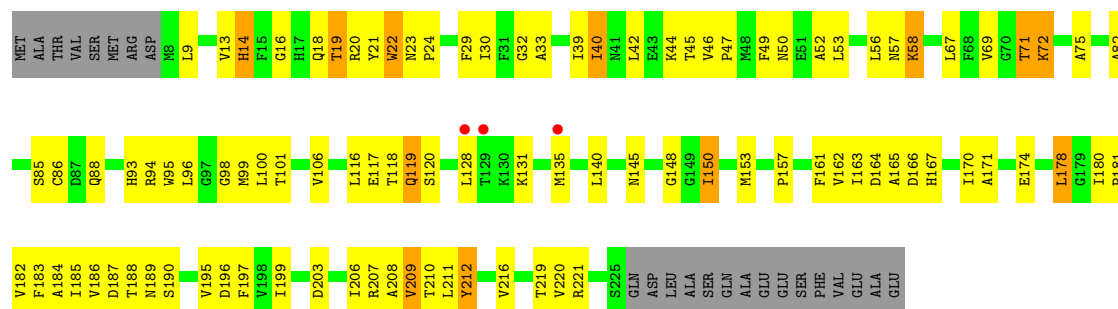


• Molecule 34: 30S ribosomal protein S2

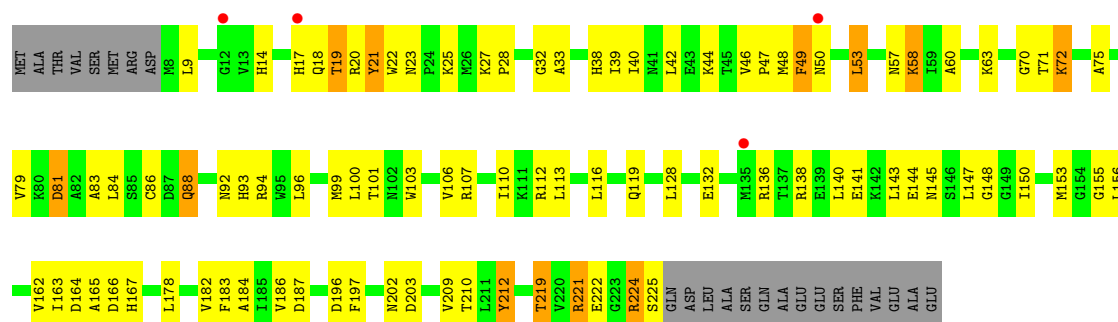


• Molecule 34: 30S ribosomal protein S2

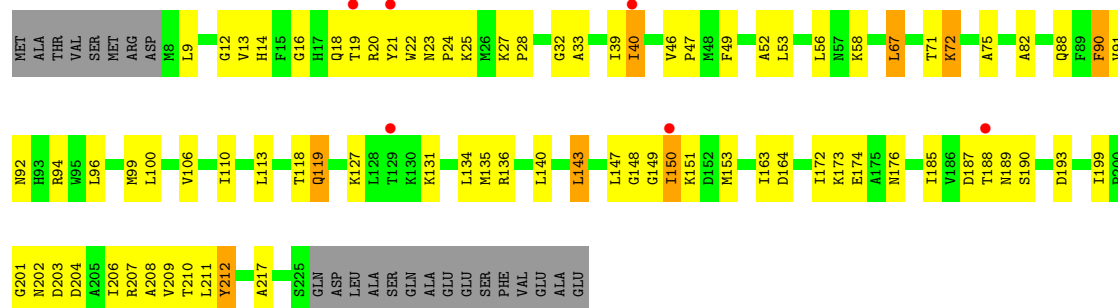




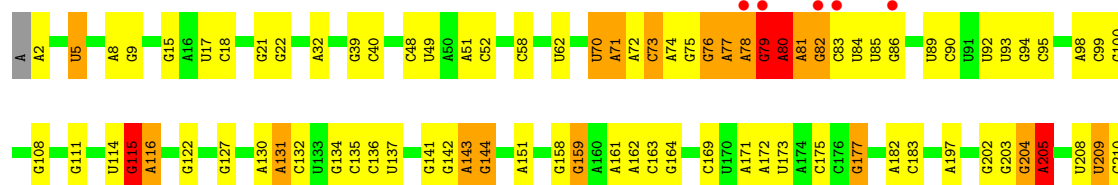
• Molecule 34: 30S ribosomal protein S2

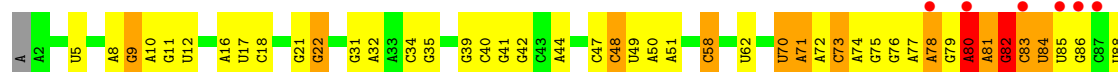


• Molecule 34: 30S ribosomal protein S2



• Molecule 35: 16S rRNA



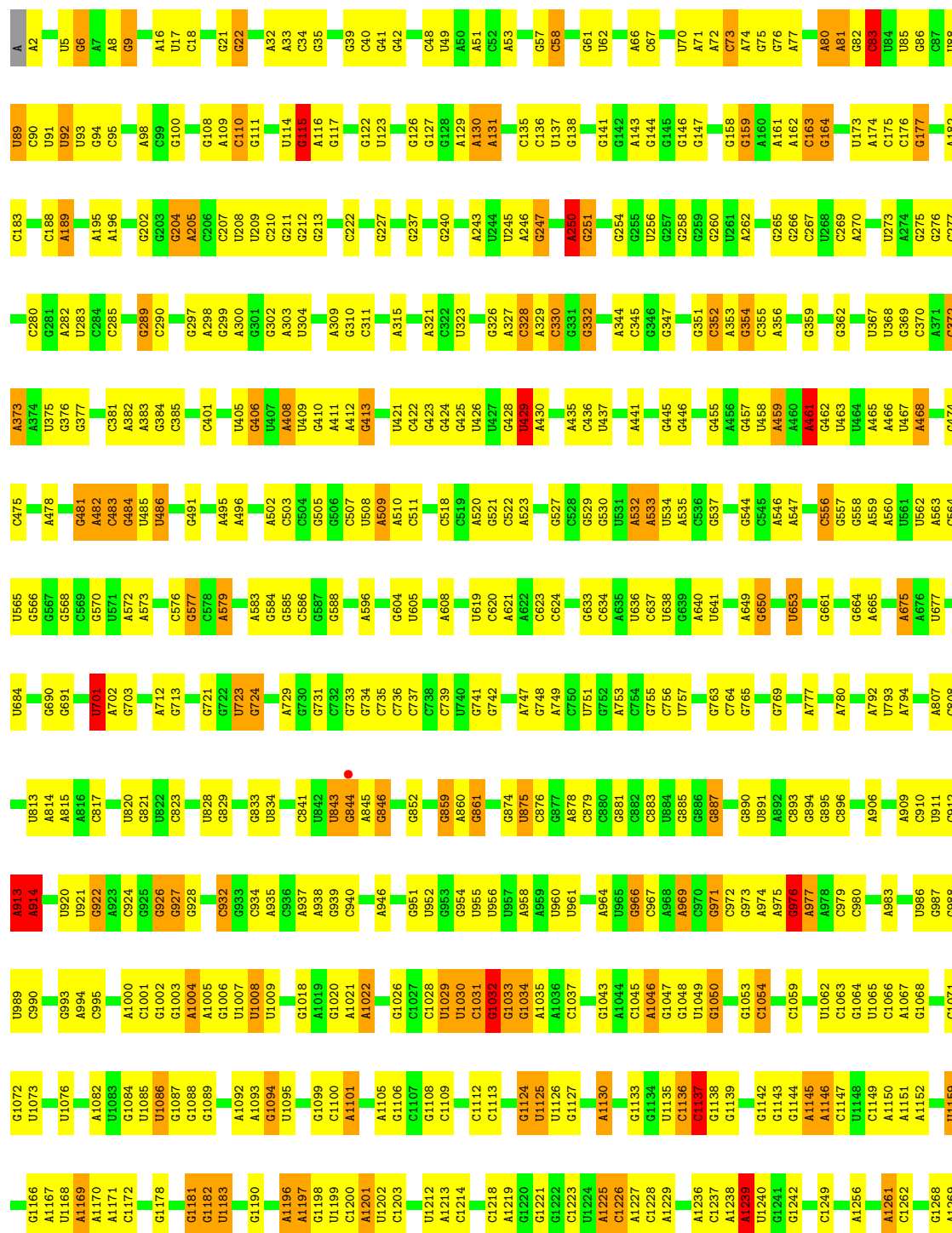


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A1375	G1310	A1238	G1144	C1066	U982	U813	A728	A608	C501	C395	C273	A195	C90
U1376	G1311	U1239	A1145	A983	A905	A814	A729	A609	U508	C396	U273	A196	A98
	G1312	U1240	A1146	A906	A907	A815	A730	U619	A509	G399	C277	A197	C99
	U1315	G1241	U1147	U1072	A909	A816	G731	U625	A510	C400	C285	G198	
G1387	G1316	G1242	U1148	U1073	C910	C817	G732	U626	C511	C401			G108
C1388	G1317	G1244	C1149	U1074	C911	G821	G733	G627		G404	G289	G201	
	C1317	G1245	U1075	U1076	C912	G824	G734	G628	C518	U405	G290	G202	G111
U1391	A1157		A1158	G1077	A914	A825	G735	U632	C525	U406	G292	G203	U114
G1392	C1159	C1249	A913	U1078	A914	C826	C736	U633	C526	U407	G293	G204	
U1393	U1160	A1250	A914	U1079	A914	C827	C737	G636	C527	U408	U294	C205	G115
C1323	C1161		G1162	U1080	U1008	U828	C738	U637	G530	U409		C207	G117
C1325	A1163		A1163	U1081	U1009	G829	C739	C637	U531	G410	A313	U208	
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	U1168	A1257	G1168	U1083	U1011	U834	G742	U642	A533	A412		C210	
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		G1260		U1085	U1013	U836	G744		G537	U420		C214	G128
		G1266		U1086	U1014	C841	G745	A649	G538	U421		G220	A129
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				U1088	U1016	U843	G747	C651		G423		C221	A131
				U1089	U1017	U844	G748	U652	A546	G424		C222	C132
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				U1092	U1020	U847	G751	G664	C549	A430		U225	
				U1093	U1021	U848	G752	A685	C556	A431			G141
				U1094	U1022	U849	G753	A686		A432		G232	G142
				U1095	U1023	U850	G754		A435	A433		G233	A143
				U1096	U1024	U851	G755	G668		A434		G234	A144
				U1097	U1025	U852	G756		A559	A441		G235	G145
				U1098	U1026	U853	G757	U672				A236	G146
				U1099	U1027	U854	G758	A673				G237	
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				U1101	U1029	U856	G760	A675		A452		G240	
				U1102	U1030	U857	G761	A676		A453			G158
				U1103	U1031	U858	G762			G457		A243	G159
				U1104	U1032	U859	G763	G683		U458		U244	A160
				U1105	U1033	U860	G764	U684		A459		A245	A161
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				U1107	U1035	U862	G766	A687		A461		G247	C163
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				U1114	U1042	U869	G773			A468			U173
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				U1118	U1046	U873	G777	U707				G260	G177
				U1119	U1047	U874	G778	C708				U261	A181
				U1120	U1048	U875	G779	G714				A262	A182
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				U1122	U1050	U877	G781	A794				C264	G184
				U1123	U1051	U878	G782					G265	U185
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				U1173	U1101	U928	G832						
				U1174	U1102	U929	G833						
				U1175	U1103	U930	G834						
				U1176	U1104	U931	G835						
				U1177	U1105	U932	G836						
				U1178	U1106	U933	G837						
				U1179	U1107	U934	G838						
				U1180	U1108	U935	G839						
				U1181	U1109	U936	G840						
				U1182	U1110	U937	G841						
				U1183	U1111	U938	G842						
				U1184	U1112	U939	G843						
				U1185	U1113	U940	G844						
				U1186	U1114	U941	G845						
				U1187	U1115	U942	G846						
				U1188	U1116	U943	G847						
				U1189	U1117	U944	G848						
				U1190	U1118	U945	G849						
				U1191	U1119	U946	G850						
				U1192	U1120	U947	G851						
				U1193	U1121	U948	G852						
				U1194	U1122	U949	G853						
				U1195	U1123	U950	G854						
				U1196	U1124	U951	G855						
				U1197	U1125	U952	G856						
				U1198	U1126	U953	G857						
				U1199	U1127	U954	G858						
				U1200	U1128	U955	G859						
				U1201	U1129	U956	G860						
				U1202	U1130	U957	G861						
				U1203	U1131	U958	G862						

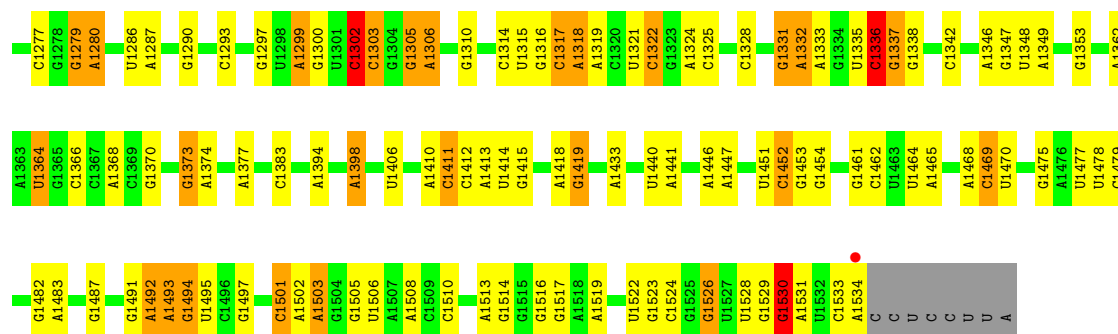


# Molecule 35: 16S rRNA

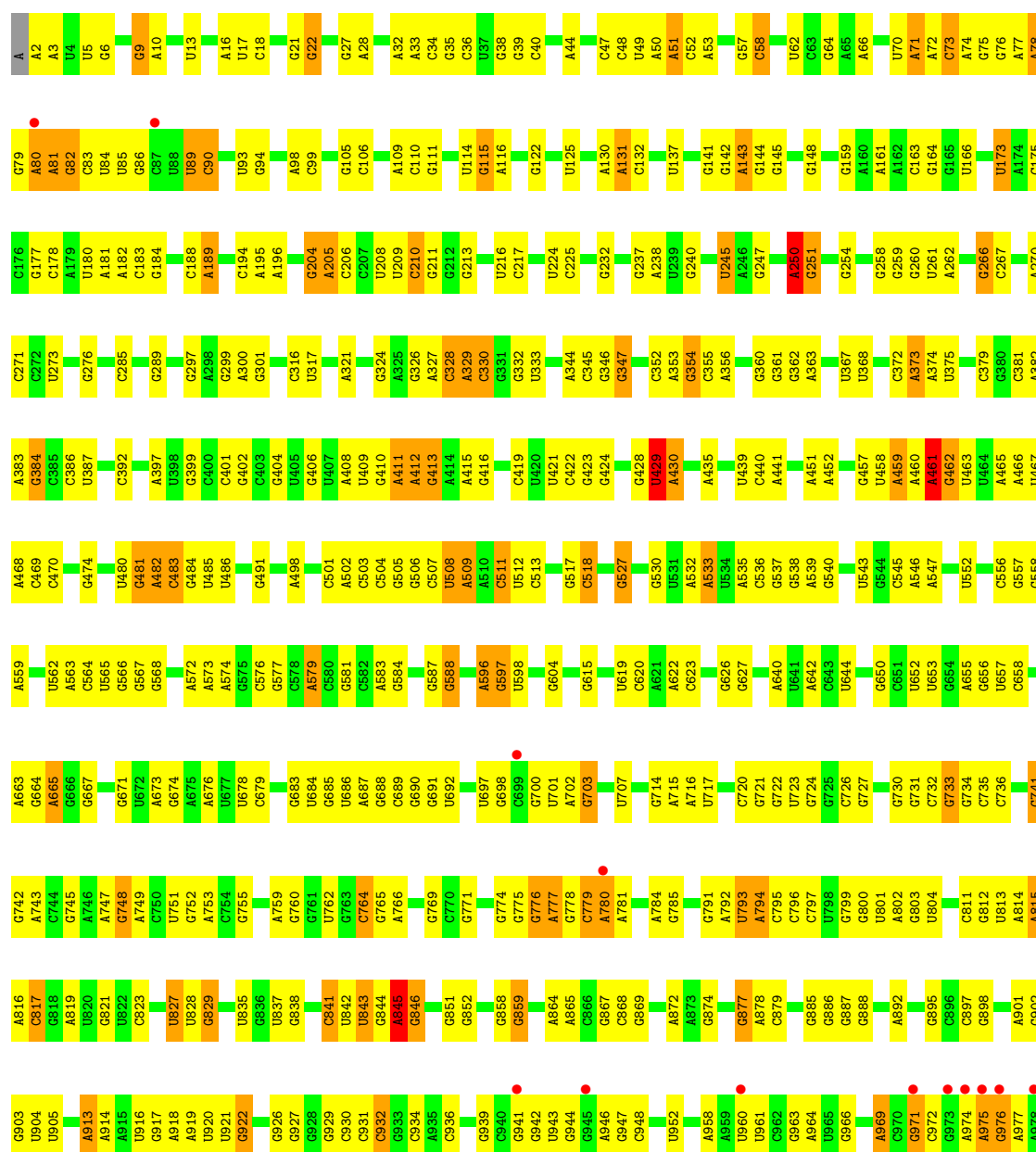
Chain FA: 56% 34% 8% ..

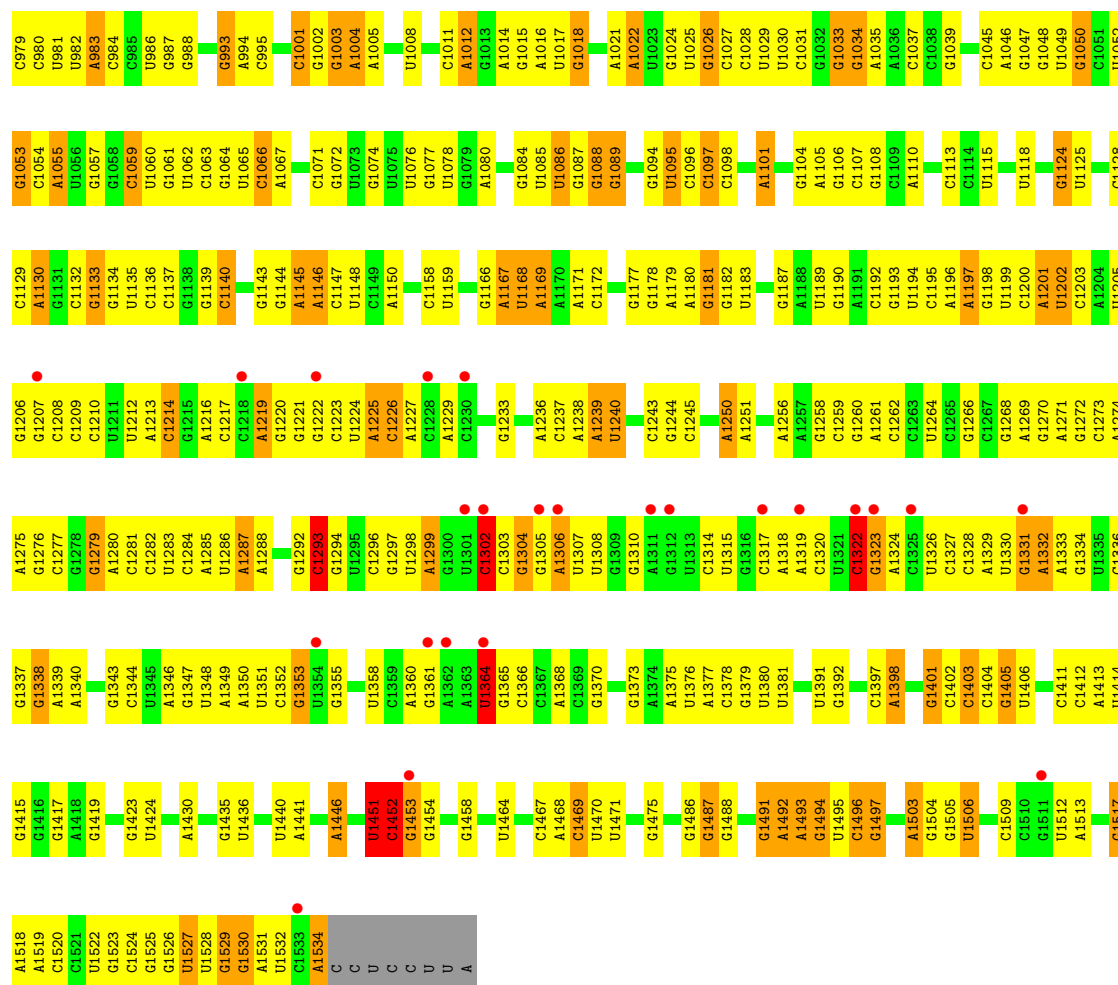






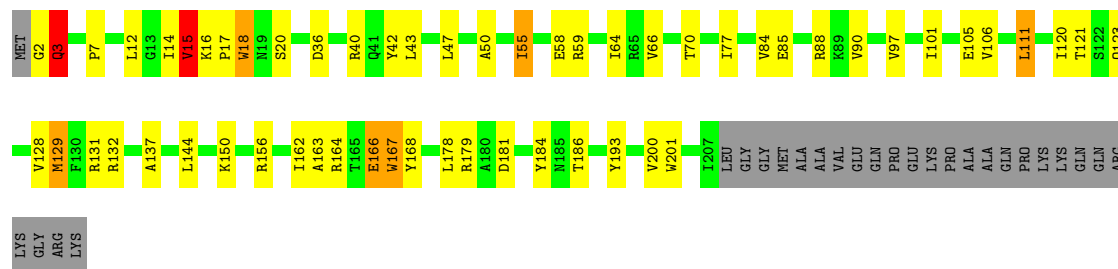
• Molecule 35: 16S rRNA





- Molecule 36: 30S ribosomal protein S3

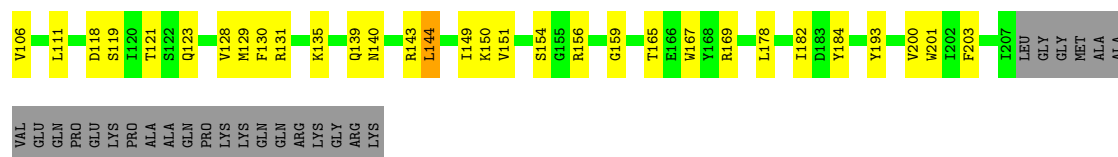
Chain BC:



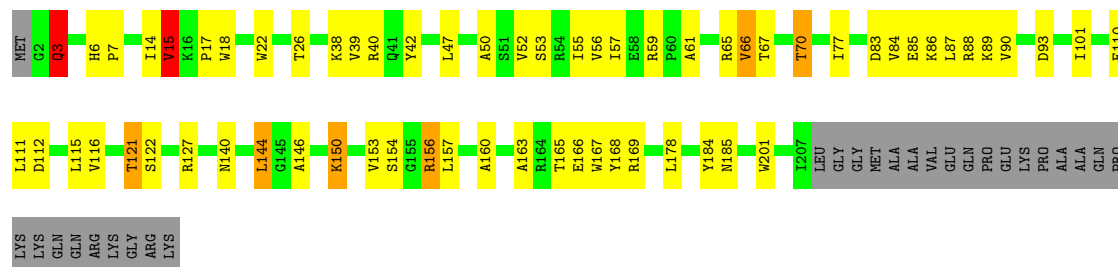
- Molecule 36: 30S ribosomal protein S3

Chain DC:

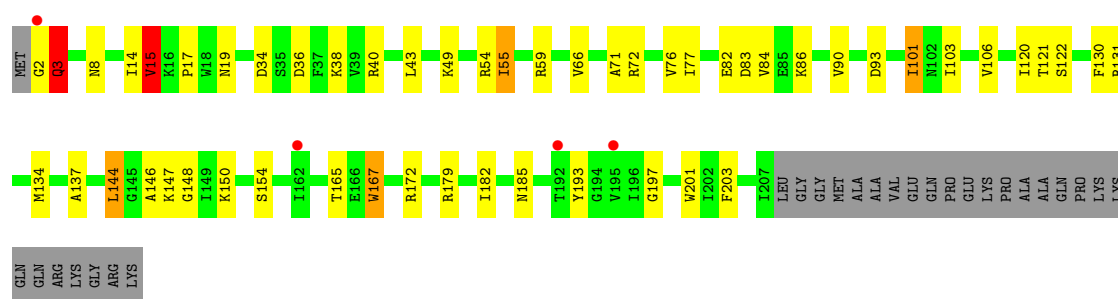




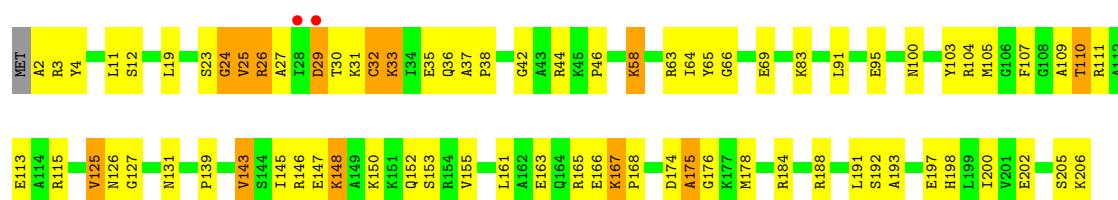
• Molecule 36: 30S ribosomal protein S3



• Molecule 36: 30S ribosomal protein S3

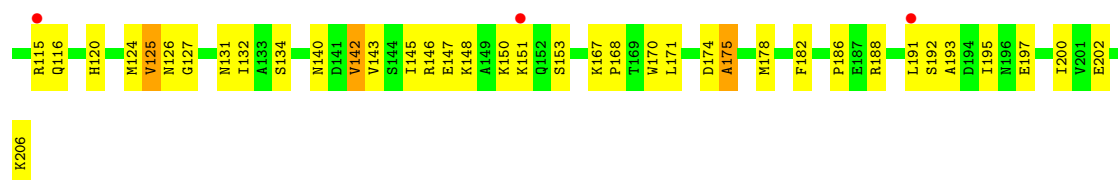


• Molecule 37: 30S ribosomal protein S4

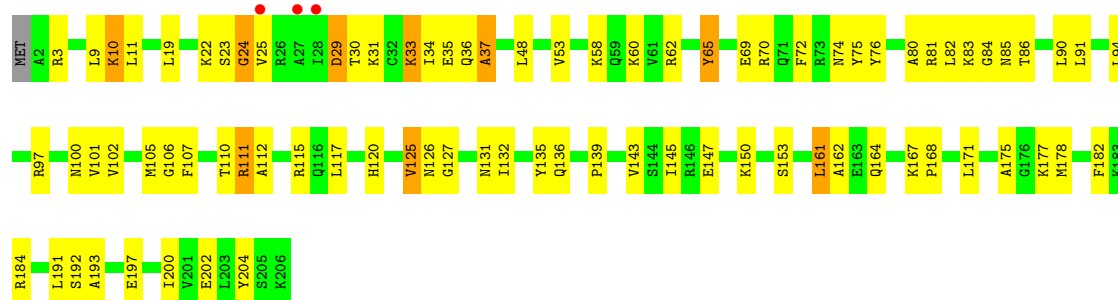


• Molecule 37: 30S ribosomal protein S4

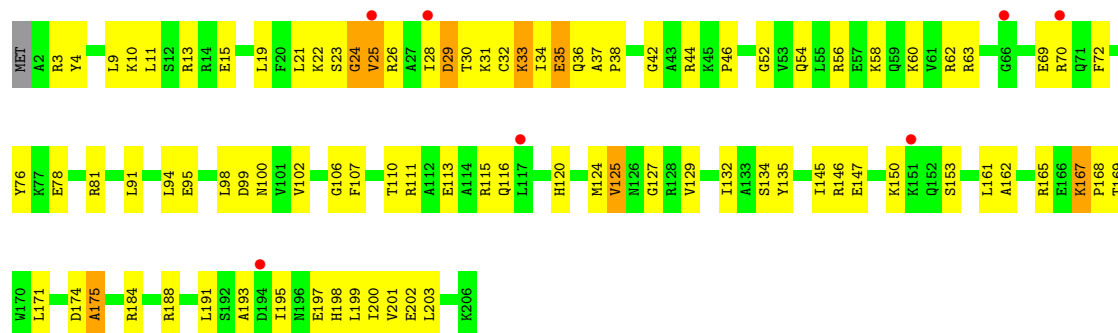




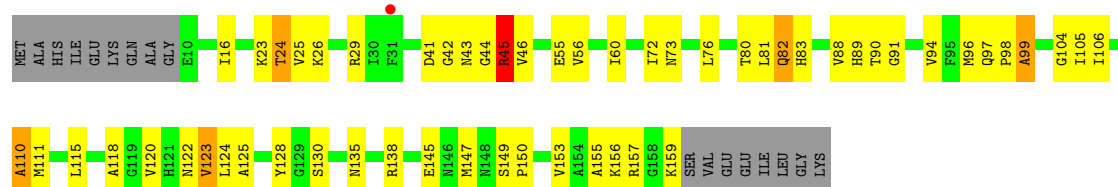
• Molecule 37: 30S ribosomal protein S4



• Molecule 37: 30S ribosomal protein S4

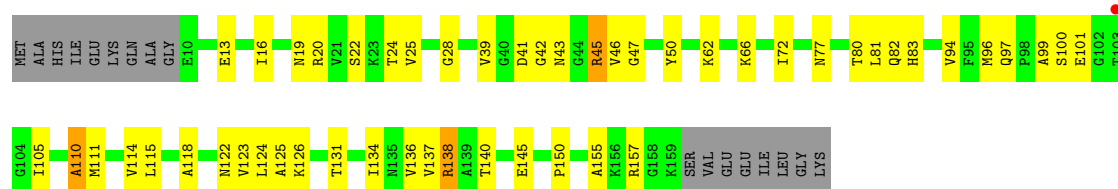


• Molecule 38: 30S ribosomal protein S5

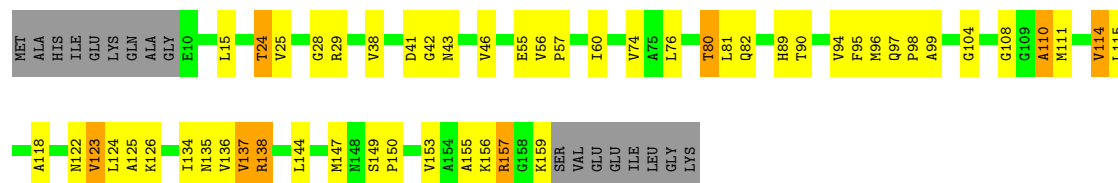


• Molecule 38: 30S ribosomal protein S5

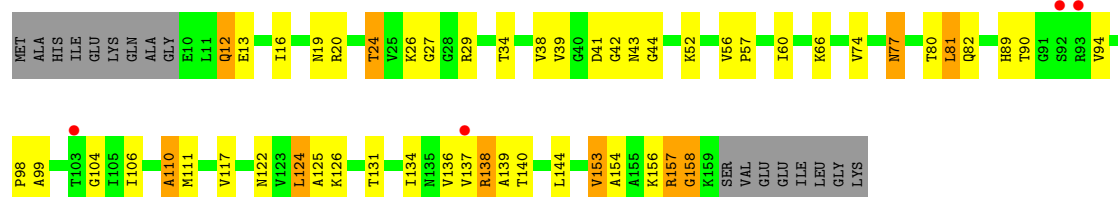




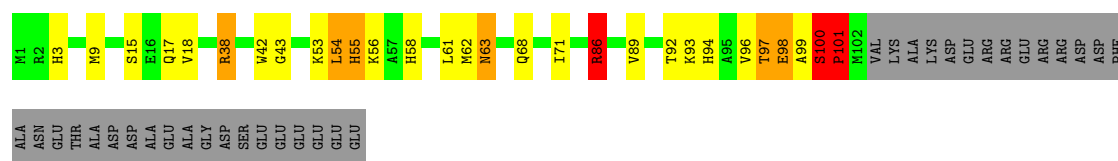
- Molecule 38: 30S ribosomal protein S5



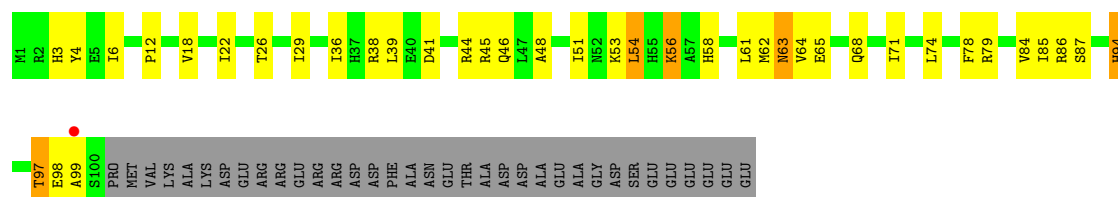
- Molecule 38: 30S ribosomal protein S5



- Molecule 39: 30S ribosomal protein S6



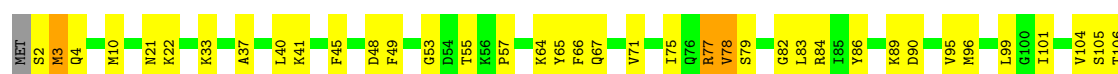
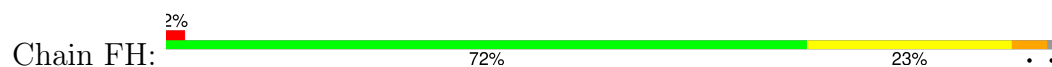
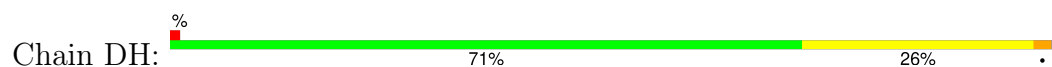
- Molecule 39: 30S ribosomal protein S6



- Molecule 39: 30S ribosomal protein S6

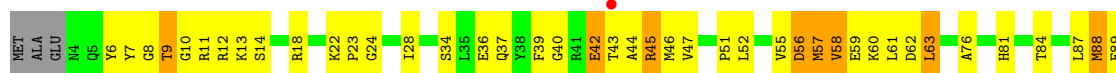


- Chain HG: 





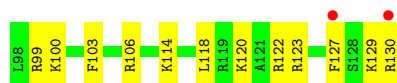
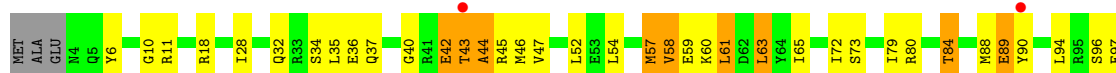
- Molecule 42: 30S ribosomal protein S9



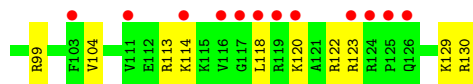
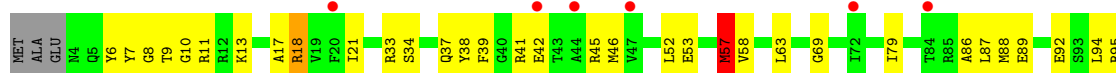
- Molecule 42: 30S ribosomal protein S9



- Molecule 42: 30S ribosomal protein S9



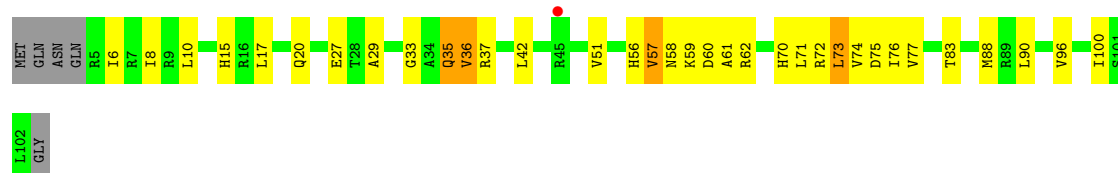
- Molecule 42: 30S ribosomal protein S9



- Molecule 43: 30S ribosomal protein S10







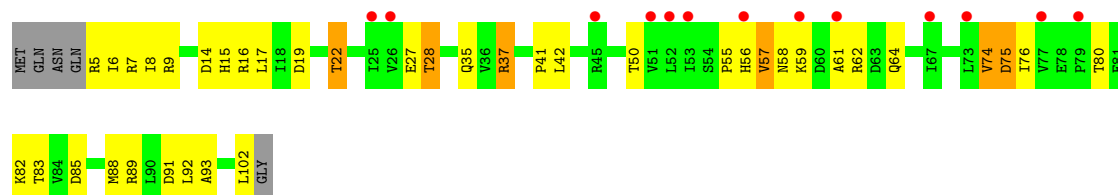
- Molecule 43: 30S ribosomal protein S10



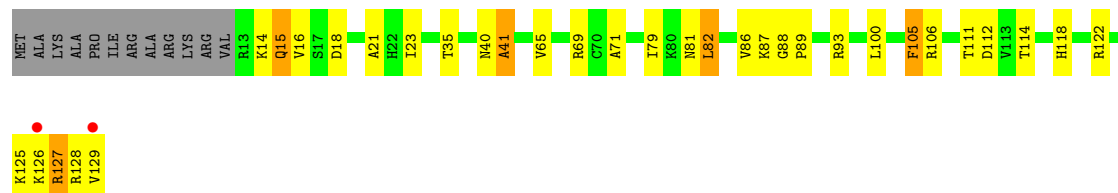
- Molecule 43: 30S ribosomal protein S10



- Molecule 43: 30S ribosomal protein S10

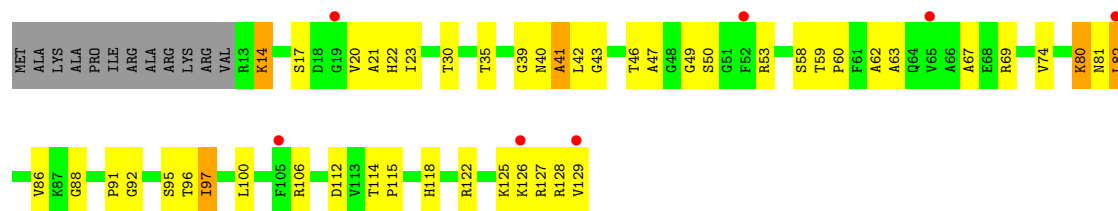


- Molecule 44: 30S ribosomal protein S11

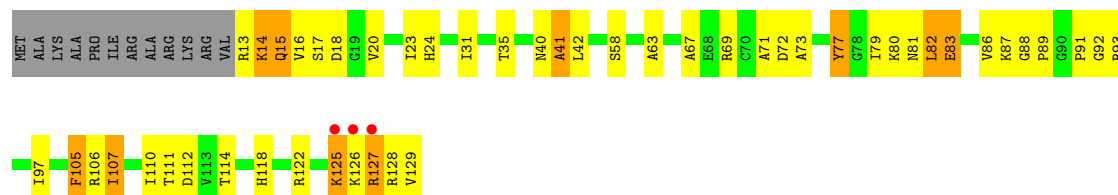


- Molecule 44: 30S ribosomal protein S11

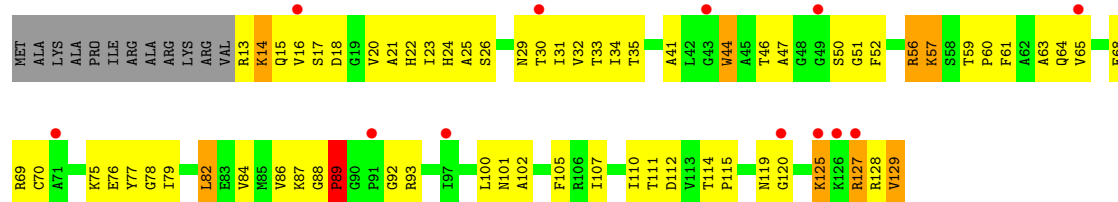




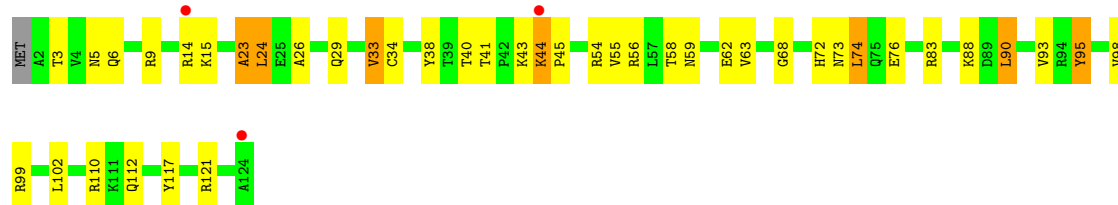
• Molecule 44: 30S ribosomal protein S11



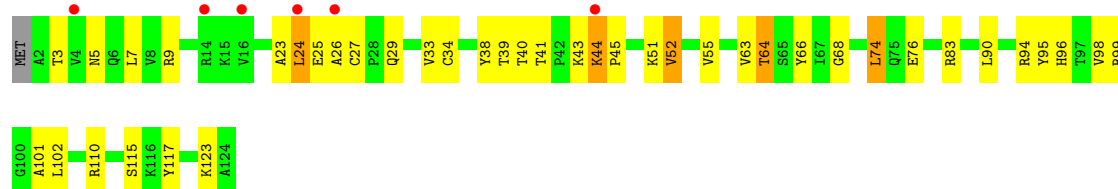
• Molecule 44: 30S ribosomal protein S11



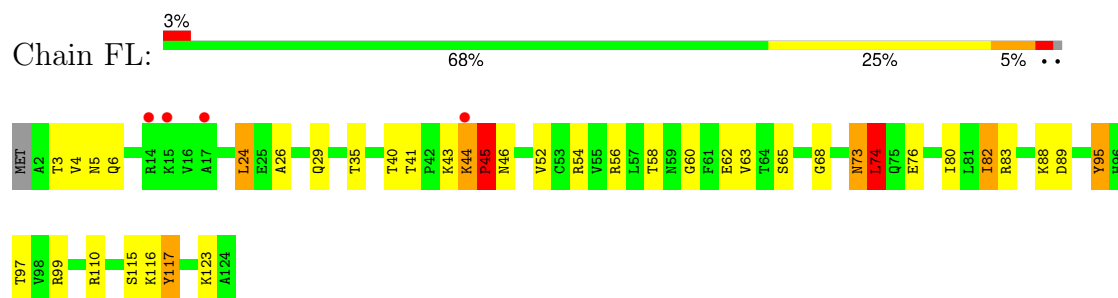
• Molecule 45: 30S ribosomal protein S12



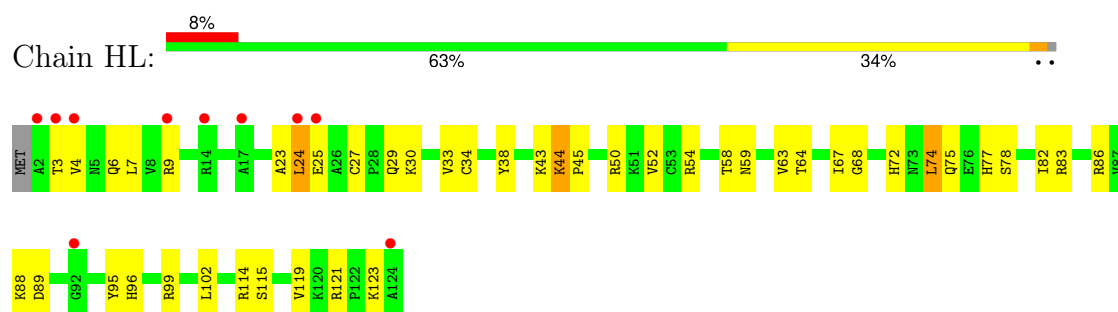
• Molecule 45: 30S ribosomal protein S12



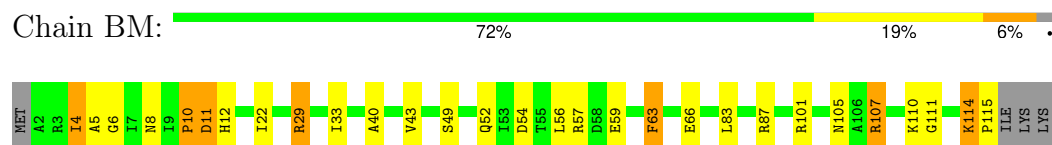
- Molecule 45: 30S ribosomal protein S12



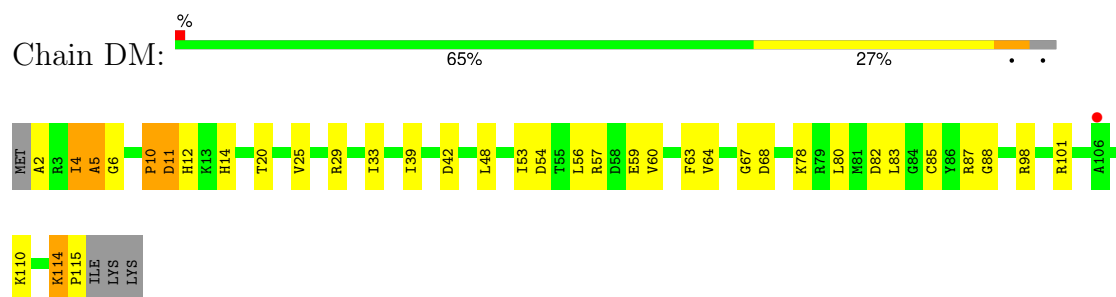
- Molecule 45: 30S ribosomal protein S12



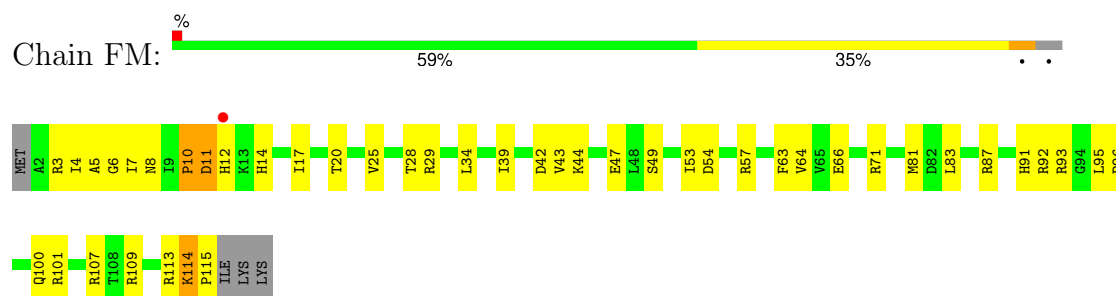
- Molecule 46: 30S ribosomal protein S13



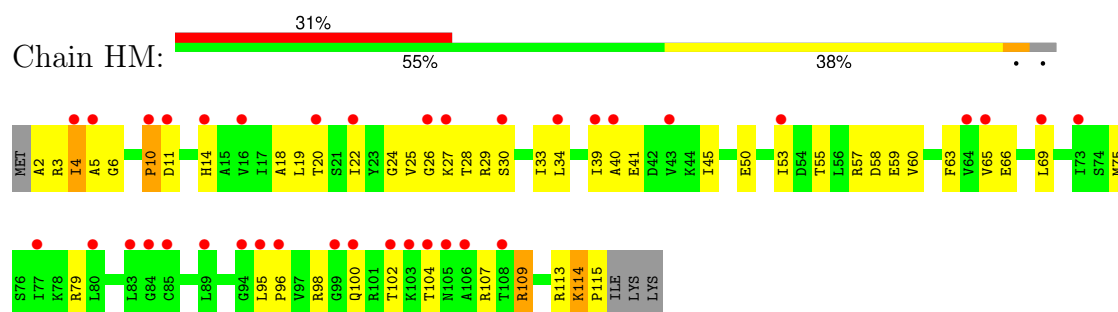
- Molecule 46: 30S ribosomal protein S13



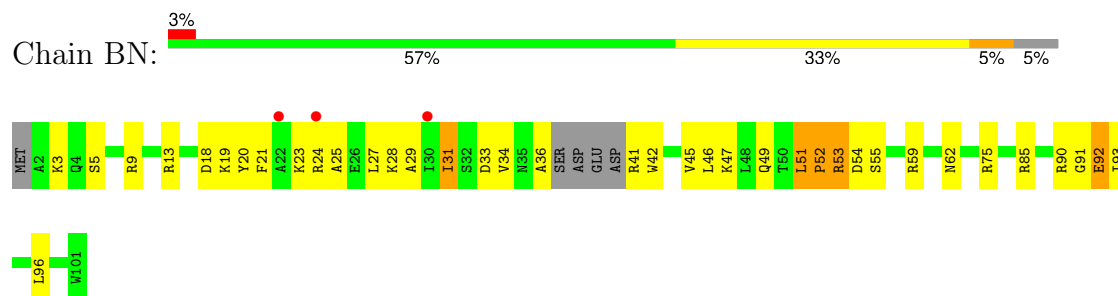
- Molecule 46: 30S ribosomal protein S13



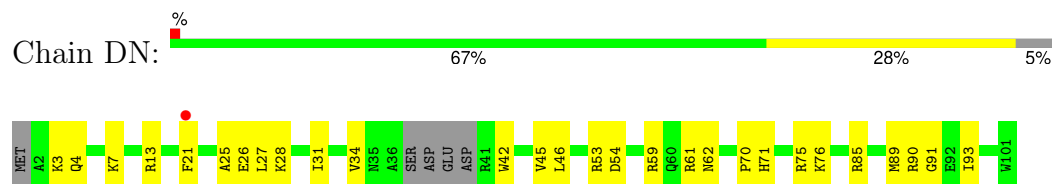
- Molecule 46: 30S ribosomal protein S13



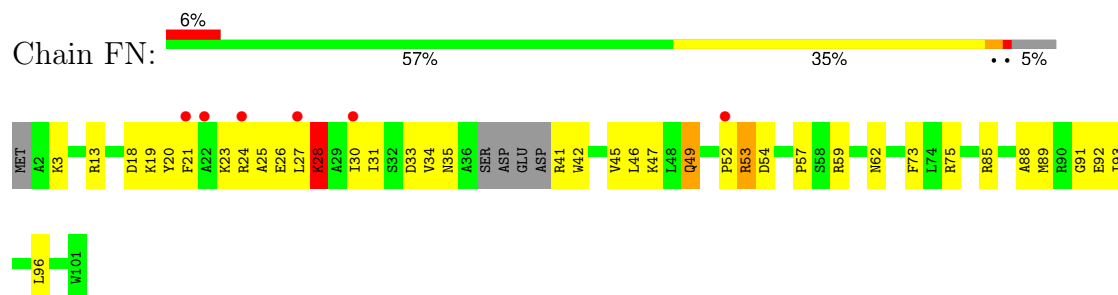
- Molecule 47: 30S ribosomal protein S14



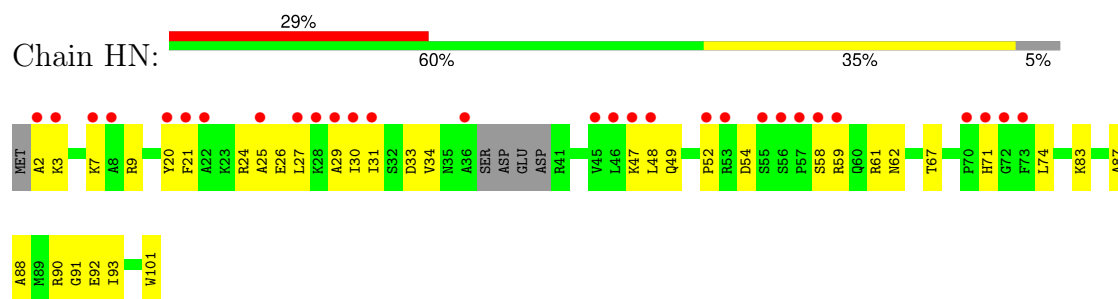
- Molecule 47: 30S ribosomal protein S14




- Molecule 47: 30S ribosomal protein S14



- Molecule 47: 30S ribosomal protein S14




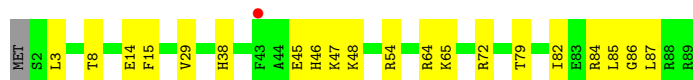
- Molecule 48: 30S ribosomal protein S15

Chain BO:  79% 19% ..




- Molecule 48: 30S ribosomal protein S15

Chain DO:  76% 22% .




- Molecule 48: 30S ribosomal protein S15

Chain FO:  75% 21% ..




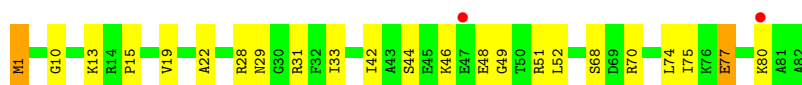
- Molecule 48: 30S ribosomal protein S15

Chain HO:  74% 24% ..



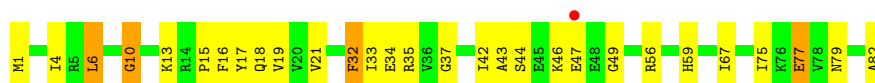
- Molecule 49: 30S ribosomal protein S16

Chain BP:  72% 26% .




- Molecule 49: 30S ribosomal protein S16

Chain DP:  65% 30% 5%

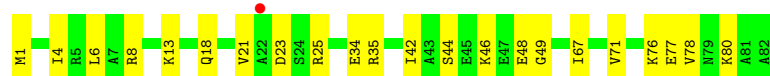
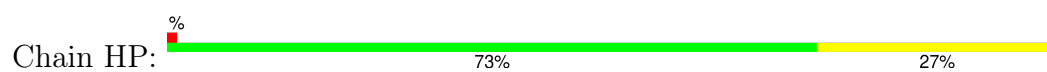


- Molecule 49: 30S ribosomal protein S16

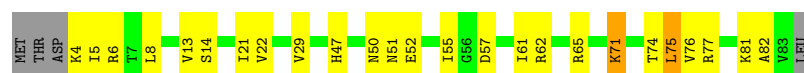
Chain FP:  72% 27% .



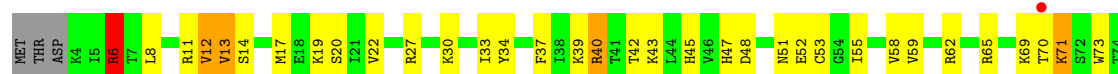
- Molecule 49: 30S ribosomal protein S16



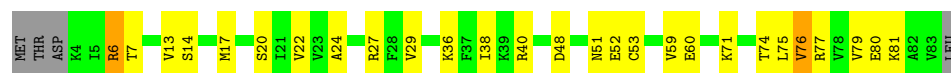
- Molecule 50: 30S ribosomal protein S17



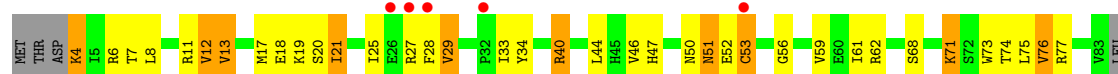
- Molecule 50: 30S ribosomal protein S17



- Molecule 50: 30S ribosomal protein S17



- Molecule 50: 30S ribosomal protein S17

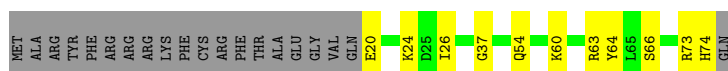


- Molecule 51: 30S ribosomal protein S18

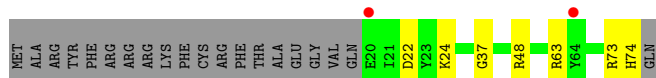


- Molecule 51: 30S ribosomal protein S18

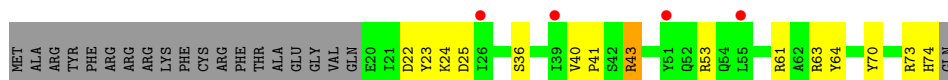




- Molecule 51: 30S ribosomal protein S18



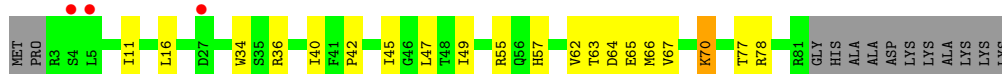
- Molecule 51: 30S ribosomal protein S18



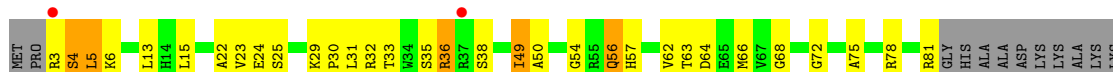
- Molecule 52: 30S ribosomal protein S19



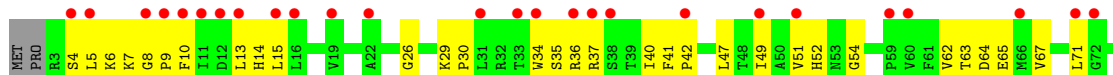
- Molecule 52: 30S ribosomal protein S19



- Molecule 52: 30S ribosomal protein S19



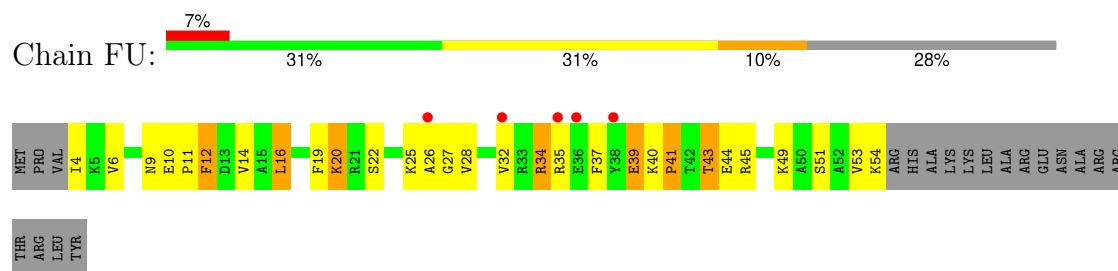
- Molecule 52: 30S ribosomal protein S19



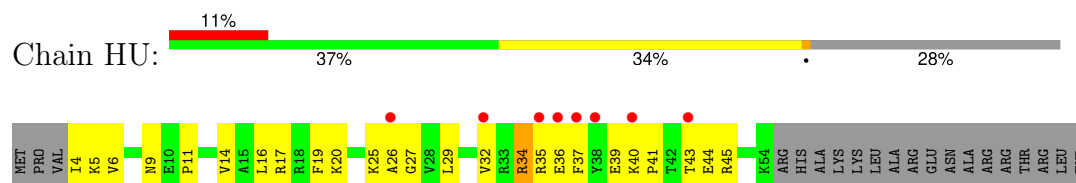




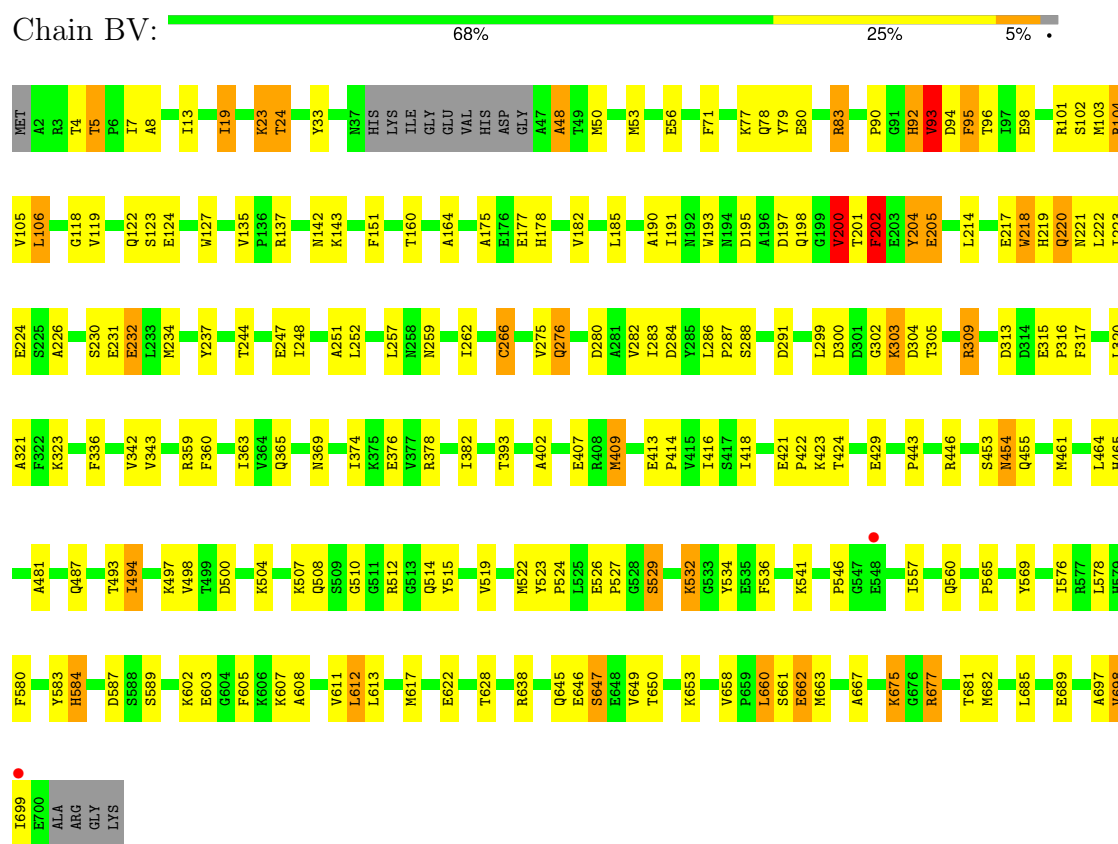
- Molecule 54: 30S ribosomal protein S21



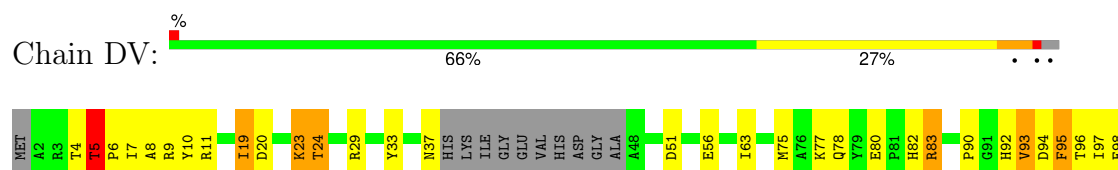
- Molecule 54: 30S ribosomal protein S21

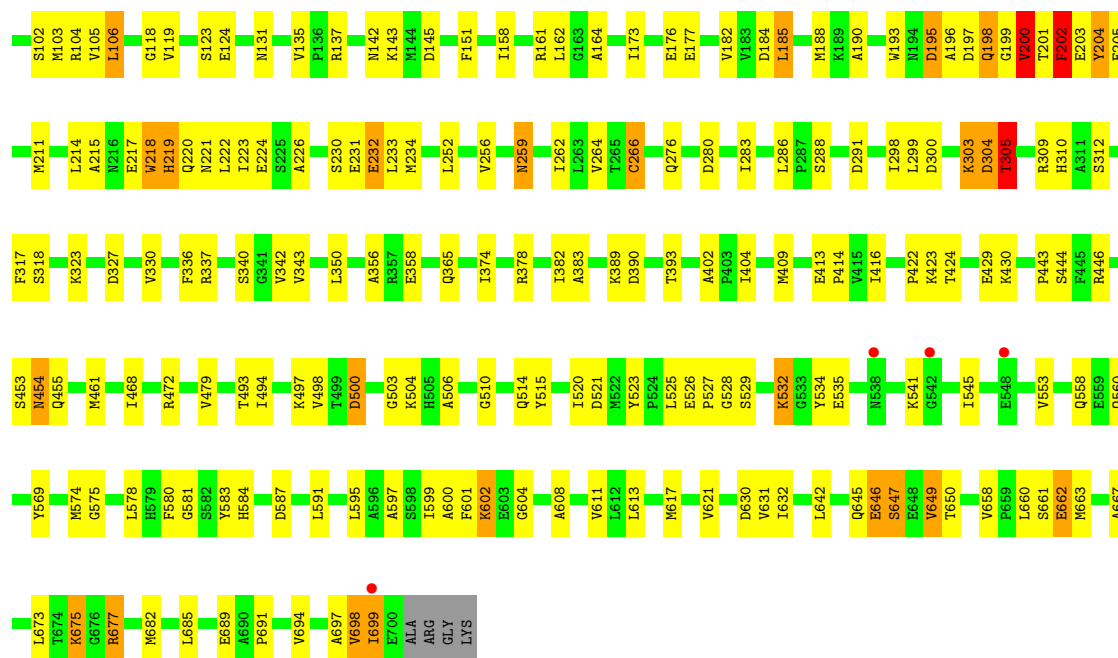


- Molecule 55: Elongation factor G



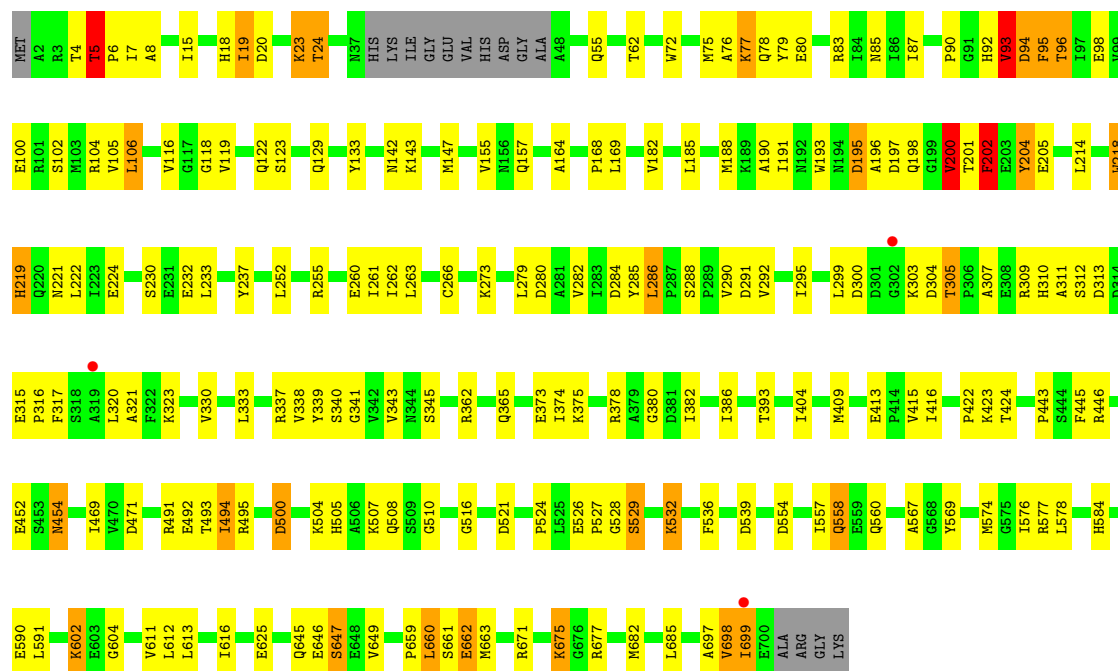
- Molecule 55: Elongation factor G





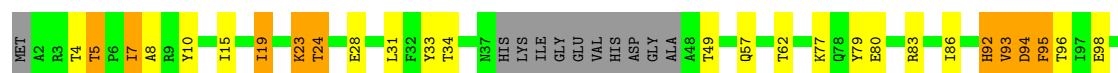
• Molecule 55: Elongation factor G

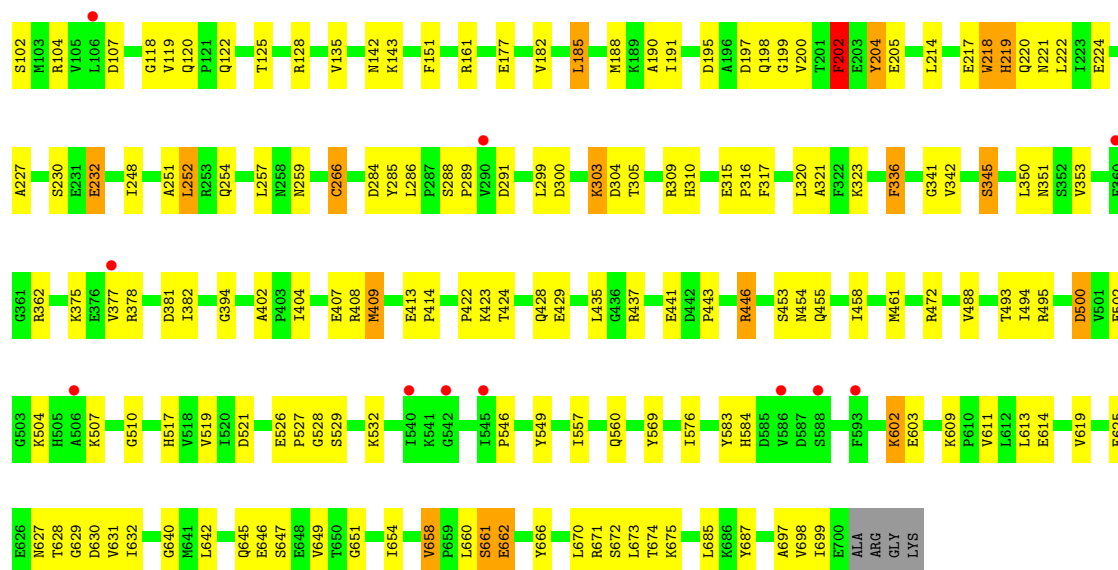
Chain FV: 69% 24%



• Molecule 55: Elongation factor G

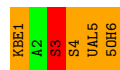
Chain HV: 2% 71% 23%





• Molecule 56: Viomycin

Chain BW: 17% 67% 17%



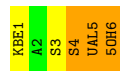
• Molecule 56: Viomycin

Chain DW: 17% 67% 17%



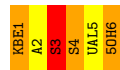
• Molecule 56: Viomycin

Chain FW: 17% 33% 50%



• Molecule 56: Viomycin

Chain HW: 33% 50% 17%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	361.60Å 361.77Å 433.20Å 90.00° 103.57° 90.00°	Depositor
Resolution (Å)	70.00 – 2.90 70.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (70.00-2.90) 78.9 (70.00-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.35 (at 2.91Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.223 , 0.272 0.222 , 0.269	Depositor DCC
$R_{free}$ test set	8388 reflections (0.45%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	73.3	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 19.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	592086	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.65 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4952e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

There are no chirality outliers.

5 of 22 planarity outliers are listed below:

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

## 5.2 Too-close contacts ⓘ

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

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

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

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

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

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

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

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

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

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 11056 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:C5:24:SER:CB	32:C5:116:GLU:HG2	1.46	1.44
32:C5:24:SER:O	32:C5:116:GLU:HB3	1.41	1.16
32:C5:24:SER:HB2	32:C5:116:GLU:CG	1.76	1.14
32:E5:24:SER:HB2	32:E5:116:GLU:HG2	1.27	1.14
3:AA:912:C:OP1	13:AM:8:LYS:NZ	1.79	1.12

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:FA:1029:U:O3'	3:GA:1508:A:N6[1_565]	2.04	0.16
43:FJ:85:ASP:OD1	3:GA:1722:A:O2'[1_565]	2.16	0.04

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	CI	139/142 (98%)	95 (68%)	38 (27%)	6 (4%)	2	8
9	EI	139/142 (98%)	97 (70%)	38 (27%)	4 (3%)	3	15
9	GI	139/142 (98%)	95 (68%)	34 (24%)	10 (7%)	1	2
10	AJ	140/142 (99%)	113 (81%)	18 (13%)	9 (6%)	1	3
10	CJ	140/142 (99%)	112 (80%)	20 (14%)	8 (6%)	1	4
10	EJ	140/142 (99%)	114 (81%)	17 (12%)	9 (6%)	1	3
10	GJ	140/142 (99%)	113 (81%)	19 (14%)	8 (6%)	1	4
11	AK	120/123 (98%)	96 (80%)	14 (12%)	10 (8%)	0	2
11	CK	120/123 (98%)	93 (78%)	21 (18%)	6 (5%)	1	6
11	EK	120/123 (98%)	92 (77%)	21 (18%)	7 (6%)	1	4
11	GK	120/123 (98%)	92 (77%)	20 (17%)	8 (7%)	1	3
12	AL	141/144 (98%)	104 (74%)	32 (23%)	5 (4%)	3	12
12	CL	141/144 (98%)	103 (73%)	33 (23%)	5 (4%)	3	12
12	EL	141/144 (98%)	108 (77%)	26 (18%)	7 (5%)	1	6
12	GL	141/144 (98%)	103 (73%)	32 (23%)	6 (4%)	2	8
13	AM	134/136 (98%)	107 (80%)	16 (12%)	11 (8%)	1	2
13	CM	134/136 (98%)	110 (82%)	16 (12%)	8 (6%)	1	4
13	EM	134/136 (98%)	106 (79%)	18 (13%)	10 (8%)	1	2
13	GM	134/136 (98%)	109 (81%)	17 (13%)	8 (6%)	1	4
14	AN	118/127 (93%)	101 (86%)	16 (14%)	1 (1%)	16	45
14	CN	118/127 (93%)	103 (87%)	14 (12%)	1 (1%)	16	45
14	EN	118/127 (93%)	100 (85%)	17 (14%)	1 (1%)	16	45
14	GN	118/127 (93%)	98 (83%)	19 (16%)	1 (1%)	16	45
15	AO	114/117 (97%)	95 (83%)	18 (16%)	1 (1%)	14	43
15	CO	114/117 (97%)	95 (83%)	15 (13%)	4 (4%)	3	12
15	EO	114/117 (97%)	95 (83%)	18 (16%)	1 (1%)	14	43
15	GO	114/117 (97%)	95 (83%)	15 (13%)	4 (4%)	3	12
16	AP	112/115 (97%)	86 (77%)	17 (15%)	9 (8%)	1	2
16	CP	112/115 (97%)	87 (78%)	16 (14%)	9 (8%)	1	2
16	EP	112/115 (97%)	84 (75%)	16 (14%)	12 (11%)	0	1
16	GP	112/115 (97%)	85 (76%)	19 (17%)	8 (7%)	1	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	AQ	115/118 (98%)	99 (86%)	12 (10%)	4 (4%)	3	12
17	CQ	115/118 (98%)	99 (86%)	12 (10%)	4 (4%)	3	12
17	EQ	115/118 (98%)	99 (86%)	12 (10%)	4 (4%)	3	12
17	GQ	115/118 (98%)	99 (86%)	14 (12%)	2 (2%)	7	27
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%)	83 (82%)	13 (13%)	5 (5%)	1	6
19	AS	108/110 (98%)	94 (87%)	9 (8%)	5 (5%)	2	8
19	CS	108/110 (98%)	95 (88%)	9 (8%)	4 (4%)	2	11
19	ES	108/110 (98%)	92 (85%)	10 (9%)	6 (6%)	1	4
19	GS	108/110 (98%)	91 (84%)	11 (10%)	6 (6%)	1	4
20	AT	91/100 (91%)	57 (63%)	24 (26%)	10 (11%)	0	1
20	CT	91/100 (91%)	55 (60%)	25 (28%)	11 (12%)	0	1
20	ET	91/100 (91%)	56 (62%)	26 (29%)	9 (10%)	0	1
20	GT	91/100 (91%)	58 (64%)	23 (25%)	10 (11%)	0	1
21	AU	100/104 (96%)	74 (74%)	16 (16%)	10 (10%)	0	1
21	CU	100/104 (96%)	75 (75%)	17 (17%)	8 (8%)	1	2
21	EU	100/104 (96%)	74 (74%)	15 (15%)	11 (11%)	0	1
21	GU	100/104 (96%)	76 (76%)	14 (14%)	10 (10%)	0	1
22	AV	92/94 (98%)	81 (88%)	11 (12%)	0	100	100
22	CV	92/94 (98%)	80 (87%)	11 (12%)	1 (1%)	12	37
22	EV	92/94 (98%)	80 (87%)	12 (13%)	0	100	100
22	GV	92/94 (98%)	78 (85%)	13 (14%)	1 (1%)	12	37
23	AW	77/85 (91%)	39 (51%)	22 (29%)	16 (21%)	0	0
23	CW	77/85 (91%)	41 (53%)	17 (22%)	19 (25%)	0	0
23	EW	77/85 (91%)	41 (53%)	21 (27%)	15 (20%)	0	0
23	GW	77/85 (91%)	40 (52%)	21 (27%)	16 (21%)	0	0
24	AX	75/78 (96%)	64 (85%)	8 (11%)	3 (4%)	2	10
24	CX	75/78 (96%)	63 (84%)	10 (13%)	2 (3%)	4	17
24	EX	75/78 (96%)	63 (84%)	9 (12%)	3 (4%)	2	10

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	E5	143/165 (87%)	79 (55%)	41 (29%)	23 (16%)	0	0
33	A6	28/121 (23%)	20 (71%)	7 (25%)	1 (4%)	3	12
34	BB	216/241 (90%)	151 (70%)	51 (24%)	14 (6%)	1	3
34	DB	216/241 (90%)	157 (73%)	47 (22%)	12 (6%)	1	4
34	FB	216/241 (90%)	153 (71%)	51 (24%)	12 (6%)	1	4
34	HB	216/241 (90%)	153 (71%)	51 (24%)	12 (6%)	1	4
36	BC	204/233 (88%)	181 (89%)	18 (9%)	5 (2%)	4	18
36	DC	204/233 (88%)	179 (88%)	20 (10%)	5 (2%)	4	18
36	FC	204/233 (88%)	180 (88%)	18 (9%)	6 (3%)	3	15
36	HC	204/233 (88%)	181 (89%)	17 (8%)	6 (3%)	3	15
37	BD	203/206 (98%)	162 (80%)	30 (15%)	11 (5%)	1	5
37	DD	203/206 (98%)	162 (80%)	29 (14%)	12 (6%)	1	4
37	FD	203/206 (98%)	163 (80%)	29 (14%)	11 (5%)	1	5
37	HD	203/206 (98%)	165 (81%)	26 (13%)	12 (6%)	1	4
38	BE	148/167 (89%)	123 (83%)	18 (12%)	7 (5%)	2	7
38	DE	148/167 (89%)	125 (84%)	18 (12%)	5 (3%)	3	13
38	FE	148/167 (89%)	122 (82%)	20 (14%)	6 (4%)	2	9
38	HE	148/167 (89%)	121 (82%)	20 (14%)	7 (5%)	2	7
39	BF	100/135 (74%)	79 (79%)	15 (15%)	6 (6%)	1	4
39	DF	98/135 (73%)	80 (82%)	13 (13%)	5 (5%)	1	6
39	FF	98/135 (73%)	81 (83%)	11 (11%)	6 (6%)	1	4
39	HF	98/135 (73%)	76 (78%)	18 (18%)	4 (4%)	2	9
40	BG	149/179 (83%)	128 (86%)	20 (13%)	1 (1%)	19	49
40	DG	149/179 (83%)	125 (84%)	22 (15%)	2 (1%)	10	33
40	FG	149/179 (83%)	127 (85%)	21 (14%)	1 (1%)	19	49
40	HG	149/179 (83%)	127 (85%)	20 (13%)	2 (1%)	10	33
41	BH	127/130 (98%)	114 (90%)	12 (9%)	1 (1%)	16	45
41	DH	127/130 (98%)	113 (89%)	12 (9%)	2 (2%)	8	28
41	FH	127/130 (98%)	112 (88%)	13 (10%)	2 (2%)	8	28
41	HH	127/130 (98%)	112 (88%)	13 (10%)	2 (2%)	8	28
42	BI	125/130 (96%)	105 (84%)	14 (11%)	6 (5%)	2	7

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

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

5 of 1342 Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AC	216/218 (99%)	202 (94%)	14 (6%)	14	40
2	CC	216/218 (99%)	197 (91%)	19 (9%)	8	26
2	EC	216/218 (99%)	194 (90%)	22 (10%)	6	19
2	GC	216/218 (99%)	203 (94%)	13 (6%)	16	44
4	AD	164/164 (100%)	151 (92%)	13 (8%)	10	30
4	CD	164/164 (100%)	152 (93%)	12 (7%)	11	34
4	ED	164/164 (100%)	152 (93%)	12 (7%)	11	34
4	GD	164/164 (100%)	151 (92%)	13 (8%)	10	30
5	AE	165/165 (100%)	146 (88%)	19 (12%)	4	15
5	CE	165/165 (100%)	157 (95%)	8 (5%)	21	54
5	EE	165/165 (100%)	153 (93%)	12 (7%)	11	34
5	GE	165/165 (100%)	152 (92%)	13 (8%)	10	30
6	AF	148/150 (99%)	138 (93%)	10 (7%)	13	38
6	CF	148/150 (99%)	140 (95%)	8 (5%)	18	49
6	EF	148/150 (99%)	133 (90%)	15 (10%)	6	20
6	GF	148/150 (99%)	146 (99%)	2 (1%)	62	86
7	AG	137/138 (99%)	122 (89%)	15 (11%)	5	17
7	CG	137/138 (99%)	125 (91%)	12 (9%)	8	26
7	EG	137/138 (99%)	119 (87%)	18 (13%)	3	10
7	GG	137/138 (99%)	128 (93%)	9 (7%)	14	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	AH	40/40 (100%)	39 (98%)	1 (2%)	42	75
8	CH	40/40 (100%)	38 (95%)	2 (5%)	20	52
8	EH	40/40 (100%)	37 (92%)	3 (8%)	11	33
8	GH	40/40 (100%)	39 (98%)	1 (2%)	42	75
9	AI	109/110 (99%)	105 (96%)	4 (4%)	29	64
9	CI	109/110 (99%)	106 (97%)	3 (3%)	38	73
9	EI	109/110 (99%)	106 (97%)	3 (3%)	38	73
9	GI	109/110 (99%)	107 (98%)	2 (2%)	54	82
10	AJ	116/116 (100%)	100 (86%)	16 (14%)	3	9
10	CJ	116/116 (100%)	101 (87%)	15 (13%)	3	11
10	EJ	116/116 (100%)	97 (84%)	19 (16%)	2	6
10	GJ	116/116 (100%)	104 (90%)	12 (10%)	6	19
11	AK	103/104 (99%)	92 (89%)	11 (11%)	5	17
11	CK	103/104 (99%)	87 (84%)	16 (16%)	2	7
11	EK	103/104 (99%)	87 (84%)	16 (16%)	2	7
11	GK	103/104 (99%)	90 (87%)	13 (13%)	3	11
12	AL	102/103 (99%)	95 (93%)	7 (7%)	13	37
12	CL	102/103 (99%)	94 (92%)	8 (8%)	10	31
12	EL	102/103 (99%)	96 (94%)	6 (6%)	16	45
12	GL	102/103 (99%)	96 (94%)	6 (6%)	16	45
13	AM	109/109 (100%)	93 (85%)	16 (15%)	2	8
13	CM	109/109 (100%)	98 (90%)	11 (10%)	6	20
13	EM	109/109 (100%)	100 (92%)	9 (8%)	9	28
13	GM	109/109 (100%)	103 (94%)	6 (6%)	18	48
14	AN	100/103 (97%)	93 (93%)	7 (7%)	12	36
14	CN	100/103 (97%)	96 (96%)	4 (4%)	27	61
14	EN	100/103 (97%)	96 (96%)	4 (4%)	27	61
14	GN	100/103 (97%)	93 (93%)	7 (7%)	12	36
15	AO	86/87 (99%)	78 (91%)	8 (9%)	7	23
15	CO	86/87 (99%)	80 (93%)	6 (7%)	12	36
15	EO	86/87 (99%)	81 (94%)	5 (6%)	17	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	GO	86/87 (99%)	81 (94%)	5 (6%)	17	46
16	AP	99/100 (99%)	91 (92%)	8 (8%)	9	29
16	CP	99/100 (99%)	90 (91%)	9 (9%)	7	25
16	EP	99/100 (99%)	88 (89%)	11 (11%)	5	16
16	GP	99/100 (99%)	90 (91%)	9 (9%)	7	25
17	AQ	89/90 (99%)	81 (91%)	8 (9%)	8	25
17	CQ	89/90 (99%)	84 (94%)	5 (6%)	17	47
17	EQ	89/90 (99%)	83 (93%)	6 (7%)	13	39
17	GQ	89/90 (99%)	83 (93%)	6 (7%)	13	39
18	AR	84/84 (100%)	78 (93%)	6 (7%)	12	36
18	CR	84/84 (100%)	79 (94%)	5 (6%)	16	44
18	ER	84/84 (100%)	76 (90%)	8 (10%)	7	22
18	GR	84/84 (100%)	79 (94%)	5 (6%)	16	44
19	AS	93/93 (100%)	84 (90%)	9 (10%)	6	22
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%)	88 (95%)	5 (5%)	18	49
20	AT	80/84 (95%)	77 (96%)	3 (4%)	28	63
20	CT	80/84 (95%)	75 (94%)	5 (6%)	15	42
20	ET	80/84 (95%)	74 (92%)	6 (8%)	11	33
20	GT	80/84 (95%)	77 (96%)	3 (4%)	28	63
21	AU	83/85 (98%)	76 (92%)	7 (8%)	9	28
21	CU	83/85 (98%)	80 (96%)	3 (4%)	30	65
21	EU	83/85 (98%)	78 (94%)	5 (6%)	16	44
21	GU	83/85 (98%)	79 (95%)	4 (5%)	21	54
22	AV	78/78 (100%)	75 (96%)	3 (4%)	28	63
22	CV	78/78 (100%)	73 (94%)	5 (6%)	14	41
22	EV	78/78 (100%)	75 (96%)	3 (4%)	28	63
22	GV	78/78 (100%)	77 (99%)	1 (1%)	65	88
23	AW	59/63 (94%)	53 (90%)	6 (10%)	6	19
23	CW	59/63 (94%)	55 (93%)	4 (7%)	13	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	EW	59/63 (94%)	49 (83%)	10 (17%)	1	5
23	GW	59/63 (94%)	57 (97%)	2 (3%)	32	67
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%)	57 (85%)	10 (15%)	2	8
24	GX	67/68 (98%)	63 (94%)	4 (6%)	16	44
25	AY	55/55 (100%)	52 (94%)	3 (6%)	18	48
25	CY	55/55 (100%)	51 (93%)	4 (7%)	11	34
25	EY	55/55 (100%)	50 (91%)	5 (9%)	7	25
25	GY	55/55 (100%)	52 (94%)	3 (6%)	18	48
26	AZ	48/49 (98%)	40 (83%)	8 (17%)	2	5
26	CZ	48/49 (98%)	39 (81%)	9 (19%)	1	4
26	EZ	48/49 (98%)	41 (85%)	7 (15%)	2	8
26	GZ	48/49 (98%)	46 (96%)	2 (4%)	25	59
27	A0	47/48 (98%)	46 (98%)	1 (2%)	48	78
27	C0	47/48 (98%)	47 (100%)	0	100	100
27	E0	47/48 (98%)	46 (98%)	1 (2%)	48	78
27	G0	47/48 (98%)	45 (96%)	2 (4%)	25	57
28	A1	45/49 (92%)	42 (93%)	3 (7%)	13	39
28	C1	45/49 (92%)	42 (93%)	3 (7%)	13	39
28	E1	45/49 (92%)	42 (93%)	3 (7%)	13	39
28	G1	45/49 (92%)	43 (96%)	2 (4%)	24	57
29	A2	38/38 (100%)	35 (92%)	3 (8%)	10	30
29	C2	38/38 (100%)	34 (90%)	4 (10%)	5	18
29	E2	38/38 (100%)	36 (95%)	2 (5%)	19	49
29	G2	38/38 (100%)	35 (92%)	3 (8%)	10	30
30	A3	51/52 (98%)	46 (90%)	5 (10%)	6	21
30	C3	51/52 (98%)	49 (96%)	2 (4%)	27	62
30	E3	51/52 (98%)	47 (92%)	4 (8%)	10	31
30	G3	51/52 (98%)	48 (94%)	3 (6%)	16	45
31	A4	34/34 (100%)	31 (91%)	3 (9%)	8	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	33 (97%)	1 (3%)	37	72
32	A5	112/123 (91%)	93 (83%)	19 (17%)	1	5
32	C5	112/123 (91%)	95 (85%)	17 (15%)	2	7
32	E5	111/123 (90%)	93 (84%)	18 (16%)	2	6
33	A6	26/85 (31%)	22 (85%)	4 (15%)	2	7
34	BB	180/199 (90%)	170 (94%)	10 (6%)	17	47
34	DB	180/199 (90%)	170 (94%)	10 (6%)	17	47
34	FB	180/199 (90%)	171 (95%)	9 (5%)	20	52
34	HB	180/199 (90%)	174 (97%)	6 (3%)	33	68
36	BC	170/190 (90%)	156 (92%)	14 (8%)	9	29
36	DC	170/190 (90%)	162 (95%)	8 (5%)	22	55
36	FC	170/190 (90%)	158 (93%)	12 (7%)	12	36
36	HC	170/190 (90%)	163 (96%)	7 (4%)	26	60
37	BD	172/173 (99%)	165 (96%)	7 (4%)	26	60
37	DD	172/173 (99%)	163 (95%)	9 (5%)	19	50
37	FD	172/173 (99%)	165 (96%)	7 (4%)	26	60
37	HD	172/173 (99%)	167 (97%)	5 (3%)	37	72
38	BE	113/126 (90%)	108 (96%)	5 (4%)	24	57
38	DE	113/126 (90%)	109 (96%)	4 (4%)	31	66
38	FE	113/126 (90%)	107 (95%)	6 (5%)	19	49
38	HE	113/126 (90%)	105 (93%)	8 (7%)	12	36
39	BF	89/116 (77%)	82 (92%)	7 (8%)	10	30
39	DF	87/116 (75%)	86 (99%)	1 (1%)	70	90
39	FF	87/116 (75%)	82 (94%)	5 (6%)	17	47
39	HF	87/116 (75%)	85 (98%)	2 (2%)	45	77
40	BG	124/147 (84%)	115 (93%)	9 (7%)	11	34
40	DG	124/147 (84%)	123 (99%)	1 (1%)	79	93
40	FG	124/147 (84%)	122 (98%)	2 (2%)	58	84
40	HG	124/147 (84%)	124 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	BH	104/105 (99%)	96 (92%)	8 (8%)	10	31
41	DH	104/105 (99%)	97 (93%)	7 (7%)	13	39
41	FH	104/105 (99%)	99 (95%)	5 (5%)	21	54
41	HH	104/105 (99%)	97 (93%)	7 (7%)	13	39
42	BI	105/107 (98%)	96 (91%)	9 (9%)	8	27
42	DI	105/107 (98%)	101 (96%)	4 (4%)	28	63
42	FI	105/107 (98%)	96 (91%)	9 (9%)	8	27
42	HI	105/107 (98%)	102 (97%)	3 (3%)	37	72
43	BJ	86/90 (96%)	83 (96%)	3 (4%)	31	66
43	DJ	86/90 (96%)	82 (95%)	4 (5%)	22	55
43	FJ	86/90 (96%)	83 (96%)	3 (4%)	31	66
43	HJ	86/90 (96%)	81 (94%)	5 (6%)	17	46
44	BK	90/99 (91%)	85 (94%)	5 (6%)	17	47
44	DK	90/99 (91%)	87 (97%)	3 (3%)	33	68
44	FK	90/99 (91%)	81 (90%)	9 (10%)	6	20
44	HK	90/99 (91%)	83 (92%)	7 (8%)	10	31
45	BL	103/104 (99%)	96 (93%)	7 (7%)	13	38
45	DL	103/104 (99%)	96 (93%)	7 (7%)	13	38
45	FL	103/104 (99%)	96 (93%)	7 (7%)	13	38
45	HL	103/104 (99%)	99 (96%)	4 (4%)	27	62
46	BM	92/96 (96%)	88 (96%)	4 (4%)	25	57
46	DM	92/96 (96%)	92 (100%)	0	100	100
46	FM	92/96 (96%)	91 (99%)	1 (1%)	70	90
46	HM	92/96 (96%)	91 (99%)	1 (1%)	70	90
47	BN	79/84 (94%)	75 (95%)	4 (5%)	20	51
47	DN	79/84 (94%)	78 (99%)	1 (1%)	65	88
47	FN	79/84 (94%)	76 (96%)	3 (4%)	28	63
47	HN	79/84 (94%)	79 (100%)	0	100	100
48	BO	76/77 (99%)	72 (95%)	4 (5%)	19	49
48	DO	76/77 (99%)	74 (97%)	2 (3%)	41	74
48	FO	76/77 (99%)	71 (93%)	5 (7%)	14	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	HO	76/77 (99%)	74 (97%)	2 (3%)	41	74
49	BP	65/65 (100%)	61 (94%)	4 (6%)	15	43
49	DP	65/65 (100%)	62 (95%)	3 (5%)	23	55
49	FP	65/65 (100%)	64 (98%)	1 (2%)	60	85
49	HP	65/65 (100%)	63 (97%)	2 (3%)	35	70
50	BQ	74/78 (95%)	66 (89%)	8 (11%)	5	17
50	DQ	74/78 (95%)	71 (96%)	3 (4%)	26	60
50	FQ	74/78 (95%)	72 (97%)	2 (3%)	40	73
50	HQ	74/78 (95%)	68 (92%)	6 (8%)	9	29
51	BR	48/65 (74%)	47 (98%)	1 (2%)	48	78
51	DR	48/65 (74%)	48 (100%)	0	100	100
51	FR	48/65 (74%)	48 (100%)	0	100	100
51	HR	48/65 (74%)	48 (100%)	0	100	100
52	BS	70/79 (89%)	64 (91%)	6 (9%)	8	27
52	DS	70/79 (89%)	67 (96%)	3 (4%)	25	57
52	FS	70/79 (89%)	67 (96%)	3 (4%)	25	57
52	HS	70/79 (89%)	69 (99%)	1 (1%)	62	86
53	BT	65/66 (98%)	60 (92%)	5 (8%)	10	31
53	DT	65/66 (98%)	58 (89%)	7 (11%)	5	17
53	FT	65/66 (98%)	58 (89%)	7 (11%)	5	17
53	HT	65/66 (98%)	57 (88%)	8 (12%)	4	12
54	BU	44/61 (72%)	36 (82%)	8 (18%)	1	4
54	DU	44/61 (72%)	42 (96%)	2 (4%)	23	56
54	FU	44/61 (72%)	39 (89%)	5 (11%)	4	15
54	HU	44/61 (72%)	43 (98%)	1 (2%)	45	77
55	BV	568/578 (98%)	521 (92%)	47 (8%)	9	28
55	DV	568/578 (98%)	527 (93%)	41 (7%)	12	35
55	FV	568/578 (98%)	528 (93%)	40 (7%)	12	36
55	HV	568/578 (98%)	535 (94%)	33 (6%)	17	46
56	BW	2/2 (100%)	1 (50%)	1 (50%)	0	0
56	DW	2/2 (100%)	1 (50%)	1 (50%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
56	FW	2/2 (100%)	1 (50%)	1 (50%)	0 0
56	HW	2/2 (100%)	0	2 (100%)	0 0
All	All	21011/21990 (96%)	19590 (93%)	1421 (7%)	13 38

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

Mol	Chain	Res	Type
18	ER	81	LYS
55	FV	602	LYS
23	EW	25	PHE
18	ER	52	PRO
38	FE	76	LEU

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

Mol	Chain	Res	Type
38	FE	89	HIS
5	GE	29	HIS
47	FN	35	ASN
55	FV	122	GLN
5	GE	97	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AB	117/120 (97%)	17 (14%)	0
1	CB	117/120 (97%)	19 (16%)	0
1	EB	117/120 (97%)	18 (15%)	0
1	GB	117/120 (97%)	20 (17%)	0
3	AA	2850/2904 (98%)	455 (15%)	40 (1%)
3	CA	2850/2904 (98%)	457 (16%)	39 (1%)
3	EA	2850/2904 (98%)	452 (15%)	36 (1%)
3	GA	2850/2904 (98%)	459 (16%)	38 (1%)
35	BA	1532/1542 (99%)	264 (17%)	17 (1%)
35	DA	1532/1542 (99%)	264 (17%)	14 (0%)
35	FA	1532/1542 (99%)	263 (17%)	16 (1%)
35	HA	1532/1542 (99%)	268 (17%)	15 (0%)
All	All	17996/18264 (98%)	2956 (16%)	215 (1%)

5 of 2956 RNA backbone outliers are listed below:

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

5 of 215 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	EA	503	A
3	EA	2423	U
3	GA	2902	C
3	EA	784	G
3	EA	1378	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
56	UAL	FW	5	56	6,8,9	2.47	3 (50%)	4,9,11	5.15	1 (25%)
56	KBE	DW	1	56	8,8,9	0.98	0	6,8,10	1.47	2 (33%)
56	5OH	HW	6	56	7,12,13	1.77	2 (28%)	4,16,18	1.42	1 (25%)
56	DPP	DW	2	56	4,5,6	0.89	0	1,5,7	0.82	0
56	UAL	BW	5	56	6,8,9	2.51	3 (50%)	4,9,11	4.46	1 (25%)
56	KBE	HW	1	56	8,8,9	0.94	0	6,8,10	1.24	1 (16%)
56	KBE	FW	1	56	8,8,9	0.96	0	6,8,10	1.09	0
56	DPP	BW	2	56	4,5,6	1.00	0	1,5,7	0.46	0
56	5OH	DW	6	56	7,12,13	1.82	2 (28%)	4,16,18	1.91	3 (75%)
56	DPP	HW	2	56	4,5,6	0.99	0	1,5,7	0.35	0
56	KBE	BW	1	56	8,8,9	1.23	2 (25%)	6,8,10	1.30	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	5OH	FW	6	56	7,12,13	2.07	2 (28%)	4,16,18	1.75	2 (50%)
56	UAL	DW	5	56	6,8,9	2.50	3 (50%)	4,9,11	4.33	2 (50%)
56	DPP	FW	2	56	4,5,6	1.23	0	1,5,7	0.88	0
56	5OH	BW	6	56	7,12,13	1.81	2 (28%)	4,16,18	2.49	2 (50%)
56	UAL	HW	5	56	6,8,9	3.19	3 (50%)	4,9,11	4.61	3 (75%)

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

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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	HW	5	UAL	C1-N1	4.85	1.47	1.40
56	HW	5	UAL	CB-N1	4.44	1.47	1.35
56	FW	5	UAL	CB-N1	4.16	1.46	1.35
56	HW	5	UAL	C-CA	4.15	1.52	1.45
56	BW	5	UAL	CB-N1	4.15	1.46	1.35

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	FW	5	UAL	O-C-CA	-10.13	112.69	125.39
56	BW	5	UAL	O-C-CA	-8.81	114.35	125.39
56	HW	5	UAL	O-C-CA	-8.73	114.45	125.39
56	DW	5	UAL	O-C-CA	-8.24	115.06	125.39
56	BW	6	5OH	O-C-CA	-3.70	115.26	124.77

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	BW	1	KBE	O-C-CA-CB
56	BW	1	KBE	C-CA-CB-N
56	BW	1	KBE	C-CA-CB-CG
56	BW	1	KBE	N-CB-CG-CD
56	BW	1	KBE	CA-CB-CG-CD

There are no ring outliers.

12 monomers are involved in 15 short contacts:

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 756 ligands modelled in this entry, 752 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
59	GCP	HV	801	57	27,34,34	2.22	6 (22%)	35,54,54	2.68	13 (37%)
59	GCP	FV	801	57	27,34,34	2.28	7 (25%)	35,54,54	2.37	9 (25%)
59	GCP	BV	801	57	27,34,34	2.30	8 (29%)	35,54,54	2.58	7 (20%)
59	GCP	DV	801	57	27,34,34	2.22	7 (25%)	35,54,54	2.64	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
59	GCP	HV	801	57	-	3/15/38/38	0/3/3/3
59	GCP	FV	801	57	-	3/15/38/38	0/3/3/3
59	GCP	BV	801	57	-	2/15/38/38	0/3/3/3
59	GCP	DV	801	57	-	1/15/38/38	0/3/3/3

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	FV	801	GCP	O4'-C1'	6.19	1.49	1.40
59	HV	801	GCP	C2-N2	5.90	1.45	1.33
59	FV	801	GCP	C2-N2	5.65	1.45	1.33
59	HV	801	GCP	O4'-C1'	5.54	1.48	1.40
59	DV	801	GCP	C2-N2	5.45	1.44	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	DV	801	GCP	C4'-O4'-C1'	-10.01	100.76	109.92
59	HV	801	GCP	C4'-O4'-C1'	-9.59	101.14	109.92
59	BV	801	GCP	C4'-O4'-C1'	-9.30	101.41	109.92
59	HV	801	GCP	N3-C2-N1	-6.43	119.04	127.21
59	FV	801	GCP	C4'-O4'-C1'	-6.27	104.18	109.92

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

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

There are no ring outliers.

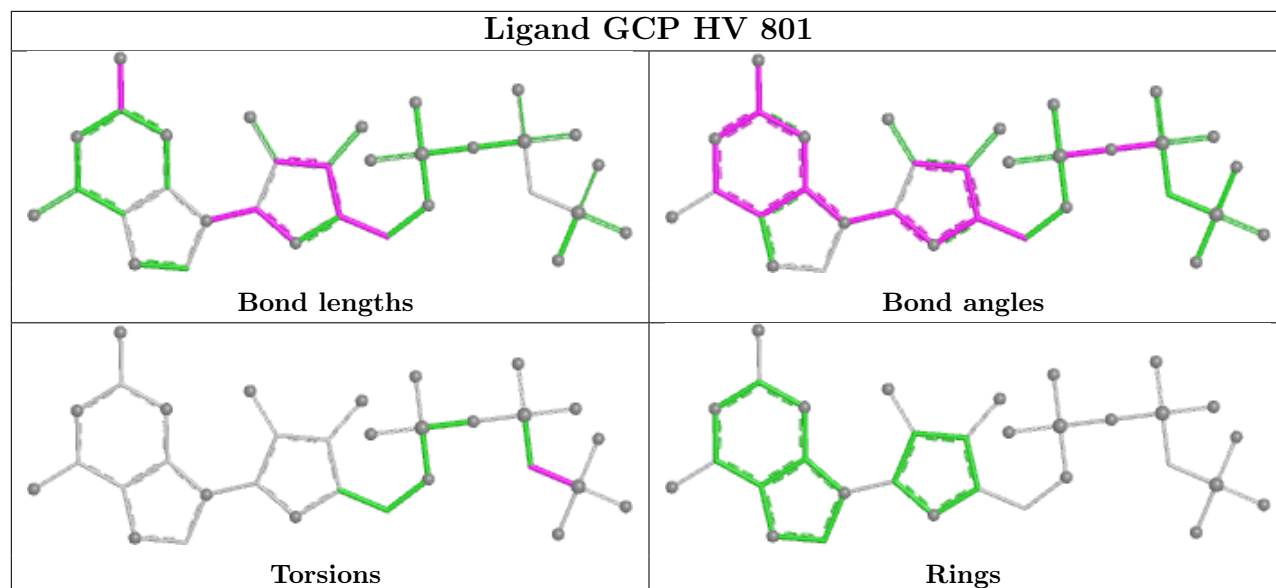
4 monomers are involved in 6 short contacts:

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

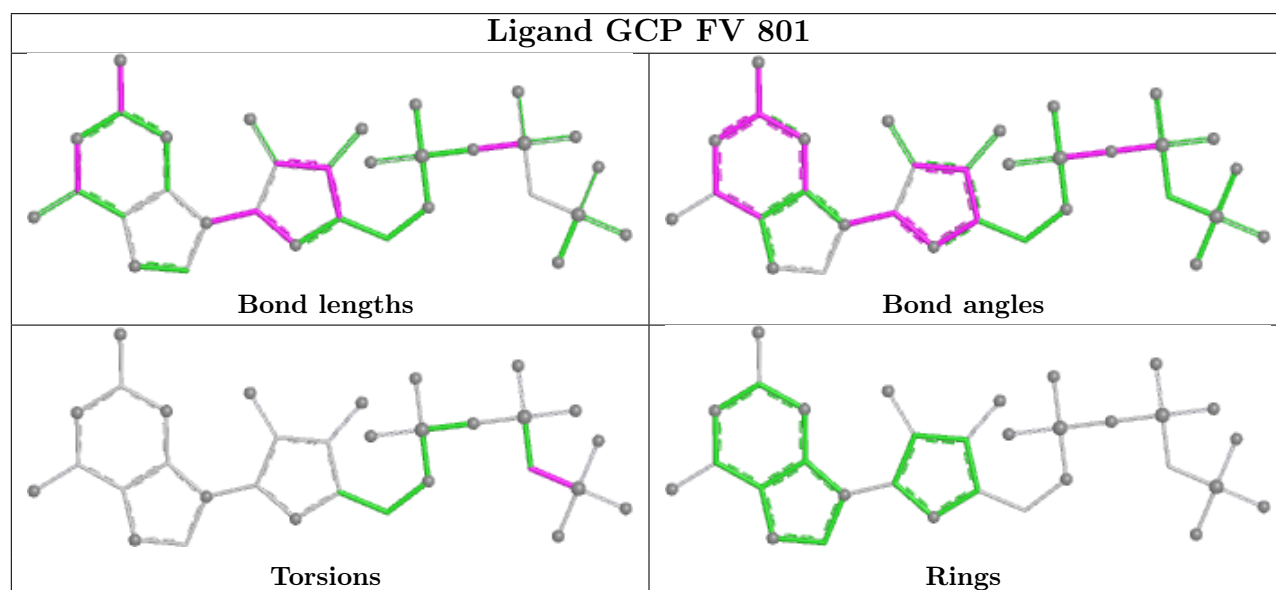
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



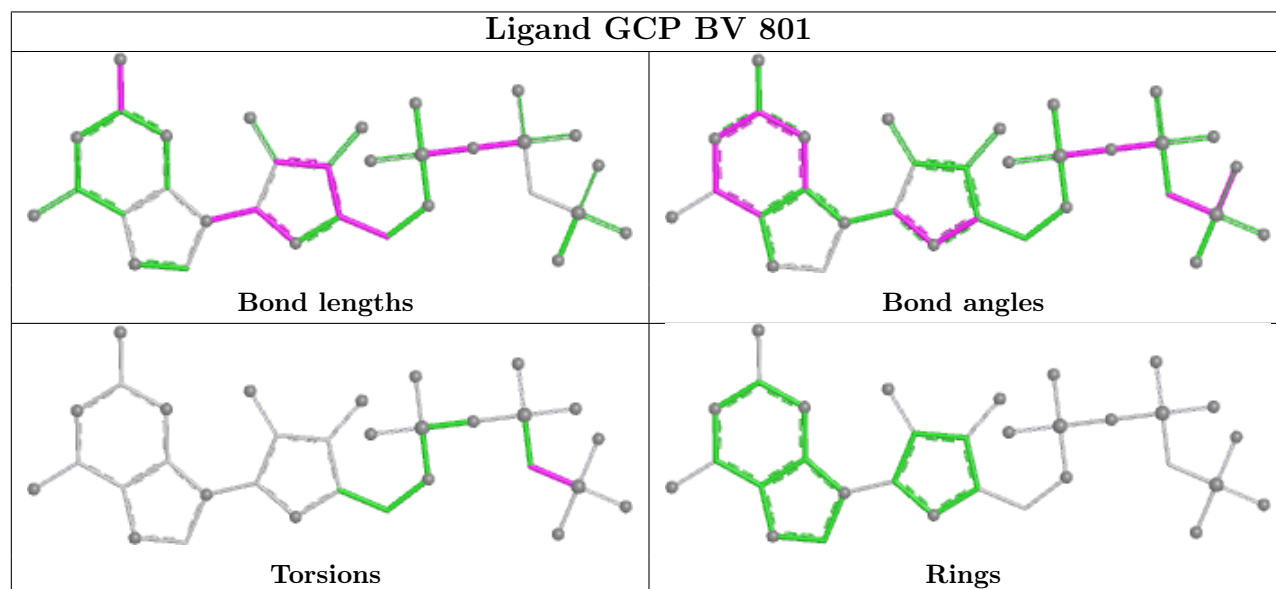
## Ligand GCP HV 801

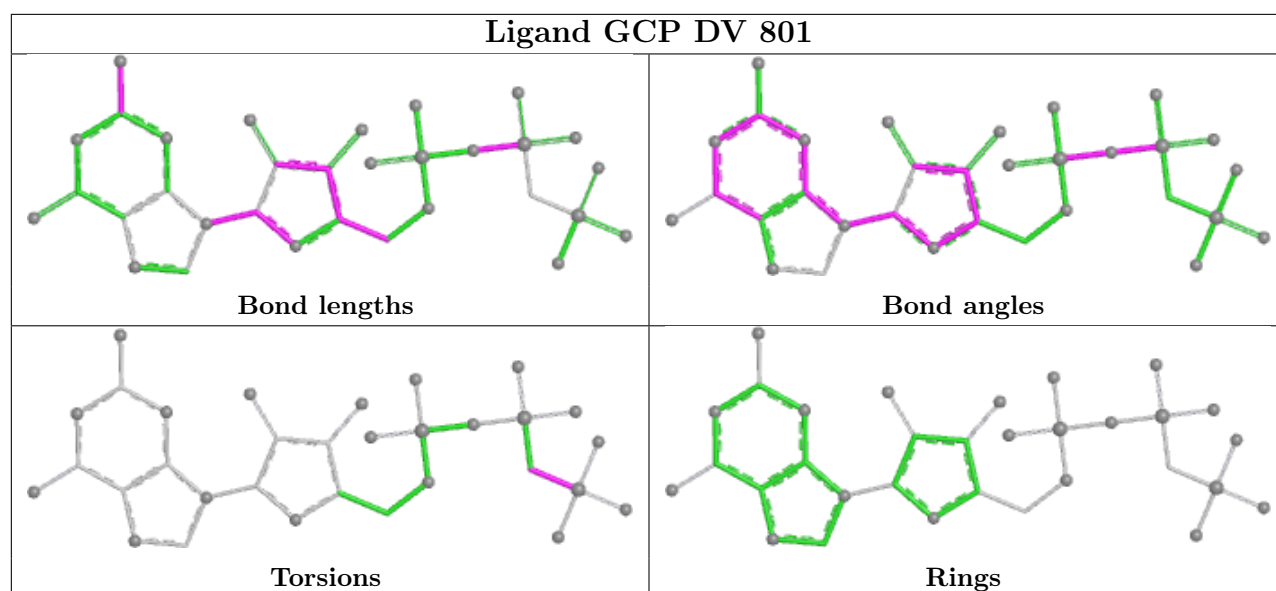


## Ligand GCP FV 801



## Ligand GCP BV 801





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AB	118/120 (98%)	-1.10	0 100 100	7, 25, 37, 49	0
1	CB	118/120 (98%)	-0.88	0 100 100	19, 41, 55, 61	0
1	EB	118/120 (98%)	-1.01	0 100 100	6, 27, 41, 51	0
1	GB	118/120 (98%)	0.13	0 100 100	34, 57, 66, 70	0
2	AC	271/273 (99%)	-0.59	3 (1%) 77 72	2, 14, 26, 50	0
2	CC	271/273 (99%)	-0.26	4 (1%) 71 66	14, 33, 45, 54	0
2	EC	271/273 (99%)	-0.51	3 (1%) 77 72	3, 17, 30, 42	0
2	GC	271/273 (99%)	-0.38	3 (1%) 77 72	12, 29, 43, 52	0
3	AA	2854/2904 (98%)	-0.87	44 (1%) 71 66	2, 14, 50, 79	0
3	CA	2854/2904 (98%)	-0.83	22 (0%) 82 78	8, 29, 57, 78	0
3	EA	2854/2904 (98%)	-0.86	29 (1%) 79 74	2, 16, 52, 83	0
3	GA	2854/2904 (98%)	-0.39	11 (0%) 89 86	10, 42, 64, 76	0
4	AD	209/209 (100%)	-0.53	3 (1%) 73 68	2, 15, 35, 57	0
4	CD	209/209 (100%)	-0.51	3 (1%) 73 68	5, 23, 42, 56	0
4	ED	209/209 (100%)	-0.47	5 (2%) 59 53	2, 20, 40, 52	0
4	GD	209/209 (100%)	-0.41	3 (1%) 73 68	10, 30, 46, 55	0
5	AE	201/201 (100%)	-0.57	0 100 100	3, 19, 40, 51	0
5	CE	201/201 (100%)	-0.46	1 (0%) 87 84	9, 34, 47, 57	0
5	EE	201/201 (100%)	-0.58	1 (0%) 87 84	2, 21, 43, 57	0
5	GE	201/201 (100%)	0.42	4 (1%) 64 58	25, 51, 61, 68	0
6	AF	177/179 (98%)	-0.62	0 100 100	19, 33, 50, 60	0
6	CF	177/179 (98%)	-0.27	0 100 100	31, 47, 56, 62	0
6	EF	177/179 (98%)	-0.36	0 100 100	16, 34, 49, 58	0
6	GF	177/179 (98%)	1.09	29 (16%) 5 5	47, 59, 67, 72	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
7	AG	176/177 (99%)	-0.39	0 100 100	9, 25, 46, 59	0
7	CG	176/177 (99%)	-0.26	2 (1%) 77 72	18, 36, 51, 61	0
7	EG	176/177 (99%)	-0.34	2 (1%) 77 72	16, 31, 44, 55	0
7	GG	176/177 (99%)	-0.05	1 (0%) 85 82	26, 43, 54, 65	0
8	AH	50/50 (100%)	-0.39	0 100 100	16, 41, 55, 57	0
8	CH	50/50 (100%)	0.83	4 (8%) 20 17	46, 57, 64, 68	0
8	EH	50/50 (100%)	-0.39	0 100 100	14, 38, 56, 62	0
8	GH	50/50 (100%)	0.54	2 (4%) 43 36	39, 52, 61, 64	0
9	AI	141/142 (99%)	0.54	8 (5%) 30 26	31, 53, 66, 78	0
9	CI	141/142 (99%)	0.50	4 (2%) 55 49	36, 54, 63, 72	0
9	EI	141/142 (99%)	0.39	7 (4%) 35 30	32, 54, 66, 76	0
9	GI	141/142 (99%)	1.33	30 (21%) 3 3	42, 59, 69, 80	0
10	AJ	142/142 (100%)	-0.50	3 (2%) 63 57	4, 11, 29, 39	0
10	CJ	142/142 (100%)	-0.56	2 (1%) 73 68	8, 24, 37, 54	0
10	EJ	142/142 (100%)	-0.37	3 (2%) 63 57	5, 14, 28, 43	0
10	GJ	142/142 (100%)	-0.00	3 (2%) 63 57	21, 36, 47, 55	0
11	AK	122/123 (99%)	-0.51	1 (0%) 82 78	4, 10, 25, 50	0
11	CK	122/123 (99%)	-0.52	0 100 100	9, 18, 35, 42	0
11	EK	122/123 (99%)	-0.54	2 (1%) 70 64	7, 18, 34, 47	0
11	GK	122/123 (99%)	-0.48	0 100 100	12, 24, 39, 53	0
12	AL	143/144 (99%)	-0.44	1 (0%) 84 80	2, 18, 34, 39	0
12	CL	143/144 (99%)	-0.33	1 (0%) 84 80	11, 31, 46, 54	0
12	EL	143/144 (99%)	-0.53	0 100 100	2, 18, 37, 49	0
12	GL	143/144 (99%)	0.48	5 (3%) 47 41	29, 46, 59, 65	0
13	AM	136/136 (100%)	-0.64	1 (0%) 84 80	2, 9, 25, 48	0
13	CM	136/136 (100%)	-0.59	0 100 100	10, 21, 36, 52	0
13	EM	136/136 (100%)	-0.62	0 100 100	4, 13, 29, 43	0
13	GM	136/136 (100%)	0.32	4 (2%) 54 48	28, 44, 56, 60	0
14	AN	120/127 (94%)	-0.69	0 100 100	5, 13, 25, 56	0
14	CN	120/127 (94%)	-0.63	0 100 100	13, 24, 35, 56	0
14	EN	120/127 (94%)	-0.66	0 100 100	9, 19, 31, 59	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
14	GN	120/127 (94%)	-0.47	1 (0%) 82 78	16, 28, 37, 58	0
15	AO	116/117 (99%)	-0.63	0 100 100	12, 24, 37, 46	0
15	CO	116/117 (99%)	-0.36	0 100 100	29, 40, 53, 59	0
15	EO	116/117 (99%)	-0.64	0 100 100	14, 27, 40, 44	0
15	GO	116/117 (99%)	0.58	4 (3%) 48 42	39, 52, 58, 65	0
16	AP	114/115 (99%)	-0.52	2 (1%) 67 61	5, 19, 36, 44	0
16	CP	114/115 (99%)	-0.37	1 (0%) 81 76	11, 25, 41, 54	0
16	EP	114/115 (99%)	-0.69	0 100 100	14, 26, 41, 60	0
16	GP	114/115 (99%)	-0.62	0 100 100	13, 27, 42, 51	0
17	AQ	117/118 (99%)	-0.43	4 (3%) 48 42	3, 10, 26, 53	0
17	CQ	117/118 (99%)	-0.45	5 (4%) 40 34	9, 23, 35, 54	0
17	EQ	117/118 (99%)	-0.43	2 (1%) 69 63	2, 12, 27, 52	0
17	GQ	117/118 (99%)	0.29	4 (3%) 48 42	24, 41, 53, 58	0
18	AR	103/103 (100%)	-0.58	1 (0%) 79 74	2, 18, 34, 47	0
18	CR	103/103 (100%)	-0.50	0 100 100	12, 31, 45, 55	0
18	ER	103/103 (100%)	-0.44	2 (1%) 66 60	3, 23, 42, 49	0
18	GR	103/103 (100%)	0.40	5 (4%) 36 30	30, 47, 56, 64	0
19	AS	110/110 (100%)	-0.54	1 (0%) 81 76	3, 12, 32, 54	0
19	CS	110/110 (100%)	-0.48	3 (2%) 56 50	13, 22, 40, 47	0
19	ES	110/110 (100%)	-0.57	0 100 100	5, 14, 36, 51	0
19	GS	110/110 (100%)	-0.23	0 100 100	20, 39, 50, 55	0
20	AT	93/100 (93%)	-0.34	1 (1%) 77 72	7, 24, 51, 55	0
20	CT	93/100 (93%)	-0.28	2 (2%) 62 55	22, 36, 52, 56	0
20	ET	93/100 (93%)	-0.25	2 (2%) 62 55	13, 26, 50, 58	0
20	GT	93/100 (93%)	0.02	1 (1%) 77 72	26, 45, 57, 64	0
21	AU	102/104 (98%)	-0.35	0 100 100	9, 22, 41, 62	0
21	CU	102/104 (98%)	-0.15	1 (0%) 79 74	25, 36, 52, 65	0
21	EU	102/104 (98%)	-0.29	2 (1%) 64 58	14, 30, 44, 59	0
21	GU	102/104 (98%)	0.79	8 (7%) 20 18	35, 53, 61, 68	0
22	AV	94/94 (100%)	-0.65	0 100 100	8, 23, 40, 46	0
22	CV	94/94 (100%)	-0.72	0 100 100	22, 31, 44, 52	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
22	EV	94/94 (100%)	-0.69	0 100 100	12, 23, 40, 48	0
22	GV	94/94 (100%)	0.20	1 (1%) 77 72	36, 49, 59, 61	0
23	AW	79/85 (92%)	0.36	8 (10%) 14 12	8, 19, 41, 49	0
23	CW	79/85 (92%)	0.37	5 (6%) 27 23	18, 32, 48, 60	0
23	EW	79/85 (92%)	0.33	10 (12%) 9 8	6, 20, 38, 51	0
23	GW	79/85 (92%)	1.15	16 (20%) 3 3	35, 49, 59, 71	0
24	AX	77/78 (98%)	-0.50	0 100 100	7, 17, 37, 41	0
24	CX	77/78 (98%)	-0.17	0 100 100	22, 37, 49, 54	0
24	EX	77/78 (98%)	-0.73	0 100 100	5, 15, 36, 37	0
24	GX	77/78 (98%)	0.25	1 (1%) 74 69	26, 44, 53, 58	0
25	AY	63/63 (100%)	-0.39	1 (1%) 70 64	16, 34, 48, 52	0
25	CY	63/63 (100%)	-0.28	0 100 100	30, 43, 55, 62	0
25	EY	63/63 (100%)	-0.22	2 (3%) 50 44	18, 33, 45, 56	0
25	GY	63/63 (100%)	0.27	1 (1%) 70 64	44, 51, 58, 60	0
26	AZ	58/59 (98%)	-0.41	1 (1%) 69 63	4, 13, 39, 51	0
26	CZ	58/59 (98%)	-0.41	1 (1%) 69 63	11, 26, 46, 59	0
26	EZ	58/59 (98%)	-0.59	0 100 100	3, 15, 37, 47	0
26	GZ	58/59 (98%)	0.84	5 (8%) 18 15	25, 48, 58, 63	0
27	A0	56/57 (98%)	-0.49	1 (1%) 67 61	3, 19, 42, 51	0
27	C0	56/57 (98%)	-0.50	0 100 100	10, 27, 44, 55	0
27	E0	56/57 (98%)	-0.64	1 (1%) 67 61	3, 22, 40, 47	0
27	G0	56/57 (98%)	-0.33	0 100 100	18, 35, 49, 57	0
28	A1	50/55 (90%)	-0.71	0 100 100	13, 24, 37, 43	0
28	C1	50/55 (90%)	-0.36	1 (2%) 64 58	25, 39, 50, 51	0
28	E1	50/55 (90%)	-0.54	0 100 100	12, 22, 36, 43	0
28	G1	50/55 (90%)	0.63	3 (6%) 29 24	38, 50, 60, 65	0
29	A2	46/46 (100%)	-0.60	1 (2%) 62 55	4, 8, 18, 44	0
29	C2	46/46 (100%)	-0.10	3 (6%) 26 22	17, 24, 34, 43	0
29	E2	46/46 (100%)	-0.63	0 100 100	5, 11, 21, 36	0
29	G2	46/46 (100%)	0.00	2 (4%) 40 34	20, 36, 43, 54	0
30	A3	64/65 (98%)	-0.51	0 100 100	3, 10, 18, 30	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
30	C3	64/65 (98%)	-0.33	0 100 100	14, 28, 36, 39	0
30	E3	64/65 (98%)	-0.40	1 (1%) 70 64	4, 9, 19, 31	0
30	G3	64/65 (98%)	0.90	7 (10%) 12 10	32, 43, 52, 60	0
31	A4	38/38 (100%)	-0.49	0 100 100	5, 11, 25, 27	0
31	C4	38/38 (100%)	-0.46	0 100 100	14, 23, 37, 39	0
31	E4	38/38 (100%)	-0.53	0 100 100	7, 16, 27, 30	0
31	G4	38/38 (100%)	-0.16	0 100 100	24, 37, 50, 53	0
32	A5	148/165 (89%)	0.92	20 (13%) 8 7	30, 49, 61, 72	0
32	C5	148/165 (89%)	1.06	22 (14%) 7 6	37, 54, 64, 72	0
32	E5	145/165 (87%)	1.03	20 (13%) 8 7	36, 53, 62, 67	0
33	A6	30/121 (24%)	1.39	8 (26%) 2 2	47, 53, 62, 65	0
34	BB	218/241 (90%)	-0.23	3 (1%) 73 68	24, 41, 56, 66	0
34	DB	218/241 (90%)	0.10	3 (1%) 73 68	35, 52, 61, 69	0
34	FB	218/241 (90%)	-0.29	4 (1%) 67 61	25, 43, 56, 66	0
34	HB	218/241 (90%)	0.40	6 (2%) 55 49	42, 56, 66, 71	0
35	BA	1533/1542 (99%)	-0.94	7 (0%) 87 84	7, 21, 52, 78	0
35	DA	1533/1542 (99%)	-0.54	8 (0%) 87 84	13, 42, 64, 78	0
35	FA	1533/1542 (99%)	-0.75	2 (0%) 92 92	9, 31, 57, 75	0
35	HA	1533/1542 (99%)	0.03	37 (2%) 59 53	20, 52, 71, 78	0
36	BC	206/233 (88%)	-0.78	0 100 100	8, 26, 39, 57	0
36	DC	206/233 (88%)	-0.30	0 100 100	30, 45, 52, 59	0
36	FC	206/233 (88%)	-0.53	0 100 100	15, 30, 44, 57	0
36	HC	206/233 (88%)	0.26	4 (1%) 66 60	36, 52, 61, 67	0
37	BD	205/206 (99%)	-0.47	2 (0%) 79 74	12, 28, 44, 51	0
37	DD	205/206 (99%)	-0.43	6 (2%) 54 48	14, 30, 47, 55	0
37	FD	205/206 (99%)	-0.07	3 (1%) 71 66	29, 45, 56, 68	0
37	HD	205/206 (99%)	0.18	7 (3%) 48 42	32, 45, 56, 65	0
38	BE	150/167 (89%)	-0.46	1 (0%) 84 80	11, 26, 45, 63	0
38	DE	150/167 (89%)	-0.25	1 (0%) 84 80	24, 38, 51, 60	0
38	FE	150/167 (89%)	-0.39	0 100 100	16, 35, 49, 64	0
38	HE	150/167 (89%)	0.21	4 (2%) 56 50	34, 49, 56, 59	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
39	BF	102/135 (75%)	-0.59	0 100 100	15, 30, 42, 51	0
39	DF	100/135 (74%)	0.05	1 (1%) 79 74	42, 52, 59, 63	0
39	FF	100/135 (74%)	-0.59	2 (2%) 64 58	13, 32, 44, 49	0
39	HF	100/135 (74%)	0.53	2 (2%) 64 58	46, 56, 65, 69	0
40	BG	151/179 (84%)	-0.40	4 (2%) 57 51	10, 27, 46, 60	0
40	DG	151/179 (84%)	0.41	5 (3%) 49 43	41, 54, 61, 67	0
40	FG	151/179 (84%)	-0.36	4 (2%) 57 51	15, 32, 50, 59	0
40	HG	151/179 (84%)	1.11	26 (17%) 5 4	46, 58, 66, 69	0
41	BH	129/130 (99%)	-0.68	0 100 100	15, 26, 40, 58	0
41	DH	129/130 (99%)	-0.26	1 (0%) 82 78	27, 43, 55, 61	0
41	FH	129/130 (99%)	-0.35	2 (1%) 70 64	19, 35, 47, 55	0
41	HH	129/130 (99%)	0.24	0 100 100	36, 50, 58, 64	0
42	BI	127/130 (97%)	-0.23	3 (2%) 59 53	8, 25, 47, 58	0
42	DI	127/130 (97%)	0.63	12 (9%) 15 13	41, 55, 62, 68	0
42	FI	127/130 (97%)	-0.21	4 (3%) 51 46	9, 27, 50, 56	0
42	HI	127/130 (97%)	1.03	18 (14%) 7 6	46, 57, 65, 68	0
43	BJ	98/103 (95%)	-0.36	1 (1%) 79 74	9, 35, 56, 61	0
43	DJ	98/103 (95%)	0.31	3 (3%) 51 46	38, 52, 60, 68	0
43	FJ	98/103 (95%)	-0.10	4 (4%) 42 35	16, 31, 53, 59	0
43	HJ	98/103 (95%)	0.86	13 (13%) 8 7	40, 54, 63, 66	0
44	BK	117/129 (90%)	-0.40	2 (1%) 69 63	14, 26, 40, 52	0
44	DK	117/129 (90%)	0.51	7 (5%) 29 24	38, 52, 60, 62	0
44	FK	117/129 (90%)	-0.58	3 (2%) 57 51	13, 24, 36, 41	0
44	HK	117/129 (90%)	0.94	12 (10%) 13 12	45, 58, 68, 73	0
45	BL	123/124 (99%)	-0.50	3 (2%) 59 53	5, 12, 29, 52	0
45	DL	123/124 (99%)	-0.33	6 (4%) 36 30	12, 24, 40, 49	0
45	FL	123/124 (99%)	-0.26	4 (3%) 49 43	11, 26, 43, 51	0
45	HL	123/124 (99%)	0.33	10 (8%) 19 16	24, 41, 53, 63	0
46	BM	114/118 (96%)	-0.58	0 100 100	11, 30, 51, 54	0
46	DM	114/118 (96%)	0.36	1 (0%) 81 76	39, 53, 62, 66	0
46	FM	114/118 (96%)	-0.46	1 (0%) 81 76	16, 36, 52, 59	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
46	HM	114/118 (96%)	1.66	37 (32%) 1 1	48, 60, 68, 76	0
47	BN	96/101 (95%)	-0.31	3 (3%) 51 46	10, 22, 46, 57	0
47	DN	96/101 (95%)	0.21	1 (1%) 79 74	31, 45, 55, 62	0
47	FN	96/101 (95%)	0.17	6 (6%) 27 23	19, 29, 50, 64	0
47	HN	96/101 (95%)	1.45	29 (30%) 1 1	41, 56, 66, 71	0
48	BO	88/89 (98%)	-0.66	0 100 100	12, 27, 40, 42	0
48	DO	88/89 (98%)	0.01	1 (1%) 77 72	36, 46, 55, 59	0
48	FO	88/89 (98%)	-0.67	0 100 100	16, 31, 44, 51	0
48	HO	88/89 (98%)	0.39	4 (4%) 39 32	37, 49, 58, 63	0
49	BP	82/82 (100%)	-0.49	2 (2%) 59 53	13, 21, 46, 63	0
49	DP	82/82 (100%)	-0.37	1 (1%) 76 71	16, 27, 48, 59	0
49	FP	82/82 (100%)	0.05	4 (4%) 36 30	24, 35, 54, 70	0
49	HP	82/82 (100%)	0.08	1 (1%) 76 71	25, 37, 49, 59	0
50	BQ	80/84 (95%)	-0.40	0 100 100	14, 26, 39, 48	0
50	DQ	80/84 (95%)	-0.30	1 (1%) 74 69	26, 37, 45, 48	0
50	FQ	80/84 (95%)	-0.23	0 100 100	18, 36, 50, 55	0
50	HQ	80/84 (95%)	0.21	5 (6%) 27 23	35, 44, 55, 62	0
51	BR	55/75 (73%)	-0.63	2 (3%) 46 40	16, 26, 39, 48	0
51	DR	55/75 (73%)	0.20	0 100 100	43, 52, 60, 62	0
51	FR	55/75 (73%)	-0.69	2 (3%) 46 40	18, 26, 37, 45	0
51	HR	55/75 (73%)	0.71	4 (7%) 22 19	43, 54, 61, 63	0
52	BS	79/92 (85%)	-0.61	1 (1%) 74 69	14, 23, 39, 65	0
52	DS	79/92 (85%)	0.19	3 (3%) 44 38	31, 49, 58, 61	0
52	FS	79/92 (85%)	-0.19	2 (2%) 58 52	22, 34, 48, 52	0
52	HS	79/92 (85%)	1.62	27 (34%) 1 1	50, 60, 70, 73	0
53	BT	85/87 (97%)	-0.48	2 (2%) 59 53	12, 23, 42, 47	0
53	DT	85/87 (97%)	-0.30	2 (2%) 59 53	17, 28, 44, 53	0
53	FT	85/87 (97%)	-0.07	2 (2%) 59 53	25, 38, 47, 63	0
53	HT	85/87 (97%)	-0.28	3 (3%) 47 41	22, 33, 46, 52	0
54	BU	51/71 (71%)	0.48	5 (9%) 14 12	22, 37, 52, 61	0
54	DU	51/71 (71%)	0.90	8 (15%) 6 5	36, 54, 60, 64	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
54	FU	51/71 (71%)	0.54	5 (9%) 14 12	25, 35, 54, 61	0
54	HU	51/71 (71%)	1.02	8 (15%) 6 5	40, 54, 65, 71	0
55	BV	690/704 (98%)	-0.62	2 (0%) 90 88	10, 30, 48, 66	0
55	DV	689/704 (97%)	-0.52	4 (0%) 85 82	16, 37, 53, 63	0
55	FV	689/704 (97%)	-0.40	3 (0%) 89 86	16, 41, 54, 63	0
55	HV	689/704 (97%)	0.10	11 (1%) 70 64	25, 51, 62, 73	0
56	BW	2/6 (33%)	-0.49	0 100 100	16, 16, 16, 20	0
56	DW	2/6 (33%)	-0.58	0 100 100	32, 32, 32, 34	0
56	FW	2/6 (33%)	-0.82	0 100 100	23, 23, 23, 29	0
56	HW	2/6 (33%)	0.89	0 100 100	51, 51, 51, 58	0
All	All	43746/45264 (96%)	-0.37	891 (2%) 64 58	2, 33, 60, 83	0

The worst 5 of 891 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	GW	51	GLY	8.1
44	FK	126	LYS	7.3
53	DT	4	ILE	7.1
26	AZ	1	ALA	6.9
47	FN	21	PHE	6.7

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	5OH	HW	6	12/13	0.71	0.13	48,54,58,60	0
56	KBE	DW	1	9/10	0.74	0.14	33,35,41,48	0
56	DPP	HW	2	6/7	0.81	0.10	30,41,49,53	0
56	KBE	HW	1	9/10	0.84	0.11	27,45,52,55	0
56	UAL	HW	5	9/10	0.85	0.07	36,48,56,60	0
56	UAL	BW	5	9/10	0.87	0.10	16,20,27,32	0
56	KBE	FW	1	9/10	0.91	0.07	17,21,37,51	0
56	UAL	DW	5	9/10	0.91	0.07	17,27,36,48	0
56	DPP	DW	2	6/7	0.91	0.06	25,37,38,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	5OH	DW	6	12/13	0.92	0.07	22,29,35,37	0
56	KBE	BW	1	9/10	0.93	0.10	4,9,22,23	0
56	5OH	BW	6	12/13	0.93	0.07	11,17,21,21	0
56	DPP	BW	2	6/7	0.94	0.08	6,12,15,22	0
56	DPP	FW	2	6/7	0.96	0.06	18,22,27,32	0
56	UAL	FW	5	9/10	0.96	0.04	15,18,29,38	0
56	5OH	FW	6	12/13	0.96	0.05	10,24,29,30	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	HA	1624	1/1	0.60	0.13	38,38,38,38	0
57	MG	DA	1629	1/1	0.62	0.15	43,43,43,43	0
57	MG	EA	3055	1/1	0.68	0.23	30,30,30,30	0
57	MG	GA	3069	1/1	0.71	0.32	70,70,70,70	0
57	MG	CA	3069	1/1	0.75	0.30	61,61,61,61	0
57	MG	AA	3069	1/1	0.76	0.21	44,44,44,44	0
57	MG	HA	1608	1/1	0.76	0.27	47,47,47,47	0
57	MG	GB	1204	1/1	0.76	0.14	37,37,37,37	0
57	MG	HA	1626	1/1	0.77	0.14	32,32,32,32	0
57	MG	FA	1635	1/1	0.78	0.25	41,41,41,41	0
57	MG	EA	3083	1/1	0.79	0.10	35,35,35,35	0
57	MG	CB	1201	1/1	0.80	0.14	28,28,28,28	0
57	MG	EA	3050	1/1	0.81	0.10	23,23,23,23	0
57	MG	EA	3076	1/1	0.82	0.07	6,6,6,6	0
57	MG	HA	1616	1/1	0.82	0.22	40,40,40,40	0
57	MG	GA	3076	1/1	0.82	0.09	34,34,34,34	0
57	MG	GA	3079	1/1	0.82	0.12	52,52,52,52	0
57	MG	AA	3078	1/1	0.83	0.26	13,13,13,13	0
57	MG	GB	1201	1/1	0.83	0.07	62,62,62,62	0
57	MG	FA	1627	1/1	0.84	0.18	53,53,53,53	0
57	MG	DA	1619	1/1	0.84	0.13	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	HA	1611	1/1	0.84	0.20	26,26,26,26	0
57	MG	GA	3005	1/1	0.85	0.11	42,42,42,42	0
57	MG	GA	3009	1/1	0.85	0.20	35,35,35,35	0
57	MG	HE	201	1/1	0.85	0.09	55,55,55,55	0
57	MG	GA	3050	1/1	0.86	0.25	26,26,26,26	0
57	MG	GL	201	1/1	0.86	0.06	47,47,47,47	0
57	MG	GB	1202	1/1	0.87	0.12	64,64,64,64	0
57	MG	HA	1615	1/1	0.87	0.13	36,36,36,36	0
57	MG	FA	1636	1/1	0.87	0.07	35,35,35,35	0
57	MG	AA	3016	1/1	0.88	0.13	11,11,11,11	0
57	MG	AA	3090	1/1	0.88	0.04	32,32,32,32	0
57	MG	GA	3136	1/1	0.88	0.16	27,27,27,27	0
57	MG	GA	3057	1/1	0.88	0.24	28,28,28,28	0
57	MG	HA	1601	1/1	0.88	0.16	27,27,27,27	0
57	MG	BE	201	1/1	0.88	0.15	31,31,31,31	0
57	MG	FA	1604	1/1	0.89	0.17	34,34,34,34	0
57	MG	DA	1626	1/1	0.89	0.29	44,44,44,44	0
57	MG	DA	1602	1/1	0.89	0.15	28,28,28,28	0
57	MG	AA	3060	1/1	0.89	0.38	34,34,34,34	0
57	MG	HA	1625	1/1	0.89	0.06	44,44,44,44	0
57	MG	EA	3091	1/1	0.89	0.08	40,40,40,40	0
57	MG	EA	3097	1/1	0.89	0.07	19,19,19,19	0
57	MG	FA	1610	1/1	0.90	0.28	33,33,33,33	0
57	MG	GA	3095	1/1	0.90	0.07	43,43,43,43	0
57	MG	GA	3135	1/1	0.90	0.28	28,28,28,28	0
57	MG	CA	3091	1/1	0.90	0.06	38,38,38,38	0
57	MG	BA	1637	1/1	0.90	0.30	15,15,15,15	0
57	MG	AA	3006	1/1	0.90	0.27	32,32,32,32	0
57	MG	HA	1634	1/1	0.90	0.05	35,35,35,35	0
57	MG	HA	1637	1/1	0.90	0.09	51,51,51,51	0
57	MG	GA	3008	1/1	0.90	0.13	24,24,24,24	0
57	MG	HA	1627	1/1	0.91	0.20	41,41,41,41	0
57	MG	HA	1628	1/1	0.91	0.05	29,29,29,29	0
57	MG	GA	3024	1/1	0.91	0.17	14,14,14,14	0
57	MG	GA	3004	1/1	0.91	0.08	25,25,25,25	0
57	MG	HA	1609	1/1	0.91	0.10	23,23,23,23	0
57	MG	FA	1618	1/1	0.92	0.09	21,21,21,21	0
57	MG	BA	1607	1/1	0.92	0.12	34,34,34,34	0
57	MG	GA	3006	1/1	0.92	0.14	29,29,29,29	0
57	MG	AA	3012	1/1	0.92	0.32	32,32,32,32	0
57	MG	GA	3133	1/1	0.92	0.27	15,15,15,15	0
57	MG	EA	3110	1/1	0.92	0.17	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	EA	3124	1/1	0.92	0.23	4,4,4,4	0
57	MG	GA	3032	1/1	0.92	0.19	22,22,22,22	0
57	MG	CA	3025	1/1	0.92	0.21	24,24,24,24	0
57	MG	DA	1636	1/1	0.92	0.12	34,34,34,34	0
57	MG	GA	3066	1/1	0.92	0.13	12,12,12,12	0
57	MG	HK	201	1/1	0.92	0.15	28,28,28,28	0
57	MG	CA	3098	1/1	0.93	0.06	29,29,29,29	0
57	MG	GA	3083	1/1	0.93	0.06	26,26,26,26	0
57	MG	CA	3110	1/1	0.93	0.20	23,23,23,23	0
57	MG	GA	3109	1/1	0.93	0.09	35,35,35,35	0
57	MG	GA	3113	1/1	0.93	0.14	32,32,32,32	0
57	MG	GA	3114	1/1	0.93	0.14	27,27,27,27	0
57	MG	GA	3131	1/1	0.93	0.06	43,43,43,43	0
57	MG	CA	3014	1/1	0.93	0.19	13,13,13,13	0
57	MG	CA	3019	1/1	0.93	0.08	27,27,27,27	0
57	MG	BA	1615	1/1	0.93	0.05	25,25,25,25	0
57	MG	EA	3125	1/1	0.93	0.16	18,18,18,18	0
57	MG	EA	3136	1/1	0.93	0.26	15,15,15,15	0
57	MG	EA	3137	1/1	0.93	0.19	11,11,11,11	0
57	MG	GA	3018	1/1	0.93	0.09	21,21,21,21	0
57	MG	DA	1628	1/1	0.93	0.14	44,44,44,44	0
57	MG	AA	3114	1/1	0.93	0.11	10,10,10,10	0
57	MG	GA	3037	1/1	0.93	0.18	18,18,18,18	0
57	MG	GA	3045	1/1	0.93	0.15	17,17,17,17	0
57	MG	CA	3005	1/1	0.93	0.21	35,35,35,35	0
57	MG	CA	3092	1/1	0.93	0.13	58,58,58,58	0
57	MG	FA	1629	1/1	0.93	0.09	30,30,30,30	0
57	MG	GA	3068	1/1	0.93	0.28	30,30,30,30	0
57	MG	CA	3094	1/1	0.93	0.06	37,37,37,37	0
57	MG	CA	3095	1/1	0.93	0.07	14,14,14,14	0
57	MG	GA	3077	1/1	0.93	0.06	55,55,55,55	0
57	MG	GA	3078	1/1	0.93	0.16	35,35,35,35	0
57	MG	GA	3127	1/1	0.94	0.09	18,18,18,18	0
57	MG	GA	3128	1/1	0.94	0.05	18,18,18,18	0
57	MG	CA	3015	1/1	0.94	0.15	25,25,25,25	0
57	MG	GA	3035	1/1	0.94	0.12	24,24,24,24	0
57	MG	EA	3057	1/1	0.94	0.11	18,18,18,18	0
57	MG	DA	1616	1/1	0.94	0.20	28,28,28,28	0
57	MG	GA	3046	1/1	0.94	0.09	35,35,35,35	0
57	MG	FA	1630	1/1	0.94	0.13	44,44,44,44	0
57	MG	HA	1606	1/1	0.94	0.12	29,29,29,29	0
57	MG	DA	1617	1/1	0.94	0.06	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	EA	3088	1/1	0.94	0.07	19,19,19,19	0
57	MG	HA	1610	1/1	0.94	0.05	31,31,31,31	0
57	MG	BA	1636	1/1	0.94	0.21	24,24,24,24	0
57	MG	HA	1613	1/1	0.94	0.21	32,32,32,32	0
57	MG	EA	3094	1/1	0.94	0.17	33,33,33,33	0
57	MG	DA	1623	1/1	0.94	0.07	42,42,42,42	0
57	MG	HA	1617	1/1	0.94	0.05	49,49,49,49	0
57	MG	HA	1618	1/1	0.94	0.13	35,35,35,35	0
57	MG	DA	1624	1/1	0.94	0.14	18,18,18,18	0
57	MG	AA	3097	1/1	0.94	0.07	34,34,34,34	0
57	MG	AB	1201	1/1	0.94	0.07	34,34,34,34	0
57	MG	CA	3077	1/1	0.94	0.15	37,37,37,37	0
57	MG	GA	3088	1/1	0.94	0.05	37,37,37,37	0
57	MG	CA	3090	1/1	0.94	0.11	19,19,19,19	0
57	MG	EA	3011	1/1	0.94	0.39	24,24,24,24	0
57	MG	CA	3135	1/1	0.94	0.20	8,8,8,8	0
57	MG	GA	3025	1/1	0.94	0.15	25,25,25,25	0
57	MG	GA	3091	1/1	0.95	0.09	28,28,28,28	0
57	MG	CA	3079	1/1	0.95	0.13	27,27,27,27	0
57	MG	GA	3100	1/1	0.95	0.15	12,12,12,12	0
57	MG	GA	3104	1/1	0.95	0.17	12,12,12,12	0
57	MG	DA	1639	1/1	0.95	0.04	30,30,30,30	0
57	MG	EA	3005	1/1	0.95	0.19	16,16,16,16	0
57	MG	CA	3088	1/1	0.95	0.05	23,23,23,23	0
57	MG	EA	3047	1/1	0.95	0.12	25,25,25,25	0
57	MG	BA	1627	1/1	0.95	0.15	19,19,19,19	0
57	MG	AA	3070	1/1	0.95	0.21	6,6,6,6	0
57	MG	AA	3100	1/1	0.95	0.19	1,1,1,1	0
57	MG	AA	3110	1/1	0.95	0.10	9,9,9,9	0
57	MG	AA	3001	1/1	0.95	0.27	20,20,20,20	0
57	MG	AA	3118	1/1	0.95	0.06	14,14,14,14	0
57	MG	CA	3009	1/1	0.95	0.13	10,10,10,10	0
57	MG	AE	301	1/1	0.95	0.27	21,21,21,21	0
57	MG	HA	1607	1/1	0.95	0.04	33,33,33,33	0
57	MG	CA	3136	1/1	0.95	0.23	22,22,22,22	0
57	MG	BA	1602	1/1	0.95	0.19	38,38,38,38	0
57	MG	DA	1611	1/1	0.95	0.16	35,35,35,35	0
57	MG	DA	1612	1/1	0.95	0.14	33,33,33,33	0
57	MG	HA	1612	1/1	0.95	0.09	20,20,20,20	0
57	MG	GA	3047	1/1	0.95	0.14	38,38,38,38	0
57	MG	DA	1614	1/1	0.95	0.06	46,46,46,46	0
57	MG	CA	3016	1/1	0.95	0.12	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	GA	3062	1/1	0.95	0.17	19,19,19,19	0
57	MG	AA	3021	1/1	0.95	0.14	6,6,6,6	0
57	MG	HA	1622	1/1	0.95	0.23	30,30,30,30	0
57	MG	GA	3067	1/1	0.95	0.19	29,29,29,29	0
57	MG	BA	1610	1/1	0.95	0.13	41,41,41,41	0
57	MG	FA	1617	1/1	0.95	0.08	40,40,40,40	0
57	MG	CA	3055	1/1	0.95	0.18	19,19,19,19	0
57	MG	FA	1620	1/1	0.95	0.06	41,41,41,41	0
57	MG	AA	3093	1/1	0.95	0.14	34,34,34,34	0
57	MG	CA	3074	1/1	0.95	0.11	13,13,13,13	0
57	MG	HA	1641	1/1	0.95	0.16	30,30,30,30	0
57	MG	CA	3076	1/1	0.95	0.04	16,16,16,16	0
57	MG	BA	1620	1/1	0.95	0.18	15,15,15,15	0
57	MG	GA	3087	1/1	0.96	0.12	23,23,23,23	0
57	MG	DA	1603	1/1	0.96	0.10	20,20,20,20	0
57	MG	DA	1604	1/1	0.96	0.12	18,18,18,18	0
57	MG	GA	3092	1/1	0.96	0.14	16,16,16,16	0
57	MG	CA	3011	1/1	0.96	0.15	31,31,31,31	0
57	MG	GA	3099	1/1	0.96	0.06	33,33,33,33	0
57	MG	GA	3003	1/1	0.96	0.10	26,26,26,26	0
57	MG	EA	3061	1/1	0.96	0.06	5,5,5,5	0
57	MG	EA	3069	1/1	0.96	0.14	25,25,25,25	0
57	MG	CA	3078	1/1	0.96	0.07	34,34,34,34	0
57	MG	AA	3019	1/1	0.96	0.13	15,15,15,15	0
57	MG	GA	3115	1/1	0.96	0.14	20,20,20,20	0
57	MG	GA	3116	1/1	0.96	0.27	22,22,22,22	0
57	MG	GA	3119	1/1	0.96	0.13	18,18,18,18	0
57	MG	GA	3121	1/1	0.96	0.05	16,16,16,16	0
57	MG	BA	1604	1/1	0.96	0.10	17,17,17,17	0
57	MG	GA	3011	1/1	0.96	0.06	46,46,46,46	0
57	MG	GA	3129	1/1	0.96	0.20	29,29,29,29	0
57	MG	GA	3013	1/1	0.96	0.06	18,18,18,18	0
57	MG	BA	1605	1/1	0.96	0.09	28,28,28,28	0
57	MG	AA	3095	1/1	0.96	0.15	4,4,4,4	0
57	MG	AA	3084	1/1	0.96	0.07	2,2,2,2	0
57	MG	GC	302	1/1	0.96	0.06	22,22,22,22	0
57	MG	GA	3030	1/1	0.96	0.14	15,15,15,15	0
57	MG	GA	3031	1/1	0.96	0.06	15,15,15,15	0
57	MG	HA	1602	1/1	0.96	0.09	26,26,26,26	0
57	MG	CA	3093	1/1	0.96	0.04	40,40,40,40	0
57	MG	EA	3122	1/1	0.96	0.16	4,4,4,4	0
57	MG	CA	3026	1/1	0.96	0.08	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	GA	3039	1/1	0.96	0.20	28,28,28,28	0
57	MG	GA	3042	1/1	0.96	0.18	20,20,20,20	0
57	MG	GA	3043	1/1	0.96	0.08	20,20,20,20	0
57	MG	GA	3044	1/1	0.96	0.09	21,21,21,21	0
57	MG	CB	1202	1/1	0.96	0.08	44,44,44,44	0
57	MG	CA	3056	1/1	0.96	0.12	27,27,27,27	0
57	MG	DA	1631	1/1	0.96	0.06	13,13,13,13	0
57	MG	EB	1201	1/1	0.96	0.08	30,30,30,30	0
57	MG	DA	1634	1/1	0.96	0.05	34,34,34,34	0
57	MG	HA	1619	1/1	0.96	0.13	19,19,19,19	0
57	MG	AA	3124	1/1	0.96	0.13	4,4,4,4	0
57	MG	HA	1623	1/1	0.96	0.16	36,36,36,36	0
57	MG	CA	3115	1/1	0.96	0.14	51,51,51,51	0
57	MG	DA	1640	1/1	0.96	0.07	24,24,24,24	0
57	MG	CA	3071	1/1	0.96	0.12	10,10,10,10	0
57	MG	FA	1621	1/1	0.96	0.12	13,13,13,13	0
57	MG	CA	3006	1/1	0.96	0.05	30,30,30,30	0
57	MG	HA	1633	1/1	0.96	0.10	46,46,46,46	0
57	MG	EA	3015	1/1	0.96	0.40	2,2,2,2	0
57	MG	EA	3042	1/1	0.96	0.20	13,13,13,13	0
57	MG	EA	3045	1/1	0.96	0.11	9,9,9,9	0
57	MG	AA	3076	1/1	0.96	0.12	13,13,13,13	0
57	MG	GA	3084	1/1	0.96	0.25	30,30,30,30	0
59	GCP	HV	801	32/32	0.96	0.05	18,36,48,55	0
57	MG	AA	3109	1/1	0.97	0.04	20,20,20,20	0
57	MG	CA	3116	1/1	0.97	0.11	7,7,7,7	0
57	MG	CA	3117	1/1	0.97	0.05	7,7,7,7	0
57	MG	EA	3070	1/1	0.97	0.10	23,23,23,23	0
57	MG	CA	3120	1/1	0.97	0.13	11,11,11,11	0
57	MG	CA	3121	1/1	0.97	0.14	8,8,8,8	0
57	MG	GA	3051	1/1	0.97	0.21	20,20,20,20	0
57	MG	GA	3055	1/1	0.97	0.08	21,21,21,21	0
57	MG	EA	3087	1/1	0.97	0.11	21,21,21,21	0
57	MG	GA	3059	1/1	0.97	0.07	25,25,25,25	0
57	MG	CA	3124	1/1	0.97	0.08	26,26,26,26	0
57	MG	CA	3131	1/1	0.97	0.11	11,11,11,11	0
57	MG	CA	3134	1/1	0.97	0.15	21,21,21,21	0
57	MG	EA	3095	1/1	0.97	0.12	6,6,6,6	0
57	MG	CA	3021	1/1	0.97	0.08	5,5,5,5	0
57	MG	EA	3109	1/1	0.97	0.06	19,19,19,19	0
57	MG	CA	3022	1/1	0.97	0.06	17,17,17,17	0
57	MG	EA	3113	1/1	0.97	0.13	7,7,7,7	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	EA	3114	1/1	0.97	0.11	17,17,17,17	0
57	MG	EA	3115	1/1	0.97	0.13	6,6,6,6	0
57	MG	EA	3121	1/1	0.97	0.17	5,5,5,5	0
57	MG	GA	3086	1/1	0.97	0.05	24,24,24,24	0
57	MG	DA	1601	1/1	0.97	0.16	26,26,26,26	0
57	MG	CA	3023	1/1	0.97	0.17	5,5,5,5	0
57	MG	AA	3082	1/1	0.97	0.09	22,22,22,22	0
57	MG	EA	3126	1/1	0.97	0.06	6,6,6,6	0
57	MG	GA	3093	1/1	0.97	0.04	21,21,21,21	0
57	MG	BA	1626	1/1	0.97	0.10	5,5,5,5	0
57	MG	DA	1606	1/1	0.97	0.12	15,15,15,15	0
57	MG	DA	1607	1/1	0.97	0.09	16,16,16,16	0
57	MG	EE	301	1/1	0.97	0.10	19,19,19,19	0
57	MG	GA	3108	1/1	0.97	0.06	38,38,38,38	0
57	MG	DA	1609	1/1	0.97	0.06	13,13,13,13	0
57	MG	GA	3110	1/1	0.97	0.09	11,11,11,11	0
57	MG	CA	3037	1/1	0.97	0.13	6,6,6,6	0
57	MG	FA	1611	1/1	0.97	0.13	7,7,7,7	0
57	MG	CA	3044	1/1	0.97	0.09	28,28,28,28	0
57	MG	CA	3049	1/1	0.97	0.11	7,7,7,7	0
57	MG	DA	1615	1/1	0.97	0.15	45,45,45,45	0
57	MG	AA	3083	1/1	0.97	0.10	18,18,18,18	0
57	MG	GA	3123	1/1	0.97	0.11	44,44,44,44	0
57	MG	GA	3124	1/1	0.97	0.03	36,36,36,36	0
57	MG	GA	3126	1/1	0.97	0.05	35,35,35,35	0
57	MG	FA	1625	1/1	0.97	0.07	21,21,21,21	0
57	MG	BA	1631	1/1	0.97	0.05	16,16,16,16	0
57	MG	AA	3115	1/1	0.97	0.16	1,1,1,1	0
57	MG	AA	3057	1/1	0.97	0.07	25,25,25,25	0
57	MG	FA	1631	1/1	0.97	0.10	24,24,24,24	0
57	MG	BA	1639	1/1	0.97	0.13	12,12,12,12	0
57	MG	AA	3122	1/1	0.97	0.04	6,6,6,6	0
57	MG	FA	1638	1/1	0.97	0.11	16,16,16,16	0
57	MG	FE	201	1/1	0.97	0.05	35,35,35,35	0
57	MG	FU	101	1/1	0.97	0.04	21,21,21,21	0
57	MG	BU	101	1/1	0.97	0.22	19,19,19,19	0
57	MG	AA	3008	1/1	0.97	0.09	19,19,19,19	0
57	MG	GB	1203	1/1	0.97	0.09	23,23,23,23	0
57	MG	AA	3129	1/1	0.97	0.17	9,9,9,9	0
57	MG	CA	3085	1/1	0.97	0.05	5,5,5,5	0
57	MG	CA	3087	1/1	0.97	0.04	23,23,23,23	0
57	MG	DA	1638	1/1	0.97	0.07	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	CA	3002	1/1	0.97	0.07	38,38,38,38	0
57	MG	GA	3007	1/1	0.97	0.07	39,39,39,39	0
57	MG	HA	1614	1/1	0.97	0.05	49,49,49,49	0
57	MG	AA	3135	1/1	0.97	0.28	12,12,12,12	0
57	MG	DA	1643	1/1	0.97	0.08	32,32,32,32	0
57	MG	AA	3091	1/1	0.97	0.11	33,33,33,33	0
57	MG	CA	3007	1/1	0.97	0.06	35,35,35,35	0
57	MG	AA	3026	1/1	0.97	0.12	4,4,4,4	0
57	MG	GA	3021	1/1	0.97	0.17	20,20,20,20	0
57	MG	EA	3018	1/1	0.97	0.15	9,9,9,9	0
57	MG	EA	3030	1/1	0.97	0.14	7,7,7,7	0
57	MG	GA	3027	1/1	0.97	0.04	17,17,17,17	0
57	MG	GA	3028	1/1	0.97	0.11	12,12,12,12	0
57	MG	GA	3029	1/1	0.97	0.07	16,16,16,16	0
57	MG	EA	3039	1/1	0.97	0.07	15,15,15,15	0
57	MG	HA	1629	1/1	0.97	0.09	45,45,45,45	0
57	MG	HA	1630	1/1	0.97	0.16	32,32,32,32	0
57	MG	HA	1632	1/1	0.97	0.06	31,31,31,31	0
57	MG	EA	3041	1/1	0.97	0.17	3,3,3,3	0
57	MG	AA	3038	1/1	0.97	0.17	3,3,3,3	0
57	MG	HA	1635	1/1	0.97	0.06	28,28,28,28	0
57	MG	GA	3034	1/1	0.97	0.10	36,36,36,36	0
57	MG	AA	3044	1/1	0.97	0.05	4,4,4,4	0
57	MG	AA	3099	1/1	0.97	0.10	13,13,13,13	0
57	MG	AA	3045	1/1	0.97	0.15	8,8,8,8	0
57	MG	HV	802	1/1	0.97	0.08	38,38,38,38	0
59	GCP	FV	801	32/32	0.97	0.06	16,28,45,57	0
57	MG	CA	3111	1/1	0.97	0.20	18,18,18,18	0
57	MG	AA	3111	1/1	0.98	0.10	3,3,3,3	0
57	MG	GA	3010	1/1	0.98	0.07	16,16,16,16	0
57	MG	BA	1629	1/1	0.98	0.16	15,15,15,15	0
57	MG	AA	3112	1/1	0.98	0.17	0,0,0,0	0
57	MG	GA	3015	1/1	0.98	0.17	27,27,27,27	0
57	MG	GA	3017	1/1	0.98	0.07	10,10,10,10	0
57	MG	BA	1635	1/1	0.98	0.08	29,29,29,29	0
57	MG	GA	3019	1/1	0.98	0.09	6,6,6,6	0
57	MG	GA	3020	1/1	0.98	0.12	3,3,3,3	0
57	MG	EA	3002	1/1	0.98	0.09	7,7,7,7	0
57	MG	EA	3004	1/1	0.98	0.10	12,12,12,12	0
57	MG	CA	3080	1/1	0.98	0.09	20,20,20,20	0
57	MG	EA	3007	1/1	0.98	0.11	12,12,12,12	0
57	MG	EA	3009	1/1	0.98	0.15	2,2,2,2	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	CA	3083	1/1	0.98	0.11	32,32,32,32	0
57	MG	EA	3012	1/1	0.98	0.12	2,2,2,2	0
57	MG	EA	3014	1/1	0.98	0.06	1,1,1,1	0
57	MG	AA	3027	1/1	0.98	0.11	15,15,15,15	0
57	MG	GA	3033	1/1	0.98	0.12	30,30,30,30	0
57	MG	AA	3046	1/1	0.98	0.18	13,13,13,13	0
57	MG	EA	3023	1/1	0.98	0.10	9,9,9,9	0
57	MG	GA	3036	1/1	0.98	0.06	38,38,38,38	0
57	MG	EA	3025	1/1	0.98	0.16	1,1,1,1	0
57	MG	EA	3028	1/1	0.98	0.07	7,7,7,7	0
57	MG	GA	3040	1/1	0.98	0.07	15,15,15,15	0
57	MG	BA	1638	1/1	0.98	0.10	13,13,13,13	0
57	MG	EA	3034	1/1	0.98	0.05	31,31,31,31	0
57	MG	CA	3089	1/1	0.98	0.13	14,14,14,14	0
57	MG	EA	3040	1/1	0.98	0.13	11,11,11,11	0
57	MG	AA	3117	1/1	0.98	0.11	11,11,11,11	0
57	MG	AA	3048	1/1	0.98	0.12	16,16,16,16	0
57	MG	GA	3048	1/1	0.98	0.09	15,15,15,15	0
57	MG	EA	3043	1/1	0.98	0.14	8,8,8,8	0
57	MG	EA	3044	1/1	0.98	0.07	15,15,15,15	0
57	MG	AA	3119	1/1	0.98	0.07	0,0,0,0	0
57	MG	GA	3056	1/1	0.98	0.11	13,13,13,13	0
57	MG	AA	3049	1/1	0.98	0.14	17,17,17,17	0
57	MG	EA	3049	1/1	0.98	0.10	8,8,8,8	0
57	MG	GA	3061	1/1	0.98	0.06	20,20,20,20	0
57	MG	AA	3088	1/1	0.98	0.09	4,4,4,4	0
57	MG	EA	3052	1/1	0.98	0.11	12,12,12,12	0
57	MG	CB	1204	1/1	0.98	0.03	15,15,15,15	0
57	MG	CA	3096	1/1	0.98	0.12	16,16,16,16	0
57	MG	AA	3125	1/1	0.98	0.09	8,8,8,8	0
57	MG	GA	3070	1/1	0.98	0.15	22,22,22,22	0
57	MG	GA	3071	1/1	0.98	0.11	16,16,16,16	0
57	MG	GA	3073	1/1	0.98	0.05	10,10,10,10	0
57	MG	CA	3103	1/1	0.98	0.03	17,17,17,17	0
57	MG	CA	3105	1/1	0.98	0.13	14,14,14,14	0
57	MG	CA	3108	1/1	0.98	0.10	11,11,11,11	0
57	MG	EA	3082	1/1	0.98	0.04	6,6,6,6	0
57	MG	CA	3109	1/1	0.98	0.11	7,7,7,7	0
57	MG	CA	3003	1/1	0.98	0.08	10,10,10,10	0
57	MG	AA	3054	1/1	0.98	0.10	3,3,3,3	0
57	MG	CA	3113	1/1	0.98	0.11	10,10,10,10	0
57	MG	AA	3131	1/1	0.98	0.03	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	GA	3089	1/1	0.98	0.14	8,8,8,8	0
57	MG	GA	3090	1/1	0.98	0.08	27,27,27,27	0
57	MG	AA	3134	1/1	0.98	0.06	21,21,21,21	0
57	MG	AA	3033	1/1	0.98	0.07	1,1,1,1	0
57	MG	EA	3098	1/1	0.98	0.04	4,4,4,4	0
57	MG	EA	3100	1/1	0.98	0.05	1,1,1,1	0
57	MG	GA	3098	1/1	0.98	0.03	15,15,15,15	0
57	MG	EA	3101	1/1	0.98	0.04	7,7,7,7	0
57	MG	EA	3108	1/1	0.98	0.08	15,15,15,15	0
57	MG	GA	3101	1/1	0.98	0.07	13,13,13,13	0
57	MG	GA	3103	1/1	0.98	0.13	12,12,12,12	0
57	MG	CA	3118	1/1	0.98	0.13	31,31,31,31	0
57	MG	CA	3119	1/1	0.98	0.12	34,34,34,34	0
57	MG	CA	3010	1/1	0.98	0.11	8,8,8,8	0
57	MG	AA	3136	1/1	0.98	0.26	11,11,11,11	0
57	MG	GA	3111	1/1	0.98	0.03	35,35,35,35	0
57	MG	CA	3123	1/1	0.98	0.08	26,26,26,26	0
57	MG	EA	3117	1/1	0.98	0.08	15,15,15,15	0
57	MG	EA	3118	1/1	0.98	0.03	17,17,17,17	0
57	MG	EA	3119	1/1	0.98	0.10	1,1,1,1	0
57	MG	GA	3117	1/1	0.98	0.05	10,10,10,10	0
57	MG	GA	3118	1/1	0.98	0.04	39,39,39,39	0
57	MG	EA	3120	1/1	0.98	0.17	5,5,5,5	0
57	MG	AA	3092	1/1	0.98	0.08	14,14,14,14	0
57	MG	CA	3127	1/1	0.98	0.08	3,3,3,3	0
57	MG	A4	101	1/1	0.98	0.06	20,20,20,20	0
57	MG	CA	3132	1/1	0.98	0.04	9,9,9,9	0
57	MG	CA	3133	1/1	0.98	0.08	13,13,13,13	0
57	MG	EA	3128	1/1	0.98	0.09	0,0,0,0	0
57	MG	EA	3133	1/1	0.98	0.13	0,0,0,0	0
57	MG	EA	3134	1/1	0.98	0.12	7,7,7,7	0
57	MG	GA	3132	1/1	0.98	0.10	28,28,28,28	0
57	MG	AA	3059	1/1	0.98	0.12	1,1,1,1	0
57	MG	GA	3134	1/1	0.98	0.08	28,28,28,28	0
57	MG	BA	1603	1/1	0.98	0.10	18,18,18,18	0
57	MG	AA	3035	1/1	0.98	0.12	5,5,5,5	0
57	MG	GC	301	1/1	0.98	0.15	26,26,26,26	0
57	MG	EB	1202	1/1	0.98	0.05	17,17,17,17	0
57	MG	EB	1203	1/1	0.98	0.14	0,0,0,0	0
57	MG	AA	3062	1/1	0.98	0.09	4,4,4,4	0
57	MG	FA	1602	1/1	0.98	0.18	18,18,18,18	0
57	MG	AA	3023	1/1	0.98	0.04	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	FA	1609	1/1	0.98	0.13	7,7,7,7	0
57	MG	CA	3024	1/1	0.98	0.14	6,6,6,6	0
57	MG	BA	1608	1/1	0.98	0.14	11,11,11,11	0
57	MG	AA	3042	1/1	0.98	0.14	8,8,8,8	0
57	MG	CA	3030	1/1	0.98	0.07	39,39,39,39	0
57	MG	CA	3034	1/1	0.98	0.05	13,13,13,13	0
57	MG	DA	1610	1/1	0.98	0.12	28,28,28,28	0
57	MG	FA	1624	1/1	0.98	0.08	27,27,27,27	0
57	MG	AA	3102	1/1	0.98	0.04	10,10,10,10	0
57	MG	CA	3038	1/1	0.98	0.11	9,9,9,9	0
57	MG	FA	1628	1/1	0.98	0.07	27,27,27,27	0
57	MG	BA	1617	1/1	0.98	0.03	21,21,21,21	0
57	MG	CA	3047	1/1	0.98	0.11	23,23,23,23	0
57	MG	HA	1620	1/1	0.98	0.09	32,32,32,32	0
57	MG	HA	1621	1/1	0.98	0.12	7,7,7,7	0
57	MG	BA	1618	1/1	0.98	0.11	1,1,1,1	0
57	MG	FA	1633	1/1	0.98	0.12	24,24,24,24	0
57	MG	FA	1634	1/1	0.98	0.10	13,13,13,13	0
57	MG	CA	3053	1/1	0.98	0.04	20,20,20,20	0
57	MG	DA	1618	1/1	0.98	0.03	37,37,37,37	0
57	MG	FA	1637	1/1	0.98	0.07	29,29,29,29	0
57	MG	AA	3075	1/1	0.98	0.04	15,15,15,15	0
57	MG	DA	1622	1/1	0.98	0.11	13,13,13,13	0
57	MG	BA	1622	1/1	0.98	0.09	17,17,17,17	0
57	MG	HA	1631	1/1	0.98	0.12	31,31,31,31	0
57	MG	CA	3061	1/1	0.98	0.06	4,4,4,4	0
57	MG	DA	1625	1/1	0.98	0.07	29,29,29,29	0
57	MG	CA	3063	1/1	0.98	0.07	4,4,4,4	0
57	MG	DA	1627	1/1	0.98	0.04	23,23,23,23	0
57	MG	GA	3002	1/1	0.98	0.03	31,31,31,31	0
57	MG	HA	1638	1/1	0.98	0.05	28,28,28,28	0
57	MG	HA	1639	1/1	0.98	0.08	22,22,22,22	0
57	MG	CA	3067	1/1	0.98	0.14	6,6,6,6	0
57	MG	BA	1624	1/1	0.98	0.17	9,9,9,9	0
57	MG	CA	3070	1/1	0.98	0.07	8,8,8,8	0
57	MG	BA	1625	1/1	0.98	0.06	23,23,23,23	0
58	ZN	E4	101	1/1	0.98	0.06	59,59,59,59	0
59	GCP	DV	801	32/32	0.98	0.05	17,28,38,41	0
57	MG	DA	1635	1/1	0.98	0.04	37,37,37,37	0
57	MG	AA	3002	1/1	0.98	0.08	25,25,25,25	0
57	MG	CA	3106	1/1	0.99	0.10	12,12,12,12	0
57	MG	CA	3107	1/1	0.99	0.10	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	EA	3127	1/1	0.99	0.05	11,11,11,11	0
57	MG	BA	1633	1/1	0.99	0.04	20,20,20,20	0
57	MG	EA	3130	1/1	0.99	0.13	0,0,0,0	0
57	MG	EA	3132	1/1	0.99	0.09	21,21,21,21	0
57	MG	BA	1634	1/1	0.99	0.03	13,13,13,13	0
57	MG	AA	3039	1/1	0.99	0.04	3,3,3,3	0
57	MG	EA	3135	1/1	0.99	0.04	25,25,25,25	0
57	MG	AA	3040	1/1	0.99	0.12	1,1,1,1	0
57	MG	CA	3112	1/1	0.99	0.10	10,10,10,10	0
57	MG	AA	3094	1/1	0.99	0.04	16,16,16,16	0
57	MG	CA	3114	1/1	0.99	0.06	26,26,26,26	0
57	MG	AA	3013	1/1	0.99	0.04	0,0,0,0	0
57	MG	ED	301	1/1	0.99	0.05	7,7,7,7	0
57	MG	AA	3043	1/1	0.99	0.09	5,5,5,5	0
57	MG	FA	1601	1/1	0.99	0.06	17,17,17,17	0
57	MG	BA	1640	1/1	0.99	0.09	11,11,11,11	0
57	MG	FA	1603	1/1	0.99	0.04	20,20,20,20	0
57	MG	AA	3015	1/1	0.99	0.12	0,0,0,0	0
57	MG	FA	1605	1/1	0.99	0.03	30,30,30,30	0
57	MG	FA	1606	1/1	0.99	0.07	15,15,15,15	0
57	MG	FA	1607	1/1	0.99	0.04	21,21,21,21	0
57	MG	BN	201	1/1	0.99	0.05	13,13,13,13	0
57	MG	AB	1203	1/1	0.99	0.08	0,0,0,0	0
57	MG	BV	802	1/1	0.99	0.07	22,22,22,22	0
57	MG	FA	1612	1/1	0.99	0.14	4,4,4,4	0
57	MG	FA	1613	1/1	0.99	0.12	6,6,6,6	0
57	MG	FA	1614	1/1	0.99	0.05	13,13,13,13	0
57	MG	FA	1615	1/1	0.99	0.04	16,16,16,16	0
57	MG	FA	1616	1/1	0.99	0.04	18,18,18,18	0
57	MG	CA	3122	1/1	0.99	0.06	5,5,5,5	0
57	MG	AA	3101	1/1	0.99	0.08	8,8,8,8	0
57	MG	FA	1619	1/1	0.99	0.07	7,7,7,7	0
57	MG	AA	3018	1/1	0.99	0.08	2,2,2,2	0
57	MG	CA	3125	1/1	0.99	0.13	11,11,11,11	0
57	MG	CA	3126	1/1	0.99	0.04	22,22,22,22	0
57	MG	CB	1203	1/1	0.99	0.07	12,12,12,12	0
57	MG	FA	1626	1/1	0.99	0.10	22,22,22,22	0
57	MG	CA	3129	1/1	0.99	0.02	9,9,9,9	0
57	MG	CA	3130	1/1	0.99	0.12	21,21,21,21	0
57	MG	AA	3104	1/1	0.99	0.10	2,2,2,2	0
57	MG	AA	3106	1/1	0.99	0.10	4,4,4,4	0
57	MG	AA	3047	1/1	0.99	0.09	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	CA	3004	1/1	0.99	0.05	24,24,24,24	0
57	MG	AA	3005	1/1	0.99	0.09	16,16,16,16	0
57	MG	AA	3020	1/1	0.99	0.03	9,9,9,9	0
57	MG	CN	201	1/1	0.99	0.15	20,20,20,20	0
57	MG	C4	101	1/1	0.99	0.04	17,17,17,17	0
57	MG	AA	3051	1/1	0.99	0.05	9,9,9,9	0
57	MG	FA	1639	1/1	0.99	0.08	20,20,20,20	0
57	MG	CA	3008	1/1	0.99	0.09	14,14,14,14	0
57	MG	FN	201	1/1	0.99	0.12	14,14,14,14	0
57	MG	AA	3113	1/1	0.99	0.02	8,8,8,8	0
57	MG	FV	802	1/1	0.99	0.08	24,24,24,24	0
57	MG	AA	3052	1/1	0.99	0.09	3,3,3,3	0
57	MG	DA	1605	1/1	0.99	0.09	18,18,18,18	0
57	MG	AA	3053	1/1	0.99	0.06	4,4,4,4	0
57	MG	CA	3012	1/1	0.99	0.04	6,6,6,6	0
57	MG	GA	3001	1/1	0.99	0.03	31,31,31,31	0
57	MG	DA	1608	1/1	0.99	0.11	30,30,30,30	0
57	MG	AA	3116	1/1	0.99	0.06	0,0,0,0	0
57	MG	AB	1204	1/1	0.99	0.03	18,18,18,18	0
57	MG	AA	3055	1/1	0.99	0.10	0,0,0,0	0
57	MG	CA	3017	1/1	0.99	0.09	7,7,7,7	0
57	MG	CA	3018	1/1	0.99	0.03	30,30,30,30	0
57	MG	AA	3022	1/1	0.99	0.02	2,2,2,2	0
57	MG	CA	3020	1/1	0.99	0.05	6,6,6,6	0
57	MG	AA	3120	1/1	0.99	0.09	9,9,9,9	0
57	MG	AA	3007	1/1	0.99	0.12	19,19,19,19	0
57	MG	GA	3012	1/1	0.99	0.09	22,22,22,22	0
57	MG	AA	3123	1/1	0.99	0.03	5,5,5,5	0
57	MG	GA	3014	1/1	0.99	0.03	15,15,15,15	0
57	MG	DA	1620	1/1	0.99	0.02	12,12,12,12	0
57	MG	GA	3016	1/1	0.99	0.08	12,12,12,12	0
57	MG	DA	1621	1/1	0.99	0.07	44,44,44,44	0
57	MG	AA	3025	1/1	0.99	0.06	0,0,0,0	0
57	MG	AA	3061	1/1	0.99	0.13	5,5,5,5	0
57	MG	AA	3126	1/1	0.99	0.04	2,2,2,2	0
57	MG	CA	3027	1/1	0.99	0.03	10,10,10,10	0
57	MG	GA	3023	1/1	0.99	0.25	27,27,27,27	0
57	MG	CA	3028	1/1	0.99	0.08	9,9,9,9	0
57	MG	CA	3029	1/1	0.99	0.06	19,19,19,19	0
57	MG	GA	3026	1/1	0.99	0.08	31,31,31,31	0
57	MG	AA	3127	1/1	0.99	0.06	10,10,10,10	0
57	MG	CA	3031	1/1	0.99	0.06	7,7,7,7	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	DA	1630	1/1	0.99	0.06	25,25,25,25	0
57	MG	CA	3032	1/1	0.99	0.05	8,8,8,8	0
57	MG	DA	1632	1/1	0.99	0.04	22,22,22,22	0
57	MG	DA	1633	1/1	0.99	0.03	29,29,29,29	0
57	MG	AA	3128	1/1	0.99	0.08	0,0,0,0	0
57	MG	CA	3036	1/1	0.99	0.06	28,28,28,28	0
57	MG	AC	301	1/1	0.99	0.04	3,3,3,3	0
57	MG	DA	1637	1/1	0.99	0.04	25,25,25,25	0
57	MG	AA	3130	1/1	0.99	0.08	3,3,3,3	0
57	MG	GA	3038	1/1	0.99	0.04	21,21,21,21	0
57	MG	CA	3039	1/1	0.99	0.12	4,4,4,4	0
57	MG	CA	3040	1/1	0.99	0.04	11,11,11,11	0
57	MG	GA	3041	1/1	0.99	0.07	10,10,10,10	0
57	MG	DA	1641	1/1	0.99	0.03	28,28,28,28	0
57	MG	DA	1642	1/1	0.99	0.11	4,4,4,4	0
57	MG	CA	3041	1/1	0.99	0.03	12,12,12,12	0
57	MG	EA	3001	1/1	0.99	0.05	11,11,11,11	0
57	MG	CA	3042	1/1	0.99	0.06	16,16,16,16	0
57	MG	EA	3003	1/1	0.99	0.07	9,9,9,9	0
57	MG	CA	3043	1/1	0.99	0.07	4,4,4,4	0
57	MG	GA	3049	1/1	0.99	0.13	12,12,12,12	0
57	MG	AA	3063	1/1	0.99	0.05	0,0,0,0	0
57	MG	EA	3006	1/1	0.99	0.07	9,9,9,9	0
57	MG	GA	3052	1/1	0.99	0.10	4,4,4,4	0
57	MG	GA	3053	1/1	0.99	0.12	6,6,6,6	0
57	MG	GA	3054	1/1	0.99	0.09	12,12,12,12	0
57	MG	CA	3045	1/1	0.99	0.10	5,5,5,5	0
57	MG	EA	3008	1/1	0.99	0.11	1,1,1,1	0
57	MG	CA	3046	1/1	0.99	0.12	21,21,21,21	0
57	MG	GA	3058	1/1	0.99	0.13	24,24,24,24	0
57	MG	EA	3010	1/1	0.99	0.04	6,6,6,6	0
57	MG	GA	3060	1/1	0.99	0.07	18,18,18,18	0
57	MG	AA	3132	1/1	0.99	0.09	0,0,0,0	0
57	MG	CA	3048	1/1	0.99	0.09	17,17,17,17	0
57	MG	GA	3063	1/1	0.99	0.04	27,27,27,27	0
57	MG	GA	3064	1/1	0.99	0.04	11,11,11,11	0
57	MG	GA	3065	1/1	0.99	0.04	20,20,20,20	0
57	MG	AA	3065	1/1	0.99	0.15	11,11,11,11	0
57	MG	CA	3050	1/1	0.99	0.06	14,14,14,14	0
57	MG	EA	3016	1/1	0.99	0.11	0,0,0,0	0
57	MG	EA	3017	1/1	0.99	0.10	8,8,8,8	0
57	MG	CA	3051	1/1	0.99	0.25	6,6,6,6	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	EA	3019	1/1	0.99	0.04	10,10,10,10	0
57	MG	GA	3072	1/1	0.99	0.04	24,24,24,24	0
57	MG	EA	3020	1/1	0.99	0.08	7,7,7,7	0
57	MG	GA	3074	1/1	0.99	0.08	10,10,10,10	0
57	MG	EA	3021	1/1	0.99	0.06	11,11,11,11	0
57	MG	EA	3022	1/1	0.99	0.07	2,2,2,2	0
57	MG	AA	3066	1/1	0.99	0.12	0,0,0,0	0
57	MG	AA	3068	1/1	0.99	0.11	2,2,2,2	0
57	MG	GA	3080	1/1	0.99	0.10	36,36,36,36	0
57	MG	GA	3081	1/1	0.99	0.11	14,14,14,14	0
57	MG	GA	3082	1/1	0.99	0.02	38,38,38,38	0
57	MG	EA	3026	1/1	0.99	0.10	0,0,0,0	0
57	MG	EA	3027	1/1	0.99	0.09	4,4,4,4	0
57	MG	GA	3085	1/1	0.99	0.04	10,10,10,10	0
57	MG	AA	3009	1/1	0.99	0.10	2,2,2,2	0
57	MG	EA	3029	1/1	0.99	0.13	2,2,2,2	0
57	MG	CA	3057	1/1	0.99	0.08	7,7,7,7	0
57	MG	EA	3033	1/1	0.99	0.12	0,0,0,0	0
57	MG	CA	3058	1/1	0.99	0.05	18,18,18,18	0
57	MG	EA	3035	1/1	0.99	0.05	12,12,12,12	0
57	MG	EA	3036	1/1	0.99	0.02	12,12,12,12	0
57	MG	EA	3037	1/1	0.99	0.11	2,2,2,2	0
57	MG	GA	3094	1/1	0.99	0.07	14,14,14,14	0
57	MG	CA	3059	1/1	0.99	0.09	10,10,10,10	0
57	MG	GA	3096	1/1	0.99	0.04	15,15,15,15	0
57	MG	GA	3097	1/1	0.99	0.12	10,10,10,10	0
57	MG	AA	3028	1/1	0.99	0.06	4,4,4,4	0
57	MG	CA	3062	1/1	0.99	0.06	15,15,15,15	0
57	MG	AA	3071	1/1	0.99	0.03	4,4,4,4	0
57	MG	CA	3064	1/1	0.99	0.10	6,6,6,6	0
57	MG	GA	3102	1/1	0.99	0.05	19,19,19,19	0
57	MG	CA	3065	1/1	0.99	0.05	11,11,11,11	0
57	MG	CA	3066	1/1	0.99	0.08	4,4,4,4	0
57	MG	GA	3106	1/1	0.99	0.11	7,7,7,7	0
57	MG	GA	3107	1/1	0.99	0.11	13,13,13,13	0
57	MG	EA	3046	1/1	0.99	0.15	9,9,9,9	0
57	MG	AA	3072	1/1	0.99	0.09	5,5,5,5	0
57	MG	EA	3048	1/1	0.99	0.09	25,25,25,25	0
57	MG	CA	3068	1/1	0.99	0.09	9,9,9,9	0
57	MG	AA	3073	1/1	0.99	0.07	2,2,2,2	0
57	MG	EA	3051	1/1	0.99	0.19	6,6,6,6	0
57	MG	AA	3029	1/1	0.99	0.13	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	EA	3053	1/1	0.99	0.12	1,1,1,1	0
57	MG	EA	3054	1/1	0.99	0.04	2,2,2,2	0
57	MG	BA	1606	1/1	0.99	0.07	14,14,14,14	0
57	MG	EA	3056	1/1	0.99	0.09	13,13,13,13	0
57	MG	GA	3120	1/1	0.99	0.08	19,19,19,19	0
57	MG	CA	3073	1/1	0.99	0.09	4,4,4,4	0
57	MG	EA	3058	1/1	0.99	0.10	5,5,5,5	0
57	MG	EA	3060	1/1	0.99	0.13	2,2,2,2	0
57	MG	GA	3125	1/1	0.99	0.05	10,10,10,10	0
57	MG	AA	3030	1/1	0.99	0.05	1,1,1,1	0
57	MG	EA	3063	1/1	0.99	0.04	2,2,2,2	0
57	MG	EA	3066	1/1	0.99	0.03	1,1,1,1	0
57	MG	EA	3067	1/1	0.99	0.10	3,3,3,3	0
57	MG	GA	3130	1/1	0.99	0.04	18,18,18,18	0
57	MG	EA	3068	1/1	0.99	0.10	2,2,2,2	0
57	MG	CA	3075	1/1	0.99	0.08	11,11,11,11	0
57	MG	AA	3077	1/1	0.99	0.05	16,16,16,16	0
57	MG	EA	3071	1/1	0.99	0.07	0,0,0,0	0
57	MG	EA	3072	1/1	0.99	0.08	2,2,2,2	0
57	MG	EA	3073	1/1	0.99	0.06	0,0,0,0	0
57	MG	EA	3074	1/1	0.99	0.10	11,11,11,11	0
57	MG	EA	3075	1/1	0.99	0.05	11,11,11,11	0
57	MG	BA	1609	1/1	0.99	0.03	7,7,7,7	0
57	MG	EA	3077	1/1	0.99	0.09	18,18,18,18	0
57	MG	EA	3078	1/1	0.99	0.12	20,20,20,20	0
57	MG	HA	1603	1/1	0.99	0.02	25,25,25,25	0
57	MG	HA	1604	1/1	0.99	0.08	31,31,31,31	0
57	MG	HA	1605	1/1	0.99	0.05	40,40,40,40	0
57	MG	EA	3080	1/1	0.99	0.07	15,15,15,15	0
57	MG	EA	3081	1/1	0.99	0.06	0,0,0,0	0
57	MG	AA	3031	1/1	0.99	0.10	5,5,5,5	0
57	MG	BA	1613	1/1	0.99	0.10	8,8,8,8	0
57	MG	EA	3085	1/1	0.99	0.09	11,11,11,11	0
57	MG	EA	3086	1/1	0.99	0.06	8,8,8,8	0
57	MG	BA	1614	1/1	0.99	0.03	7,7,7,7	0
57	MG	CA	3081	1/1	0.99	0.10	6,6,6,6	0
57	MG	EA	3089	1/1	0.99	0.04	6,6,6,6	0
57	MG	EA	3090	1/1	0.99	0.02	11,11,11,11	0
57	MG	AA	3080	1/1	0.99	0.09	0,0,0,0	0
57	MG	EA	3092	1/1	0.99	0.10	22,22,22,22	0
57	MG	EA	3093	1/1	0.99	0.07	11,11,11,11	0
57	MG	CA	3084	1/1	0.99	0.12	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	1616	1/1	0.99	0.11	3,3,3,3	0
57	MG	EA	3096	1/1	0.99	0.09	9,9,9,9	0
57	MG	CA	3086	1/1	0.99	0.06	15,15,15,15	0
57	MG	AA	3081	1/1	0.99	0.03	1,1,1,1	0
57	MG	EA	3099	1/1	0.99	0.09	3,3,3,3	0
57	MG	AA	3010	1/1	0.99	0.12	8,8,8,8	0
57	MG	AA	3034	1/1	0.99	0.10	4,4,4,4	0
57	MG	EA	3102	1/1	0.99	0.03	23,23,23,23	0
57	MG	EA	3103	1/1	0.99	0.16	0,0,0,0	0
57	MG	EA	3104	1/1	0.99	0.11	0,0,0,0	0
57	MG	EA	3107	1/1	0.99	0.04	5,5,5,5	0
57	MG	BA	1621	1/1	0.99	0.03	11,11,11,11	0
57	MG	AA	3011	1/1	0.99	0.12	6,6,6,6	0
57	MG	AA	3086	1/1	0.99	0.03	14,14,14,14	0
57	MG	EA	3112	1/1	0.99	0.09	2,2,2,2	0
57	MG	AA	3087	1/1	0.99	0.07	19,19,19,19	0
57	MG	HA	1636	1/1	0.99	0.03	28,28,28,28	0
57	MG	AA	3036	1/1	0.99	0.08	2,2,2,2	0
57	MG	AA	3089	1/1	0.99	0.03	4,4,4,4	0
57	MG	EA	3116	1/1	0.99	0.08	6,6,6,6	0
57	MG	HA	1640	1/1	0.99	0.10	18,18,18,18	0
57	MG	AA	3037	1/1	0.99	0.15	30,30,30,30	0
57	MG	BA	1630	1/1	0.99	0.12	26,26,26,26	0
57	MG	CA	3099	1/1	0.99	0.04	5,5,5,5	0
57	MG	CA	3101	1/1	0.99	0.06	5,5,5,5	0
58	ZN	A4	102	1/1	0.99	0.02	42,42,42,42	0
57	MG	CA	3102	1/1	0.99	0.11	9,9,9,9	0
58	ZN	G4	101	1/1	0.99	0.03	66,66,66,66	0
59	GCP	BV	801	32/32	0.99	0.04	9,25,32,35	0
57	MG	AB	1202	1/1	0.99	0.03	25,25,25,25	0
57	MG	EA	3123	1/1	0.99	0.07	3,3,3,3	0
57	MG	BA	1632	1/1	0.99	0.08	14,14,14,14	0
57	MG	EA	3106	1/1	1.00	0.02	9,9,9,9	0
57	MG	AA	3085	1/1	1.00	0.01	7,7,7,7	0
57	MG	DV	802	1/1	1.00	0.08	14,14,14,14	0
57	MG	GA	3122	1/1	1.00	0.04	16,16,16,16	0
57	MG	BA	1611	1/1	1.00	0.02	7,7,7,7	0
57	MG	FA	1632	1/1	1.00	0.06	24,24,24,24	0
57	MG	CA	3097	1/1	1.00	0.03	3,3,3,3	0
57	MG	EA	3111	1/1	1.00	0.01	5,5,5,5	0
57	MG	BA	1612	1/1	1.00	0.07	3,3,3,3	0
57	MG	CA	3060	1/1	1.00	0.03	7,7,7,7	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	CA	3100	1/1	1.00	0.04	16,16,16,16	0
57	MG	AA	3103	1/1	1.00	0.06	0,0,0,0	0
57	MG	AA	3024	1/1	1.00	0.06	5,5,5,5	0
57	MG	AA	3105	1/1	1.00	0.03	2,2,2,2	0
57	MG	EA	3059	1/1	1.00	0.06	10,10,10,10	0
57	MG	FN	202	1/1	1.00	0.06	26,26,26,26	0
57	MG	CA	3104	1/1	1.00	0.06	8,8,8,8	0
57	MG	AA	3050	1/1	1.00	0.10	2,2,2,2	0
57	MG	EA	3062	1/1	1.00	0.07	4,4,4,4	0
57	MG	AA	3107	1/1	1.00	0.08	4,4,4,4	0
57	MG	EA	3064	1/1	1.00	0.05	2,2,2,2	0
57	MG	EA	3065	1/1	1.00	0.04	5,5,5,5	0
57	MG	AA	3108	1/1	1.00	0.10	1,1,1,1	0
57	MG	EA	3013	1/1	1.00	0.03	1,1,1,1	0
57	MG	BA	1619	1/1	1.00	0.09	13,13,13,13	0
57	MG	DA	1613	1/1	1.00	0.03	23,23,23,23	0
57	MG	EA	3129	1/1	1.00	0.09	2,2,2,2	0
57	MG	CA	3001	1/1	1.00	0.02	16,16,16,16	0
57	MG	GA	3075	1/1	1.00	0.03	16,16,16,16	0
57	MG	EA	3131	1/1	1.00	0.05	3,3,3,3	0
57	MG	CA	3033	1/1	1.00	0.06	6,6,6,6	0
57	MG	AA	3003	1/1	1.00	0.05	11,11,11,11	0
57	MG	CA	3035	1/1	1.00	0.04	7,7,7,7	0
57	MG	CA	3072	1/1	1.00	0.05	14,14,14,14	0
57	MG	AA	3074	1/1	1.00	0.04	5,5,5,5	0
57	MG	AA	3133	1/1	1.00	0.05	10,10,10,10	0
57	MG	BA	1623	1/1	1.00	0.01	25,25,25,25	0
57	MG	EA	3024	1/1	1.00	0.07	2,2,2,2	0
57	MG	EA	3079	1/1	1.00	0.07	8,8,8,8	0
57	MG	EB	1204	1/1	1.00	0.06	8,8,8,8	0
57	MG	AA	3017	1/1	1.00	0.03	0,0,0,0	0
57	MG	AA	3032	1/1	1.00	0.05	0,0,0,0	0
57	MG	AA	3064	1/1	1.00	0.02	3,3,3,3	0
57	MG	AA	3014	1/1	1.00	0.03	2,2,2,2	0
57	MG	GA	3022	1/1	1.00	0.07	30,30,30,30	0
57	MG	EA	3084	1/1	1.00	0.09	7,7,7,7	0
57	MG	BA	1628	1/1	1.00	0.05	18,18,18,18	0
57	MG	AA	3079	1/1	1.00	0.05	4,4,4,4	0
57	MG	EA	3031	1/1	1.00	0.04	1,1,1,1	0
57	MG	EA	3032	1/1	1.00	0.06	1,1,1,1	0
57	MG	FA	1608	1/1	1.00	0.05	13,13,13,13	0
57	MG	CA	3082	1/1	1.00	0.05	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	1601	1/1	1.00	0.11	23,23,23,23	0
57	MG	CA	3013	1/1	1.00	0.03	9,9,9,9	0
57	MG	AA	3004	1/1	1.00	0.09	20,20,20,20	0
57	MG	AA	3096	1/1	1.00	0.03	0,0,0,0	0
57	MG	EA	3038	1/1	1.00	0.07	2,2,2,2	0
57	MG	CA	3128	1/1	1.00	0.05	17,17,17,17	0
57	MG	GA	3105	1/1	1.00	0.05	16,16,16,16	0
57	MG	AA	3067	1/1	1.00	0.07	2,2,2,2	0
57	MG	AA	3098	1/1	1.00	0.06	0,0,0,0	0
57	MG	AA	3056	1/1	1.00	0.03	11,11,11,11	0
57	MG	CA	3052	1/1	1.00	0.06	4,4,4,4	0
57	MG	AA	3121	1/1	1.00	0.07	3,3,3,3	0
57	MG	CA	3054	1/1	1.00	0.03	14,14,14,14	0
57	MG	GA	3112	1/1	1.00	0.09	13,13,13,13	0
58	ZN	C4	102	1/1	1.00	0.01	41,41,41,41	0
57	MG	FA	1622	1/1	1.00	0.07	9,9,9,9	0
57	MG	FA	1623	1/1	1.00	0.08	6,6,6,6	0
57	MG	AA	3041	1/1	1.00	0.07	7,7,7,7	0
57	MG	AA	3058	1/1	1.00	0.04	9,9,9,9	0
57	MG	CE	301	1/1	1.00	0.06	19,19,19,19	0
57	MG	EA	3105	1/1	1.00	0.08	5,5,5,5	0

## 6.5 Other polymers

There are no such residues in this entry.