



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 26, 2023 – 10:20 AM EDT

PDB ID : 6C5L  
Title : Conformation of methylated GGQ in the Peptidyl Transferase Center during translation termination (*T. thermophilus*)  
Authors : Zeng, F.; Jin, H.  
Deposited on : 2018-01-16  
Resolution : 3.20 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>.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

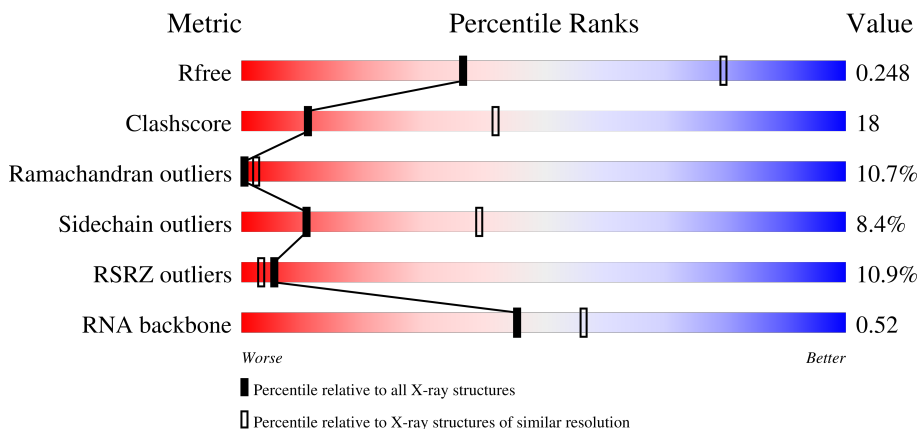
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


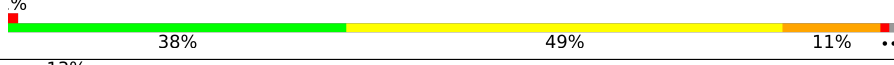
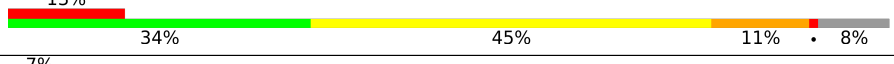
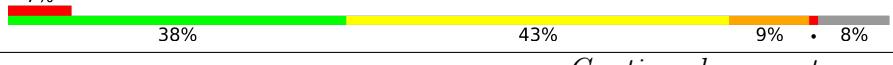
The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)
RNA backbone	3102	1010 (3.50-2.90)

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

Mol	Chain	Length	Quality of chain
1	AA	1522	 38% 49% 10% ..
1	CA	1522	 38% 49% 11% ..
2	AB	256	 13% 34% 45% 11% • 8%
2	CB	256	 7% 38% 43% 9% • 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	132	
12	CL	132	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	CO	89	2% 58% 38% ..
16	AP	88	18% 38% 53% 5% 5%
16	CP	88	43% 41% 51% 5%
17	AQ	105	10% 54% 37% 5%
17	CQ	105	15% 52% 40% 5%
18	AR	88	20% 42% 33% .. 20%
18	CR	88	8% 44% 31% 5% 20%
19	AS	93	38% 39% 34% 10% 15%
19	CS	93	43% 35% 37% 11% 15%
20	AT	106	8% 60% 28% 5% 7%
20	CT	106	23% 66% 23% .. 7%
21	AU	27	89% 44% 41% 7% 7%
21	CU	27	70% 33% 48% 11% 7%
22	AV	76	49% 39% 9% .
22	AW	76	17% 26% 53% 13% 7% .
22	CV	76	3% 46% 43% 8% .
22	CW	76	14% 25% 49% 21% ..
23	AX	25	4% 12% 16% . 68%
23	CX	25	16% 8% 8% 68%
24	AY	357	40% 61% 34% ..
24	CY	357	45% 52% 41% ..
25	B0	85	20% 56% 38% ..
25	D0	85	20% 66% 28% ..
26	B1	98	5% 42% 44% 8% ..
26	D1	98	5% 50% 41% .. .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
27	B2	72	7% 38% 46% 15%
27	D2	72	6% 56% 29% 10%
28	B3	60	42% 58% 38%
28	D3	60	22% 62% 35%
29	B4	71	4% 17% 25% 56%
29	D4	71	% 15% 24% 56%
30	B5	60	8% 53% 30% 7% 8%
30	D5	60	8% 48% 35% 7% 8%
31	B6	54	74% 17% 43% 19% 6% 17%
31	D6	54	76% 19% 33% 20% 11% 17%
32	B7	49	12% 63% 37%
32	D7	49	4% 71% 29%
33	B8	65	11% 38% 48% 5% 8%
33	D8	65	5% 46% 38% 8% 6%
34	B9	37	95% 59% 32% 5%
34	D9	37	97% 59% 32% 5%
35	BA	2915	% 43% 44% 12%
35	DA	2915	2% 44% 43% 12%
36	BB	122	51% 36% 10%
36	DB	122	% 45% 39% 13%
37	BC	229	34% 24% 25% 48%
37	DC	229	37% 27% 24% 48%
38	BD	276	3% 49% 37% 11%
38	DD	276	2% 51% 37% 9%
39	BE	206	9% 50% 37% 11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
39	DE	206	
40	BF	210	
40	DF	210	
41	BG	182	
41	DG	182	
42	BH	180	
42	DH	180	
43	BI	148	
43	DI	148	
44	BJ	130	
44	DJ	130	
45	BK	147	
45	DK	147	
46	BN	140	
46	DN	140	
47	BO	122	
47	DO	122	
48	BP	150	
48	DP	150	
49	BQ	141	
49	DQ	141	
50	BR	118	
50	DR	118	
51	BS	112	
51	DS	112	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
52	BT	146	
52	DT	146	
53	BU	118	
53	DU	118	
54	BV	101	
54	DV	101	
55	BW	113	
55	DW	113	
56	BX	96	
56	DX	96	
57	BY	110	
57	DY	110	
58	BZ	206	
58	DZ	206	

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
24	MEQ	CY	240	-	-	-	X
59	MG	AA	1617	-	-	-	X
59	MG	AA	1622	-	-	-	X
59	MG	BA	3082	-	-	-	X
59	MG	BA	3105	-	-	-	X
59	MG	BA	3120	-	-	-	X
59	MG	BA	3125	-	-	-	X
59	MG	BA	3144	-	-	-	X
59	MG	BA	3155	-	-	-	X
59	MG	BA	3162	-	-	-	X
59	MG	BA	3174	-	-	-	X
59	MG	BA	3179	-	-	-	X
59	MG	BB	202	-	-	-	X

Continued on next page...

*Continued from previous page...*

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
59	MG	BQ	201	-	-	-	X
59	MG	BT	201	-	-	-	X
59	MG	CA	1606	-	-	-	X
59	MG	CA	1617	-	-	-	X
59	MG	DA	3104	-	-	-	X
59	MG	DA	3163	-	-	-	X
59	MG	DA	3176	-	-	-	X
60	ZN	B9	101	-	-	-	X



## 2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 304459 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 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	AA	1504	Total 32329	C 14390	N 5992	O 10444	P 1503	0	0	0
1	CA	1504	Total 32329	C 14390	N 5992	O 10444	P 1503	0	0	0

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	AB	235	Total 1901	C 1213	N 342	O 341	S 5	0	0	1
2	CB	235	Total 1901	C 1213	N 342	O 341	S 5	0	0	1

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	AC	207	Total 1613	C 1016	N 315	O 281	S 1	0	0	1
3	CC	207	Total 1613	C 1016	N 315	O 281	S 1	0	0	1

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	AD	208	Total 1703	C 1066	N 339	O 291	S 7	0	0	0
4	CD	208	Total 1703	C 1066	N 339	O 291	S 7	0	0	0

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			
5	CE	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
6	CF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
7	CG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
8	CH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O	0	0	0
			1011	639	198	174			
9	CI	127	Total	C	N	O	0	0	0
			1011	639	198	174			

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	CJ	99	795	499	157	138	1	0	0	1

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	AK	119	885	549	168	165	3	0	0	0
11	CK	119	885	549	168	165	3	0	0	0

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	AL	125	971	611	196	163	1	0	0	1
12	CL	125	971	611	196	163	1	0	0	1

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	AM	125	988	611	206	169	2	0	0	1
13	CM	125	988	611	206	169	2	0	0	1

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	AN	60	492	312	104	72	4	0	0	0
14	CN	60	492	312	104	72	4	0	0	0

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	AO	88	734	459	147	126	2	0	0	0
15	CO	88	734	459	147	126	2	0	0	0

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			
16	CP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			
17	CQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	70	Total	C	N	O	0	0	0
			574	367	112	95			
18	CR	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			
19	CS	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			
20	CT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 21 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	25	Total	C	N	O	0	0	1
			209	128	51	30			
21	CU	25	Total	C	N	O	0	0	1
			209	128	51	30			

- Molecule 22 is a RNA chain called E-site tRNA PHE OR P-site tRNA PHE (unmodified bases).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			
22	AW	75	Total	C	N	O	P	0	0	0
			1597	713	285	525	74			
22	CV	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			
22	CW	75	Total	C	N	O	P	0	0	0
			1597	713	285	525	74			

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
23	AX	8	Total	C	N	O	P	0	0	0
			166	76	29	54	7			
23	CX	8	Total	C	N	O	P	0	0	0
			166	76	29	54	7			

- Molecule 24 is a protein called Peptide chain release factor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AY	351	Total	C	N	O	S	0	0	0
			2802	1753	506	535	8			
24	CY	351	Total	C	N	O	S	0	0	0
			2802	1753	506	535	8			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AY	0	HIS	-	expression tag	UNP F6DD48
AY	1	HIS	-	expression tag	UNP F6DD48
AY	2	HIS	-	expression tag	UNP F6DD48
AY	3	HIS	-	expression tag	UNP F6DD48
AY	4	HIS	-	expression tag	UNP F6DD48
AY	5	HIS	-	expression tag	UNP F6DD48

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
CY	0	HIS	-	expression tag	UNP F6DD48
CY	1	HIS	-	expression tag	UNP F6DD48
CY	2	HIS	-	expression tag	UNP F6DD48
CY	3	HIS	-	expression tag	UNP F6DD48
CY	4	HIS	-	expression tag	UNP F6DD48
CY	5	HIS	-	expression tag	UNP F6DD48

- Molecule 25 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
25	B0	83	657	407	139	110	1	0	0	0
25	D0	83	657	407	139	110	1	0	0	0

- Molecule 26 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	B1	94	732	460	146	125	1	0	0	1
26	D1	94	732	460	146	125	1	0	0	1

- Molecule 27 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
27	B2	71	598	370	121	106	1	0	0	0
27	D2	71	598	370	121	106	1	0	0	0

- Molecule 28 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
28	B3	60	468	298	91	78	1	0	0	1
28	D3	60	468	298	91	78	1	0	0	1

- Molecule 29 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	B4	31	Total	C	N	O	S	0	0	1
			226	142	37	43	4			
29	D4	31	Total	C	N	O	S	0	0	1
			226	142	37	43	4			

- Molecule 30 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	B5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
30	D5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 31 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	B6	45	Total	C	N	O	S	0	0	1
			381	235	78	64	4			
31	D6	45	Total	C	N	O	S	0	0	1
			381	235	78	64	4			

- Molecule 32 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	B7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			
32	D7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			

- Molecule 33 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	B8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			
33	D8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			

- Molecule 34 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	B9	36	Total	C	N	O	S	0	0	0
			299	183	67	46	3			

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	D9	36	Total	C	N	O	S	0	0	0
			299	183	67	46	3			

- Molecule 35 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BA	2901	Total	C	N	O	P	0	0	0
			62474	27806	11681	20087	2900			
35	DA	2901	Total	C	N	O	P	0	0	0
			62474	27806	11681	20087	2900			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	1227	G	UNK	conflict	GB 37223181
DA	1227	G	UNK	conflict	GB 37223181

- Molecule 36 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			
36	DB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

- Molecule 37 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BC	120	Total	C	N	O	S	0	0	0
			937	590	174	172	1			
37	DC	120	Total	C	N	O	S	0	0	0
			937	590	174	172	1			

- Molecule 38 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BD	273	Total	C	N	O	S	0	0	0
			2120	1338	421	358	3			
38	DD	273	Total	C	N	O	S	0	0	0
			2120	1338	421	358	3			

- Molecule 39 is a protein called 50S ribosomal protein L3.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BE	205	Total	C	N	O	S	0	0	1
			1564	988	300	270	6			
39	DE	205	Total	C	N	O	S	0	0	1
			1564	988	300	270	6			

- Molecule 40 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BF	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			
40	DF	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			

- Molecule 41 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			
41	DG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 42 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BH	165	Total	C	N	O	S	0	0	1
			1248	788	234	225	1			
42	DH	165	Total	C	N	O	S	0	0	1
			1248	788	234	225	1			

- Molecule 43 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BI	146	Total	C	N	O	S	0	0	1
			1132	723	201	207	1			
43	DI	146	Total	C	N	O	S	0	0	1
			1132	723	201	207	1			

- Molecule 44 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
44	BJ	130	Total	C	N	O	0	0	0
			651	390	130	131			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
44	DJ	130	Total	C	N	O	0	0	0
			651	390	130	131			

- Molecule 45 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BK	141	Total	C	N	O	S	0	0	1
			1038	661	184	187	6			
45	DK	141	Total	C	N	O	S	0	0	1
			1038	661	184	187	6			

- Molecule 46 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			
46	DN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			

- Molecule 47 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
47	DO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 48 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			
48	DP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 49 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
49	DQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
50	BR	117	960	599	202	159	0	0	0
50	DR	117	960	599	202	159	0	0	0

- Molecule 51 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
51	BS	99	771	486	155	130	0	0	1
51	DS	99	771	486	155	130	0	0	1

- Molecule 52 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
52	BT	138	1142	710	235	196	1	0	0	1
52	DT	138	1142	710	235	196	1	0	0	1

- Molecule 53 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
53	BU	117	958	604	202	151	1	0	0	0
53	DU	117	958	604	202	151	1	0	0	0

- Molecule 54 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
54	BV	101	779	501	142	135	1	0	0	0
54	DV	101	779	501	142	135	1	0	0	0

- Molecule 55 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	BW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			
55	DW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			

- Molecule 56 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	BX	93	Total	C	N	O	S	0	0	1
			726	471	132	123				
56	DX	93	Total	C	N	O	S	0	0	1
			726	471	132	123				

- Molecule 57 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	BY	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			
57	DY	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			

- Molecule 58 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	BZ	185	Total	C	N	O	S	0	0	1
			1468	936	262	268	2			
58	DZ	185	Total	C	N	O	S	0	0	1
			1468	936	262	268	2			

- Molecule 59 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	AA	30	Total	Mg	0	0
			30	30		
59	B5	1	Total	Mg	0	0
			1	1		
59	BA	180	Total	Mg	0	0
			180	180		
59	BB	2	Total	Mg	0	0
			2	2		
59	BD	1	Total	Mg	0	0
			1	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	BE	1	Total Mg 1 1	0	0
59	BF	1	Total Mg 1 1	0	0
59	BQ	1	Total Mg 1 1	0	0
59	BT	1	Total Mg 1 1	0	0
59	CA	26	Total Mg 26 26	0	0
59	D5	2	Total Mg 2 2	0	0
59	DA	221	Total Mg 221 221	0	0
59	DB	2	Total Mg 2 2	0	0
59	DD	2	Total Mg 2 2	0	0
59	DP	1	Total Mg 1 1	0	0
59	DU	1	Total Mg 1 1	0	0
59	DW	1	Total Mg 1 1	0	0

- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	AD	1	Total Zn 1 1	0	0
60	AN	1	Total Zn 1 1	0	0
60	B9	1	Total Zn 1 1	0	0
60	CD	1	Total Zn 1 1	0	0
60	CN	1	Total Zn 1 1	0	0
60	D9	1	Total Zn 1 1	0	0

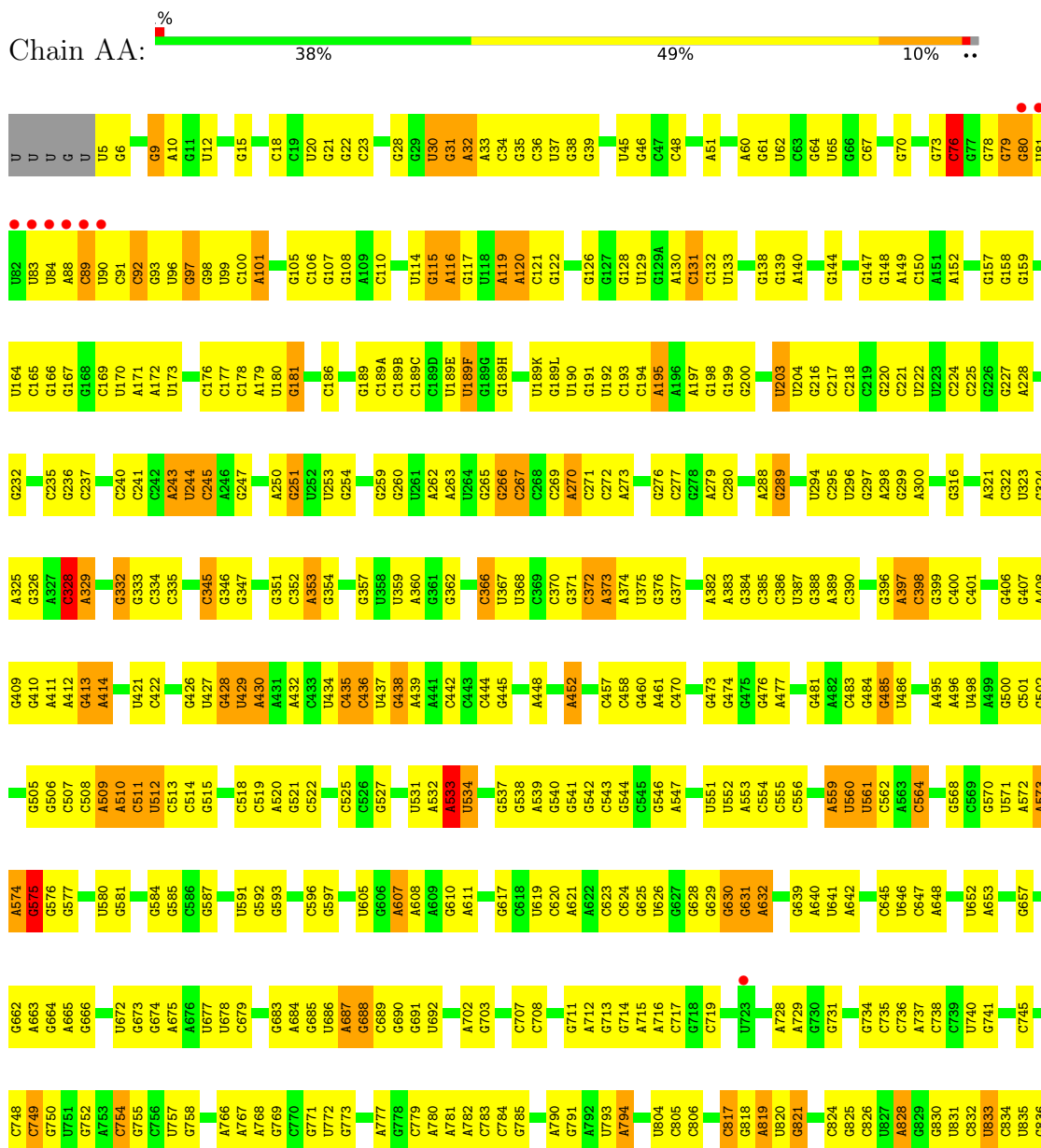
- Molecule 61 is water.

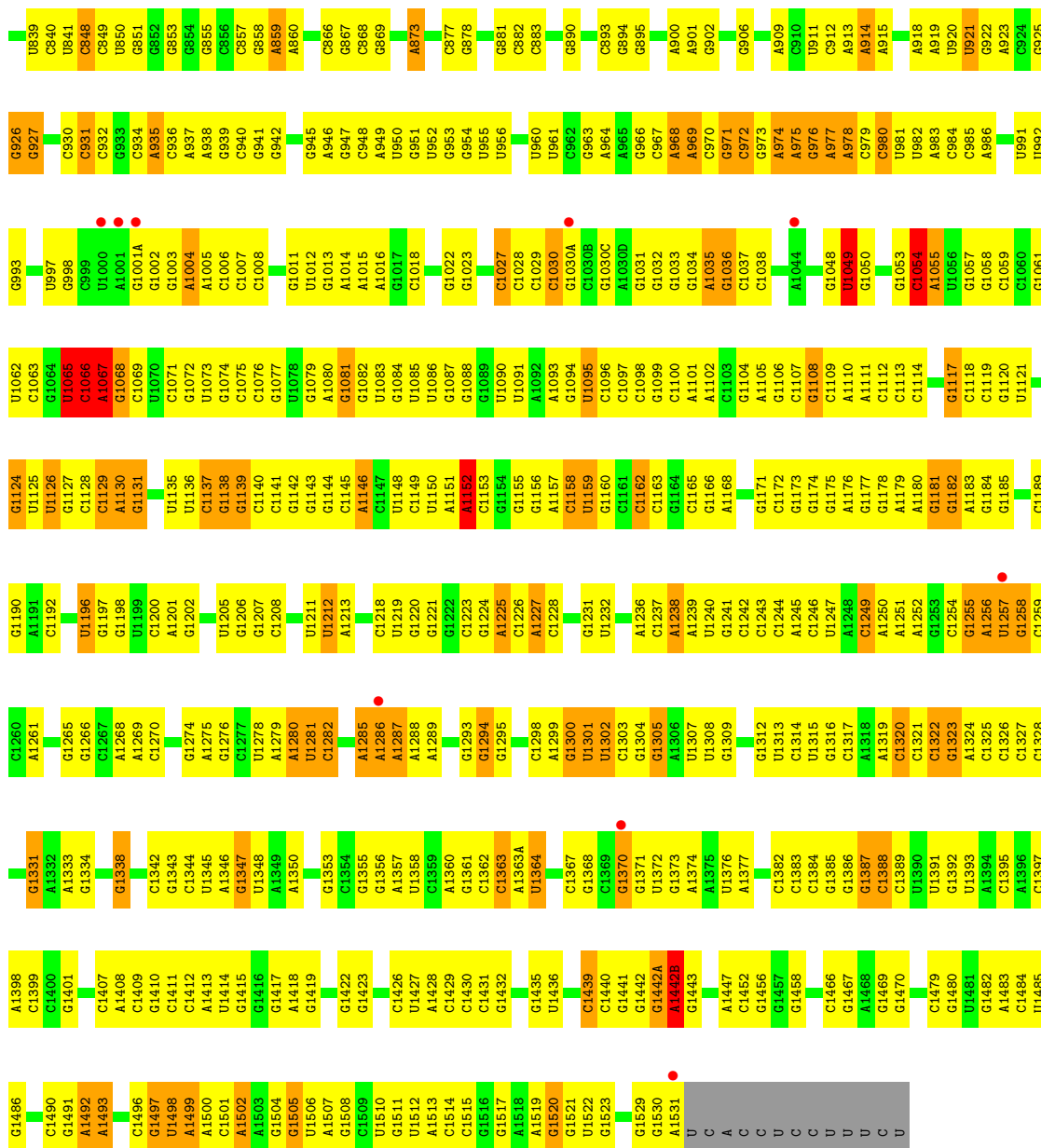
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
61	AA	2	Total O 2 2	0	0
61	BA	6	Total O 6 6	0	0
61	BE	1	Total O 1 1	0	0
61	DA	7	Total O 7 7	0	0
61	DE	1	Total O 1 1	0	0
61	DS	1	Total O 1 1	0	0
61	DZ	1	Total O 1 1	0	0

### 3 Residue-property plots

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

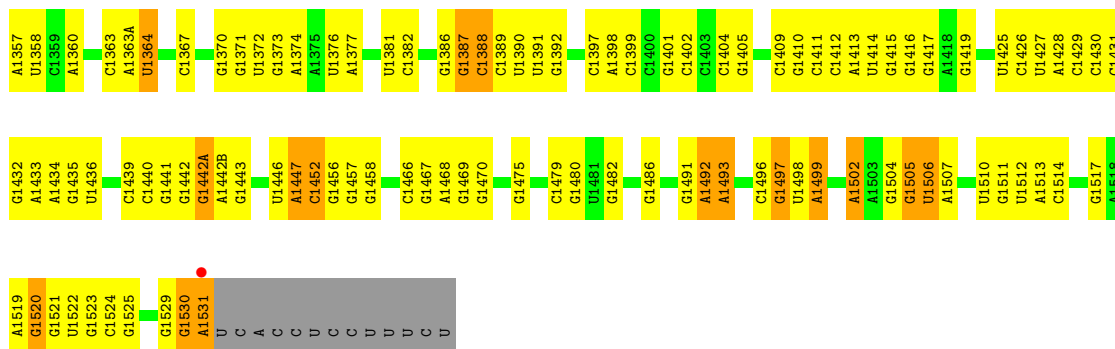
- Molecule 1: 16S rRNA



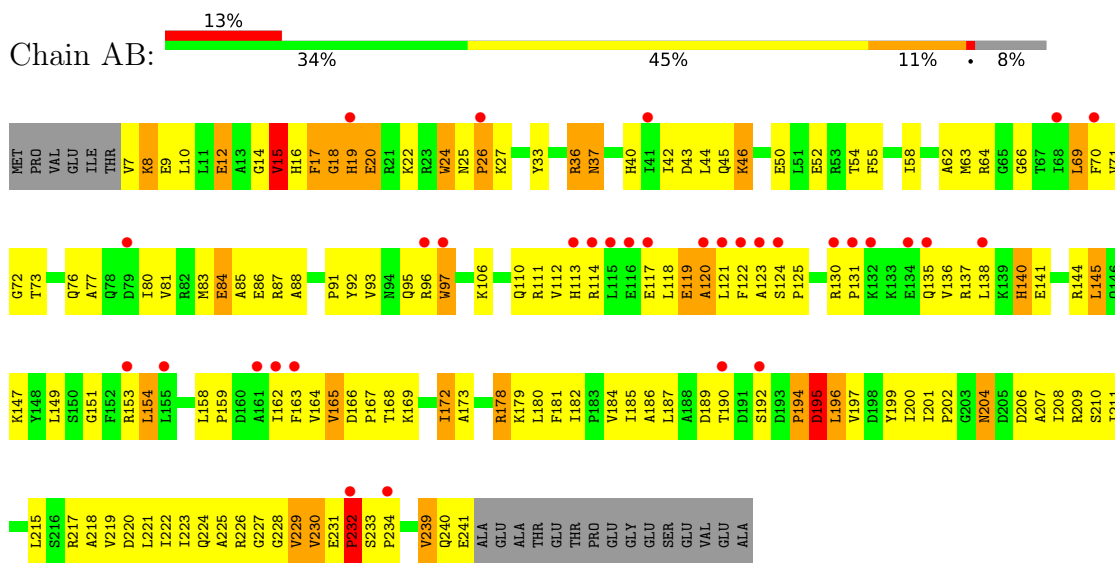




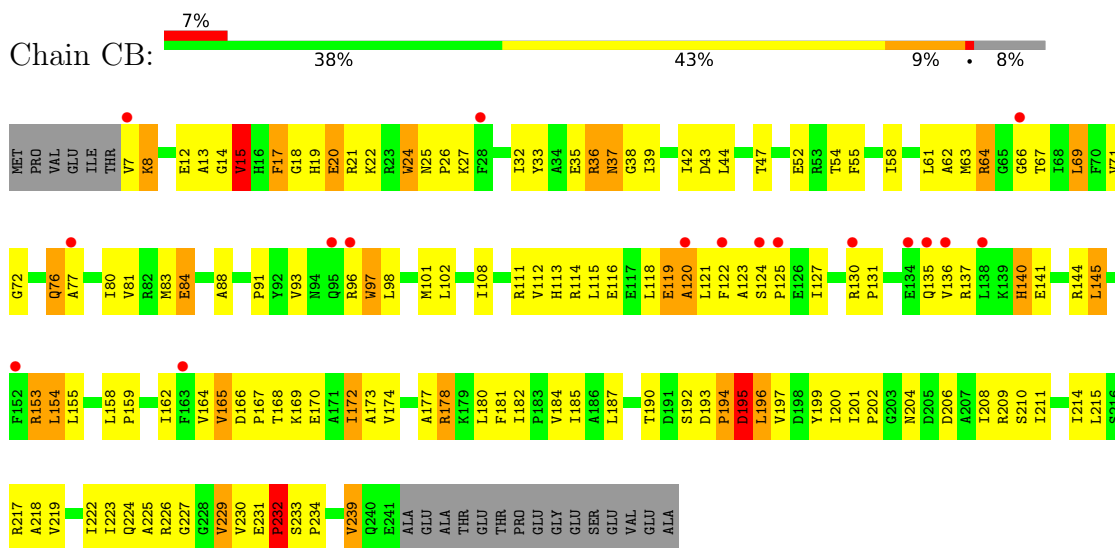




• Molecule 2: 30S ribosomal protein S2



• Molecule 2: 30S ribosomal protein S2



• Molecule 3: 30S ribosomal protein S3

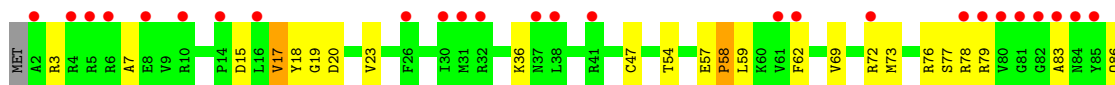








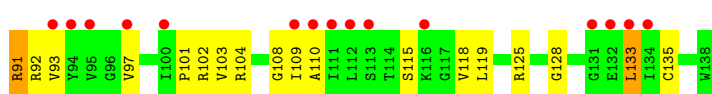
- Molecule 7: 30S ribosomal protein S7



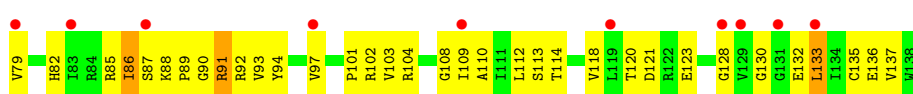
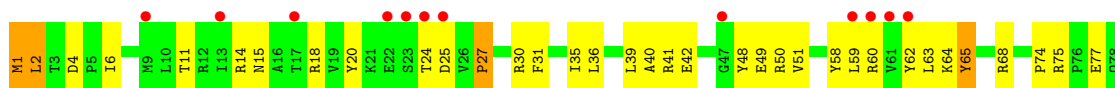
- Molecule 7: 30S ribosomal protein S7



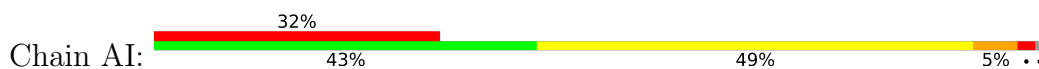
- Molecule 8: 30S ribosomal protein S8

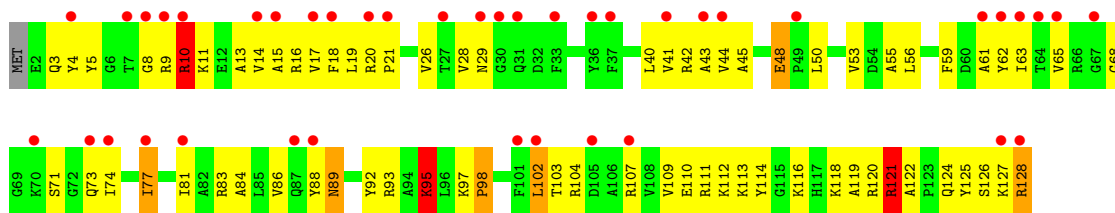


- Molecule 8: 30S ribosomal protein S8

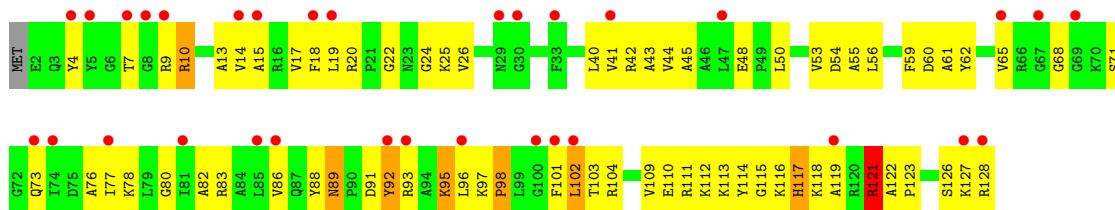


- Molecule 9: 30S ribosomal protein S9

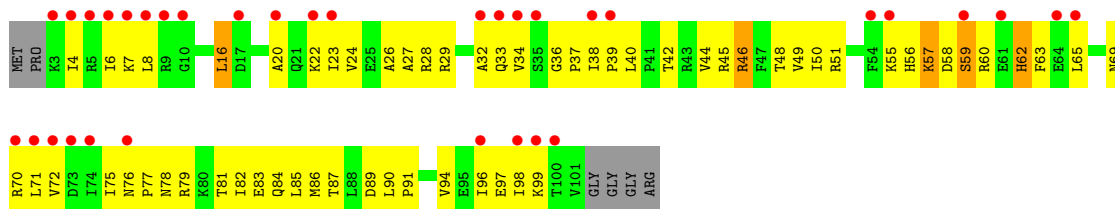




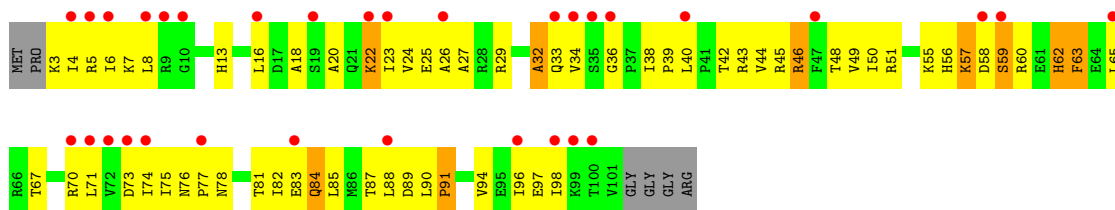
● Molecule 9: 30S ribosomal protein S9



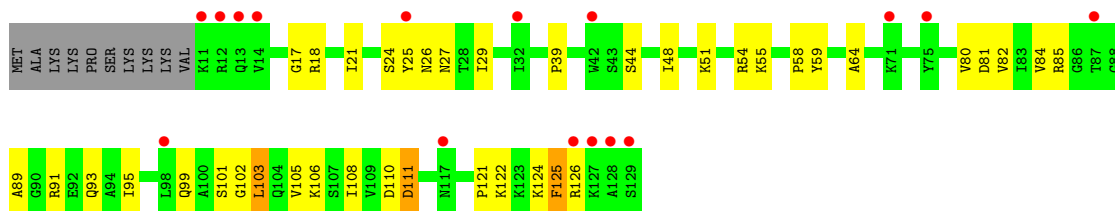
● Molecule 10: 30S ribosomal protein S10



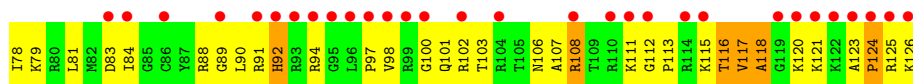
● Molecule 10: 30S ribosomal protein S10



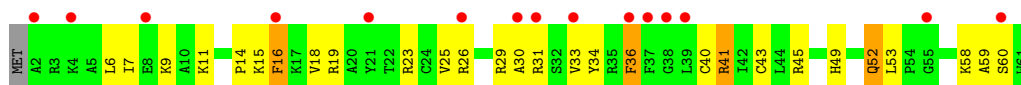
● Molecule 11: 30S ribosomal protein S11



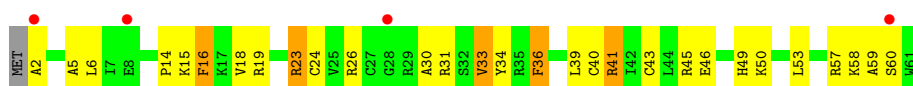




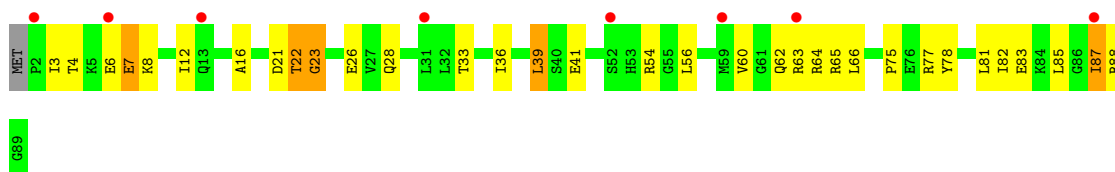
- Molecule 14: 30S ribosomal protein S14 type Z



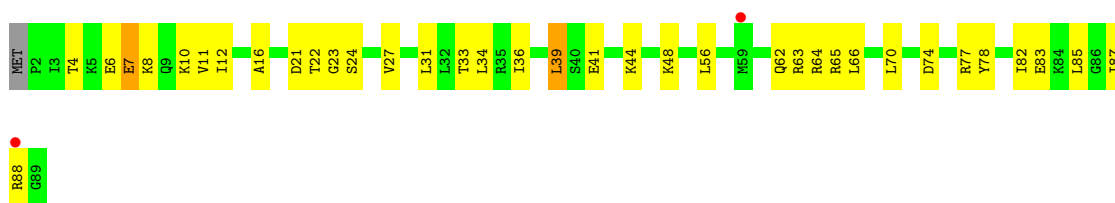
- Molecule 14: 30S ribosomal protein S14 type Z



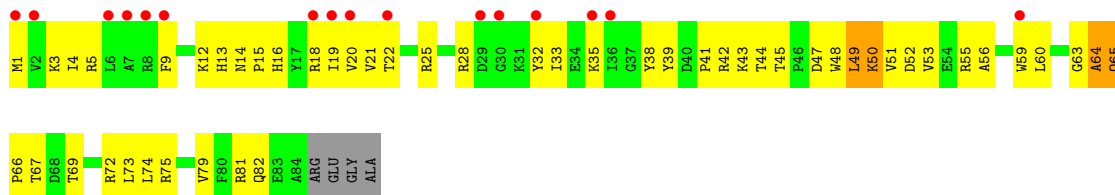
- Molecule 15: 30S ribosomal protein S15



- Molecule 15: 30S ribosomal protein S15

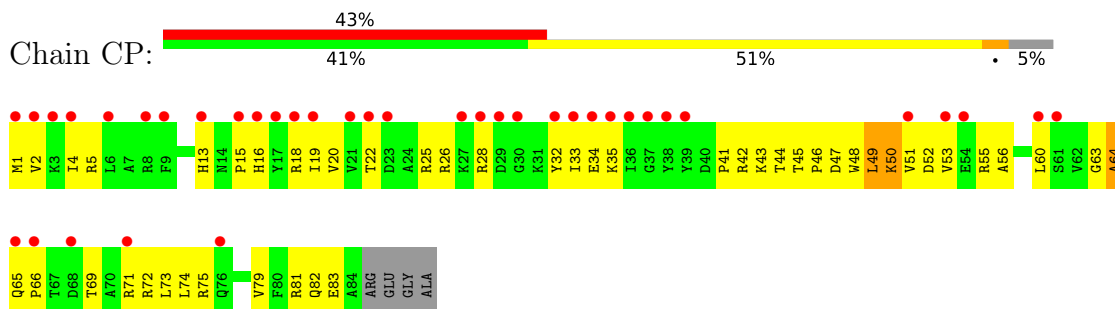


- Molecule 16: 30S ribosomal protein S16

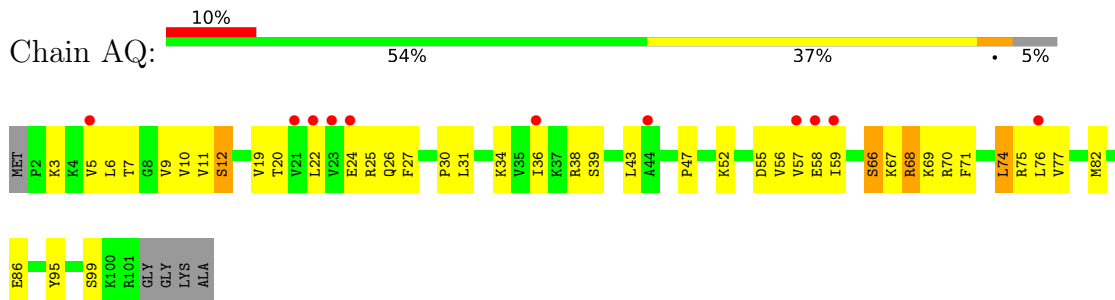


- Molecule 16: 30S ribosomal protein S16

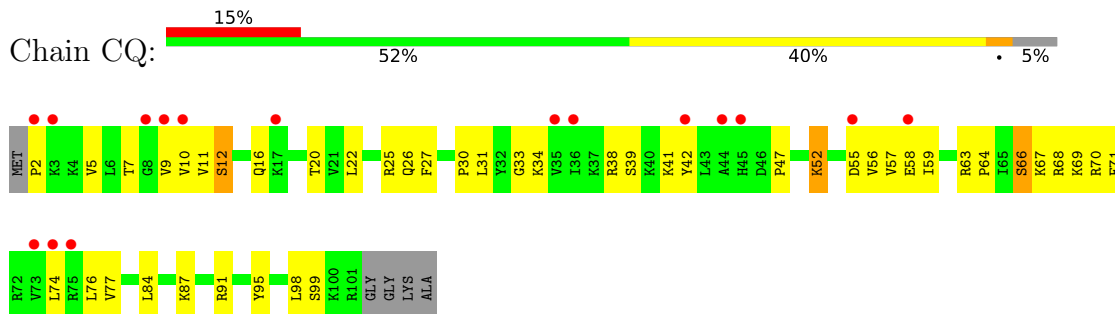




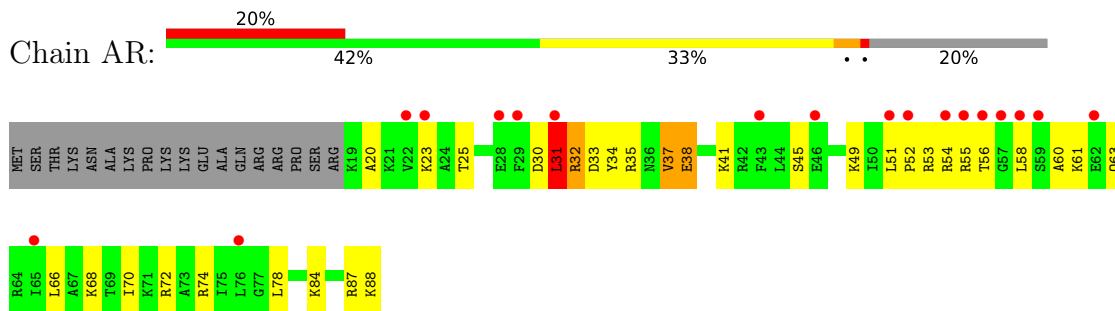
- Molecule 17: 30S ribosomal protein S17



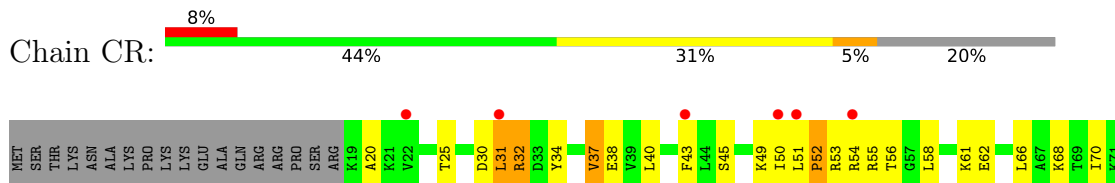
- Molecule 17: 30S ribosomal protein S17

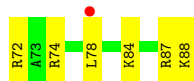


- Molecule 18: 30S ribosomal protein S18

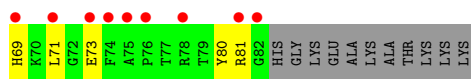
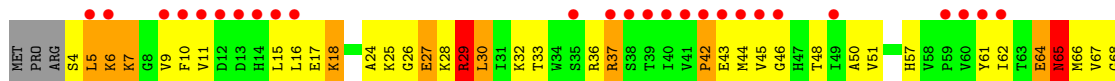
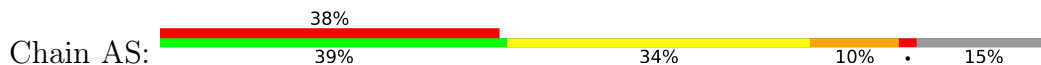


- Molecule 18: 30S ribosomal protein S18

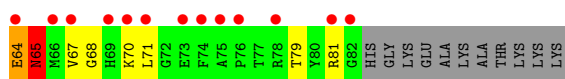
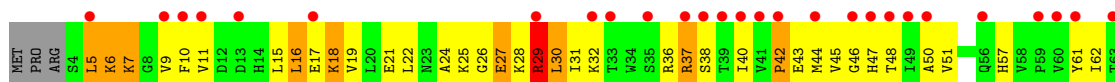




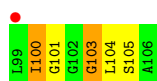
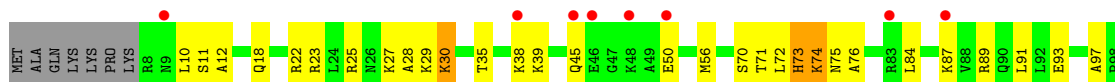
- Molecule 19: 30S ribosomal protein S19



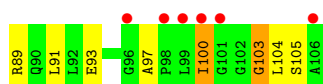
- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20

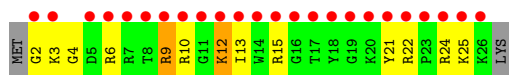


- Molecule 20: 30S ribosomal protein S20

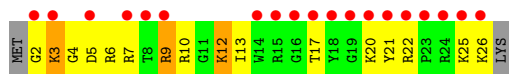
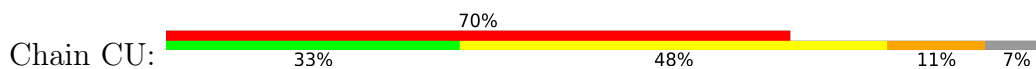


- Molecule 21: 30S ribosomal protein Thx

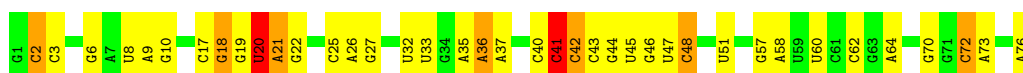




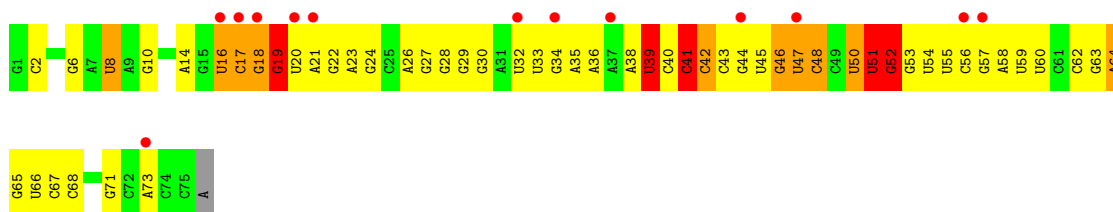
- Molecule 21: 30S ribosomal protein Thx



- Molecule 22: E-site tRNA PHE OR P-site tRNA PHE (unmodified bases)



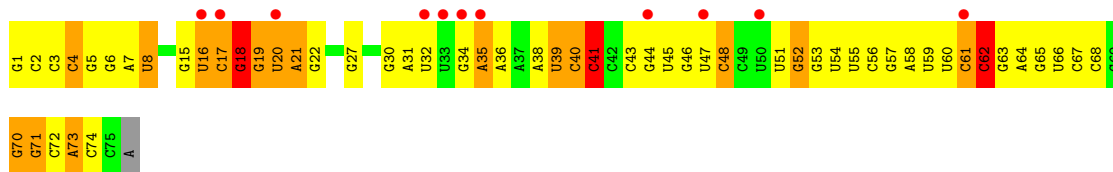
- Molecule 22: E-site tRNA PHE OR P-site tRNA PHE (unmodified bases)



- Molecule 22: E-site tRNA PHE OR P-site tRNA PHE (unmodified bases)



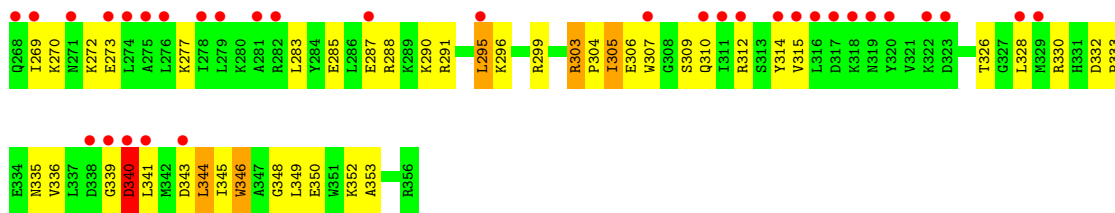
- Molecule 22: E-site tRNA PHE OR P-site tRNA PHE (unmodified bases)



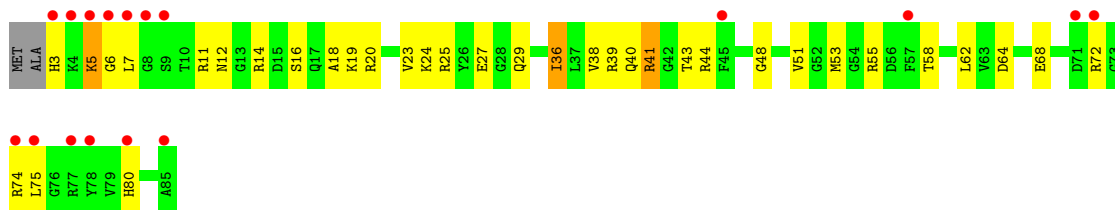
- Molecule 23: mRNA



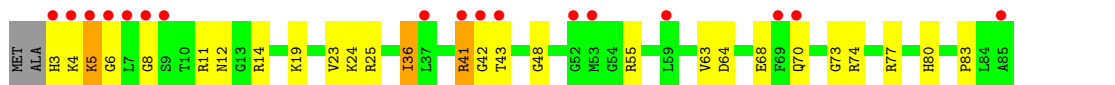




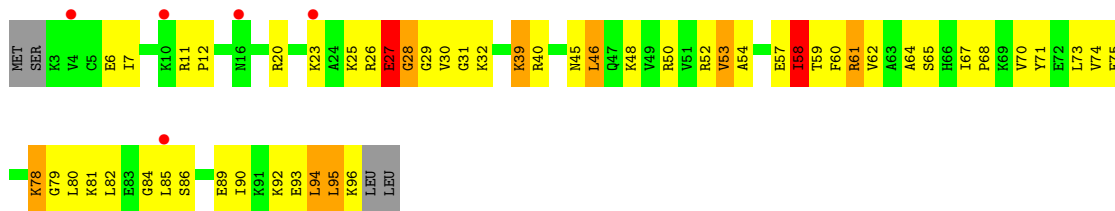
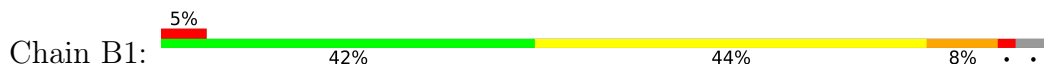
● Molecule 25: 50S ribosomal protein L27



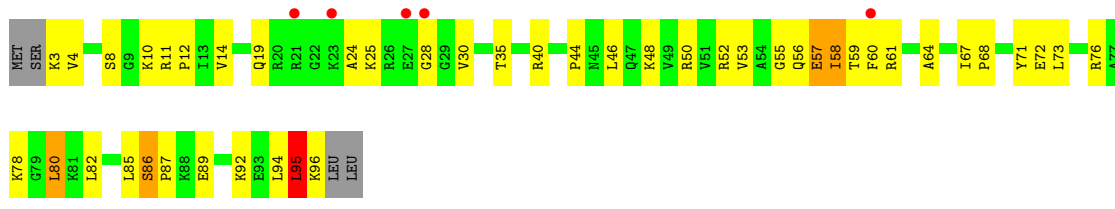
● Molecule 25: 50S ribosomal protein L27



● Molecule 26: 50S ribosomal protein L28

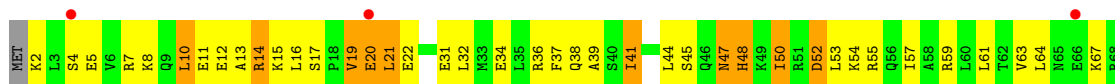


● Molecule 26: 50S ribosomal protein L28



● Molecule 27: 50S ribosomal protein L29

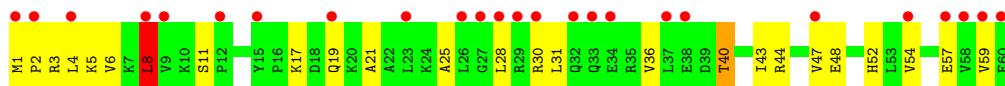
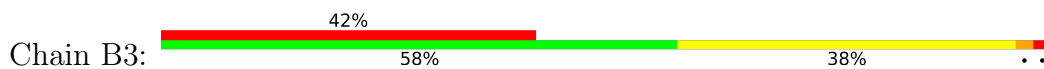




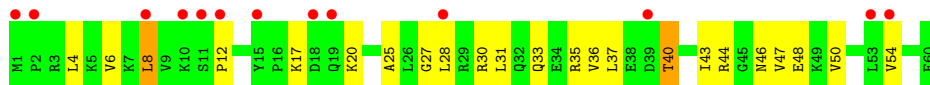
- Molecule 27: 50S ribosomal protein L29



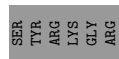
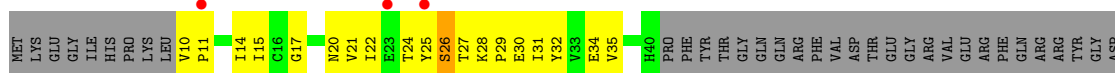
- Molecule 28: 50S ribosomal protein L30



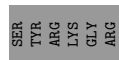
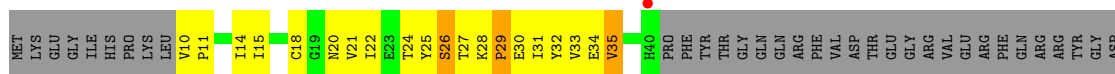
- Molecule 28: 50S ribosomal protein L30



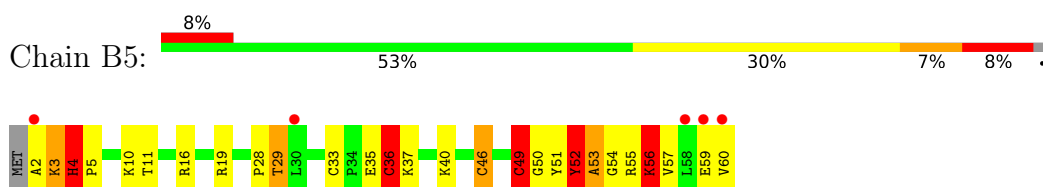
- Molecule 29: 50S ribosomal protein L31



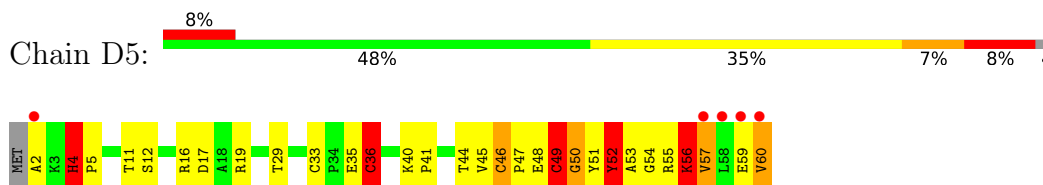
- Molecule 29: 50S ribosomal protein L31



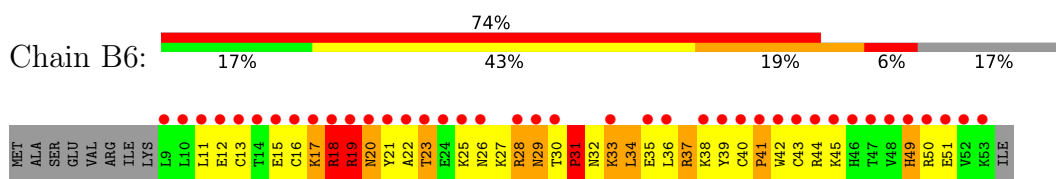
- Molecule 30: 50S ribosomal protein L32



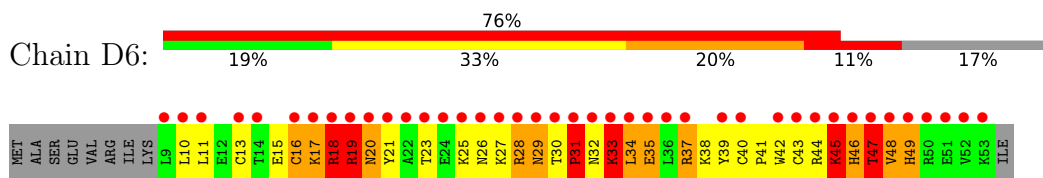
- Molecule 30: 50S ribosomal protein L32



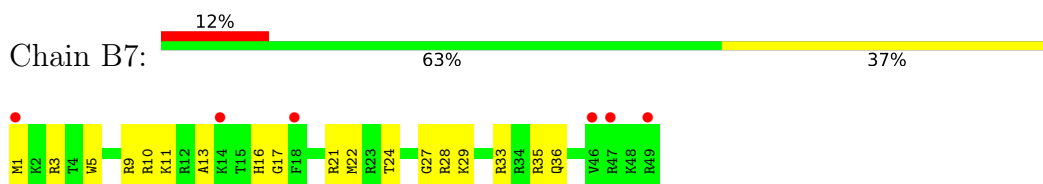
- Molecule 31: 50S ribosomal protein L33



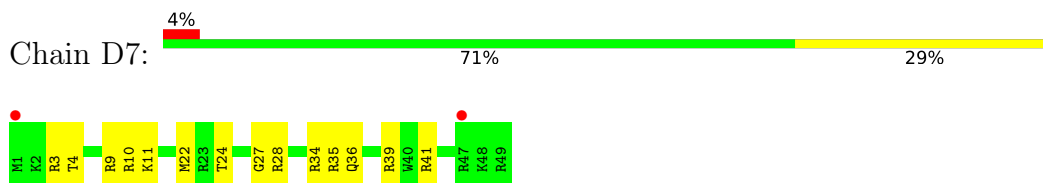
- Molecule 31: 50S ribosomal protein L33



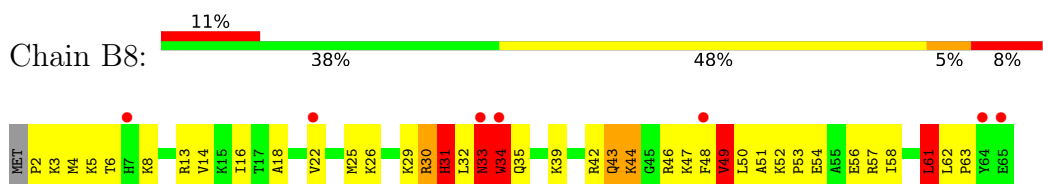
- Molecule 32: 50S ribosomal protein L34



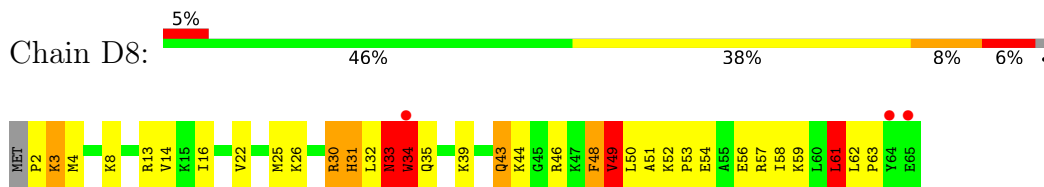
- Molecule 32: 50S ribosomal protein L34



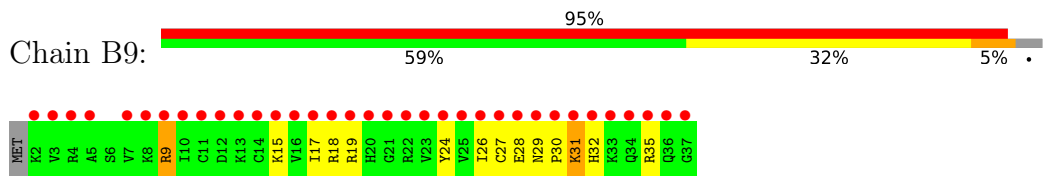
- Molecule 33: 50S ribosomal protein L35



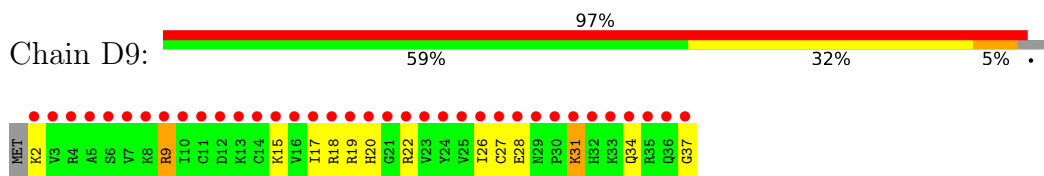
• Molecule 33: 50S ribosomal protein L35



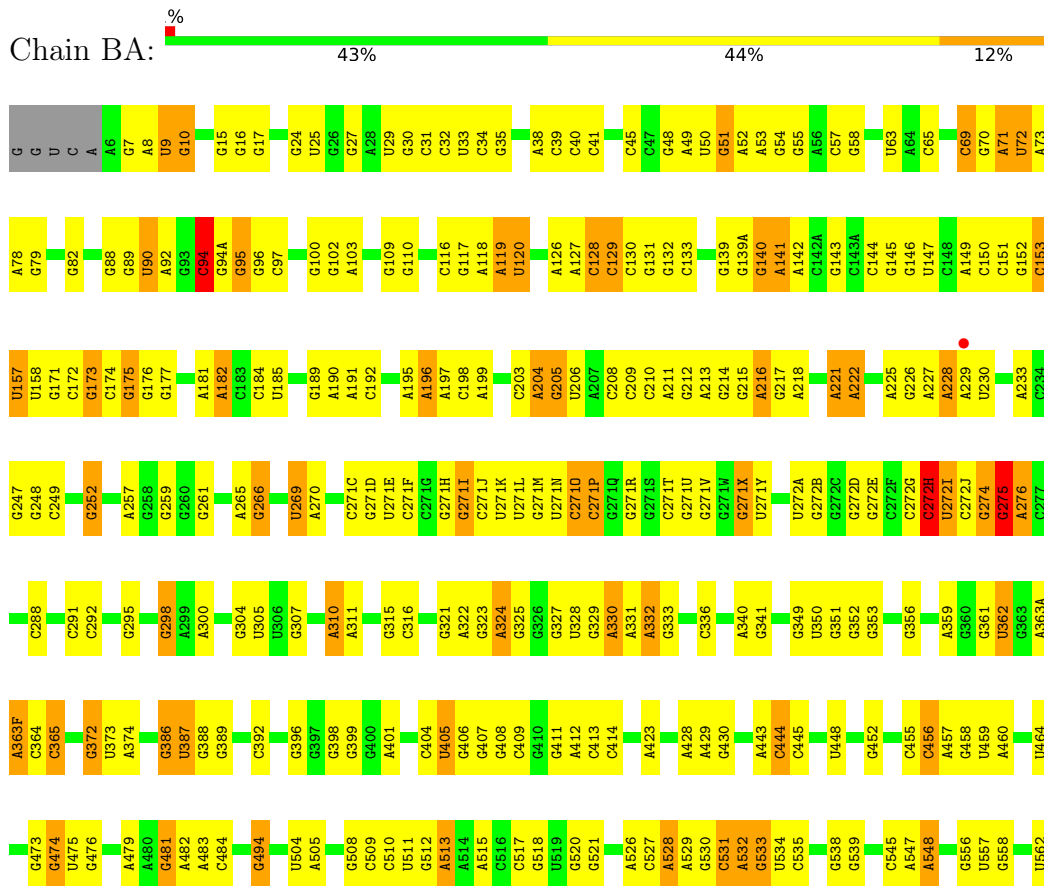
• Molecule 34: 50S ribosomal protein L36



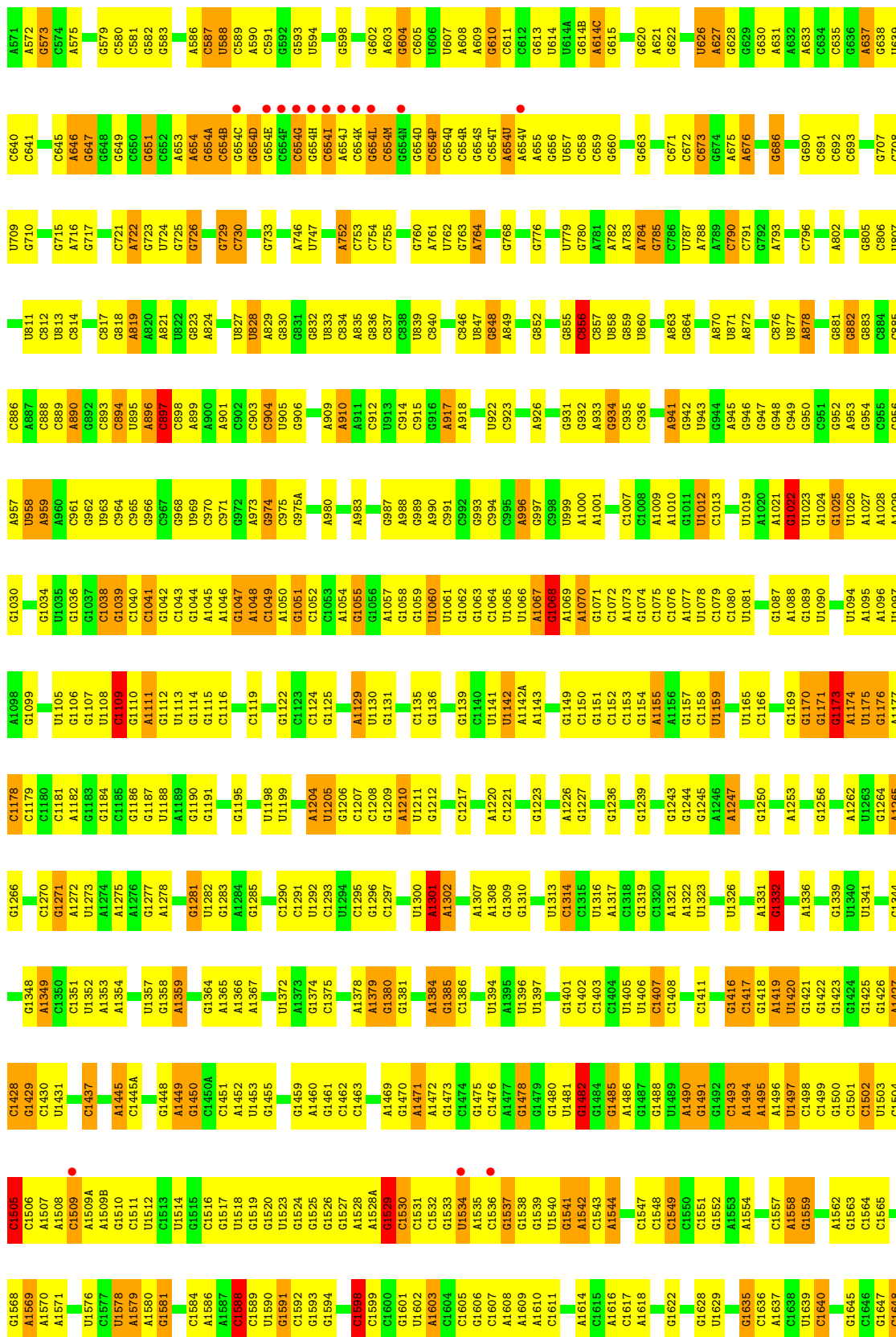
• Molecule 34: 50S ribosomal protein L36



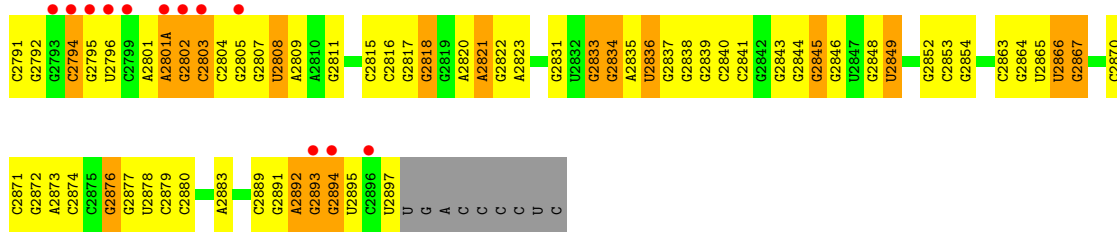
• Molecule 35: 23S rRNA



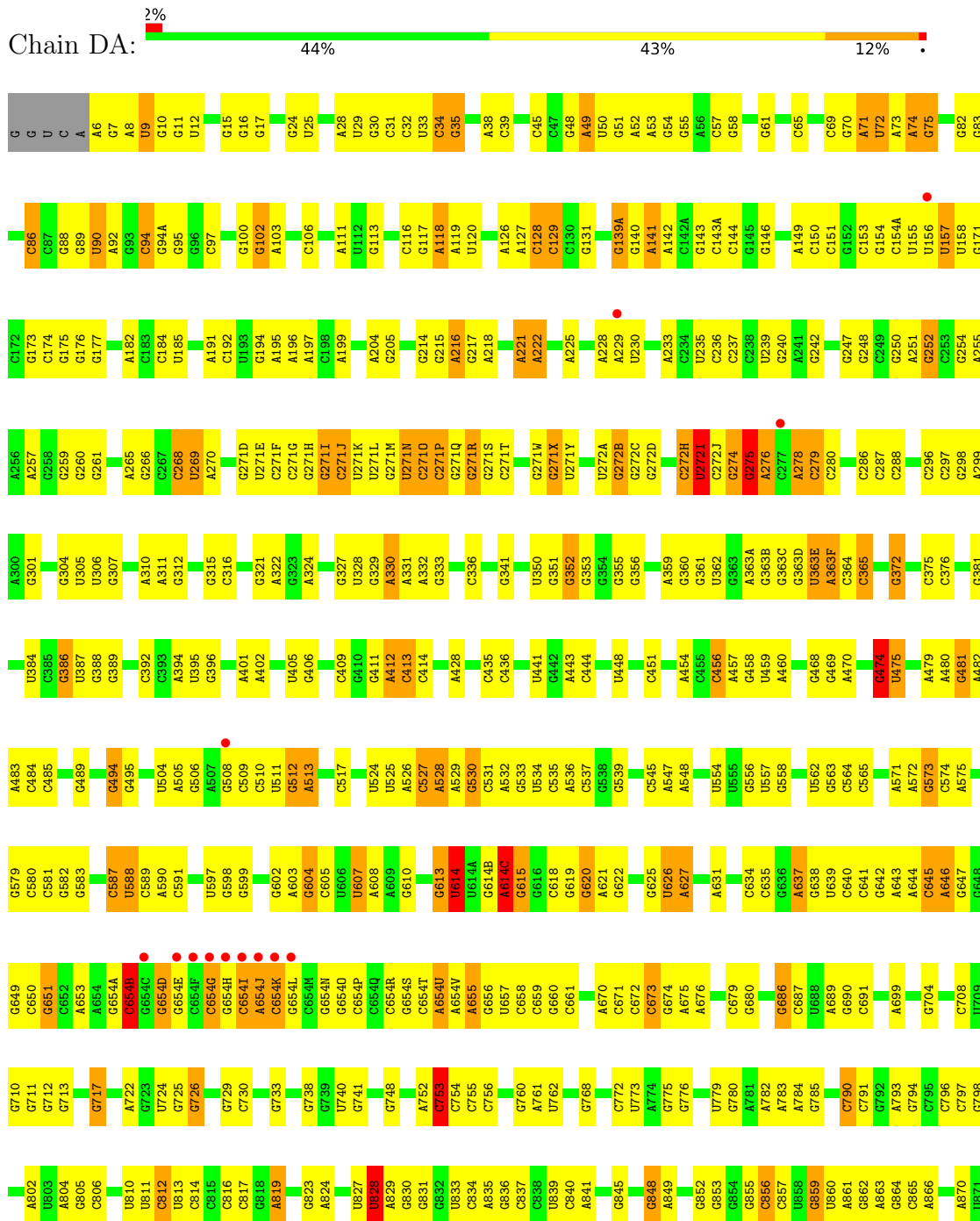




G2714	G1649
C2715	G1650
G2719	G1651
G2652	A1652
A2566	G1653
G2657	A1654
G2668	A1655
G2669	G1656
G2723	G1657
G2724	G1666
A2725	G1667
G2726	G1668
G2727	G1669
G2730	G1670
G2731	G1674
G2732	G1675
A2733	A1676
G2734	A1677
G2735	A1678
G2736	G1681
A2740	G1682
A2741	G1683
G2744	G1684
G2745	C1685
G2746	C1686
G2747	A1689
C2752	C1694
A2753	G1695
A2757	G1696
A2758	G1697
G2761	A1698
G2762	G1702
A2765	U1709
G2766	C1710
C2767	C1711
C2768	C1712
C2769	G1717
G2770	G1718
C2773	U1719
G2777	C1720
A2778	G1721
G2779	A1722
G2780	U1739
A2781	G1740
G2782	A1741
A2785	G1742
G2786	A1825
C2787	G1826
C2788	G1827
C2789	G1828
A2790	A1829
U1923	C1830
C1924	G1831
G1929	C1832
G1930	G1835
A1936	G1836
A1937	C1837
A1938	U1841
A1939	G1842
G1947	C1843
G1948	G1844
A1952	G1845
G1955	G1846
G1959	A1847
A1960	A1848
U1963	G1852
G1964	A1853
C1967	A1854
G1968	G1857
A1969	G1858
A1970	A1859
A1971	G1860
A1972	U1864
G1975	G1865
G1976	A1787
G1977	C1788
A1979	A1789
A2057	A1785
A2058	A1786
A2059	C1787
A2060	C1788
G2061	C1789
A2062	A1791
C2063	G1792
C2064	C1793
C2065	A1981
C2066	G1982
G2067	A1883
U1991	A1884
G1992	A1885
G1993	A1886
C1996	G1887
G1997	C1888
G1998	G1889
G1999	A1890
A2004	U1898
A2042	G1899
A2043	A1900
A2044	A1901
U2047	G1902
G2048	G1906
A2051	G2004
G2055	A1912
G2056	A1913
A2057	C2006
A2058	C2007
A2059	C2008
A2060	G2009
G2061	G2010
A2062	U1899
C2063	A1812
C2064	G1813
C2065	G1816
C2066	G1817
G2067	U1818
U1991	U1819
U1992	U1820
U1993	A1821
C1996	G1825
G1997	G1826
G1998	G1827
G1999	G1828
A2004	A1829
A2042	G2083
A2043	C2084
A2044	C2085
U2047	U2086
G2048	G2087
A2051	G2090
G2055	U2091
G2056	G2092
A2057	G2093
A2058	G2094
A2059	G2095
A2060	G2096
G2061	G2097
A2062	G2098
C2063	G2099
C2064	G2100
C2065	G2101
C2066	G2102
G2067	G2103
U1991	G2104
U1992	C2107
U1993	C2108
C1996	G2109
G1997	G2110
G1998	C2111
G1999	G2112
A2004	G2113
A2042	A2114
A2043	G2115
A2044	G2116
U2047	A2117
G2048	U2118
A2051	A2119
G2055	G2120
G2056	G2121
A2057	G2122
A2058	G2123
A2059	G2124
A2060	G2125
G2061	A2126
A2062	G2127
C2063	C2128
C2064	G2129
C2065	U2130
C2066	G2131
G2067	U2132
U1991	G2133
U1992	G2134
U1993	A2135
C1996	C2136
G1997	C2137
G1998	C2138
G1999	C2139
A2004	C2140
A2042	G2141
A2043	C2142
A2044	C2143
U2047	U2144
G2048	G2145
A2051	A2146
G2055	G2147
G2056	G2148
A2057	G2149
A2058	U2150
A2059	G2151
A2060	G2152
G2061	C2203
A2062	G2204
C2063	G2205
C2064	G2206
C2065	G2207
C2066	G2208
G2067	G2209
U1991	G2210
U1992	G2211
U1993	G2212
C1996	G2213
G1997	G2214
G1998	G2215
G1999	G2216
A2004	G2217
A2042	G2218
A2043	G2219
A2044	G2220
U2047	G2221
G2048	G2222
A2051	G2223
G2055	G2224
G2056	G2225
A2057	G2226
A2058	G2227
A2059	G2228
A2060	G2229
G2061	G2230
A2062	G2231
C2063	G2232
C2064	G2233
C2065	G2234
C2066	G2235
G2067	G2236
U1991	G2237
U1992	G2238
U1993	G2239
C1996	G2240
G1997	G2241
G1998	G2242
G1999	G2243
A2004	G2244
A2042	G2245
A2043	G2246
A2044	G2247
U2047	G2248
G2048	G2249
A2051	G2250
G2055	G2251
G2056	G2252
A2057	G2253
A2058	G2254
A2059	G2255
A2060	G2256
G2061	G2257
A2062	G2258
C2063	G2259
C2064	G2260
C2065	G2261
C2066	G2262
G2067	G2263
U1991	G2264
U1992	G2265
U1993	G2266
C1996	G2267
G1997	G2268
G1998	G2269
G1999	G2270
A2004	G2271
A2042	G2272
A2043	G2273
A2044	G2274
U2047	G2275
G2048	G2276
A2051	G2277
G2055	G2278
G2056	G2279
A2057	G2280
A2058	G2281
A2059	G2282
A2060	G2283
G2061	G2284
A2062	G2285
C2063	G2286
C2064	G2287
C2065	G2288
C2066	G2289
G2067	G2290
U1991	G2291
U1992	G2292
U1993	G2293
C1996	G2294
G1997	G2295
G1998	G2296
G1999	G2297
A2004	G2298
A2042	G2299
A2043	G2300
A2044	G2301
U2047	G2302
G2048	G2303
A2051	G2304
G2055	G2305
G2056	G2306
A2057	G2307
A2058	G2308
A2059	G2309
A2060	G2310
G2061	G2311
A2062	G2312
C2063	G2313
C2064	G2314
C2065	G2315
C2066	G2316
G2067	G2317
U1991	G2318
U1992	G2319
U1993	G2320
C1996	G2321
G1997	G2322
G1998	G2323
G1999	G2324
A2004	G2325
A2042	G2326
A2043	G2327
A2044	G2328
U2047	G2329
G2048	G2330
A2051	G2331
G2055	G2332
G2056	G2333
A2057	G2334
A2058	G2335
A2059	G2336
A2060	G2337
G2061	G2338
A2062	G2339
C2063	G2340
C2064	G2341
C2065	G2342
C2066	G2343
G2067	G2344
U1991	G2345
U1992	G2346
U1993	G2347
C1996	G2348
G1997	G2349
G1998	G2350
G1999	G2351
A2004	G2352
A2042	G2353
A2043	G2354
A2044	G2355
U2047	G2356
G2048	G2357
A2051	G2358
G2055	G2359
G2056	G2360
A2057	G2361
A2058	G2362
A2059	G2363
A2060	G2364
G2061	G2365
A2062	G2366
C2063	G2367
C2064	G2368
C2065	G2369
C2066	G2370
G2067	G2371
U1991	G2372
U1992	G2373
U1993	G2374
C1996	G2375
G1997	G2376
G1998	G2377
G1999	G2378
A2004	G2379
A2042	G2380
A2043	G2381
A2044	G2382
U2047	G2383
G2048	G2384
A2051	G2385
G2055	G2386
G2056	G2387
A2057	G2388
A2058	G2389
A2059	G2390
A2060	G2391
G2061	G2392
A2062	G2393
C2063	G2394
C2064	G2395
C2065	G2396
C2066	G2397
G2067	G2398
U1991	G2399
U1992	G2400
U1993	G2401
C1996	G2402
G1997	G2403
G1998	G2404
G1999	G2405
A2004	G2406
A2042	G2407
A2043	G2410
A2044	G2411
U2047	G2412
G2048	G2413
A2051	G2414
G2055	G2415
G2056	G2416
A2057	G2417
A2058	G2418
A2059	G2419
A2060	G2420
G2061	G2421
A2062	G2422
C2063	G2423
C2064	G2424
C2065	G2425
C2066	G2426
G2067	G2427
U1991	G2428
U1992	G2429
U1993	G2430
C1996	G2431
G1997	G2432
G1998	G2433
G1999	G2434
A2004	G2435
A2042	G2436
A2043	G2437
A2044	G2438
U2047	G2439
G2048	G2440
A2051	G2441
G2055	G2442
G2056	G2443
A2057	G2444
A2058	G2445
A2059	G2446
A2060	G2447
G2061	G2448
A2062	G2449
C2063	G2450
C2064	G2451
C2065	G2452
C2066	G2453
G2067	G2454
U1991	G2455
U1992	G2456
U1993	G2457
C1996	G2458
G1997	G2459
G1998	G2460
G1999	G2461
A2004	G2462
A2042	G2463
A2043	G2464
A2044	G2465
U2047	G2466
G2048	G2467
A2051	G2468
G2055	G2469
G2056	G2470
A2057	G2471
A2058	G2472
A2059	G2473
A2060	G2474
G2061	G2475
A2062	G2476
C2063	G2477
C2064	G2478
C2065	G2479
C2066	G2480
G2067	G2481
U1991	G2482
U1992	G2483
U1993	G2484
C1996	G2485
G1997	G2486
G1998	G2487
G1999	G2488
A2004	G2489
A2042	G2490
A2043	G2491
A2044	G2492
U2047	G2493
G2048	G2494
A2051	G2495
G2055	G2496
G2056	G2500
A2057	G2501
A2058	G2502
A2059	G2503
A2060	G2504
G2061	G2505
A2062	G2506
C2063	G2507
C2064	G2508
C2065	G2509
C2066	G2510
G2067	G2511
U1991	G2512
U1992	G2513
U1993	G2514
C1996	G2515
G1997	G2516
G1998	G2517
G1999	G2518
A2004	G2519
A2042	G2520
A2043	G2521
A2044	G2522
U2047	G2523
G2048	G2524
A2051	G2525
G2055	G2526
G2056	G2527
A2057	G2528
A2058	G2529
A2059	G2530
A2060	G2531
G2061	G2532
A2062	G2533
C2063	G2534
C2064	G2535
C2065	G2536
C2066	G2537
G2067	G2538
U1991	G2539
U1992	G2540
U1993	G2541
C1996	G2542
G1997	G2543
G1998	G2544
G1999	G2545
A2004	G2546
A2042	

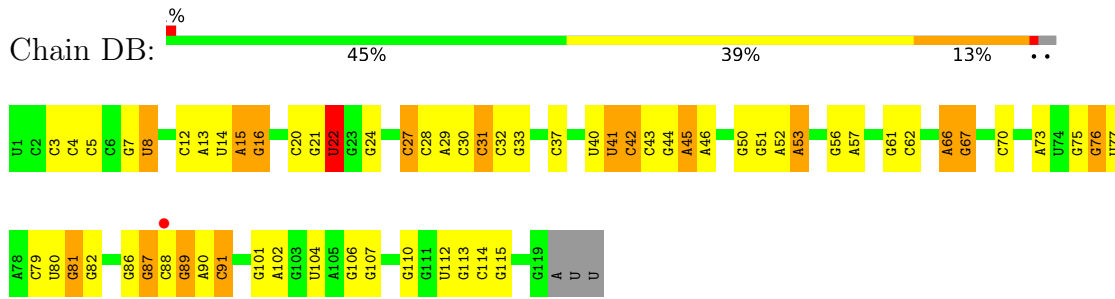


• Molecule 35: 23S rRNA

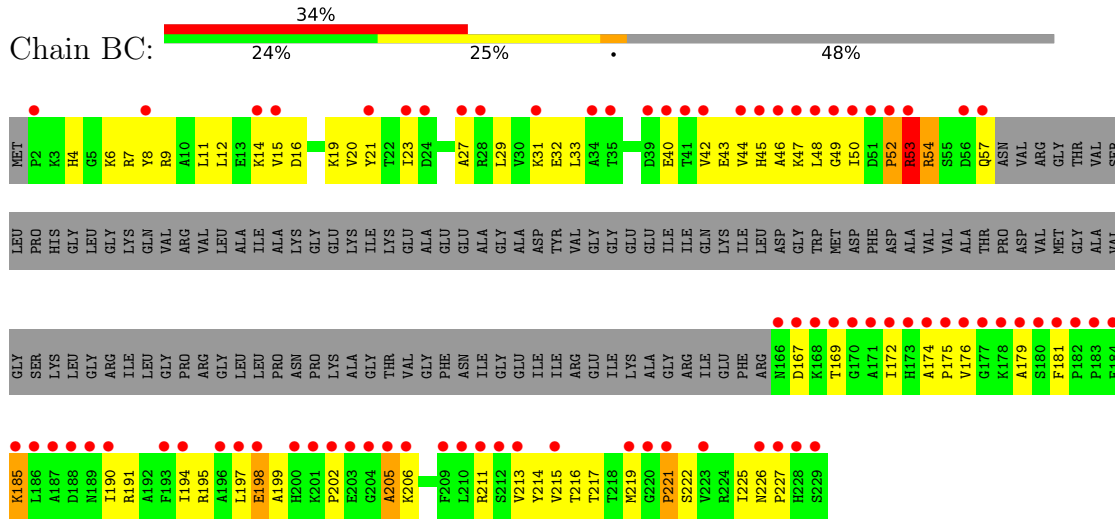


U1956	A1859	A1677	C1589	C1445A	G1358	A1269	G1173	G1099	A1028	A872
U1963	G1860	G1678	U1512	G1448	A1359	C1271	A1174	C1100	A1029	C948
G1964	U1679	U1679	C1516	G1449	G1364	G1270	U1175	U1101	G1030	C949
C1967	G1865	G1680	U1517	G1450	G1365	A1272	G1176	C1102	U876	U877
G1968	C1866	G1682	G1518	G1450A	A1366	U1273	A1177	A1103	U1033	A878
A1969	A1876	C1683	G1519	C1451	A1367	U1280	C1178	C1104	G1034	C954
A1970	G1878	C1685	G1520	A1452	U1372	G1281	C1180	U1105	G956	G882
A1971	C1881	G1686	G1525	U1453	A1373	G1281	C1180	G1107	U958	G883
A1972	G1881	G1687	U1526	G1455	A1378	A1287	G1186	U1108	C1040	U958
C1982	C1882	U1688	G1527	G1458	A1378	U1288	G1187	C1109	C1041	C884
G1973	G1883	C1604	A1528	G1459	A1379	C1289	U1188	G1110	A960	C885
A1974	A1884	C1605	A1528A	A1460	G1380	C1290	G1044	G1111	C961	C886
G1975	A1885	G1606	G1529	G1461	U1390	C1291	A1045	G1112	U963	A887
G1980	A1888	G1607	C1531	G1466	A1384	U1292	A1046	U1113	C964	C888
A1981	G1888	G1695	G1532	G1467	G1385	U1293	G1047	G1114	C965	A890
C1982	A1889	A1609	C1533	A1471	G1386	U1294	A1048	G1115	A1048	A890
C1983	A1890	A1610	U1534	A1472	U1390	G1299	C1049	G1120	U969	C893
G1984	G1897	A1614	A1535	A1473	A1395	U1300	A1050	C1121	C970	C894
G1985	U1898	G1700	C1536	C1474	U1396	A1301	C1052	G1122	C971	U895
A1986	G1899	A1701	G1537	G1475	U1397	A1302	A1054	G1125	A973	A896
G1987	G1899	G1702	G1538	G1476	U1397	A1302	A1054	G1125	G974	C897
C1988	A1900	G1703	G1539	C1476	U1400	C1306	C1055	G1055	C975	A900
A1901	G1801	G1703	U1540	A1477	G1400	A1307	A1210	G1056	A901	A901
G1989	A1802	U1709	U1541	G1478	G1401	A1308	U1211	A1057	C902	C902
G1990	A1802	C1710	A1542	G1479	G1402	G1309	G1212	A1058	C903	C903
G1991	A1803	C1711	C1543	G1480	C1403	G1309	C1217	G1059	C904	C904
G1992	G1813	C1712	A1544	U1481	C1404	U1313	C1221	U1060	U905	U905
U1993	G1816	G1717	G1545	G1482	U1405	U1314	C1221A	U1061	G906	G906
G1996	A1912	G1718	C1546	G1484	U1406	C1315	C1222	G1062	U907	U907
C1997	C1914	G1718	C1547	G1485	U1407	G1316	C1222	G1063	C988	C988
G1998	U1915	U1820	C1548	G1486	C1408	U1317	U1141	U1065	A909	A909
G1999	U1916	U1720	G1549	A1487	C1409	C1318	U1142	U1066	A910	A910
G1999	U1917	A1641	C1550	G1488	C1409	G1319	U1142	U1066	A911	A911
G2000	A1918	G1642	A1554	U1489	G1416	C1320	A1142A	A1067	A996	A996
G2003	A1919	U1739	A1558	A1490	G1417	A1321	G1230	A1068	C977	C977
G2004	C1920	G1740	G1559	G1491	G1418	A1322	G1231	A1069	C998	C998
C2008	U1923	G1742	G1564	G1492	A1419	U1323	U1234	A1070	A917	A917
G2009	C1924	G1742	C1565	C1493	U1420	U1323	G1235	G1071	A918	A918
G2010	G1929	G1746	C1566	A1494	G1421	A1331	G1236	C1072	U922	U922
G2011	G1930	G1747	C1565	A1495	G1422	G1332	C1150	A1073	C923	C923
A2013	U1841	G1747A	U1665	U1497	G1423	G1337	C1151	C1006	C924	C924
A2014	G1842	G1747A	G1666	C1498	G1424	G1338	C1152	C1007	C925	C925
A2015	G1845	U1749	C1667	C1499	A1427	U1338	C1153	C1080	G928	G928
A2019	A1937	G1752	A1668	C1499	C1428	U1341	C1154	C1080	U1012	U1012
A2020	U1939	G1753	A1669	G1500	G1429	U1341	A1155	U1081	C1013	C1013
C2021	A1847	C1754	A1670	C1501	G1430	C1345	G1244	U1082	C1013	C1013
U1946	A1848	A1755	G1674	C1502	U1430	U1345	G1245	A1156	U1014	U1014
C1947	G1849	G1756	A1675	C1503	U1431	G1348	A1246	G1157	G1015	G1015
G2023	C1947	G1756	U1578	C1504	C1432	A1348	A1247	C1158	G1016	G1016
G2024	G1948	A1668	A1579	C1505	U1433	A1349	A1253	U1159	U1019	U1019
G1949	U1851	A1669	U1579	A1507	A1434	U1352	G1256	G1160	G939	G939
C2025	C1852	C1670	A1579	A1508	G1435	U1352	G1257	G1165	G940	G940
C2026	G1853	C1670	C1584	A1509	G1436	A1354	C1257	U1166	A941	A941
U1951	A1854	G1764	A1586	C1509	C1437	A1354	G1265	C1166	G942	G942
A1952	G1857	A1773	A1587	A1509A	G1444	G1355	G1266	U1169	A1096	A1096
U1955	G1858	C1774	C1588	G1510	A1445	G1356	G1266	G1170	A1097	A1097
								G1171	U1023	U1023
								G1024	G1024	G1024
								U1025	U1025	U1025
								A1026	A1026	A1026
								A1027	A1027	A1027

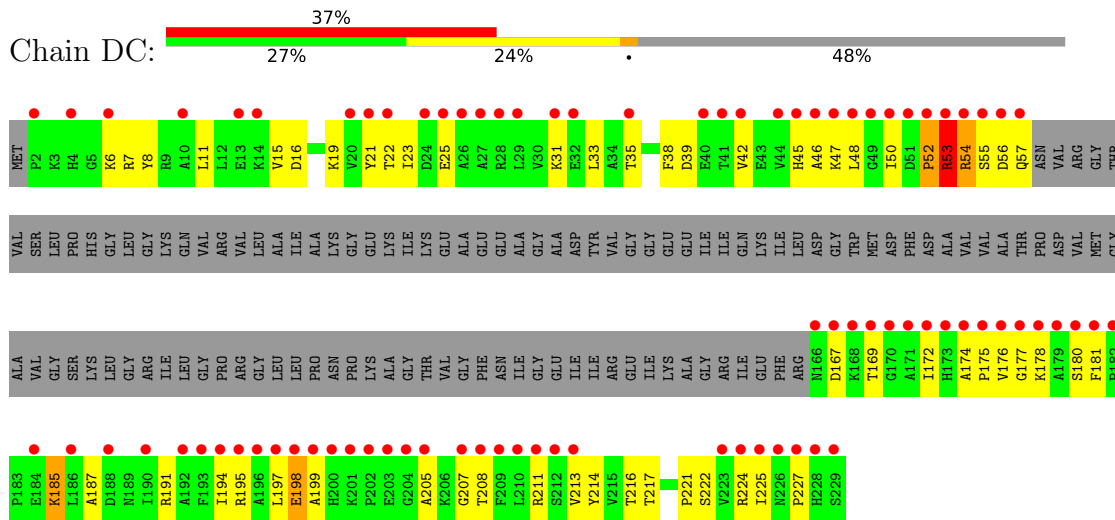




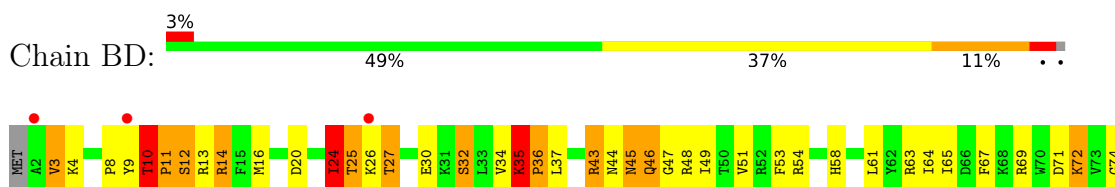
• Molecule 37: 50S ribosomal protein L1

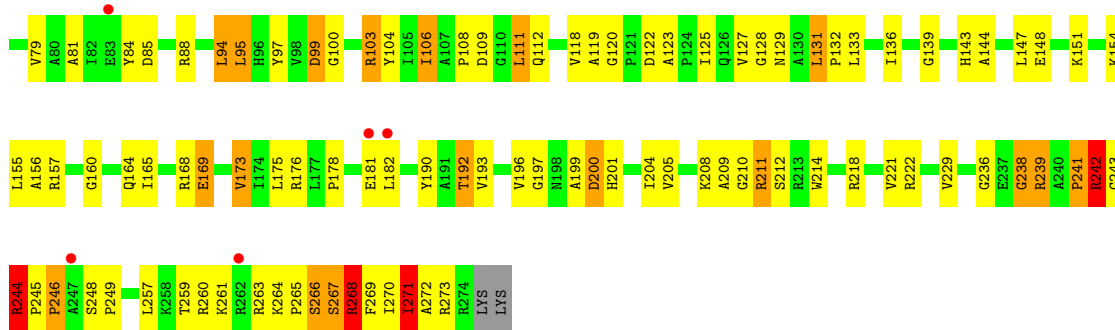


• Molecule 37: 50S ribosomal protein L1

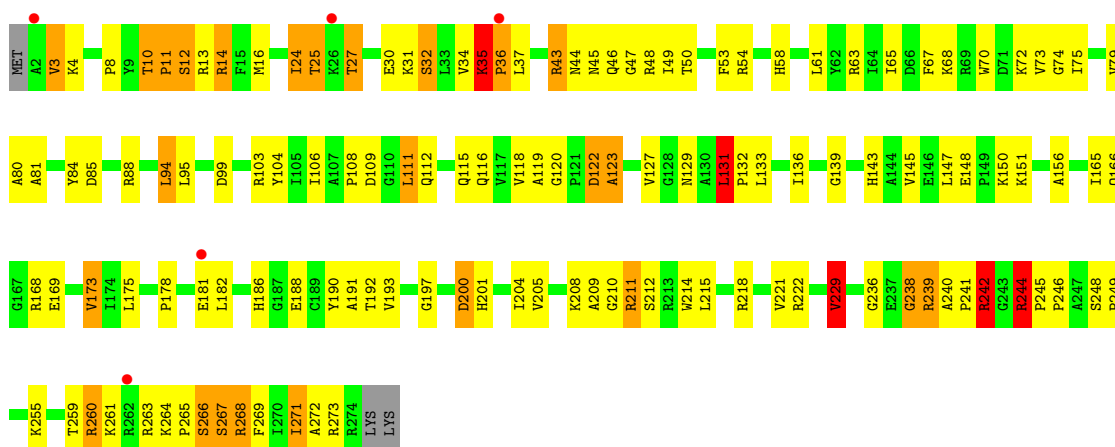


• Molecule 38: 50S ribosomal protein L2

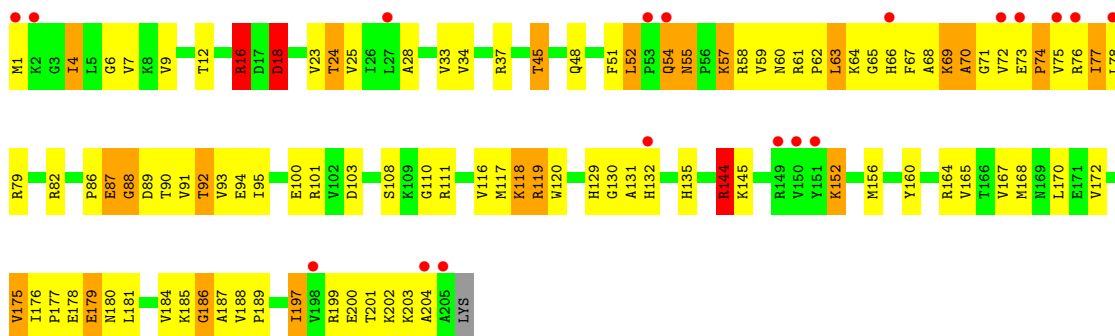




• Molecule 38: 50S ribosomal protein L2

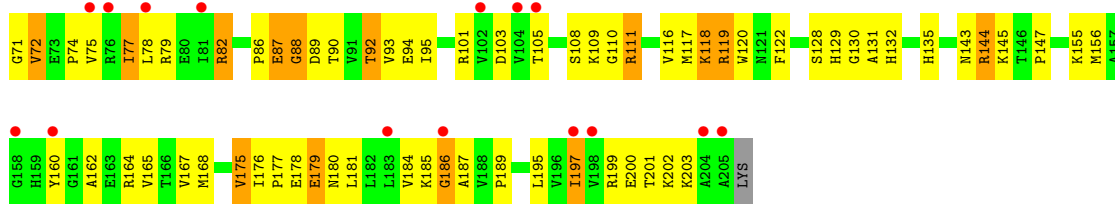


• Molecule 39: 50S ribosomal protein L3

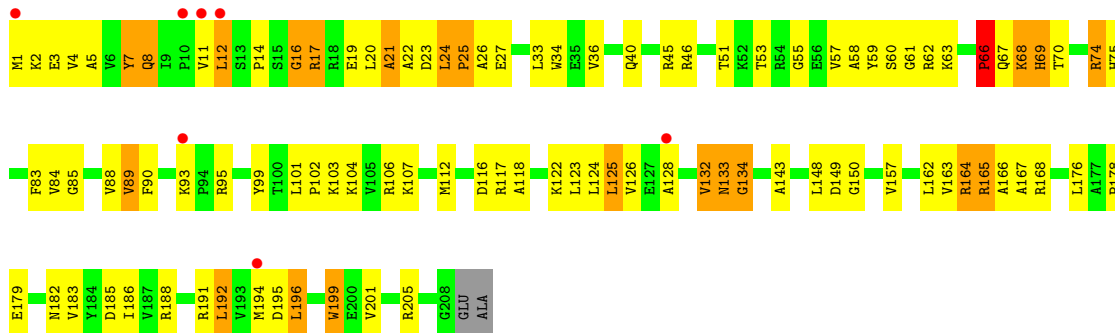


• Molecule 39: 50S ribosomal protein L3

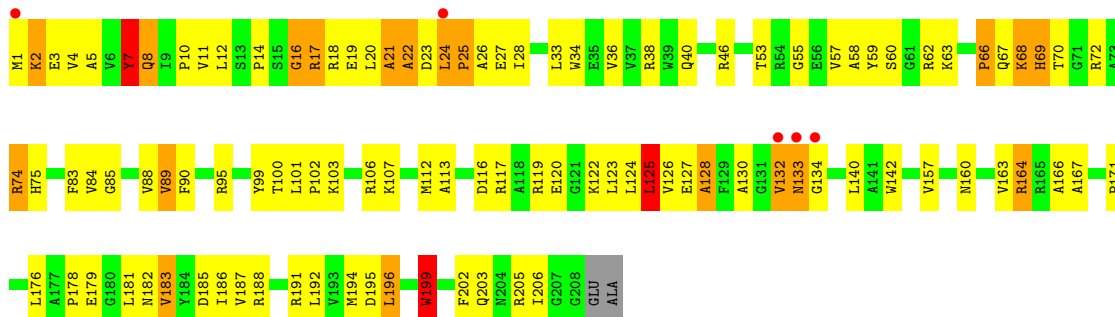




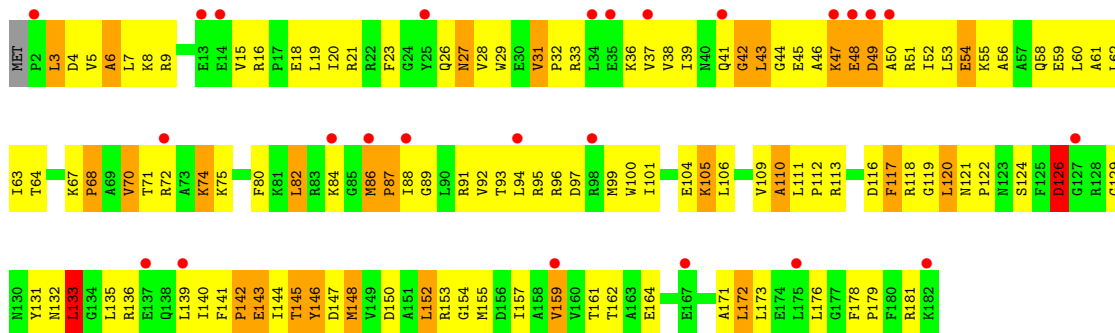
• Molecule 40: 50S ribosomal protein L4



• Molecule 40: 50S ribosomal protein L4

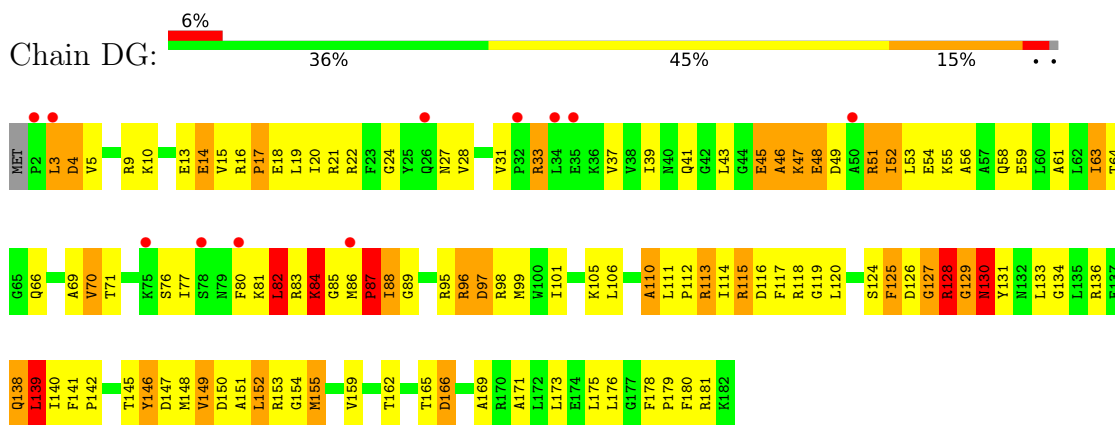


• Molecule 41: 50S ribosomal protein L5

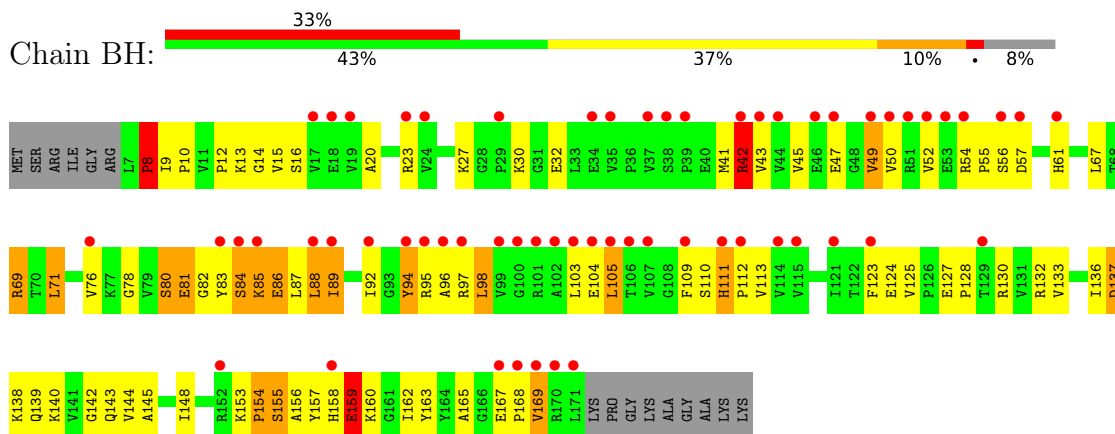




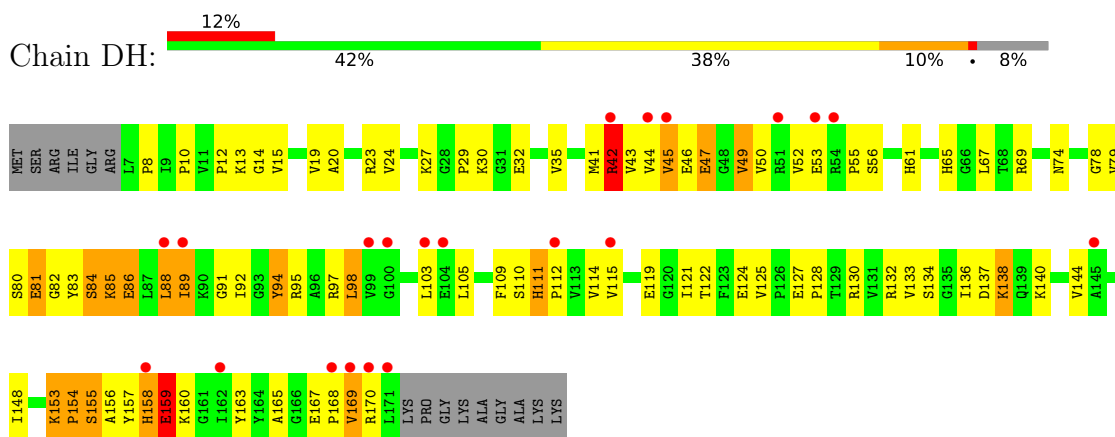
- Molecule 41: 50S ribosomal protein L5



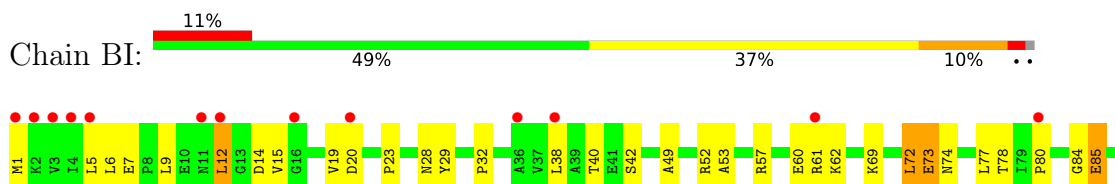
- Molecule 42: 50S ribosomal protein L6

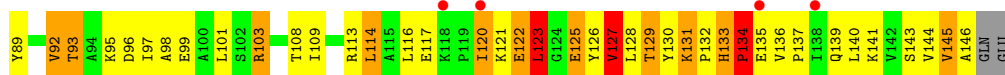


- Molecule 42: 50S ribosomal protein L6



- Molecule 43: 50S ribosomal protein L9

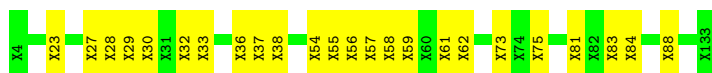
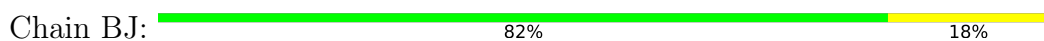




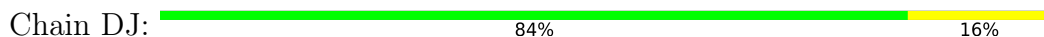
• Molecule 43: 50S ribosomal protein L9



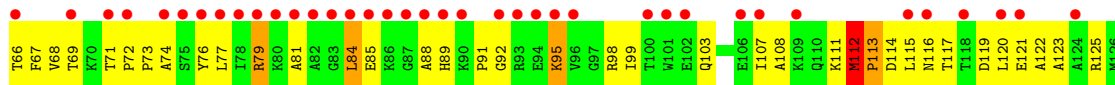
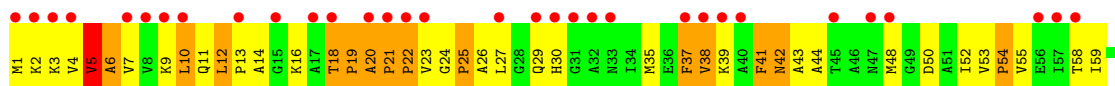
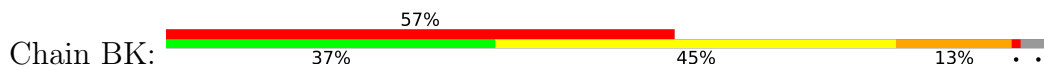
• Molecule 44: 50S ribosomal protein L10



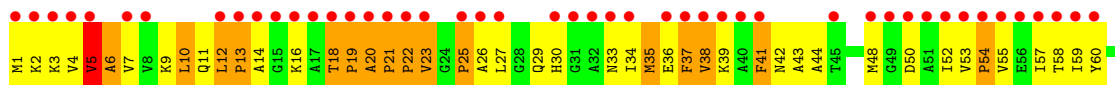
• Molecule 44: 50S ribosomal protein L10

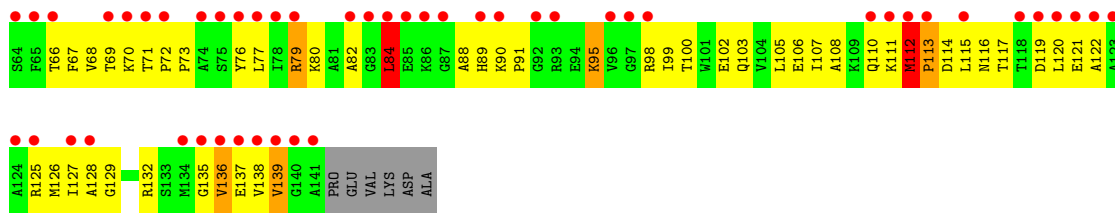


• Molecule 45: 50S ribosomal protein L11

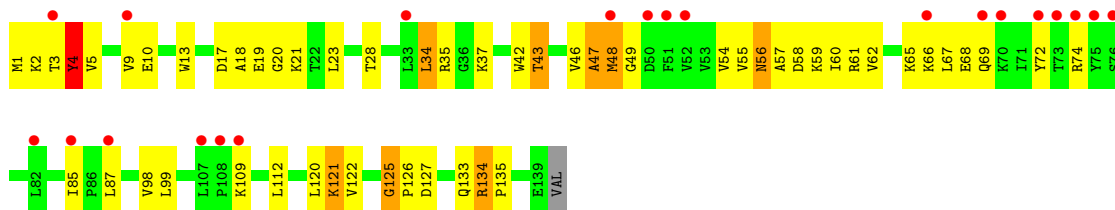


• Molecule 45: 50S ribosomal protein L11

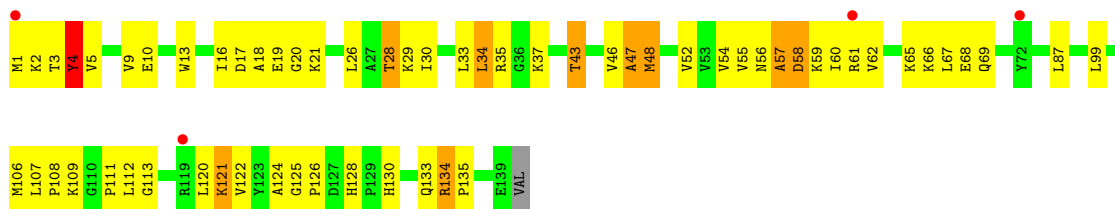




- Molecule 46: 50S ribosomal protein L13



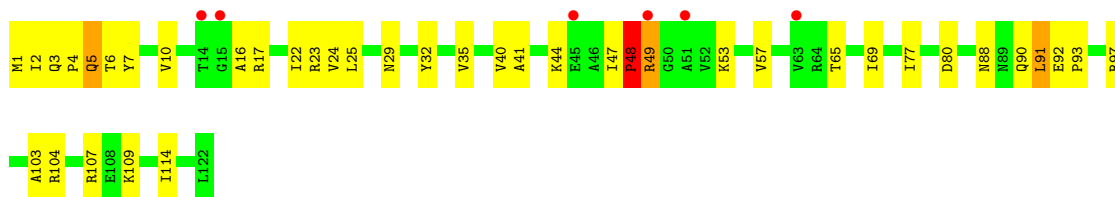
- Molecule 46: 50S ribosomal protein L13



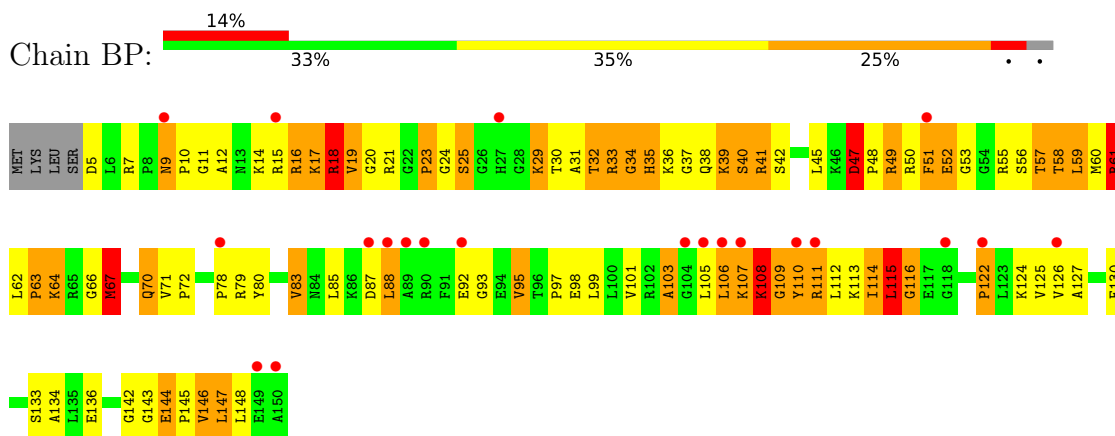
- Molecule 47: 50S ribosomal protein L14



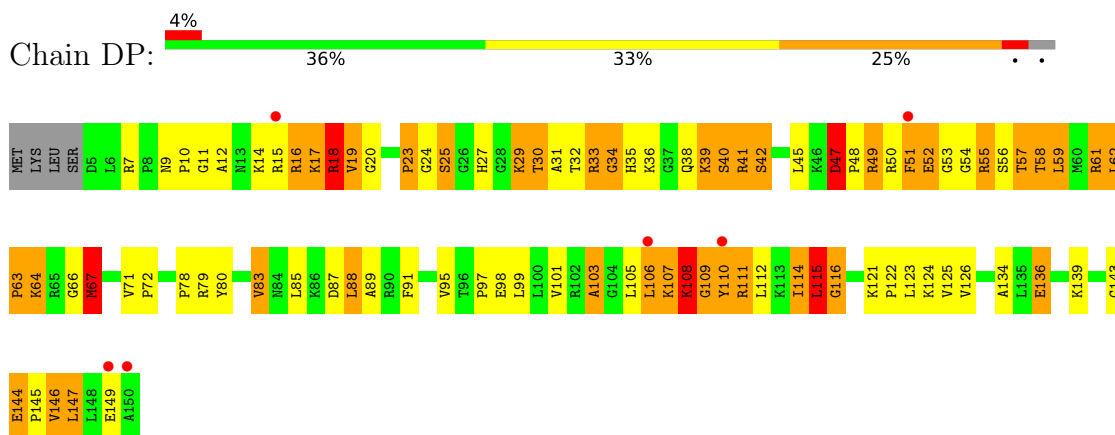
- Molecule 47: 50S ribosomal protein L14



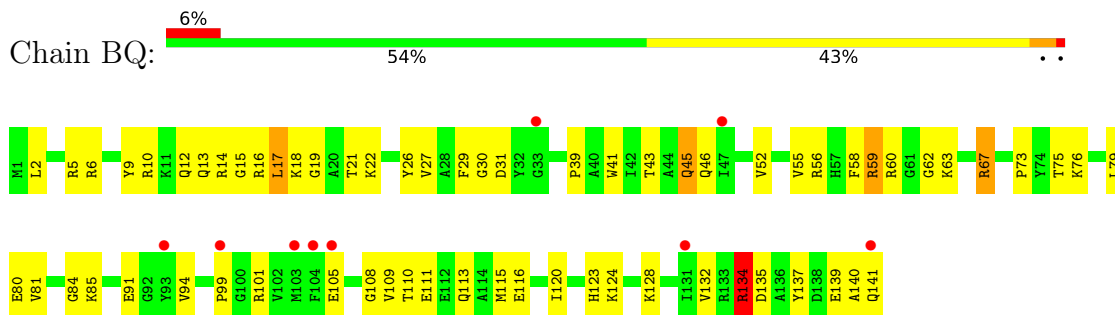
- Molecule 48: 50S ribosomal protein L15



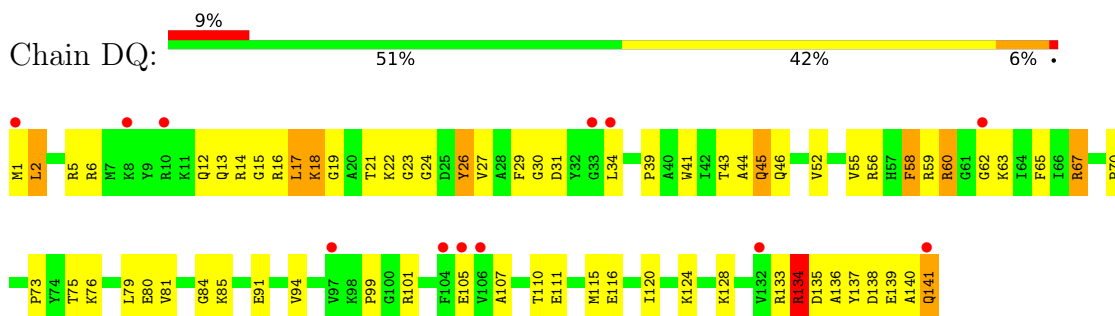
- Molecule 48: 50S ribosomal protein L15



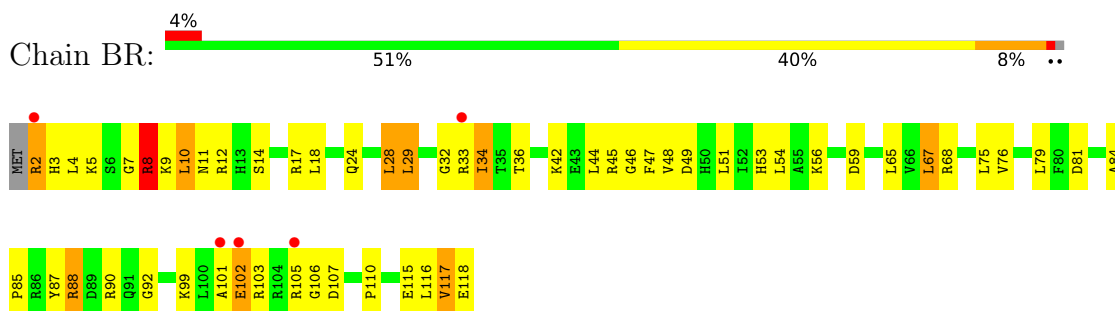
- Molecule 49: 50S ribosomal protein L16



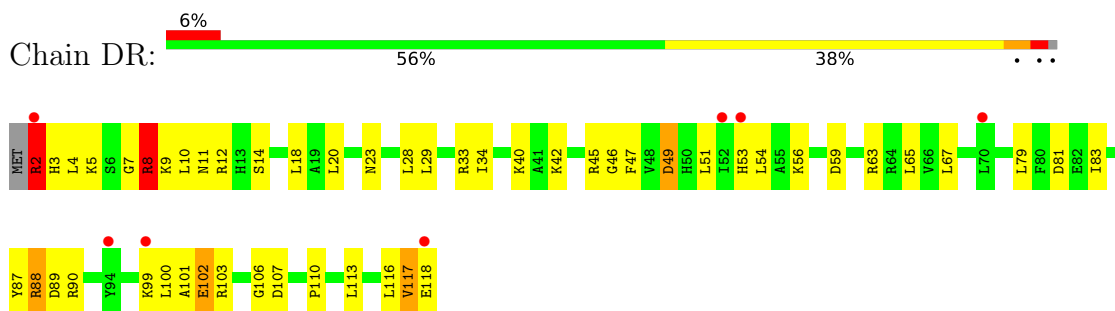
- Molecule 49: 50S ribosomal protein L16



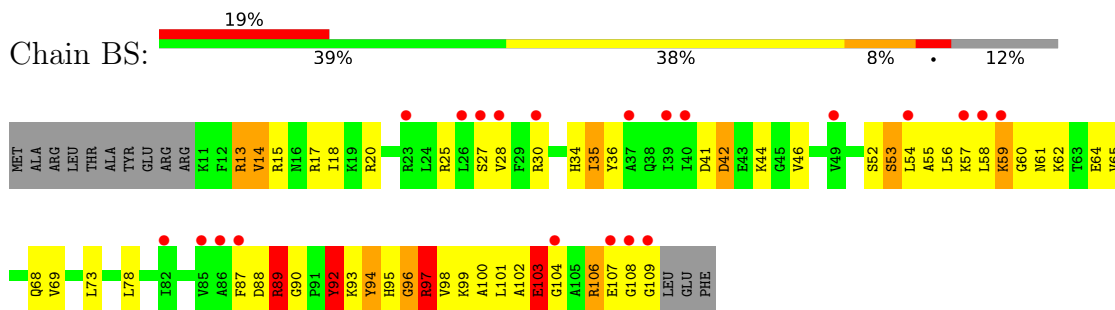
- Molecule 50: 50S ribosomal protein L17



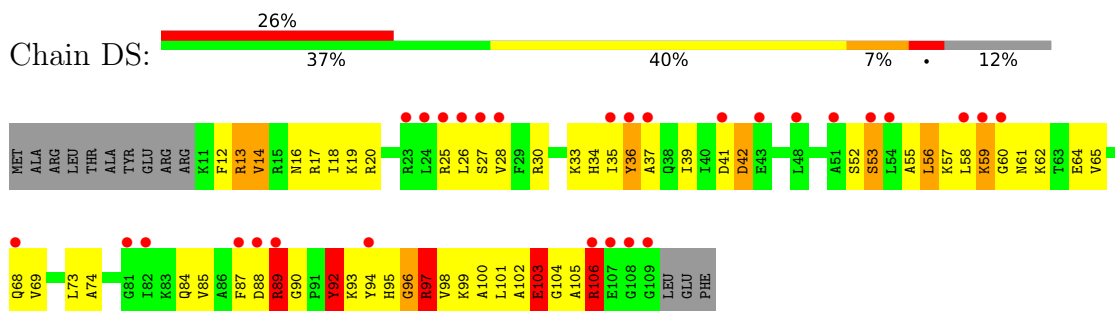
- Molecule 50: 50S ribosomal protein L17



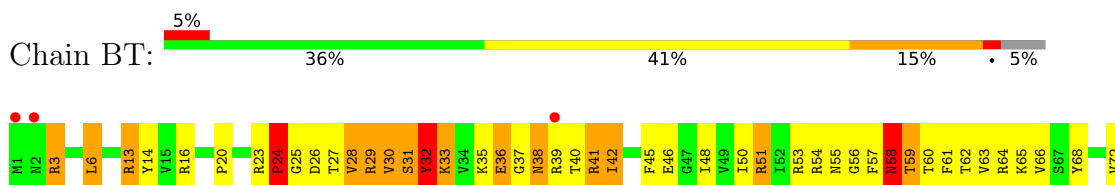
- Molecule 51: 50S ribosomal protein L18

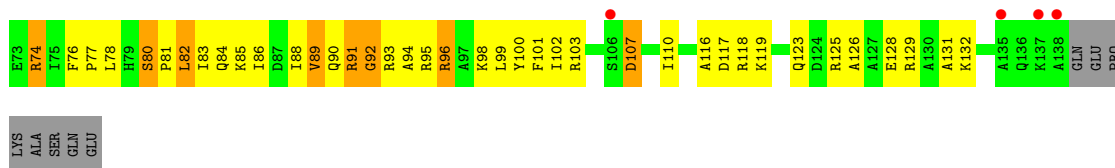


- Molecule 51: 50S ribosomal protein L18

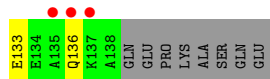


- Molecule 52: 50S ribosomal protein L19

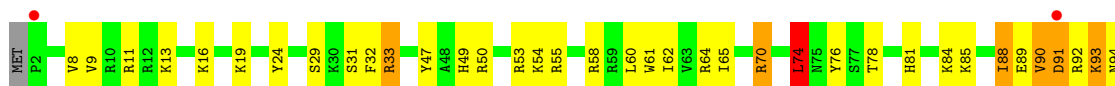




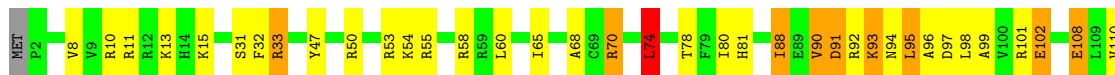
• Molecule 52: 50S ribosomal protein L19



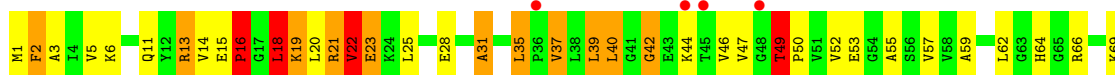
• Molecule 53: 50S ribosomal protein L20



• Molecule 53: 50S ribosomal protein L20

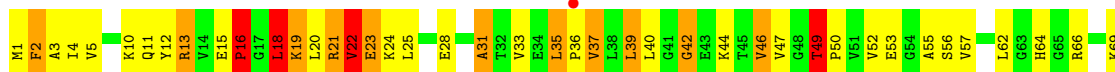
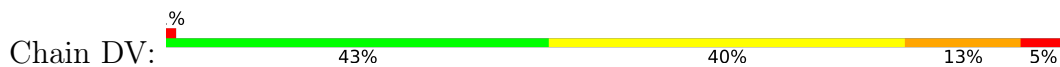


• Molecule 54: 50S ribosomal protein L21

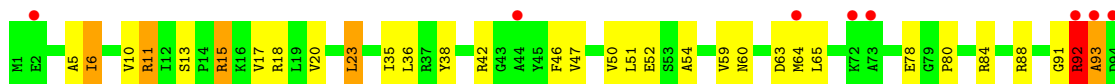




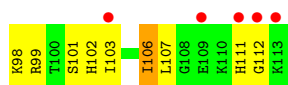
- Molecule 54: 50S ribosomal protein L21



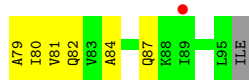
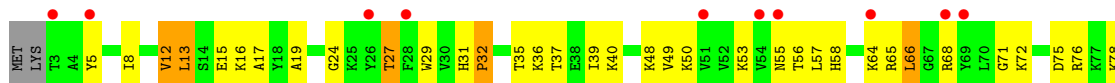
- Molecule 55: 50S ribosomal protein L22



- Molecule 55: 50S ribosomal protein L22

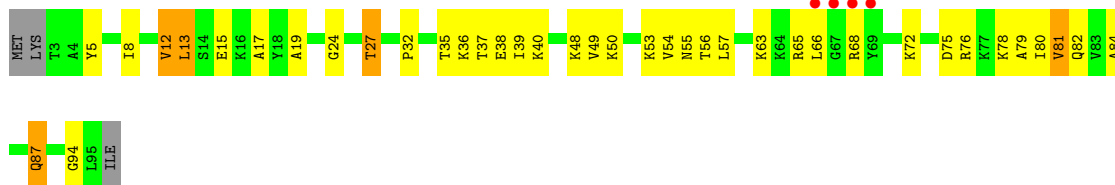


- Molecule 56: 50S ribosomal protein L23

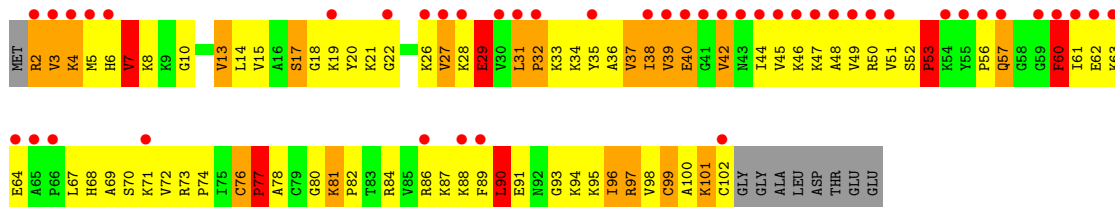
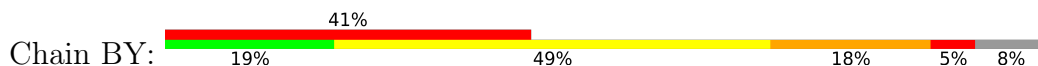


- Molecule 56: 50S ribosomal protein L23

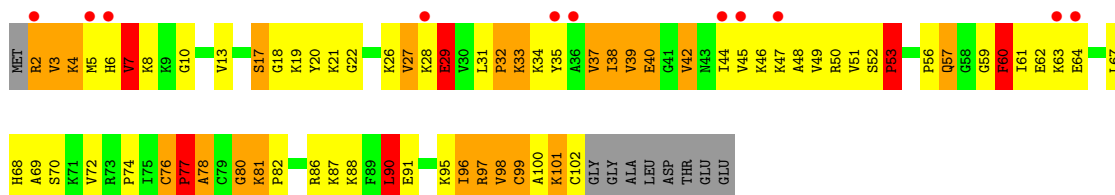




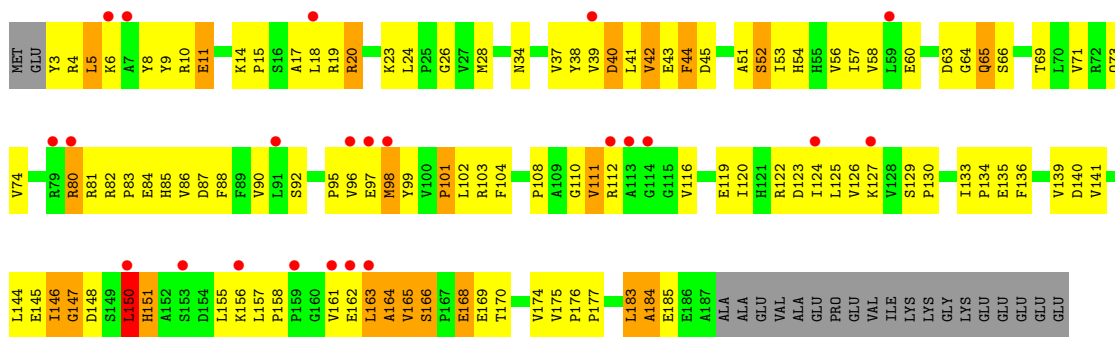
• Molecule 57: 50S ribosomal protein L24



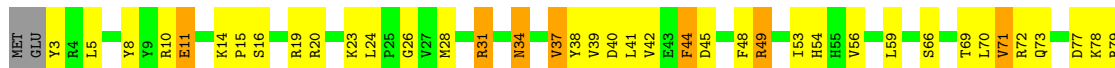
• Molecule 57: 50S ribosomal protein L24



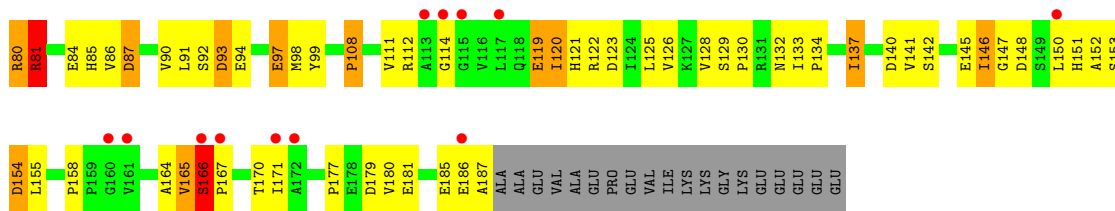
• Molecule 58: 50S ribosomal protein L25



• Molecule 58: 50S ribosomal protein L25







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.02Å 452.53Å 623.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.98 – 3.20 49.97 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.98-3.20) 100.0 (49.97-3.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.16 (at 3.19Å)	Xtrriage
Refinement program	PHENIX 1.12_2829	Depositor
R, $R_{free}$	0.223 , 0.247 0.223 , 0.248	Depositor DCC
$R_{free}$ test set	48519 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	128.7	Xtrriage
Anisotropy	0.019	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 121.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.25$ , $\langle L^2 \rangle = 0.12$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	304459	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	160.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MEQ, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	AA	0.36	3/36190 (0.0%)	1.02	60/56486 (0.1%)
1	CA	0.36	2/36190 (0.0%)	1.04	81/56486 (0.1%)
2	AB	0.32	0/1936	0.71	0/2611
2	CB	0.31	0/1936	0.71	0/2611
3	AC	0.30	0/1637	0.69	0/2207
3	CC	0.30	0/1637	0.69	1/2207 (0.0%)
4	AD	0.30	0/1733	0.73	2/2318 (0.1%)
4	CD	0.32	0/1733	0.74	2/2318 (0.1%)
5	AE	0.31	0/1163	0.68	0/1566
5	CE	0.30	0/1163	0.65	0/1566
6	AF	0.32	0/856	0.77	2/1154 (0.2%)
6	CF	0.33	0/856	0.77	1/1154 (0.1%)
7	AG	0.29	0/1276	0.63	0/1709
7	CG	0.30	0/1276	0.66	0/1709
8	AH	0.30	0/1136	0.68	0/1527
8	CH	0.29	0/1136	0.68	0/1527
9	AI	0.31	0/1028	0.71	0/1375
9	CI	0.31	0/1028	0.72	0/1375
10	AJ	0.29	0/808	0.69	1/1087 (0.1%)
10	CJ	0.31	0/808	0.68	0/1087
11	AK	0.28	0/900	0.64	1/1213 (0.1%)
11	CK	0.28	0/900	0.64	0/1213
12	AL	0.34	0/987	0.71	0/1322
12	CL	0.34	0/987	0.73	1/1322 (0.1%)
13	AM	0.32	0/996	0.73	1/1328 (0.1%)
13	CM	0.32	0/996	0.73	0/1328
14	AN	0.30	0/501	0.61	0/664
14	CN	0.32	0/501	0.64	0/664
15	AO	0.30	0/745	0.62	0/992
15	CO	0.28	0/745	0.59	0/992
16	AP	0.29	0/717	0.65	0/965
16	CP	0.30	0/717	0.66	0/965

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AQ	0.29	0/837	0.64	0/1119
17	CQ	0.29	0/837	0.64	0/1119
18	AR	0.33	0/579	0.73	1/768 (0.1%)
18	CR	0.30	0/579	0.79	1/768 (0.1%)
19	AS	0.30	0/643	0.73	0/867
19	CS	0.28	0/643	0.75	1/867 (0.1%)
20	AT	0.29	0/765	0.66	0/1007
20	CT	0.28	0/765	0.62	0/1007
21	AU	0.26	0/213	0.76	0/279
21	CU	0.29	0/213	0.59	0/279
22	AV	0.41	0/1809	1.14	9/2819 (0.3%)
22	AW	0.44	0/1784	1.13	7/2780 (0.3%)
22	CV	0.42	0/1809	1.09	6/2819 (0.2%)
22	CW	0.44	0/1784	1.23	14/2780 (0.5%)
23	AX	0.53	0/185	1.23	0/286
23	CX	0.54	0/185	1.22	0/286
24	AY	0.30	0/2839	0.62	1/3833 (0.0%)
24	CY	0.32	0/2839	0.64	3/3833 (0.1%)
25	B0	0.31	0/666	0.67	0/885
25	D0	0.30	0/666	0.67	0/885
26	B1	0.33	0/739	0.78	1/983 (0.1%)
26	D1	0.35	0/739	0.74	0/983
27	B2	0.29	0/600	0.69	0/793
27	D2	0.32	0/600	0.79	1/793 (0.1%)
28	B3	0.37	0/473	0.72	1/636 (0.2%)
28	D3	0.31	0/473	0.60	0/636
29	B4	0.30	0/229	0.73	0/311
29	D4	0.33	0/229	0.73	0/311
30	B5	0.44	0/473	0.96	2/639 (0.3%)
30	D5	0.39	0/473	0.90	2/639 (0.3%)
31	B6	0.44	0/387	0.95	0/517
31	D6	0.46	0/388	1.11	1/520 (0.2%)
32	B7	0.27	0/427	0.64	0/563
32	D7	0.27	0/427	0.65	0/563
33	B8	0.34	0/516	0.78	0/681
33	D8	0.35	0/516	0.78	0/681
34	B9	0.29	0/302	0.62	0/397
34	D9	0.30	0/302	0.68	0/397
35	BA	0.40	10/69972 (0.0%)	1.09	201/109237 (0.2%)
35	DA	0.41	8/69972 (0.0%)	1.10	197/109237 (0.2%)
36	BB	0.38	0/2853	1.07	6/4451 (0.1%)
36	DB	0.39	0/2853	1.14	10/4451 (0.2%)
37	BC	0.30	0/956	0.67	0/1288

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
37	DC	0.29	0/956	0.67	0/1288
38	BD	0.33	0/2170	0.73	1/2926 (0.0%)
38	DD	0.34	0/2170	0.76	3/2926 (0.1%)
39	BE	0.38	0/1597	0.83	3/2155 (0.1%)
39	DE	0.35	0/1597	0.76	0/2155
40	BF	0.35	0/1659	0.75	2/2246 (0.1%)
40	DF	0.37	1/1659 (0.1%)	0.75	2/2246 (0.1%)
41	BG	0.31	0/1498	0.79	1/2013 (0.0%)
41	DG	0.35	0/1499	0.80	2/2016 (0.1%)
42	BH	0.31	0/1271	0.78	2/1720 (0.1%)
42	DH	0.33	0/1271	0.80	2/1720 (0.1%)
43	BI	0.34	0/1147	0.76	0/1553
43	DI	0.33	0/1147	0.79	0/1553
45	BK	0.31	0/1057	0.73	0/1432
45	DK	0.34	0/1057	0.76	1/1432 (0.1%)
46	BN	0.32	0/1132	0.74	0/1527
46	DN	0.31	0/1132	0.73	0/1527
47	BO	0.32	0/943	0.66	0/1269
47	DO	0.30	0/943	0.65	0/1269
48	BP	0.42	1/1131 (0.1%)	1.03	1/1504 (0.1%)
48	DP	0.39	0/1131	1.05	3/1504 (0.2%)
49	BQ	0.32	0/1143	0.69	1/1527 (0.1%)
49	DQ	0.32	0/1143	0.71	1/1527 (0.1%)
50	BR	0.31	0/974	0.71	1/1302 (0.1%)
50	DR	0.31	0/974	0.76	2/1302 (0.2%)
51	BS	0.33	0/779	0.80	0/1038
51	DS	0.35	0/779	0.85	4/1038 (0.4%)
52	BT	0.34	0/1156	0.84	1/1544 (0.1%)
52	DT	0.35	0/1156	0.87	1/1544 (0.1%)
53	BU	0.33	0/975	0.66	1/1297 (0.1%)
53	DU	0.35	0/975	0.72	2/1297 (0.2%)
54	BV	0.35	0/790	0.81	1/1057 (0.1%)
54	DV	0.38	0/790	0.85	1/1057 (0.1%)
55	BW	0.37	0/907	0.70	0/1216
55	DW	0.32	0/907	0.66	0/1216
56	BX	0.32	0/740	0.74	0/995
56	DX	0.34	0/740	0.74	0/995
57	BY	0.58	2/789 (0.3%)	0.88	0/1053
57	DY	0.39	0/789	0.88	0/1053
58	BZ	0.33	0/1500	0.78	1/2037 (0.0%)
58	DZ	0.32	0/1500	0.76	1/2037 (0.0%)
All	All	0.37	27/328430 (0.0%)	0.99	659/490154 (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
13	AM	0	1
13	CM	0	1
35	BA	0	1
All	All	0	3

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	BY	7	VAL	CB-CG2	10.35	1.74	1.52
35	BA	1649	G	N7-C5	-10.02	1.33	1.39
1	AA	452	A	C5-C4	9.08	1.45	1.38
35	DA	2484	G	N7-C5	-8.84	1.33	1.39
35	DA	2279	G	N3-C4	-8.53	1.29	1.35

The worst 5 of 659 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	BA	2155	G	N1-C6-O6	-15.32	110.71	119.90
35	BA	2155	G	C5-C6-O6	13.90	136.94	128.60
35	BA	1899	G	N3-C4-N9	-12.56	118.46	126.00
35	DA	2279	G	C2-N3-C4	12.45	118.12	111.90
35	DA	859	G	C8-N9-C4	10.90	110.76	106.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	AM	118	ALA	Peptide
35	BA	2379	G	Sidechain
13	CM	118	ALA	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32329	0	16318	846	0
1	CA	32329	0	16318	862	0
2	AB	1901	0	1951	121	0
2	CB	1901	0	1951	106	0
3	AC	1613	0	1677	86	0
3	CC	1613	0	1677	85	0
4	AD	1703	0	1763	112	0
4	CD	1703	0	1763	101	0
5	AE	1147	0	1207	50	0
5	CE	1147	0	1207	48	0
6	AF	843	0	857	49	0
6	CF	843	0	857	54	0
7	AG	1257	0	1296	44	0
7	CG	1257	0	1296	51	0
8	AH	1116	0	1177	49	0
8	CH	1116	0	1177	55	0
9	AI	1011	0	1042	78	0
9	CI	1011	0	1042	62	0
10	AJ	795	0	840	62	0
10	CJ	795	0	840	68	0
11	AK	885	0	904	36	0
11	CK	885	0	904	30	0
12	AL	971	0	1057	54	0
12	CL	971	0	1057	59	0
13	AM	988	0	1057	88	0
13	CM	988	0	1057	66	0
14	AN	492	0	530	22	0
14	CN	492	0	529	24	0
15	AO	734	0	771	26	0
15	CO	734	0	771	23	0
16	AP	701	0	720	38	0
16	CP	701	0	720	36	0
17	AQ	824	0	891	34	0
17	CQ	824	0	891	30	0
18	AR	574	0	644	32	0
18	CR	574	0	644	28	0
19	AS	630	0	652	31	0
19	CS	630	0	652	32	0
20	AT	763	0	861	23	0
20	CT	763	0	861	23	0
21	AU	209	0	221	14	0
21	CU	209	0	221	15	0
22	AV	1619	0	822	19	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	AW	1597	0	811	63	0
22	CV	1619	0	822	29	0
22	CW	1597	0	811	59	0
23	AX	166	0	87	3	0
23	CX	166	0	87	9	0
24	AY	2802	0	2818	109	0
24	CY	2802	0	2818	141	0
25	B0	657	0	683	36	0
25	D0	657	0	683	33	0
26	B1	732	0	808	36	0
26	D1	732	0	808	33	0
27	B2	598	0	653	42	0
27	D2	598	0	653	24	0
28	B3	468	0	523	19	0
28	D3	468	0	523	18	0
29	B4	226	0	229	18	0
29	D4	226	0	229	19	0
30	B5	459	0	477	25	0
30	D5	459	0	477	27	0
31	B6	381	0	390	45	0
31	D6	381	0	391	49	0
32	B7	419	0	467	13	0
32	D7	419	0	467	10	0
33	B8	508	0	576	42	0
33	D8	508	0	576	41	0
34	B9	299	0	323	15	0
34	D9	299	0	324	14	0
35	BA	62474	0	31495	1332	0
35	DA	62474	0	31497	1254	0
36	BB	2551	0	1295	56	0
36	DB	2551	0	1295	55	0
37	BC	937	0	957	64	0
37	DC	937	0	957	60	0
38	BD	2120	0	2197	117	0
38	DD	2120	0	2197	110	0
39	BE	1564	0	1629	78	0
39	DE	1564	0	1629	84	0
40	BF	1624	0	1677	83	0
40	DF	1624	0	1677	86	0
41	BG	1474	0	1534	118	0
41	DG	1474	0	1535	116	0
42	BH	1248	0	1289	59	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	DH	1248	0	1289	64	0
43	BI	1132	0	1218	46	0
43	DI	1132	0	1218	57	0
44	BJ	651	0	155	14	0
44	DJ	651	0	157	12	0
45	BK	1038	0	1089	76	0
45	DK	1038	0	1089	96	0
46	BN	1105	0	1180	41	0
46	DN	1105	0	1180	59	0
47	BO	933	0	996	38	0
47	DO	933	0	996	35	0
48	BP	1114	0	1186	131	0
48	DP	1114	0	1187	121	0
49	BQ	1122	0	1179	64	0
49	DQ	1122	0	1179	65	0
50	BR	960	0	1021	51	0
50	DR	960	0	1021	43	0
51	BS	771	0	832	55	0
51	DS	771	0	832	61	0
52	BT	1142	0	1202	86	0
52	DT	1142	0	1202	99	0
53	BU	958	0	1015	52	0
53	DU	958	0	1015	49	0
54	BV	779	0	852	46	0
54	DV	779	0	852	60	0
55	BW	896	0	953	26	0
55	DW	896	0	953	30	0
56	BX	726	0	778	29	0
56	DX	726	0	778	27	0
57	BY	776	0	870	89	0
57	DY	776	0	870	73	0
58	BZ	1468	0	1492	102	0
58	DZ	1468	0	1492	72	0
59	AA	30	0	0	0	0
59	B5	1	0	0	0	0
59	BA	180	0	0	0	0
59	BB	2	0	0	0	0
59	BD	1	0	0	0	0
59	BE	1	0	0	0	0
59	BF	1	0	0	0	0
59	BQ	1	0	0	0	0
59	BT	1	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	CA	26	0	0	0	0
59	D5	2	0	0	0	0
59	DA	221	0	0	0	0
59	DB	2	0	0	0	0
59	DD	2	0	0	0	0
59	DP	1	0	0	0	0
59	DU	1	0	0	0	0
59	DW	1	0	0	0	0
60	AD	1	0	0	0	0
60	AN	1	0	0	0	0
60	B9	1	0	0	0	0
60	CD	1	0	0	0	0
60	CN	1	0	0	0	0
60	D9	1	0	0	0	0
61	AA	2	0	0	1	0
61	BA	6	0	0	2	0
61	BE	1	0	0	0	0
61	DA	7	0	0	3	0
61	DE	1	0	0	1	0
61	DS	1	0	0	0	0
61	DZ	1	0	0	0	0
All	All	304459	0	208395	9132	0

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 18.

The worst 5 of 9132 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)
57:BY:7:VAL:CB	57:BY:7:VAL:CG2	1.74	1.61
23:AX:20:G:N2	24:AY:203:THR:O	1.69	1.24
35:BA:1048:A:H62	35:BA:1052:C:N4	1.39	1.19
31:D6:35:GLU:HG3	31:D6:37:ARG:HH22	1.10	1.16
35:BA:1048:A:N6	35:BA:1052:C:H42	1.54	1.06

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	233/256 (91%)	128 (55%)	71 (30%)	34 (15%)	0	1
2	CB	233/256 (91%)	131 (56%)	67 (29%)	35 (15%)	0	1
3	AC	205/239 (86%)	131 (64%)	39 (19%)	35 (17%)	0	0
3	CC	205/239 (86%)	130 (63%)	41 (20%)	34 (17%)	0	0
4	AD	206/209 (99%)	138 (67%)	45 (22%)	23 (11%)	0	2
4	CD	206/209 (99%)	141 (68%)	42 (20%)	23 (11%)	0	2
5	AE	149/162 (92%)	116 (78%)	23 (15%)	10 (7%)	1	9
5	CE	149/162 (92%)	117 (78%)	22 (15%)	10 (7%)	1	9
6	AF	99/101 (98%)	71 (72%)	21 (21%)	7 (7%)	1	8
6	CF	99/101 (98%)	73 (74%)	19 (19%)	7 (7%)	1	8
7	AG	153/156 (98%)	116 (76%)	29 (19%)	8 (5%)	2	15
7	CG	153/156 (98%)	118 (77%)	27 (18%)	8 (5%)	2	15
8	AH	136/138 (99%)	106 (78%)	23 (17%)	7 (5%)	2	15
8	CH	136/138 (99%)	106 (78%)	23 (17%)	7 (5%)	2	15
9	AI	123/128 (96%)	86 (70%)	27 (22%)	10 (8%)	1	5
9	CI	123/128 (96%)	86 (70%)	26 (21%)	11 (9%)	1	4
10	AJ	97/105 (92%)	69 (71%)	23 (24%)	5 (5%)	2	15
10	CJ	97/105 (92%)	72 (74%)	20 (21%)	5 (5%)	2	15
11	AK	117/129 (91%)	87 (74%)	26 (22%)	4 (3%)	3	24
11	CK	117/129 (91%)	87 (74%)	26 (22%)	4 (3%)	3	24
12	AL	123/132 (93%)	85 (69%)	21 (17%)	17 (14%)	0	1
12	CL	123/132 (93%)	84 (68%)	20 (16%)	19 (15%)	0	1
13	AM	117/126 (93%)	72 (62%)	30 (26%)	15 (13%)	0	1
13	CM	117/126 (93%)	72 (62%)	28 (24%)	17 (14%)	0	1
14	AN	58/61 (95%)	40 (69%)	12 (21%)	6 (10%)	0	3

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	CN	58/61 (95%)	41 (71%)	11 (19%)	6 (10%)	0	3
15	AO	86/89 (97%)	68 (79%)	16 (19%)	2 (2%)	6	34
15	CO	86/89 (97%)	67 (78%)	17 (20%)	2 (2%)	6	34
16	AP	82/88 (93%)	58 (71%)	17 (21%)	7 (8%)	1	4
16	CP	82/88 (93%)	58 (71%)	16 (20%)	8 (10%)	0	3
17	AQ	98/105 (93%)	75 (76%)	14 (14%)	9 (9%)	1	3
17	CQ	98/105 (93%)	76 (78%)	12 (12%)	10 (10%)	0	3
18	AR	68/88 (77%)	45 (66%)	16 (24%)	7 (10%)	0	3
18	CR	68/88 (77%)	43 (63%)	19 (28%)	6 (9%)	1	4
19	AS	77/93 (83%)	44 (57%)	22 (29%)	11 (14%)	0	1
19	CS	77/93 (83%)	43 (56%)	22 (29%)	12 (16%)	0	1
20	AT	97/106 (92%)	64 (66%)	25 (26%)	8 (8%)	1	5
20	CT	97/106 (92%)	63 (65%)	26 (27%)	8 (8%)	1	5
21	AU	23/27 (85%)	15 (65%)	6 (26%)	2 (9%)	1	4
21	CU	23/27 (85%)	16 (70%)	6 (26%)	1 (4%)	2	20
24	AY	348/357 (98%)	303 (87%)	37 (11%)	8 (2%)	6	34
24	CY	348/357 (98%)	297 (85%)	40 (12%)	11 (3%)	4	26
25	B0	81/85 (95%)	69 (85%)	11 (14%)	1 (1%)	13	49
25	D0	81/85 (95%)	69 (85%)	11 (14%)	1 (1%)	13	49
26	B1	92/98 (94%)	64 (70%)	15 (16%)	13 (14%)	0	1
26	D1	92/98 (94%)	72 (78%)	11 (12%)	9 (10%)	0	3
27	B2	69/72 (96%)	45 (65%)	14 (20%)	10 (14%)	0	1
27	D2	69/72 (96%)	42 (61%)	18 (26%)	9 (13%)	0	1
28	B3	58/60 (97%)	51 (88%)	7 (12%)	0	100	100
28	D3	58/60 (97%)	52 (90%)	6 (10%)	0	100	100
29	B4	29/71 (41%)	16 (55%)	10 (34%)	3 (10%)	0	3
29	D4	29/71 (41%)	16 (55%)	10 (34%)	3 (10%)	0	3
30	B5	57/60 (95%)	41 (72%)	6 (10%)	10 (18%)	0	0
30	D5	57/60 (95%)	41 (72%)	5 (9%)	11 (19%)	0	0
31	B6	41/54 (76%)	19 (46%)	7 (17%)	15 (37%)	0	0
31	D6	43/54 (80%)	19 (44%)	7 (16%)	17 (40%)	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	B7	47/49 (96%)	47 (100%)	0	0	100	100
32	D7	47/49 (96%)	47 (100%)	0	0	100	100
33	B8	62/65 (95%)	43 (69%)	12 (19%)	7 (11%)	0	2
33	D8	62/65 (95%)	42 (68%)	12 (19%)	8 (13%)	0	1
34	B9	34/37 (92%)	31 (91%)	2 (6%)	1 (3%)	4	28
34	D9	34/37 (92%)	31 (91%)	2 (6%)	1 (3%)	4	28
37	BC	116/229 (51%)	89 (77%)	18 (16%)	9 (8%)	1	6
37	DC	116/229 (51%)	88 (76%)	20 (17%)	8 (7%)	1	8
38	BD	271/276 (98%)	205 (76%)	35 (13%)	31 (11%)	0	2
38	DD	271/276 (98%)	205 (76%)	38 (14%)	28 (10%)	0	3
39	BE	203/206 (98%)	147 (72%)	32 (16%)	24 (12%)	0	2
39	DE	203/206 (98%)	149 (73%)	32 (16%)	22 (11%)	0	2
40	BF	206/210 (98%)	152 (74%)	30 (15%)	24 (12%)	0	2
40	DF	206/210 (98%)	149 (72%)	35 (17%)	22 (11%)	0	2
41	BG	177/182 (97%)	99 (56%)	48 (27%)	30 (17%)	0	0
41	DG	179/182 (98%)	126 (70%)	23 (13%)	30 (17%)	0	0
42	BH	163/180 (91%)	107 (66%)	31 (19%)	25 (15%)	0	1
42	DH	163/180 (91%)	109 (67%)	31 (19%)	23 (14%)	0	1
43	BI	144/148 (97%)	85 (59%)	36 (25%)	23 (16%)	0	0
43	DI	144/148 (97%)	91 (63%)	39 (27%)	14 (10%)	0	3
45	BK	139/147 (95%)	80 (58%)	37 (27%)	22 (16%)	0	1
45	DK	139/147 (95%)	81 (58%)	36 (26%)	22 (16%)	0	1
46	BN	137/140 (98%)	106 (77%)	25 (18%)	6 (4%)	2	19
46	DN	137/140 (98%)	104 (76%)	26 (19%)	7 (5%)	2	15
47	BO	120/122 (98%)	101 (84%)	14 (12%)	5 (4%)	3	20
47	DO	120/122 (98%)	101 (84%)	15 (12%)	4 (3%)	4	25
48	BP	144/150 (96%)	72 (50%)	32 (22%)	40 (28%)	0	0
48	DP	144/150 (96%)	72 (50%)	31 (22%)	41 (28%)	0	0
49	BQ	139/141 (99%)	109 (78%)	23 (16%)	7 (5%)	2	16
49	DQ	139/141 (99%)	110 (79%)	22 (16%)	7 (5%)	2	16
50	BR	115/118 (98%)	93 (81%)	14 (12%)	8 (7%)	1	8

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	DR	115/118 (98%)	93 (81%)	15 (13%)	7 (6%)	1	12
51	BS	97/112 (87%)	52 (54%)	28 (29%)	17 (18%)	0	0
51	DS	97/112 (87%)	52 (54%)	28 (29%)	17 (18%)	0	0
52	BT	136/146 (93%)	86 (63%)	31 (23%)	19 (14%)	0	1
52	DT	136/146 (93%)	87 (64%)	30 (22%)	19 (14%)	0	1
53	BU	115/118 (98%)	96 (84%)	13 (11%)	6 (5%)	2	15
53	DU	115/118 (98%)	97 (84%)	11 (10%)	7 (6%)	1	12
54	BV	99/101 (98%)	72 (73%)	11 (11%)	16 (16%)	0	0
54	DV	99/101 (98%)	72 (73%)	11 (11%)	16 (16%)	0	0
55	BW	111/113 (98%)	94 (85%)	10 (9%)	7 (6%)	1	10
55	DW	111/113 (98%)	94 (85%)	9 (8%)	8 (7%)	1	7
56	BX	91/96 (95%)	74 (81%)	10 (11%)	7 (8%)	1	6
56	DX	91/96 (95%)	75 (82%)	8 (9%)	8 (9%)	1	4
57	BY	99/110 (90%)	55 (56%)	18 (18%)	26 (26%)	0	0
57	DY	99/110 (90%)	54 (54%)	18 (18%)	27 (27%)	0	0
58	BZ	183/206 (89%)	109 (60%)	43 (24%)	31 (17%)	0	0
58	DZ	183/206 (89%)	125 (68%)	39 (21%)	19 (10%)	0	3
All	All	12544/13594 (92%)	8912 (71%)	2295 (18%)	1337 (11%)	0	2

5 of 1337 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	12	GLU
2	AB	15	VAL
2	AB	20	GLU
2	AB	64	ARG
2	AB	97	TRP

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	202/220 (92%)	185 (92%)	17 (8%)	11	39
2	CB	202/220 (92%)	186 (92%)	16 (8%)	12	43
3	AC	160/188 (85%)	148 (92%)	12 (8%)	13	45
3	CC	160/188 (85%)	149 (93%)	11 (7%)	15	49
4	AD	180/181 (99%)	162 (90%)	18 (10%)	7	30
4	CD	180/181 (99%)	162 (90%)	18 (10%)	7	30
5	AE	115/123 (94%)	114 (99%)	1 (1%)	78	91
5	CE	115/123 (94%)	114 (99%)	1 (1%)	78	91
6	AF	90/90 (100%)	87 (97%)	3 (3%)	38	71
6	CF	90/90 (100%)	87 (97%)	3 (3%)	38	71
7	AG	126/127 (99%)	123 (98%)	3 (2%)	49	77
7	CG	126/127 (99%)	123 (98%)	3 (2%)	49	77
8	AH	119/119 (100%)	115 (97%)	4 (3%)	37	70
8	CH	119/119 (100%)	114 (96%)	5 (4%)	30	65
9	AI	98/99 (99%)	92 (94%)	6 (6%)	18	54
9	CI	98/99 (99%)	91 (93%)	7 (7%)	14	47
10	AJ	88/92 (96%)	85 (97%)	3 (3%)	37	70
10	CJ	88/92 (96%)	83 (94%)	5 (6%)	20	56
11	AK	90/99 (91%)	88 (98%)	2 (2%)	52	79
11	CK	90/99 (91%)	88 (98%)	2 (2%)	52	79
12	AL	104/109 (95%)	93 (89%)	11 (11%)	6	27
12	CL	104/109 (95%)	92 (88%)	12 (12%)	5	24
13	AM	99/101 (98%)	94 (95%)	5 (5%)	24	60
13	CM	99/101 (98%)	93 (94%)	6 (6%)	18	54
14	AN	49/50 (98%)	45 (92%)	4 (8%)	11	41
14	CN	49/50 (98%)	45 (92%)	4 (8%)	11	41
15	AO	79/80 (99%)	74 (94%)	5 (6%)	18	52
15	CO	79/80 (99%)	74 (94%)	5 (6%)	18	52
16	AP	72/74 (97%)	69 (96%)	3 (4%)	30	65
16	CP	72/74 (97%)	69 (96%)	3 (4%)	30	65
17	AQ	94/97 (97%)	92 (98%)	2 (2%)	53	79
17	CQ	94/97 (97%)	92 (98%)	2 (2%)	53	79

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	AR	61/77 (79%)	59 (97%)	2 (3%)	38	71
18	CR	61/77 (79%)	59 (97%)	2 (3%)	38	71
19	AS	69/80 (86%)	60 (87%)	9 (13%)	4	19
19	CS	69/80 (86%)	59 (86%)	10 (14%)	3	15
20	AT	76/82 (93%)	71 (93%)	5 (7%)	16	51
20	CT	76/82 (93%)	71 (93%)	5 (7%)	16	51
21	AU	19/22 (86%)	17 (90%)	2 (10%)	7	28
21	CU	19/22 (86%)	17 (90%)	2 (10%)	7	28
24	AY	297/303 (98%)	282 (95%)	15 (5%)	24	60
24	CY	297/303 (98%)	283 (95%)	14 (5%)	26	62
25	B0	66/67 (98%)	61 (92%)	5 (8%)	13	45
25	D0	66/67 (98%)	61 (92%)	5 (8%)	13	45
26	B1	78/83 (94%)	70 (90%)	8 (10%)	7	29
26	D1	78/83 (94%)	72 (92%)	6 (8%)	13	44
27	B2	66/67 (98%)	63 (96%)	3 (4%)	27	63
27	D2	66/67 (98%)	60 (91%)	6 (9%)	9	34
28	B3	51/52 (98%)	49 (96%)	2 (4%)	32	67
28	D3	51/52 (98%)	49 (96%)	2 (4%)	32	67
29	B4	27/63 (43%)	26 (96%)	1 (4%)	34	68
29	D4	27/63 (43%)	26 (96%)	1 (4%)	34	68
30	B5	51/52 (98%)	43 (84%)	8 (16%)	2	12
30	D5	51/52 (98%)	43 (84%)	8 (16%)	2	12
31	B6	43/52 (83%)	37 (86%)	6 (14%)	3	16
31	D6	43/52 (83%)	34 (79%)	9 (21%)	1	6
32	B7	41/42 (98%)	40 (98%)	1 (2%)	49	77
32	D7	41/42 (98%)	40 (98%)	1 (2%)	49	77
33	B8	53/55 (96%)	43 (81%)	10 (19%)	1	8
33	D8	53/55 (96%)	44 (83%)	9 (17%)	2	10
34	B9	33/34 (97%)	32 (97%)	1 (3%)	41	73
34	D9	33/34 (97%)	32 (97%)	1 (3%)	41	73
37	BC	99/181 (55%)	96 (97%)	3 (3%)	41	73

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	DC	99/181 (55%)	96 (97%)	3 (3%)	41	73
38	BD	214/218 (98%)	187 (87%)	27 (13%)	4	21
38	DD	214/218 (98%)	190 (89%)	24 (11%)	6	25
39	BE	165/166 (99%)	145 (88%)	20 (12%)	5	22
39	DE	165/166 (99%)	145 (88%)	20 (12%)	5	22
40	BF	165/166 (99%)	154 (93%)	11 (7%)	16	50
40	DF	165/166 (99%)	151 (92%)	14 (8%)	10	38
41	BG	155/156 (99%)	142 (92%)	13 (8%)	11	39
41	DG	155/156 (99%)	137 (88%)	18 (12%)	5	24
42	BH	132/148 (89%)	121 (92%)	11 (8%)	11	40
42	DH	132/148 (89%)	121 (92%)	11 (8%)	11	40
43	BI	122/124 (98%)	113 (93%)	9 (7%)	13	46
43	DI	122/124 (98%)	108 (88%)	14 (12%)	5	24
45	BK	106/111 (96%)	93 (88%)	13 (12%)	4	21
45	DK	106/111 (96%)	94 (89%)	12 (11%)	6	25
46	BN	117/119 (98%)	108 (92%)	9 (8%)	13	44
46	DN	117/119 (98%)	108 (92%)	9 (8%)	13	44
47	BO	100/100 (100%)	95 (95%)	5 (5%)	24	60
47	DO	100/100 (100%)	95 (95%)	5 (5%)	24	60
48	BP	112/116 (97%)	94 (84%)	18 (16%)	2	11
48	DP	112/116 (97%)	92 (82%)	20 (18%)	2	9
49	BQ	111/111 (100%)	101 (91%)	10 (9%)	9	34
49	DQ	111/111 (100%)	99 (89%)	12 (11%)	6	27
50	BR	100/101 (99%)	88 (88%)	12 (12%)	5	22
50	DR	100/101 (99%)	89 (89%)	11 (11%)	6	26
51	BS	77/88 (88%)	69 (90%)	8 (10%)	7	28
51	DS	77/88 (88%)	68 (88%)	9 (12%)	5	23
52	BT	120/127 (94%)	102 (85%)	18 (15%)	3	14
52	DT	120/127 (94%)	100 (83%)	20 (17%)	2	10
53	BU	92/94 (98%)	86 (94%)	6 (6%)	17	51
53	DU	92/94 (98%)	87 (95%)	5 (5%)	22	58

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	BV	82/82 (100%)	67 (82%)	15 (18%)	1	8
54	DV	82/82 (100%)	68 (83%)	14 (17%)	2	10
55	BW	91/92 (99%)	81 (89%)	10 (11%)	6	26
55	DW	91/92 (99%)	82 (90%)	9 (10%)	8	30
56	BX	74/78 (95%)	65 (88%)	9 (12%)	5	22
56	DX	74/78 (95%)	65 (88%)	9 (12%)	5	22
57	BY	84/91 (92%)	70 (83%)	14 (17%)	2	10
57	DY	84/91 (92%)	70 (83%)	14 (17%)	2	10
58	BZ	162/179 (90%)	154 (95%)	8 (5%)	25	61
58	DZ	162/179 (90%)	143 (88%)	19 (12%)	5	23
All	All	10552/11256 (94%)	9670 (92%)	882 (8%)	11	39

5 of 882 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	CD	107	ARG
27	D2	32	LEU
58	DZ	145	GLU
52	DT	41	ARG
7	CG	72	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
40	DF	160	ASN
43	DI	133	HIS
48	DP	35	HIS
51	BS	34	HIS
45	BK	103	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	233 (15%)	31 (2%)
1	CA	1503/1522 (98%)	238 (15%)	32 (2%)
22	AV	75/76 (98%)	22 (29%)	0

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
22	AW	74/76 (97%)	22 (29%)	0
22	CV	75/76 (98%)	18 (24%)	0
22	CW	74/76 (97%)	21 (28%)	1 (1%)
23	AX	7/25 (28%)	3 (42%)	0
23	CX	7/25 (28%)	2 (28%)	1 (14%)
35	BA	2900/2915 (99%)	574 (19%)	38 (1%)
35	DA	2900/2915 (99%)	588 (20%)	36 (1%)
36	BB	118/122 (96%)	16 (13%)	1 (0%)
36	DB	118/122 (96%)	17 (14%)	1 (0%)
All	All	9354/9472 (98%)	1754 (18%)	141 (1%)

5 of 1754 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	31	G
1	AA	32	A
1	AA	39	G
1	AA	48	C

5 of 141 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	DA	603	A
35	DA	1022	G
35	DA	1970	A
35	BA	1210	A
35	BA	1048	A

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

2 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
24	MEQ	CY	240	24	8,9,10	1.34	2 (25%)	5,10,12	1.82	2 (40%)
24	MEQ	AY	240	24	8,9,10	1.36	2 (25%)	5,10,12	1.83	2 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	MEQ	CY	240	24	-	3/8/9/11	-
24	MEQ	AY	240	24	-	2/8/9/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AY	240	MEQ	CD-NE2	2.40	1.45	1.34
24	CY	240	MEQ	CD-NE2	2.37	1.45	1.34
24	CY	240	MEQ	OE1-CD	-2.17	1.18	1.23
24	AY	240	MEQ	OE1-CD	-2.15	1.18	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AY	240	MEQ	CG-CD-NE2	3.19	120.71	116.29
24	CY	240	MEQ	CG-CD-NE2	2.93	120.36	116.29
24	CY	240	MEQ	CB-CG-CD	-2.50	107.45	113.04
24	AY	240	MEQ	CB-CG-CD	-2.05	108.47	113.04

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	AY	240	MEQ	N-CA-CB-CG
24	AY	240	MEQ	C-CA-CB-CG
24	CY	240	MEQ	N-CA-CB-CG
24	CY	240	MEQ	C-CA-CB-CG
24	CY	240	MEQ	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 480 ligands modelled in this entry, 480 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	AM	3
13	CM	3
31	B6	1
9	AI	1
41	BG	1
9	CI	1
48	BP	1

The worst 5 of 11 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B6	46:HIS	C	47:THR	N	7.71
1	AM	112:GLY	C	113:PRO	N	4.87
1	CM	112:GLY	C	113:PRO	N	4.87
1	AI	104:ARG	C	105:ASP	N	4.73
1	AM	65:LYS	C	66:LEU	N	4.57

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AA	1504/1522 (98%)	-0.31	18 (1%) 79 67	101, 160, 266, 374	0
1	CA	1504/1522 (98%)	-0.32	13 (0%) 84 75	99, 164, 261, 390	0
2	AB	235/256 (91%)	0.68	33 (14%) 2 1	171, 220, 260, 279	0
2	CB	235/256 (91%)	0.34	17 (7%) 15 9	135, 195, 239, 253	0
3	AC	207/239 (86%)	0.59	29 (14%) 2 1	160, 205, 242, 281	0
3	CC	207/239 (86%)	0.67	42 (20%) 1 1	146, 179, 215, 234	0
4	AD	208/209 (99%)	0.35	12 (5%) 23 13	122, 157, 189, 209	0
4	CD	208/209 (99%)	0.80	31 (14%) 2 1	141, 181, 208, 229	0
5	AE	151/162 (93%)	0.41	10 (6%) 18 11	129, 168, 201, 221	0
5	CE	151/162 (93%)	0.30	10 (6%) 18 11	120, 152, 184, 213	0
6	AF	101/101 (100%)	0.39	11 (10%) 5 3	157, 189, 218, 247	0
6	CF	101/101 (100%)	-0.12	1 (0%) 82 72	128, 162, 192, 226	0
7	AG	155/156 (99%)	0.93	30 (19%) 1 1	166, 199, 235, 255	0
7	CG	155/156 (99%)	0.59	22 (14%) 2 1	136, 188, 223, 253	0
8	AH	138/138 (100%)	0.71	20 (14%) 2 1	143, 170, 199, 216	0
8	CH	138/138 (100%)	0.86	22 (15%) 1 1	136, 162, 186, 202	0
9	AI	127/128 (99%)	1.56	41 (32%) 0 0	172, 227, 248, 264	0
9	CI	127/128 (99%)	1.12	32 (25%) 0 0	145, 202, 241, 246	0
10	AJ	99/105 (94%)	1.67	34 (34%) 0 0	174, 216, 246, 256	0
10	CJ	99/105 (94%)	1.60	32 (32%) 0 0	164, 201, 235, 250	0
11	AK	119/129 (92%)	0.79	16 (13%) 3 2	135, 176, 211, 255	0
11	CK	119/129 (92%)	0.53	10 (8%) 11 6	130, 159, 197, 249	0
12	AL	125/132 (94%)	0.37	7 (5%) 24 13	112, 136, 173, 203	0
12	CL	125/132 (94%)	0.76	23 (18%) 1 1	118, 140, 180, 220	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AM	125/126 (99%)	1.02	28 (22%) 0 0	173, 220, 245, 273	0
13	CM	125/126 (99%)	1.18	37 (29%) 0 0	151, 197, 224, 244	0
14	AN	60/61 (98%)	1.45	15 (25%) 0 0	179, 202, 223, 232	0
14	CN	60/61 (98%)	0.53	4 (6%) 17 10	146, 177, 200, 208	0
15	AO	88/89 (98%)	0.39	8 (9%) 9 5	132, 161, 202, 213	0
15	CO	88/89 (98%)	0.32	2 (2%) 60 47	120, 151, 187, 202	0
16	AP	84/88 (95%)	0.94	16 (19%) 1 1	123, 143, 182, 198	0
16	CP	84/88 (95%)	1.99	38 (45%) 0 0	154, 185, 231, 243	0
17	AQ	100/105 (95%)	0.54	11 (11%) 5 3	123, 150, 178, 188	0
17	CQ	100/105 (95%)	0.74	16 (16%) 1 1	121, 152, 181, 200	0
18	AR	70/88 (79%)	1.17	18 (25%) 0 0	162, 190, 227, 235	0
18	CR	70/88 (79%)	0.71	7 (10%) 7 4	120, 161, 192, 205	0
19	AS	79/93 (84%)	2.40	35 (44%) 0 0	180, 225, 257, 264	0
19	CS	79/93 (84%)	2.29	40 (50%) 0 0	152, 200, 248, 260	0
20	AT	99/106 (93%)	0.65	9 (9%) 9 5	112, 149, 188, 211	0
20	CT	99/106 (93%)	1.14	24 (24%) 0 0	133, 171, 215, 243	0
21	AU	25/27 (92%)	5.70	24 (96%) 0 0	187, 213, 239, 242	0
21	CU	25/27 (92%)	3.33	19 (76%) 0 0	156, 181, 195, 199	0
22	AV	76/76 (100%)	-0.10	0 100 100	152, 210, 242, 302	0
22	AW	75/76 (98%)	0.89	13 (17%) 1 1	323, 391, 436, 444	0
22	CV	76/76 (100%)	-0.03	2 (2%) 56 40	141, 191, 230, 296	0
22	CW	75/76 (98%)	0.87	11 (14%) 2 1	342, 398, 492, 499	0
23	AX	8/25 (32%)	0.84	1 (12%) 3 2	93, 149, 231, 248	0
23	CX	8/25 (32%)	0.53	0 100 100	91, 140, 225, 232	0
24	AY	350/357 (98%)	2.04	143 (40%) 0 0	154, 199, 282, 305	0
24	CY	350/357 (98%)	2.42	161 (46%) 0 0	149, 202, 279, 297	0
25	B0	83/85 (97%)	1.58	17 (20%) 1 1	114, 138, 194, 242	0
25	D0	83/85 (97%)	1.22	17 (20%) 1 1	104, 125, 189, 229	0
26	B1	94/98 (95%)	0.63	5 (5%) 26 14	94, 124, 167, 203	0
26	D1	94/98 (95%)	0.50	5 (5%) 26 14	88, 120, 172, 191	0
27	B2	71/72 (98%)	0.33	5 (7%) 16 9	132, 166, 193, 229	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
27	D2	71/72 (98%)	0.11	4 (5%) 24 13	87, 125, 166, 194	0
28	B3	60/60 (100%)	1.84	25 (41%) 0 0	113, 142, 177, 204	0
28	D3	60/60 (100%)	1.01	13 (21%) 0 0	106, 122, 158, 204	0
29	B4	31/71 (43%)	0.75	3 (9%) 7 4	200, 226, 244, 255	0
29	D4	31/71 (43%)	-0.28	1 (3%) 47 31	173, 195, 213, 223	0
30	B5	59/60 (98%)	0.46	5 (8%) 10 6	102, 134, 247, 283	0
30	D5	59/60 (98%)	0.56	5 (8%) 10 6	85, 122, 245, 254	0
31	B6	45/54 (83%)	5.45	40 (88%) 0 0	199, 239, 256, 271	0
31	D6	45/54 (83%)	4.93	41 (91%) 0 0	206, 233, 253, 260	0
32	B7	49/49 (100%)	0.60	6 (12%) 4 2	90, 105, 164, 187	0
32	D7	49/49 (100%)	0.19	2 (4%) 37 24	70, 90, 135, 203	0
33	B8	64/65 (98%)	0.89	7 (10%) 5 3	95, 125, 170, 193	0
33	D8	64/65 (98%)	0.71	3 (4%) 31 19	100, 121, 164, 195	0
34	B9	36/37 (97%)	6.43	35 (97%) 0 0	147, 185, 220, 226	0
34	D9	36/37 (97%)	6.47	36 (100%) 0 0	140, 159, 201, 218	0
35	BA	2901/2915 (99%)	-0.31	42 (1%) 75 63	84, 127, 274, 441	0
35	DA	2901/2915 (99%)	-0.26	51 (1%) 68 55	74, 114, 282, 427	0
36	BB	119/122 (97%)	-0.57	0 100 100	134, 193, 232, 248	0
36	DB	119/122 (97%)	-0.66	1 (0%) 86 78	122, 159, 190, 222	0
37	BC	120/229 (52%)	3.83	79 (65%) 0 0	214, 309, 343, 358	0
37	DC	120/229 (52%)	3.57	84 (70%) 0 0	227, 322, 369, 374	0
38	BD	273/276 (98%)	0.28	8 (2%) 51 36	80, 117, 153, 183	0
38	DD	273/276 (98%)	0.08	5 (1%) 68 55	78, 106, 143, 194	0
39	BE	205/206 (99%)	0.53	18 (8%) 10 5	88, 126, 179, 217	0
39	DE	205/206 (99%)	0.64	21 (10%) 6 4	84, 126, 183, 224	0
40	BF	208/210 (99%)	0.27	7 (3%) 45 29	88, 134, 196, 257	0
40	DF	208/210 (99%)	0.10	5 (2%) 59 44	71, 118, 193, 245	0
41	BG	181/182 (99%)	0.55	25 (13%) 2 2	157, 199, 231, 260	0
41	DG	181/182 (99%)	0.27	11 (6%) 21 12	133, 165, 214, 276	0
42	BH	165/180 (91%)	1.55	60 (36%) 0 0	146, 198, 246, 270	0
42	DH	165/180 (91%)	0.54	21 (12%) 3 2	98, 145, 186, 222	0

Continued on next page...



Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
43	BI	146/148 (98%)	0.53	17 (11%) 4 3	117, 175, 202, 218	0
43	DI	146/148 (98%)	0.16	3 (2%) 63 49	119, 157, 195, 216	0
44	BJ	0/130	-	-	-	-
44	DJ	0/130	-	-	-	-
45	BK	141/147 (95%)	3.33	84 (59%) 0 0	224, 266, 287, 294	0
45	DK	141/147 (95%)	3.37	96 (68%) 0 0	233, 278, 303, 327	0
46	BN	139/140 (99%)	0.65	21 (15%) 2 1	106, 144, 181, 204	0
46	DN	139/140 (99%)	0.17	4 (2%) 51 36	95, 123, 166, 192	0
47	BO	122/122 (100%)	0.25	6 (4%) 29 17	88, 118, 144, 157	0
47	DO	122/122 (100%)	0.39	6 (4%) 29 17	89, 119, 150, 168	0
48	BP	146/150 (97%)	0.83	21 (14%) 2 1	85, 148, 190, 235	0
48	DP	146/150 (97%)	0.39	6 (4%) 37 24	82, 134, 170, 225	0
49	BQ	141/141 (100%)	0.49	9 (6%) 19 11	113, 141, 176, 223	0
49	DQ	141/141 (100%)	0.54	12 (8%) 10 6	91, 127, 164, 214	0
50	BR	117/118 (99%)	0.36	5 (4%) 35 22	98, 125, 162, 200	0
50	DR	117/118 (99%)	0.54	7 (5%) 21 12	95, 123, 158, 187	0
51	BS	99/112 (88%)	1.05	21 (21%) 0 1	131, 183, 209, 216	0
51	DS	99/112 (88%)	1.35	29 (29%) 0 0	122, 163, 196, 216	0
52	BT	138/146 (94%)	0.28	7 (5%) 28 16	91, 137, 214, 284	0
52	DT	138/146 (94%)	0.42	12 (8%) 10 5	106, 145, 229, 264	0
53	BU	117/118 (99%)	0.35	4 (3%) 45 29	100, 138, 184, 207	0
53	DU	117/118 (99%)	-0.06	1 (0%) 84 75	79, 112, 163, 196	0
54	BV	101/101 (100%)	0.19	5 (4%) 28 16	96, 159, 197, 229	0
54	DV	101/101 (100%)	0.25	1 (0%) 82 72	90, 141, 180, 211	0
55	BW	113/113 (100%)	0.78	15 (13%) 3 2	94, 122, 155, 225	0
55	DW	113/113 (100%)	0.48	7 (6%) 20 11	81, 106, 145, 264	0
56	BX	93/96 (96%)	0.61	11 (11%) 4 2	111, 142, 163, 204	0
56	DX	93/96 (96%)	0.19	4 (4%) 35 22	84, 113, 145, 172	0
57	BY	101/110 (91%)	1.97	45 (44%) 0 0	122, 163, 211, 239	0
57	DY	101/110 (91%)	0.61	11 (10%) 5 3	101, 137, 193, 221	0
58	BZ	185/206 (89%)	0.51	23 (12%) 4 2	146, 176, 218, 239	0
58	DZ	185/206 (89%)	0.19	12 (6%) 18 11	117, 165, 209, 235	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	22142/23326 (94%)	0.41	2416 (10%) <b>5</b> <b>3</b>	70, 153, 269, 499	0

The worst 5 of 2416 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
30	D5	59	GLU	18.4
45	BK	87	GLY	17.6
31	B6	13	CYS	17.3
24	CY	262	CYS	17.1
37	BC	174	ALA	15.7

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
24	MEQ	CY	240	10/11	0.78	0.55	149,152,186,247	0
24	MEQ	AY	240	10/11	0.83	0.51	143,154,163,163	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(Å <sup>2</sup> )	Q<0.9
59	MG	BA	3114	1/1	0.41	0.21	110,110,110,110	0
60	ZN	B9	101	1/1	0.53	0.65	205,205,205,205	1
59	MG	BQ	201	1/1	0.57	1.22	104,104,104,104	0
59	MG	BB	202	1/1	0.59	0.59	95,95,95,95	0
59	MG	BA	3125	1/1	0.62	0.64	100,100,100,100	0

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
59	MG	AA	1622	1/1	0.62	0.61	96,96,96,96	0
59	MG	BA	3144	1/1	0.64	1.56	91,91,91,91	0
59	MG	DA	3219	1/1	0.65	0.15	115,115,115,115	0
59	MG	CA	1619	1/1	0.67	0.35	87,87,87,87	0
59	MG	BT	201	1/1	0.70	0.44	108,108,108,108	0
59	MG	CA	1606	1/1	0.71	0.42	75,75,75,75	0
59	MG	DA	3073	1/1	0.71	0.17	129,129,129,129	0
59	MG	BA	3174	1/1	0.72	0.73	87,87,87,87	0
59	MG	DA	3176	1/1	0.72	1.58	87,87,87,87	0
59	MG	BA	3105	1/1	0.72	1.32	85,85,85,85	0
59	MG	BA	3151	1/1	0.72	0.27	87,87,87,87	0
59	MG	DA	3205	1/1	0.73	0.26	86,86,86,86	0
59	MG	BA	3155	1/1	0.73	0.53	93,93,93,93	0
59	MG	DA	3190	1/1	0.73	0.30	91,91,91,91	0
59	MG	BA	3166	1/1	0.76	0.21	80,80,80,80	0
59	MG	BA	3179	1/1	0.76	0.65	104,104,104,104	0
59	MG	DA	3163	1/1	0.76	0.94	84,84,84,84	0
59	MG	CA	1617	1/1	0.76	1.07	125,125,125,125	0
59	MG	DA	3104	1/1	0.77	0.97	82,82,82,82	0
59	MG	AA	1617	1/1	0.78	0.60	73,73,73,73	0
59	MG	BA	3120	1/1	0.78	0.56	81,81,81,81	0
59	MG	DA	3213	1/1	0.78	0.28	101,101,101,101	0
59	MG	BA	3162	1/1	0.78	0.53	79,79,79,79	0
59	MG	BA	3145	1/1	0.78	0.40	114,114,114,114	0
59	MG	BA	3082	1/1	0.79	0.97	75,75,75,75	0
59	MG	AA	1629	1/1	0.79	0.13	120,120,120,120	0
59	MG	BA	3152	1/1	0.80	0.61	91,91,91,91	0
59	MG	DA	3141	1/1	0.81	0.45	67,67,67,67	0
59	MG	DA	3086	1/1	0.81	0.70	65,65,65,65	0
59	MG	DA	3128	1/1	0.82	0.30	72,72,72,72	0
59	MG	DA	3195	1/1	0.82	0.57	100,100,100,100	0
59	MG	DA	3199	1/1	0.82	0.37	81,81,81,81	0
59	MG	DA	3202	1/1	0.82	0.93	97,97,97,97	0
59	MG	BA	3112	1/1	0.82	1.26	84,84,84,84	0
59	MG	CA	1610	1/1	0.82	0.40	71,71,71,71	0
59	MG	CA	1621	1/1	0.82	0.22	136,136,136,136	0
59	MG	DA	3182	1/1	0.82	0.52	80,80,80,80	0
59	MG	DA	3136	1/1	0.83	0.51	71,71,71,71	0
59	MG	BA	3163	1/1	0.83	0.51	104,104,104,104	0
59	MG	DA	3147	1/1	0.83	0.44	91,91,91,91	0
59	MG	BA	3147	1/1	0.83	0.18	70,70,70,70	0
59	MG	CA	1624	1/1	0.83	0.47	91,91,91,91	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	DA	3119	1/1	0.83	0.29	85,85,85,85	0
59	MG	DA	3033	1/1	0.83	0.65	77,77,77,77	0
59	MG	BA	3148	1/1	0.84	0.51	90,90,90,90	0
59	MG	AA	1628	1/1	0.84	1.30	99,99,99,99	0
59	MG	CA	1625	1/1	0.84	0.41	110,110,110,110	0
59	MG	DA	3016	1/1	0.84	0.54	58,58,58,58	0
59	MG	AA	1612	1/1	0.84	0.80	75,75,75,75	0
59	MG	AA	1630	1/1	0.84	0.54	86,86,86,86	0
59	MG	BF	301	1/1	0.85	0.23	120,120,120,120	0
59	MG	DA	3212	1/1	0.85	1.09	92,92,92,92	0
59	MG	DA	3116	1/1	0.85	0.40	71,71,71,71	0
59	MG	DA	3137	1/1	0.85	0.51	92,92,92,92	0
59	MG	BA	3154	1/1	0.85	1.04	92,92,92,92	0
59	MG	DA	3204	1/1	0.86	0.68	85,85,85,85	0
59	MG	BA	3116	1/1	0.86	0.55	75,75,75,75	0
59	MG	BA	3091	1/1	0.86	0.51	71,71,71,71	0
59	MG	DA	3156	1/1	0.86	0.24	59,59,59,59	0
59	MG	DA	3111	1/1	0.86	0.42	80,80,80,80	0
59	MG	BA	3088	1/1	0.86	0.76	83,83,83,83	0
59	MG	BA	3159	1/1	0.87	0.50	81,81,81,81	0
59	MG	DA	3193	1/1	0.87	0.30	96,96,96,96	0
59	MG	DA	3208	1/1	0.87	0.35	87,87,87,87	0
59	MG	DA	3170	1/1	0.87	0.58	80,80,80,80	0
59	MG	BA	3164	1/1	0.87	0.45	84,84,84,84	0
59	MG	BA	3086	1/1	0.87	0.52	69,69,69,69	0
59	MG	DB	201	1/1	0.87	0.48	78,78,78,78	0
59	MG	DB	202	1/1	0.87	0.39	101,101,101,101	0
59	MG	DA	3203	1/1	0.87	0.41	93,93,93,93	0
59	MG	BA	3126	1/1	0.88	0.26	108,108,108,108	0
59	MG	BA	3143	1/1	0.88	1.00	86,86,86,86	0
59	MG	DA	3206	1/1	0.88	0.46	67,67,67,67	0
59	MG	DA	3131	1/1	0.88	1.38	91,91,91,91	0
59	MG	BA	3038	1/1	0.88	0.35	63,63,63,63	0
59	MG	BA	3052	1/1	0.88	0.45	62,62,62,62	0
59	MG	DA	3217	1/1	0.88	0.55	56,56,56,56	0
59	MG	AA	1626	1/1	0.88	0.45	132,132,132,132	0
59	MG	BA	3121	1/1	0.88	0.34	65,65,65,65	0
59	MG	DA	3113	1/1	0.88	0.58	74,74,74,74	0
59	MG	AA	1618	1/1	0.88	0.51	94,94,94,94	0
59	MG	DA	3164	1/1	0.89	0.62	91,91,91,91	0
59	MG	BA	3169	1/1	0.89	0.23	94,94,94,94	0
59	MG	DA	3138	1/1	0.89	0.39	64,64,64,64	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	CA	1616	1/1	0.89	0.35	98,98,98,98	0
59	MG	DA	3220	1/1	0.89	0.81	99,99,99,99	0
59	MG	DA	3129	1/1	0.89	0.71	75,75,75,75	0
59	MG	DA	3114	1/1	0.89	0.28	107,107,107,107	0
59	MG	AA	1602	1/1	0.89	0.25	87,87,87,87	0
59	MG	DA	3112	1/1	0.90	0.28	75,75,75,75	0
59	MG	BA	3168	1/1	0.90	0.48	78,78,78,78	0
59	MG	BA	3078	1/1	0.90	0.39	65,65,65,65	0
59	MG	AA	1605	1/1	0.90	0.44	76,76,76,76	0
59	MG	DA	3207	1/1	0.90	0.23	104,104,104,104	0
59	MG	DA	3027	1/1	0.90	0.80	57,57,57,57	0
59	MG	DA	3123	1/1	0.90	0.19	77,77,77,77	0
59	MG	CA	1614	1/1	0.90	0.78	81,81,81,81	0
59	MG	DA	3064	1/1	0.90	0.38	48,48,48,48	0
59	MG	BA	3047	1/1	0.90	0.43	72,72,72,72	0
59	MG	DA	3132	1/1	0.90	0.78	72,72,72,72	0
59	MG	BA	3137	1/1	0.90	0.46	80,80,80,80	0
59	MG	AA	1611	1/1	0.90	0.67	69,69,69,69	0
59	MG	BA	3061	1/1	0.90	0.87	74,74,74,74	0
59	MG	DA	3196	1/1	0.91	0.77	69,69,69,69	0
59	MG	CA	1615	1/1	0.91	0.96	98,98,98,98	0
59	MG	BA	3177	1/1	0.91	1.02	80,80,80,80	0
59	MG	BA	3075	1/1	0.91	0.48	78,78,78,78	0
59	MG	BB	201	1/1	0.91	0.26	85,85,85,85	0
59	MG	DA	3148	1/1	0.91	0.31	87,87,87,87	0
59	MG	AA	1608	1/1	0.91	0.34	90,90,90,90	0
59	MG	BE	301	1/1	0.91	0.44	73,73,73,73	0
59	MG	BA	3098	1/1	0.91	0.68	66,66,66,66	0
59	MG	BA	3103	1/1	0.91	0.37	88,88,88,88	0
59	MG	BA	3131	1/1	0.91	0.20	76,76,76,76	0
59	MG	BA	3171	1/1	0.91	0.31	91,91,91,91	0
59	MG	DA	3183	1/1	0.91	0.26	82,82,82,82	0
59	MG	BA	3172	1/1	0.91	0.50	78,78,78,78	0
59	MG	DA	3192	1/1	0.91	0.42	86,86,86,86	0
59	MG	CA	1613	1/1	0.91	0.60	80,80,80,80	0
59	MG	BA	3133	1/1	0.91	0.29	83,83,83,83	0
59	MG	CA	1601	1/1	0.92	0.22	78,78,78,78	0
59	MG	AA	1623	1/1	0.92	0.77	83,83,83,83	0
59	MG	AA	1619	1/1	0.92	0.59	90,90,90,90	0
59	MG	CA	1618	1/1	0.92	0.44	105,105,105,105	0
59	MG	DA	3184	1/1	0.92	0.54	85,85,85,85	0
59	MG	DA	3058	1/1	0.92	0.30	54,54,54,54	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
59	MG	CA	1612	1/1	0.92	0.36	77,77,77,77	0
59	MG	BA	3160	1/1	0.92	0.61	98,98,98,98	0
59	MG	DA	3120	1/1	0.92	0.46	83,83,83,83	0
59	MG	BA	3175	1/1	0.92	0.44	69,69,69,69	0
59	MG	DA	3157	1/1	0.92	0.51	80,80,80,80	0
59	MG	DA	3088	1/1	0.92	0.25	75,75,75,75	0
59	MG	DA	3096	1/1	0.92	0.70	62,62,62,62	0
59	MG	DA	3159	1/1	0.93	0.41	89,89,89,89	0
59	MG	BA	3097	1/1	0.93	0.58	69,69,69,69	0
59	MG	BA	3041	1/1	0.93	0.46	63,63,63,63	0
59	MG	DA	3023	1/1	0.93	0.46	51,51,51,51	0
59	MG	DA	3173	1/1	0.93	0.21	102,102,102,102	0
59	MG	BA	3009	1/1	0.93	0.46	46,46,46,46	0
59	MG	BA	3084	1/1	0.93	0.45	87,87,87,87	0
59	MG	DA	3210	1/1	0.93	0.47	77,77,77,77	0
59	MG	DA	3035	1/1	0.93	0.37	50,50,50,50	0
59	MG	DA	3036	1/1	0.93	0.42	40,40,40,40	0
59	MG	DA	3057	1/1	0.93	0.32	52,52,52,52	0
59	MG	BA	3016	1/1	0.93	0.70	69,69,69,69	0
59	MG	DA	3063	1/1	0.93	0.37	54,54,54,54	0
59	MG	DA	3153	1/1	0.93	0.77	66,66,66,66	0
59	MG	BA	3027	1/1	0.93	0.43	76,76,76,76	0
59	MG	AA	1625	1/1	0.93	0.38	78,78,78,78	0
59	MG	BA	3109	1/1	0.94	0.25	74,74,74,74	0
59	MG	BA	3110	1/1	0.94	0.40	75,75,75,75	0
59	MG	AA	1604	1/1	0.94	0.91	76,76,76,76	0
59	MG	DA	3158	1/1	0.94	0.23	71,71,71,71	0
59	MG	DA	3049	1/1	0.94	0.67	64,64,64,64	0
59	MG	DA	3161	1/1	0.94	0.19	58,58,58,58	0
59	MG	BA	3081	1/1	0.94	0.21	107,107,107,107	0
59	MG	BA	3044	1/1	0.94	0.51	81,81,81,81	0
59	MG	BA	3117	1/1	0.94	0.44	100,100,100,100	0
59	MG	CA	1602	1/1	0.94	0.28	64,64,64,64	0
59	MG	DA	3175	1/1	0.94	0.28	60,60,60,60	0
59	MG	DA	3071	1/1	0.94	0.25	66,66,66,66	0
59	MG	DA	3181	1/1	0.94	0.24	82,82,82,82	0
59	MG	CA	1604	1/1	0.94	0.66	58,58,58,58	0
59	MG	DA	3080	1/1	0.94	0.46	68,68,68,68	0
59	MG	BA	3119	1/1	0.94	0.90	80,80,80,80	0
59	MG	DA	3188	1/1	0.94	0.71	87,87,87,87	0
59	MG	CA	1609	1/1	0.94	0.17	110,110,110,110	0
59	MG	DA	3092	1/1	0.94	0.33	70,70,70,70	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	BA	3083	1/1	0.94	0.55	64,64,64,64	0
59	MG	BA	3022	1/1	0.94	0.79	68,68,68,68	0
59	MG	BA	3123	1/1	0.94	0.10	105,105,105,105	0
59	MG	DA	3198	1/1	0.94	0.45	85,85,85,85	0
59	MG	BA	3006	1/1	0.94	0.51	41,41,41,41	0
59	MG	DA	3201	1/1	0.94	0.36	82,82,82,82	0
59	MG	BA	3053	1/1	0.94	0.66	71,71,71,71	0
59	MG	BA	3130	1/1	0.94	0.44	63,63,63,63	0
59	MG	BA	3058	1/1	0.94	0.44	66,66,66,66	0
59	MG	BA	3093	1/1	0.94	0.29	110,110,110,110	0
59	MG	BA	3037	1/1	0.94	0.23	98,98,98,98	0
59	MG	CA	1620	1/1	0.94	0.43	121,121,121,121	0
59	MG	BA	3066	1/1	0.94	0.29	75,75,75,75	0
59	MG	CA	1623	1/1	0.94	0.30	151,151,151,151	0
59	MG	BA	3176	1/1	0.94	0.18	98,98,98,98	0
59	MG	BA	3101	1/1	0.94	0.13	86,86,86,86	0
59	MG	CA	1626	1/1	0.94	0.46	97,97,97,97	0
59	MG	D5	102	1/1	0.94	0.90	82,82,82,82	0
59	MG	BA	3178	1/1	0.94	0.56	96,96,96,96	0
59	MG	AA	1603	1/1	0.94	0.30	102,102,102,102	0
59	MG	BA	3076	1/1	0.94	0.32	68,68,68,68	0
59	MG	DW	201	1/1	0.94	0.50	70,70,70,70	0
59	MG	DA	3031	1/1	0.94	0.36	48,48,48,48	0
59	MG	DA	3168	1/1	0.95	0.08	72,72,72,72	0
59	MG	BA	3032	1/1	0.95	0.45	69,69,69,69	0
59	MG	DA	3172	1/1	0.95	0.15	66,66,66,66	0
59	MG	BD	301	1/1	0.95	0.23	71,71,71,71	0
59	MG	DA	3099	1/1	0.95	1.05	71,71,71,71	0
59	MG	BA	3034	1/1	0.95	0.40	75,75,75,75	0
59	MG	DA	3178	1/1	0.95	0.16	79,79,79,79	0
59	MG	BA	3100	1/1	0.95	0.30	102,102,102,102	0
59	MG	AA	1627	1/1	0.95	0.45	90,90,90,90	0
59	MG	AA	1624	1/1	0.95	0.27	110,110,110,110	0
59	MG	DA	3012	1/1	0.95	0.45	60,60,60,60	0
59	MG	DA	3185	1/1	0.95	0.57	76,76,76,76	0
59	MG	BA	3165	1/1	0.95	0.27	111,111,111,111	0
59	MG	BA	3104	1/1	0.95	0.38	80,80,80,80	0
59	MG	CA	1603	1/1	0.95	0.49	89,89,89,89	0
59	MG	DA	3030	1/1	0.95	0.31	42,42,42,42	0
59	MG	DA	3124	1/1	0.95	0.35	97,97,97,97	0
59	MG	BA	3011	1/1	0.95	0.30	58,58,58,58	0
59	MG	DA	3197	1/1	0.95	0.18	84,84,84,84	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
59	MG	CA	1605	1/1	0.95	0.27	94,94,94,94	0
59	MG	BA	3106	1/1	0.95	0.68	90,90,90,90	0
59	MG	BA	3170	1/1	0.95	0.32	77,77,77,77	0
59	MG	DA	3042	1/1	0.95	0.34	45,45,45,45	0
59	MG	DA	3046	1/1	0.95	0.55	74,74,74,74	0
59	MG	BA	3043	1/1	0.95	0.15	67,67,67,67	0
59	MG	DA	3055	1/1	0.95	0.38	62,62,62,62	0
59	MG	AA	1613	1/1	0.95	0.19	117,117,117,117	0
59	MG	AA	1607	1/1	0.95	0.39	83,83,83,83	0
59	MG	DA	3150	1/1	0.95	0.09	100,100,100,100	0
59	MG	BA	3113	1/1	0.95	0.28	74,74,74,74	0
59	MG	BA	3051	1/1	0.95	0.43	75,75,75,75	0
59	MG	DA	3068	1/1	0.95	0.25	56,56,56,56	0
59	MG	BA	3003	1/1	0.95	0.50	62,62,62,62	0
59	MG	BA	3030	1/1	0.95	0.67	62,62,62,62	0
59	MG	BA	3057	1/1	0.95	0.36	61,61,61,61	0
59	MG	DA	3162	1/1	0.95	0.43	70,70,70,70	0
59	MG	BA	3180	1/1	0.95	0.08	99,99,99,99	0
59	MG	DD	302	1/1	0.95	0.29	54,54,54,54	0
59	MG	DP	201	1/1	0.95	0.24	57,57,57,57	0
59	MG	BA	3031	1/1	0.95	0.64	82,82,82,82	0
59	MG	DA	3165	1/1	0.95	0.34	60,60,60,60	0
60	ZN	D9	101	1/1	0.95	0.28	223,223,223,223	0
59	MG	DA	3133	1/1	0.96	0.28	91,91,91,91	0
59	MG	DA	3078	1/1	0.96	0.18	90,90,90,90	0
59	MG	DA	3187	1/1	0.96	0.23	92,92,92,92	0
59	MG	BA	3010	1/1	0.96	0.82	54,54,54,54	0
59	MG	DA	3189	1/1	0.96	0.35	75,75,75,75	0
59	MG	DA	3082	1/1	0.96	0.18	73,73,73,73	0
59	MG	DA	3085	1/1	0.96	0.62	52,52,52,52	0
59	MG	BA	3153	1/1	0.96	0.40	98,98,98,98	0
59	MG	BA	3005	1/1	0.96	0.56	59,59,59,59	0
59	MG	BA	3132	1/1	0.96	0.17	71,71,71,71	0
59	MG	AA	1609	1/1	0.96	1.08	83,83,83,83	0
59	MG	BA	3134	1/1	0.96	0.30	86,86,86,86	0
59	MG	DA	3038	1/1	0.96	0.32	62,62,62,62	0
59	MG	DA	3200	1/1	0.96	0.24	79,79,79,79	0
59	MG	DA	3110	1/1	0.96	0.30	77,77,77,77	0
59	MG	BA	3161	1/1	0.96	0.34	80,80,80,80	0
59	MG	BA	3017	1/1	0.96	0.74	59,59,59,59	0
59	MG	BA	3085	1/1	0.96	0.28	76,76,76,76	0
59	MG	AA	1620	1/1	0.96	0.51	69,69,69,69	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
59	MG	BA	3070	1/1	0.96	0.26	87,87,87,87	0
59	MG	CA	1611	1/1	0.96	0.70	72,72,72,72	0
59	MG	DA	3166	1/1	0.96	0.66	55,55,55,55	0
59	MG	DA	3004	1/1	0.96	0.32	52,52,52,52	0
59	MG	DA	3169	1/1	0.96	0.21	62,62,62,62	0
59	MG	DA	3122	1/1	0.96	0.15	56,56,56,56	0
59	MG	DA	3214	1/1	0.96	0.33	80,80,80,80	0
59	MG	DA	3215	1/1	0.96	0.42	54,54,54,54	0
59	MG	BA	3048	1/1	0.96	0.56	54,54,54,54	0
59	MG	DA	3218	1/1	0.96	0.17	82,82,82,82	0
59	MG	DA	3065	1/1	0.96	0.33	79,79,79,79	0
59	MG	DA	3174	1/1	0.96	0.31	77,77,77,77	0
59	MG	DA	3126	1/1	0.96	0.37	71,71,71,71	0
59	MG	DA	3127	1/1	0.96	0.56	78,78,78,78	0
59	MG	BA	3036	1/1	0.96	0.30	76,76,76,76	0
59	MG	DA	3180	1/1	0.96	0.29	86,86,86,86	0
59	MG	DA	3017	1/1	0.96	0.36	45,45,45,45	0
59	MG	BA	3025	1/1	0.96	0.21	73,73,73,73	0
59	MG	DA	3077	1/1	0.96	0.17	70,70,70,70	0
59	MG	DA	3171	1/1	0.97	0.42	104,104,104,104	0
59	MG	DA	3007	1/1	0.97	0.50	53,53,53,53	0
59	MG	DA	3097	1/1	0.97	0.30	77,77,77,77	0
59	MG	BA	3049	1/1	0.97	0.31	63,63,63,63	0
59	MG	BA	3015	1/1	0.97	0.47	59,59,59,59	0
59	MG	DA	3107	1/1	0.97	0.23	66,66,66,66	0
59	MG	BA	3033	1/1	0.97	0.54	65,65,65,65	0
59	MG	DA	3021	1/1	0.97	0.36	56,56,56,56	0
59	MG	AA	1621	1/1	0.97	0.40	81,81,81,81	0
59	MG	BA	3054	1/1	0.97	0.32	74,74,74,74	0
59	MG	BA	3007	1/1	0.97	0.68	54,54,54,54	0
59	MG	BA	3092	1/1	0.97	0.42	80,80,80,80	0
59	MG	BA	3018	1/1	0.97	0.49	52,52,52,52	0
59	MG	CA	1608	1/1	0.97	1.16	78,78,78,78	0
59	MG	BA	3059	1/1	0.97	0.34	66,66,66,66	0
59	MG	BA	3060	1/1	0.97	0.46	76,76,76,76	0
59	MG	BA	3008	1/1	0.97	0.54	58,58,58,58	0
59	MG	BA	3039	1/1	0.97	0.67	60,60,60,60	0
59	MG	DA	3047	1/1	0.97	0.16	63,63,63,63	0
59	MG	DA	3048	1/1	0.97	0.69	51,51,51,51	0
59	MG	BA	3102	1/1	0.97	0.26	78,78,78,78	0
59	MG	DA	3050	1/1	0.97	0.23	49,49,49,49	0
59	MG	DA	3054	1/1	0.97	0.35	68,68,68,68	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
59	MG	BA	3023	1/1	0.97	0.44	45,45,45,45	0
59	MG	DA	3134	1/1	0.97	0.35	64,64,64,64	0
59	MG	BA	3136	1/1	0.97	0.36	67,67,67,67	0
59	MG	BA	3074	1/1	0.97	0.59	69,69,69,69	0
59	MG	DA	3061	1/1	0.97	0.38	50,50,50,50	0
59	MG	DA	3139	1/1	0.97	0.35	90,90,90,90	0
59	MG	BA	3139	1/1	0.97	0.47	61,61,61,61	0
59	MG	DA	3146	1/1	0.97	0.64	92,92,92,92	0
59	MG	BA	3141	1/1	0.97	0.32	72,72,72,72	0
59	MG	AA	1614	1/1	0.97	0.36	105,105,105,105	0
59	MG	AA	1616	1/1	0.97	0.30	77,77,77,77	0
59	MG	BA	3108	1/1	0.97	0.46	67,67,67,67	0
59	MG	DA	3154	1/1	0.97	0.10	80,80,80,80	0
59	MG	CA	1622	1/1	0.97	0.12	104,104,104,104	0
59	MG	DA	3075	1/1	0.97	0.45	74,74,74,74	0
59	MG	BA	3045	1/1	0.97	0.48	63,63,63,63	0
59	MG	BA	3080	1/1	0.97	0.39	77,77,77,77	0
59	MG	DA	3079	1/1	0.97	0.38	66,66,66,66	0
59	MG	BA	3150	1/1	0.97	0.34	94,94,94,94	0
59	MG	DA	3221	1/1	0.97	0.11	92,92,92,92	0
59	MG	BA	3111	1/1	0.97	0.32	71,71,71,71	0
59	MG	DA	3084	1/1	0.97	0.31	56,56,56,56	0
59	MG	DD	301	1/1	0.97	0.33	53,53,53,53	0
59	MG	AA	1601	1/1	0.97	0.26	69,69,69,69	0
59	MG	DA	3001	1/1	0.97	0.43	36,36,36,36	0
59	MG	BA	3012	1/1	0.97	0.45	72,72,72,72	0
59	MG	DA	3090	1/1	0.97	0.54	47,47,47,47	0
60	ZN	CN	101	1/1	0.97	0.16	170,170,170,170	0
59	MG	DA	3005	1/1	0.97	0.43	44,44,44,44	0
59	MG	BA	3079	1/1	0.98	0.38	83,83,83,83	0
59	MG	BA	3028	1/1	0.98	0.43	56,56,56,56	0
59	MG	BA	3055	1/1	0.98	0.35	85,85,85,85	0
59	MG	BA	3056	1/1	0.98	0.47	76,76,76,76	0
59	MG	DA	3051	1/1	0.98	0.23	60,60,60,60	0
59	MG	DA	3052	1/1	0.98	0.49	51,51,51,51	0
59	MG	DA	3053	1/1	0.98	0.44	72,72,72,72	0
59	MG	BA	3029	1/1	0.98	0.50	59,59,59,59	0
59	MG	DA	3151	1/1	0.98	0.34	70,70,70,70	0
59	MG	BA	3115	1/1	0.98	0.43	90,90,90,90	0
59	MG	BA	3156	1/1	0.98	0.27	62,62,62,62	0
59	MG	BA	3157	1/1	0.98	0.23	107,107,107,107	0
59	MG	DA	3060	1/1	0.98	0.49	57,57,57,57	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	AA	1610	1/1	0.98	0.46	64,64,64,64	0
59	MG	AA	1615	1/1	0.98	0.41	87,87,87,87	0
59	MG	BA	3118	1/1	0.98	0.23	80,80,80,80	0
59	MG	BA	3020	1/1	0.98	0.22	69,69,69,69	0
59	MG	DA	3067	1/1	0.98	0.29	57,57,57,57	0
59	MG	BA	3087	1/1	0.98	0.35	74,74,74,74	0
59	MG	BA	3001	1/1	0.98	0.48	56,56,56,56	0
59	MG	DA	3072	1/1	0.98	0.35	61,61,61,61	0
59	MG	BA	3122	1/1	0.98	0.57	67,67,67,67	0
59	MG	DA	3074	1/1	0.98	0.40	61,61,61,61	0
59	MG	BA	3089	1/1	0.98	0.32	60,60,60,60	0
59	MG	DA	3076	1/1	0.98	0.28	73,73,73,73	0
59	MG	BA	3090	1/1	0.98	0.37	60,60,60,60	0
59	MG	BA	3062	1/1	0.98	0.52	70,70,70,70	0
59	MG	BA	3127	1/1	0.98	0.24	63,63,63,63	0
59	MG	BA	3129	1/1	0.98	0.18	69,69,69,69	0
59	MG	DA	3081	1/1	0.98	0.21	62,62,62,62	0
59	MG	DA	3177	1/1	0.98	0.29	86,86,86,86	0
59	MG	BA	3063	1/1	0.98	0.32	74,74,74,74	0
59	MG	DA	3179	1/1	0.98	1.14	93,93,93,93	0
59	MG	D5	101	1/1	0.98	0.14	78,78,78,78	0
59	MG	BA	3173	1/1	0.98	0.28	84,84,84,84	0
59	MG	BA	3064	1/1	0.98	0.56	51,51,51,51	0
59	MG	DA	3087	1/1	0.98	0.36	73,73,73,73	0
59	MG	DA	3002	1/1	0.98	0.50	58,58,58,58	0
59	MG	DA	3003	1/1	0.98	0.54	53,53,53,53	0
59	MG	DA	3186	1/1	0.98	0.23	93,93,93,93	0
59	MG	BA	3095	1/1	0.98	0.35	69,69,69,69	0
59	MG	DA	3093	1/1	0.98	0.29	74,74,74,74	0
59	MG	DA	3094	1/1	0.98	0.75	64,64,64,64	0
59	MG	BA	3013	1/1	0.98	0.35	62,62,62,62	0
59	MG	DA	3191	1/1	0.98	0.38	83,83,83,83	0
59	MG	BA	3067	1/1	0.98	0.19	67,67,67,67	0
59	MG	DA	3098	1/1	0.98	0.66	60,60,60,60	0
59	MG	BA	3135	1/1	0.98	0.32	71,71,71,71	0
59	MG	DA	3100	1/1	0.98	0.22	57,57,57,57	0
59	MG	DA	3102	1/1	0.98	0.57	77,77,77,77	0
59	MG	DA	3015	1/1	0.98	0.43	51,51,51,51	0
59	MG	DA	3106	1/1	0.98	0.35	43,43,43,43	0
59	MG	BA	3068	1/1	0.98	0.44	76,76,76,76	0
59	MG	DA	3108	1/1	0.98	0.43	69,69,69,69	0
59	MG	DA	3109	1/1	0.98	0.23	80,80,80,80	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
59	MG	BA	3035	1/1	0.98	0.48	51,51,51,51	0
59	MG	DA	3019	1/1	0.98	0.43	66,66,66,66	0
59	MG	BA	3138	1/1	0.98	0.60	93,93,93,93	0
59	MG	DA	3022	1/1	0.98	0.38	40,40,40,40	0
59	MG	BA	3072	1/1	0.98	0.41	80,80,80,80	0
59	MG	DA	3024	1/1	0.98	0.42	53,53,53,53	0
59	MG	DA	3209	1/1	0.98	0.21	64,64,64,64	0
59	MG	DA	3118	1/1	0.98	0.28	67,67,67,67	0
59	MG	DA	3211	1/1	0.98	0.15	80,80,80,80	0
59	MG	DA	3025	1/1	0.98	0.59	44,44,44,44	0
59	MG	BA	3140	1/1	0.98	0.21	85,85,85,85	0
59	MG	DA	3121	1/1	0.98	0.48	50,50,50,50	0
59	MG	BA	3073	1/1	0.98	0.27	91,91,91,91	0
59	MG	BA	3050	1/1	0.98	0.58	66,66,66,66	0
59	MG	BA	3002	1/1	0.98	0.47	50,50,50,50	0
59	MG	DA	3125	1/1	0.98	0.43	80,80,80,80	0
59	MG	DA	3034	1/1	0.98	0.32	47,47,47,47	0
59	MG	BA	3026	1/1	0.98	0.41	58,58,58,58	0
59	MG	BA	3146	1/1	0.98	0.12	104,104,104,104	0
59	MG	BA	3077	1/1	0.98	0.29	93,93,93,93	0
59	MG	DA	3130	1/1	0.98	0.18	63,63,63,63	0
59	MG	DA	3040	1/1	0.98	0.67	63,63,63,63	0
59	MG	AA	1606	1/1	0.98	0.29	87,87,87,87	0
59	MG	DU	201	1/1	0.98	0.49	62,62,62,62	0
59	MG	DA	3044	1/1	0.98	0.51	56,56,56,56	0
60	ZN	AD	301	1/1	0.98	0.34	117,117,117,117	0
60	ZN	AN	101	1/1	0.98	0.19	165,165,165,165	0
59	MG	DA	3045	1/1	0.98	0.59	43,43,43,43	0
60	ZN	CD	301	1/1	0.98	0.30	107,107,107,107	0
59	MG	DA	3135	1/1	0.98	0.18	56,56,56,56	0
59	MG	BA	3149	1/1	0.98	0.33	84,84,84,84	0
59	MG	DA	3056	1/1	0.99	0.23	54,54,54,54	0
59	MG	DA	3018	1/1	0.99	0.49	56,56,56,56	0
59	MG	BA	3069	1/1	0.99	0.51	72,72,72,72	0
59	MG	DA	3059	1/1	0.99	0.30	66,66,66,66	0
59	MG	DA	3020	1/1	0.99	0.57	35,35,35,35	0
59	MG	BA	3094	1/1	0.99	0.24	62,62,62,62	0
59	MG	DA	3062	1/1	0.99	0.31	51,51,51,51	0
59	MG	BA	3128	1/1	0.99	0.23	83,83,83,83	0
59	MG	DA	3115	1/1	0.99	0.26	55,55,55,55	0
59	MG	BA	3167	1/1	0.99	0.33	79,79,79,79	0
59	MG	DA	3117	1/1	0.99	0.50	53,53,53,53	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	BA	3014	1/1	0.99	0.38	50,50,50,50	0
59	MG	DA	3066	1/1	0.99	0.44	58,58,58,58	0
59	MG	BA	3096	1/1	0.99	0.19	76,76,76,76	0
59	MG	DA	3026	1/1	0.99	0.41	44,44,44,44	0
59	MG	DA	3069	1/1	0.99	0.40	71,71,71,71	0
59	MG	DA	3070	1/1	0.99	0.36	71,71,71,71	0
59	MG	BA	3071	1/1	0.99	0.19	84,84,84,84	0
59	MG	DA	3028	1/1	0.99	0.37	51,51,51,51	0
59	MG	DA	3029	1/1	0.99	0.45	63,63,63,63	0
59	MG	BA	3042	1/1	0.99	0.59	66,66,66,66	0
59	MG	BA	3099	1/1	0.99	0.40	67,67,67,67	0
59	MG	DA	3032	1/1	0.99	0.50	57,57,57,57	0
59	MG	BA	3004	1/1	0.99	0.32	49,49,49,49	0
59	MG	DA	3194	1/1	0.99	0.27	67,67,67,67	0
59	MG	CA	1607	1/1	0.99	0.46	55,55,55,55	0
59	MG	BA	3024	1/1	0.99	0.35	50,50,50,50	0
59	MG	BA	3019	1/1	0.99	0.39	64,64,64,64	0
59	MG	DA	3037	1/1	0.99	0.47	58,58,58,58	0
59	MG	BA	3046	1/1	0.99	0.32	77,77,77,77	0
59	MG	DA	3083	1/1	0.99	0.26	78,78,78,78	0
59	MG	DA	3039	1/1	0.99	0.33	60,60,60,60	0
59	MG	BA	3065	1/1	0.99	0.36	74,74,74,74	0
59	MG	DA	3041	1/1	0.99	0.28	44,44,44,44	0
59	MG	DA	3140	1/1	0.99	0.32	69,69,69,69	0
59	MG	BA	3158	1/1	0.99	0.53	89,89,89,89	0
59	MG	DA	3142	1/1	0.99	0.55	84,84,84,84	0
59	MG	DA	3143	1/1	0.99	0.30	72,72,72,72	0
59	MG	DA	3144	1/1	0.99	0.36	70,70,70,70	0
59	MG	DA	3145	1/1	0.99	0.25	58,58,58,58	0
59	MG	DA	3043	1/1	0.99	0.42	53,53,53,53	0
59	MG	DA	3089	1/1	0.99	0.24	67,67,67,67	0
59	MG	DA	3006	1/1	0.99	0.34	51,51,51,51	0
59	MG	DA	3149	1/1	0.99	0.41	59,59,59,59	0
59	MG	DA	3091	1/1	0.99	0.28	56,56,56,56	0
59	MG	B5	101	1/1	0.99	0.12	73,73,73,73	0
59	MG	DA	3216	1/1	0.99	0.11	62,62,62,62	0
59	MG	DA	3152	1/1	0.99	0.26	61,61,61,61	0
59	MG	DA	3008	1/1	0.99	0.30	61,61,61,61	0
59	MG	DA	3009	1/1	0.99	0.44	45,45,45,45	0
59	MG	DA	3155	1/1	0.99	0.21	59,59,59,59	0
59	MG	DA	3095	1/1	0.99	0.26	59,59,59,59	0
59	MG	DA	3010	1/1	0.99	0.51	47,47,47,47	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	DA	3011	1/1	0.99	0.43	67,67,67,67	0
59	MG	BA	3021	1/1	0.99	0.34	66,66,66,66	0
59	MG	DA	3160	1/1	0.99	0.24	85,85,85,85	0
59	MG	DA	3013	1/1	0.99	0.51	46,46,46,46	0
59	MG	DA	3014	1/1	0.99	0.35	61,61,61,61	0
59	MG	DA	3101	1/1	0.99	0.56	71,71,71,71	0
59	MG	BA	3107	1/1	0.99	0.20	91,91,91,91	0
59	MG	DA	3103	1/1	0.99	0.38	59,59,59,59	0
59	MG	BA	3124	1/1	0.99	0.36	90,90,90,90	0
59	MG	DA	3167	1/1	0.99	0.29	58,58,58,58	0
59	MG	DA	3105	1/1	0.99	0.29	60,60,60,60	0
59	MG	BA	3040	1/1	0.99	0.36	55,55,55,55	0
59	MG	BA	3142	1/1	1.00	0.44	74,74,74,74	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.