



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 12:39 AM UTC

PDB ID : 6C5L / pdb_00006c5l
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

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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

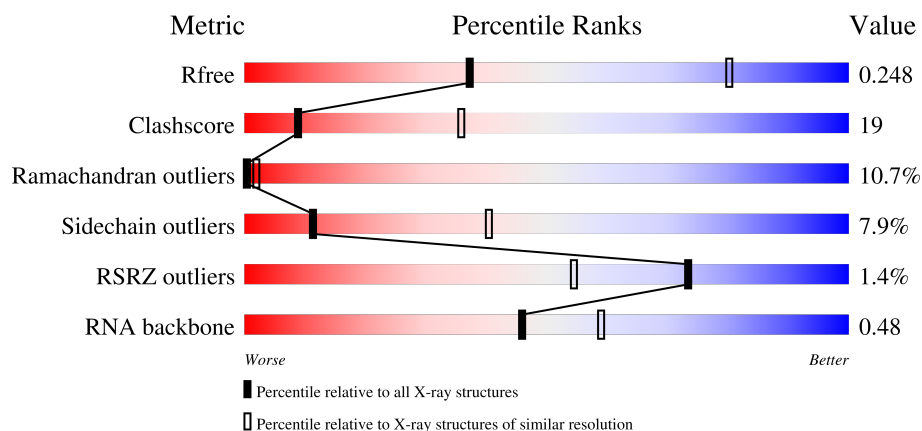
1 Overall quality at a glance

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.



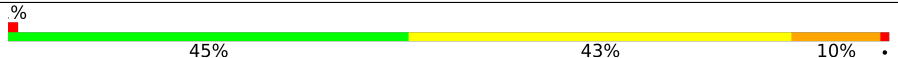
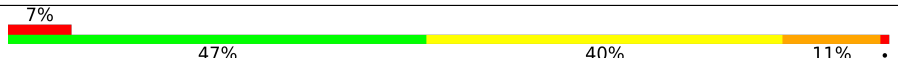
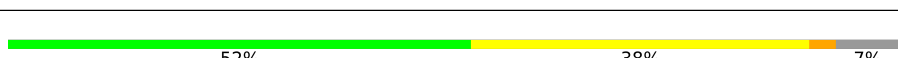
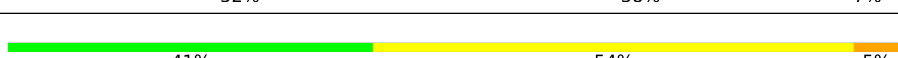
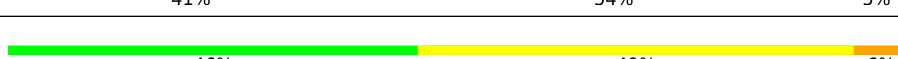
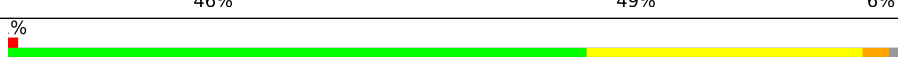
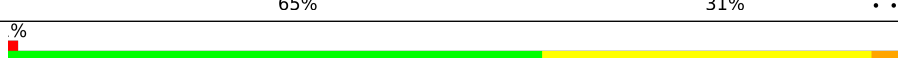
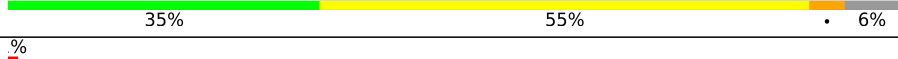
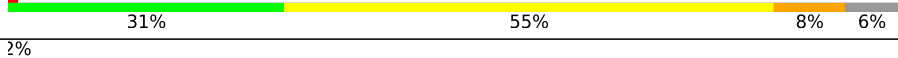
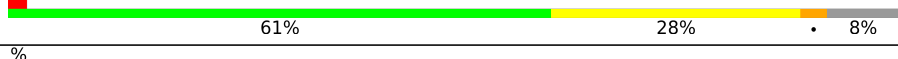
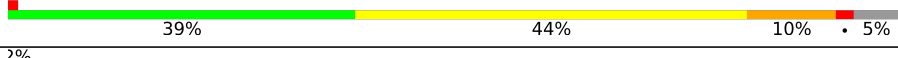
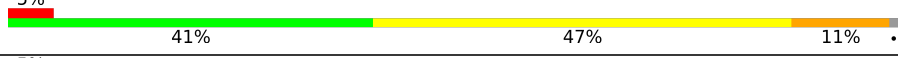
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)
RNA backbone	3983	1222 (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 ≥ 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	39%49%11%
1	CA	1522	38%50%11%
2	AB	256	% 34%47%10%8%
2	CB	256	% 34%48%9%8%

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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	

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Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	76	
22	AW	76	
22	CV	76	
22	CW	76	
23	AX	25	
23	CX	25	
24	AY	357	
24	CY	357	
25	B0	85	
25	D0	85	
26	B1	98	
26	D1	98	

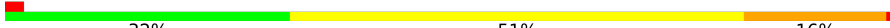
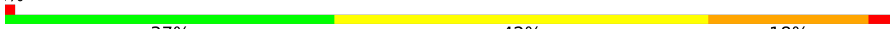
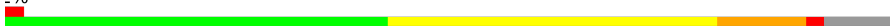
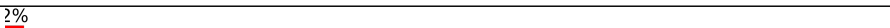
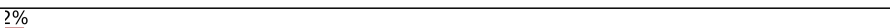
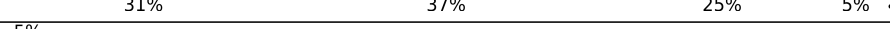
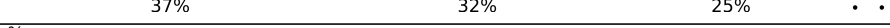
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Mol	Chain	Length	Quality of chain
27	B2	72	
27	D2	72	
28	B3	60	
28	D3	60	
29	B4	71	
29	D4	71	
30	B5	60	
30	D5	60	
31	B6	54	
31	D6	54	
32	B7	49	
32	D7	49	
33	B8	65	
33	D8	65	
34	B9	37	
34	D9	37	
35	BA	2915	
35	DA	2915	
36	BB	122	
36	DB	122	
37	BC	229	
37	DC	229	
38	BD	276	
38	DD	276	
39	BE	206	

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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	

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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	

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
1	AA	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			
1	CA	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			

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

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

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

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

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

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

- 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			

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

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

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

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

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

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

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

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

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

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

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

- 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

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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
25	B0	83	Total	C	N	O	S	0	0	0
			657	407	139	110	1			
25	D0	83	Total	C	N	O	S	0	0	0
			657	407	139	110	1			

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

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

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

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

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

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

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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				

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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 1114	C 692	N 227	O 193	S 2	0	0	0
48	DP	146	Total 1114	C 692	N 227	O 193	S 2	0	0	0

- 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
50	BR	117	Total	C	N	O	0	0	0
			960	599	202	159			
50	DR	117	Total	C	N	O	0	0	0
			960	599	202	159			

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

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

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

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

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

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

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

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

- 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 (CCD ID: 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		

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

- Molecule 60 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

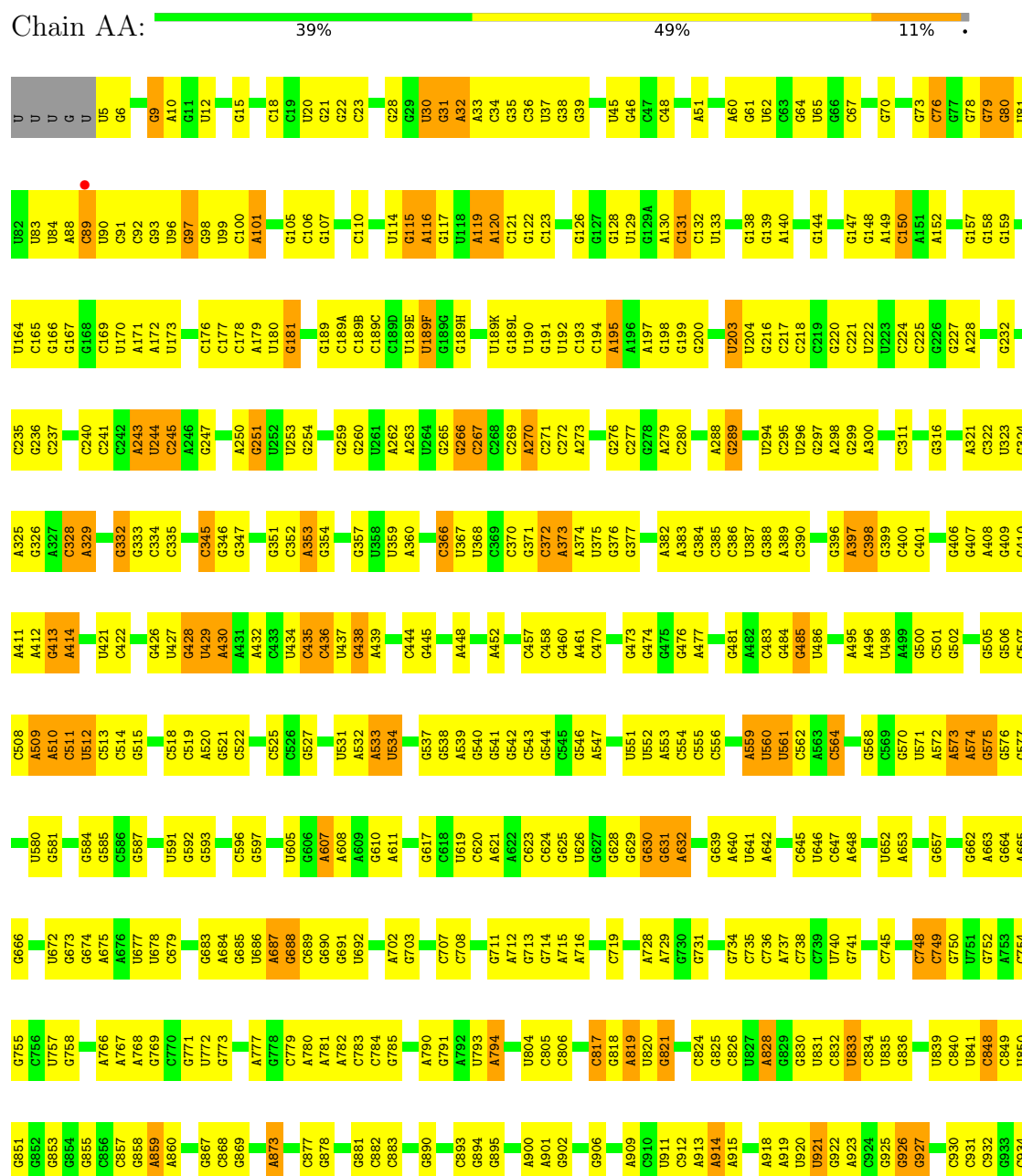
- Molecule 61 is water.

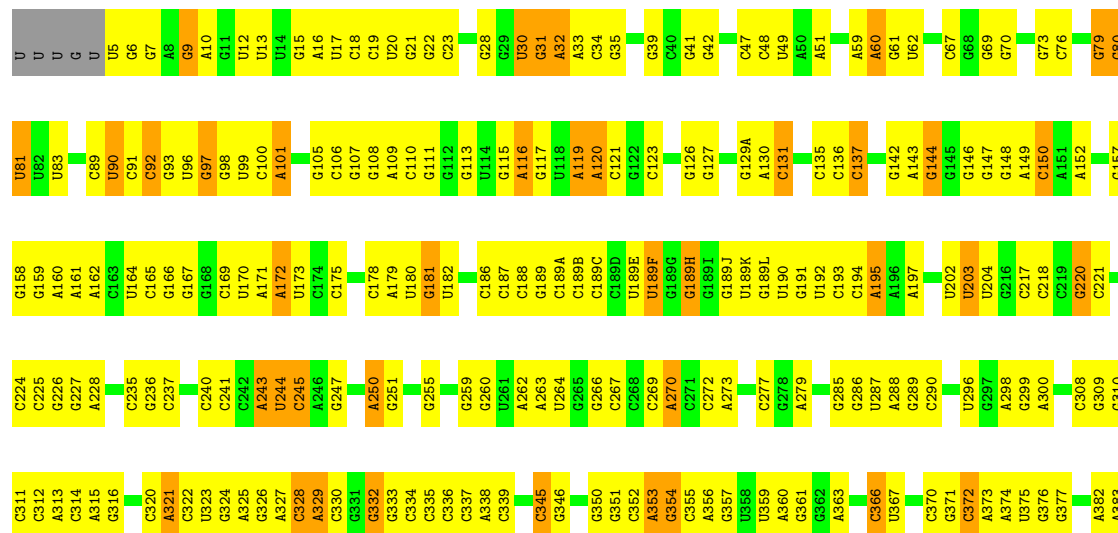
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	AA	2	Total 2	O 2	0	0
61	BA	6	Total 6	O 6	0	0
61	BE	1	Total 1	O 1	0	0
61	DA	7	Total 7	O 7	0	0
61	DE	1	Total 1	O 1	0	0
61	DS	1	Total 1	O 1	0	0
61	DZ	1	Total 1	O 1	0	0

3 Residue-property plots

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

• Molecule 1: 16S rRNA

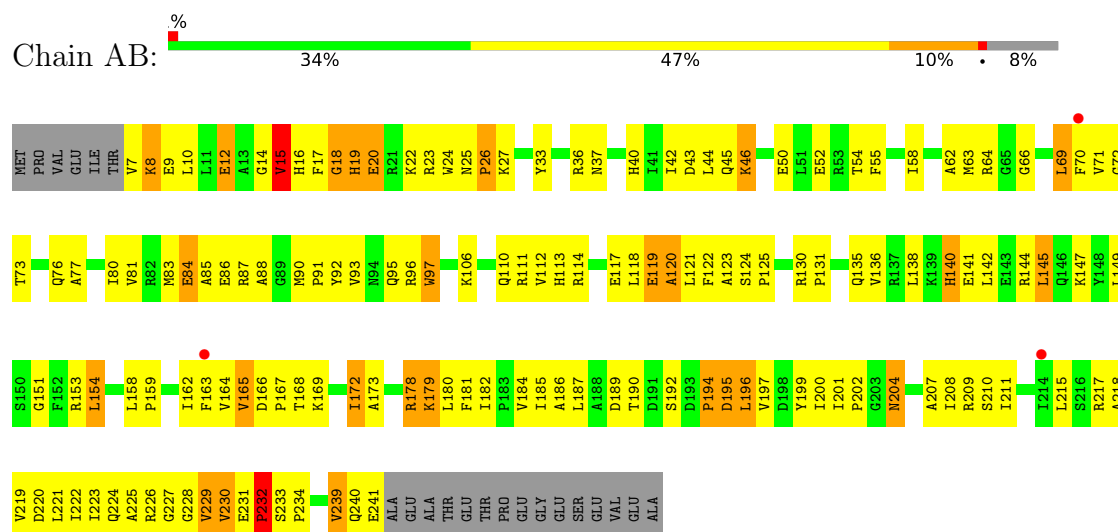




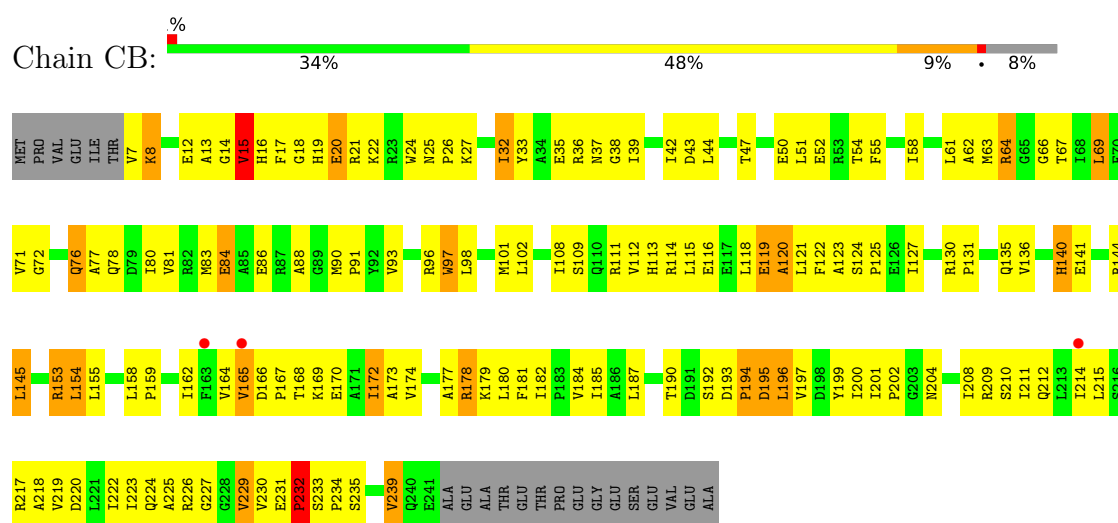
G1442	G1443	A1442B	U1446	A1447	C1452	G1456	G1457	G1458	C1466	G1467	A1468	G1469	G1470	G1475	C1479	G1480	U1481	G1482	G1486	G1491	A1492	A1493	C1496	G1497	U1498	A1499	A1502	A1503	G1504	G1505	U1506	A1507	U1510	G1511	U1512	A1513	C1514	G1517	A1518	A1519	G1520	U1521	U1522	A1523	A1524	G1525	G1529	G1530						
C1298	A1299	G1300	U1301	U1302	C1303	G1304	A1305	A1306	G1309	G1310	G1311	G1312	U1313	G1314	U1315	G1316	C1317	C1320	C1321	C1322	G1323	A1324	C1325	G1326	C1327	C1328	A1329	U1330	G1331	A1332	A1333	G1334	G1338	G1343	C1344	U1345	A1346	G1347	U1348	A1349	A1350	U1351	G1352	C1353	C1354	G1355	U1356	A1357	U1358	A1359	C1360	G1363	A1363A	U1364
C1367	G1370	U1371	U1372	G1373	A1374	G1375	A1376	A1377	U1381	G1382	G1386	G1387	C1388	C1389	U1390	U1391	G1392	C1397	A1398	C1399	G1400	G1401	C1402	G1403	C1404	G1405	C1409	G1410	C1411	C1412	A1413	U1414	G1415	U1416	G1417	A1418	U1419	U1425	C1426	U1427	A1428	U1429	C1430	U1431	G1432	A1433	A1434	G1435	U1436	C1440	G1441			
G1220	C1223	G1224	A1225	C1226	A1227	G1231	C1234	U1235	A1236	C1237	A1238	U1239	U1240	G1241	C1242	C1243	C1244	A1245	C1246	C1249	A1250	C1254	G1255	A1256	U1257	C1258	C1259	G1265	G1266	A1269	G1276	U1277	C1278	U1279	A1280	U1281	C1282	G1283	C1284	A1285	C1286	A1287	U1288	A1289	G1290	U1291	U1292	G1293	G1294	G1295	U1219			
C1145	A1146	U1147	U1148	C1149	U1150	A1151	A1152	C1153	A1157	U1158	U1159	C1163	A1164	A1168	A1169	A1170	G1171	G1172	G1173	G1174	G1175	A1176	G1177	C1178	A1179	A1180	G1181	G1182	A1183	G1184	C1189	G1190	U1196	G1197	U1198	U1199	C1200	A1201	G1202	G1206	G1207	C1208	G1209	C1210	U1211	U1212	U1213	C1214	G1215	G1216	C1217	U1218	U1219	
C1071	U1072	U1073	C1074	C1075	C1076	U1077	U1078	A1079	A1080	G1081	G1082	U1083	A1092	A1093	G1094	U1095	C1096	C1097	C1100	A1101	A1102	C1103	G1104	A1105	G1106	C1107	G1108	C1109	A1110	A1111	C1112	C1116	G1117	C1118	C1119	G1120	G1124	U1125	U1126	C1127	C1128	A1129	A1130	G1131	C1132	U1136	C1137	G1138	G1139	G1142				
G1006	C1007	G1010	U1011	U1012	G1013	A1014	A1015	G944	G945	U950	G951	U952	G953	G954	U955	U956	U957	U960	U961	C962	G963	C966	C967	A968	C969	C970	G971	C972	A901	G973	A974	A975	A976	C977	A978	C979	C980	U981	U982	A983	A986	G987	C990	U991	U992	G993	A994	G1001A	G1002	G1003	A1004	A1005		
A859	A860	G861	C868	G869	U870	U871	A872	A873	G874	U875	A876	C877	G878	G881	C882	C883	U884	G885	G886	G887	G888	C883	G884	C885	C886	U887	C888	C883	G884	A908	A909	C910	U911	C912	A913	A914	A915	A918	A919	U920	U921	G922	A923	C924	G925	U926	G927	C931	C932					
G778	C779	A781	C784	G785	G786	A790	A791	U792	U793	A794	G798	A802	C803	U804	C806	G807	C808	U813	A816	C817	C818	C819	U820	G821	C824	G825	A828	C832	U833	C834	U835	G836	G837	G838	U839	C840	U841	C848	C849	U850	G851	C852	G853	G854	C855	C856	G858							
C615	G616	G617	C620	A621	A622	G623	G624	U626	G629	G630	A632	U633	U636	G637	A642	G643	G644	C645	U646	C647	C735	C736	A737	U652	A653	C656	A665	G666	G667	G668	G673	G674	A675	A676	U677	U678	C679	G683	A684	A687	G688	C689	G690	G691	U692	G693	A694	A695	A696					
C701	A702	G703	A704	C707	C708	G711	A712	G713	G714	A715	A716	C719	A722	U723	A728	A729	G730	G731	C732	C735	C736	A737	U652	A653	C739	U740	G741	C742	U743	C744	C745	C748	G749	U750	U751	G752	G755	U756	G757	U758	A759	G760	A766	A767	G768	G769	G773	A777						
C457	C458	G460	A461	C470	A471	A472	G473	G474	A476	A477	C479	U480	A481	A482	C483	G484	C485	U486	A487	C488	C489	U494	A495	A496	U498	C501	C502	C503	A509	A510	C511	U512	C513	G515	C518	C519	A520	G521	G524	C525	C526	G527	C528	U531	A448	A532	A533	U534	A451	A452	A453	G537	G538	
A539	G540	G541	C542	C543	G544	A547	U551	U552	A553	C554	C555	C556	A559	U560	C561	C562	A563	U564	U565	G566	G570	U571	A572	U498	C501	C502	C503	U580	G581	U582	A583	G584	G585	G588	U591	G592	G593	G594	C595	C596	G597	U598	C599	U605	G606	A607	A608	A609	G610	A611				
C384	C385	C386	A389	C390	G391	C392	A393	G396	A397	C398	C399	C400	C401	G402	U404	U405	G406	G407	A408	G409	G410	A411	A412	G413	A414	A415	G416	C417	C422	G423	G424	G425	G426	U427	G428	U429	A430	A431	A432	C433	U434	C435	C436	U437	G438	A439	G447	A448	A449	G450	A451	A452	A453	G454



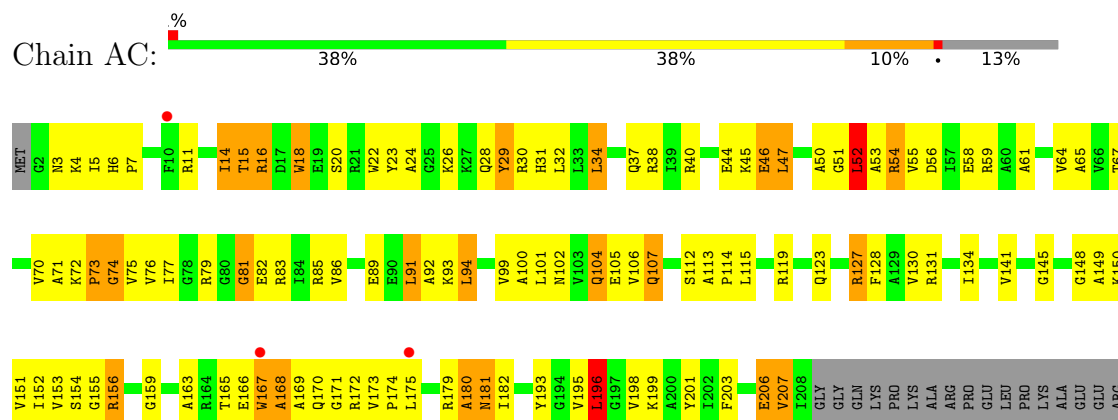
• Molecule 2: 30S ribosomal protein S2



• Molecule 2: 30S ribosomal protein S2

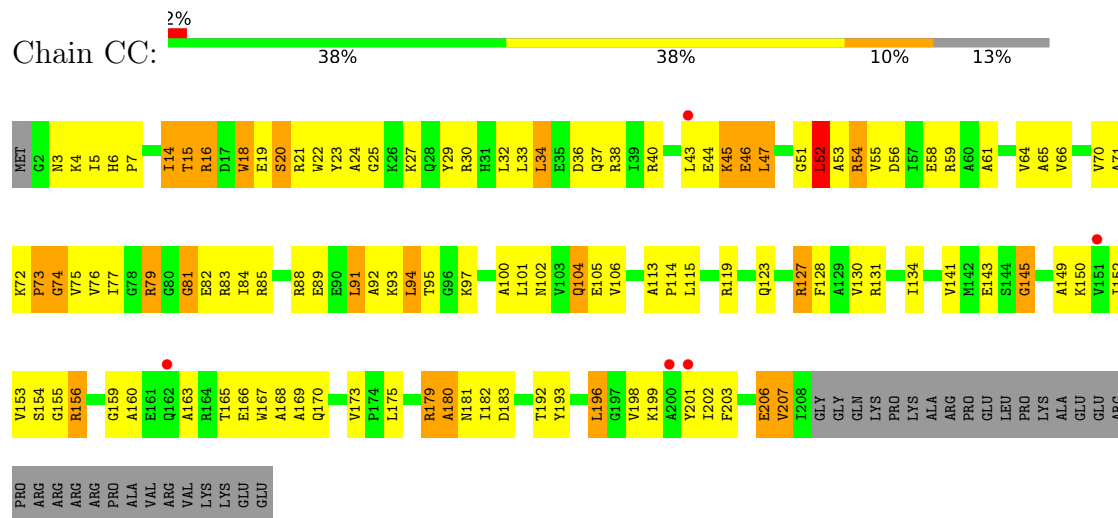


• Molecule 3: 30S ribosomal protein S3

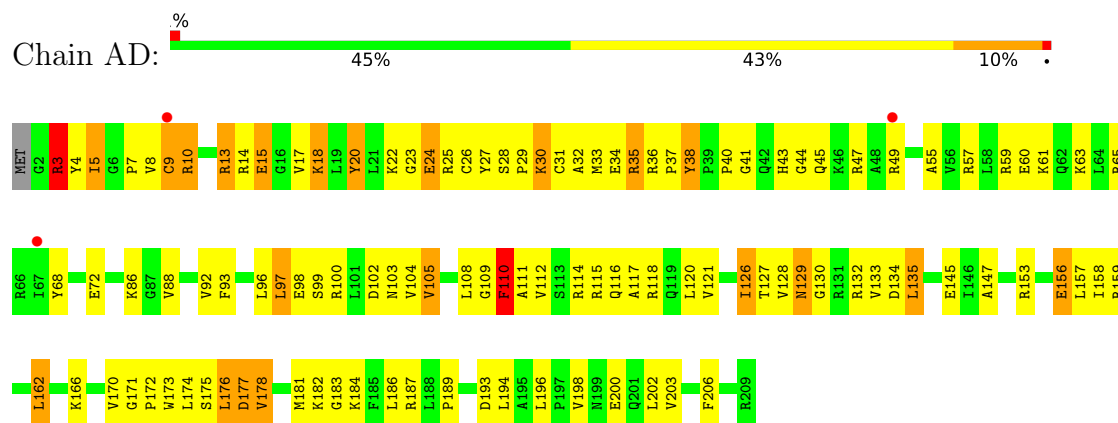


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ARG
ARG
ARG
VAL
VAL
LVS
LVS
GLU
GLU

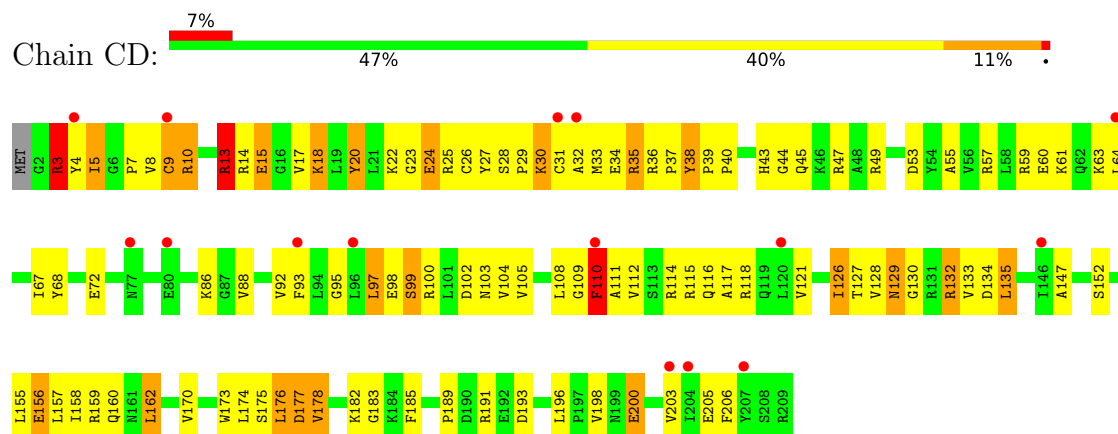
• Molecule 3: 30S ribosomal protein S3



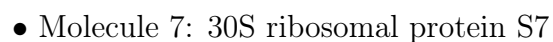
• Molecule 4: 30S ribosomal protein S4

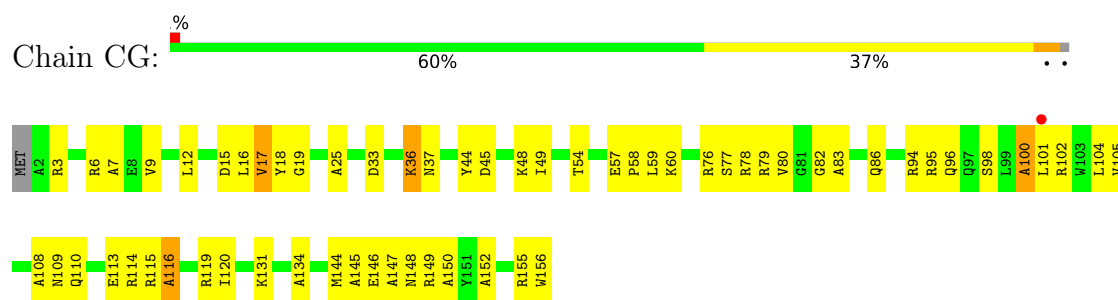


• Molecule 4: 30S ribosomal protein S4

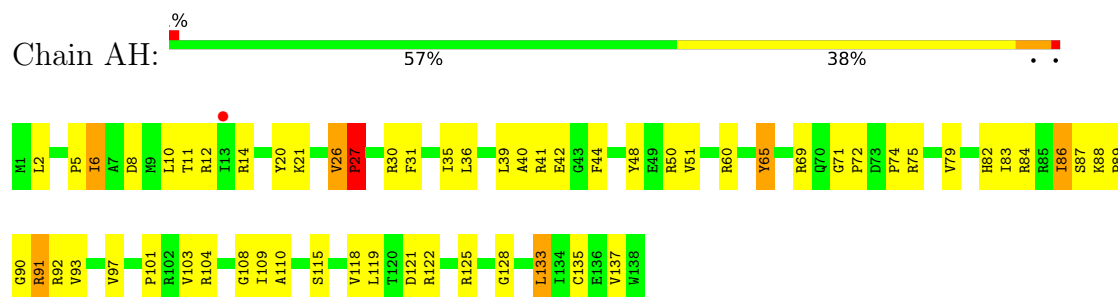


• Molecule 5: 30S ribosomal protein S5

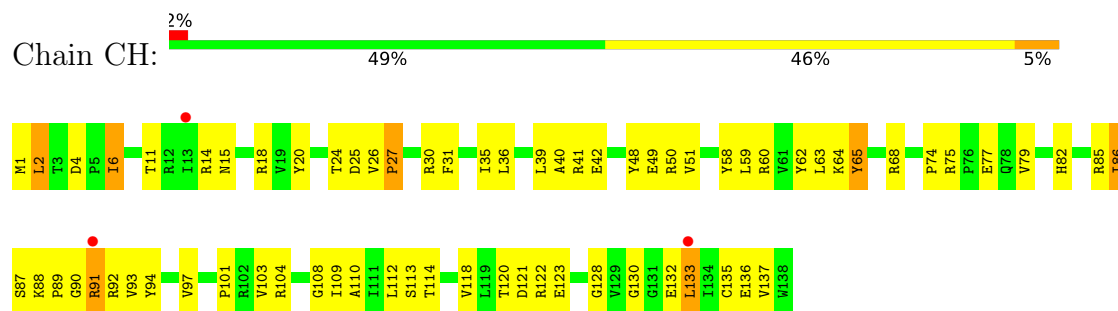




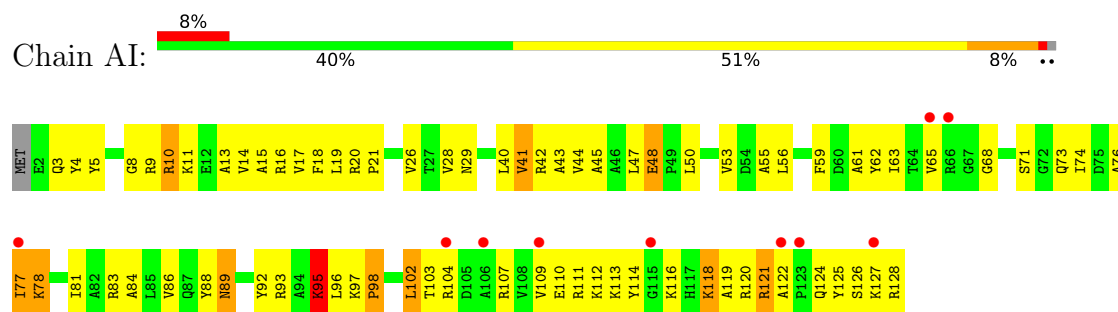
• Molecule 8: 30S ribosomal protein S8



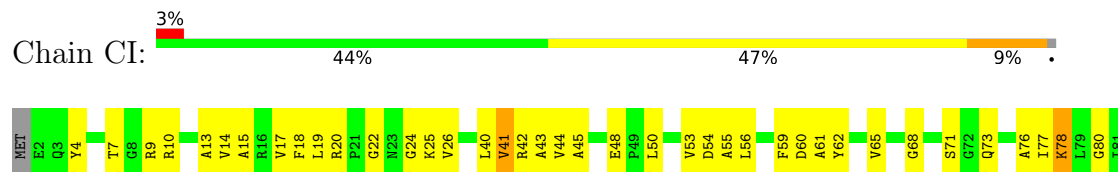
• Molecule 8: 30S ribosomal protein S8

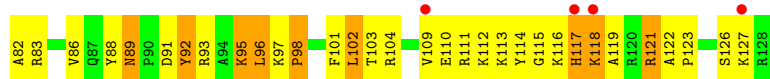


• Molecule 9: 30S ribosomal protein S9



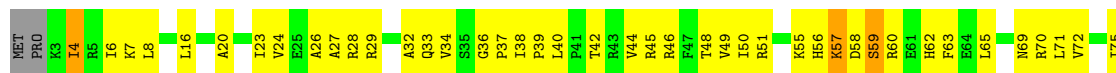
• Molecule 9: 30S ribosomal protein S9





- Molecule 10: 30S ribosomal protein S10

Chain AJ: 35% 55% 6%



- Molecule 10: 30S ribosomal protein S10

Chain CJ: 31% 55% 8% 6%



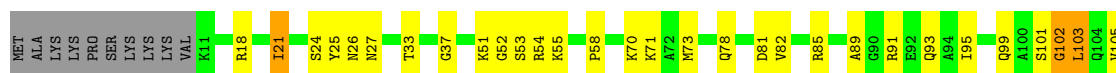
- Molecule 11: 30S ribosomal protein S11

Chain AK: 2% 60% 29% 8%



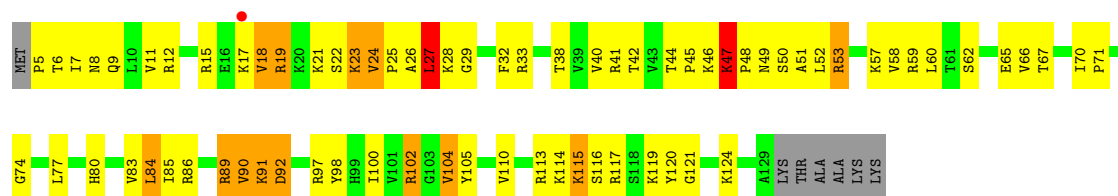
- Molecule 11: 30S ribosomal protein S11

Chain CK: 2% 61% 28% 8%

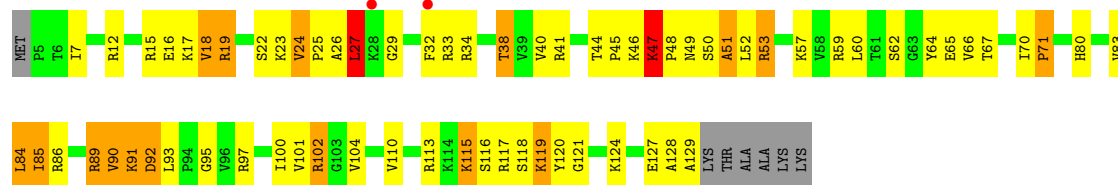
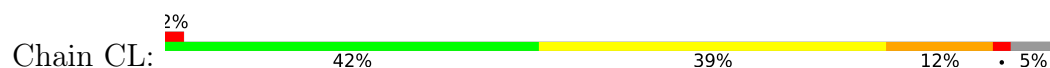


- Molecule 12: 30S ribosomal protein S12

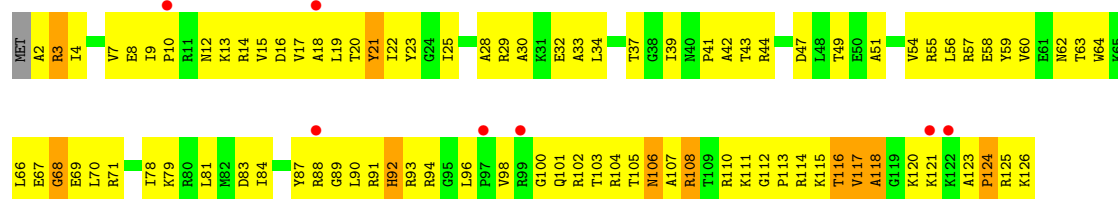
Chain AL: 39% 44% 10% 5%



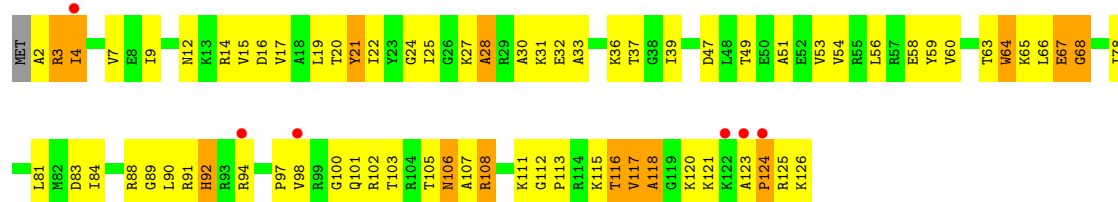
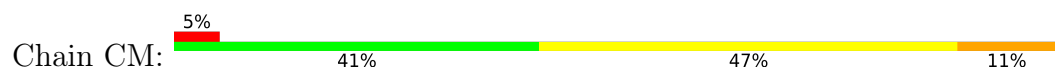
• Molecule 12: 30S ribosomal protein S12



• Molecule 13: 30S ribosomal protein S13



• Molecule 13: 30S ribosomal protein S13



• Molecule 14: 30S ribosomal protein S14 type Z



• Molecule 14: 30S ribosomal protein S14 type Z

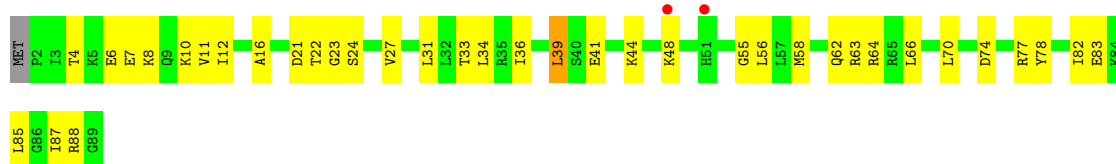




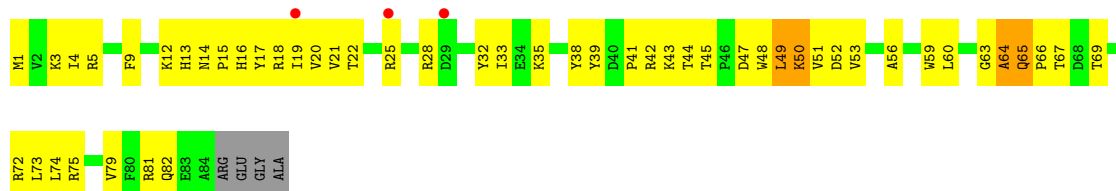
- Molecule 15: 30S ribosomal protein S15



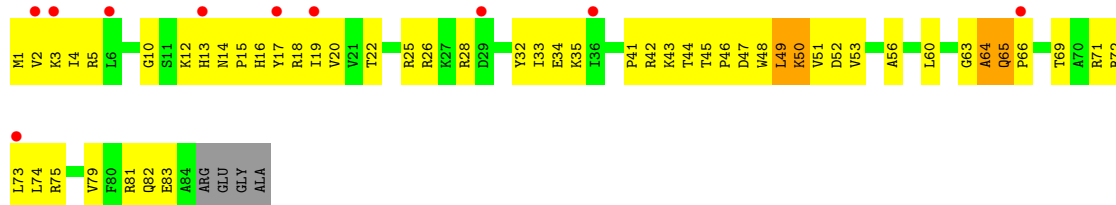
- Molecule 15: 30S ribosomal protein S15



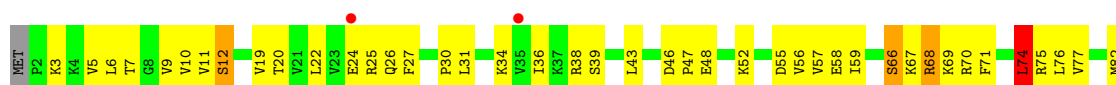
- Molecule 16: 30S ribosomal protein S16



- Molecule 16: 30S ribosomal protein S16

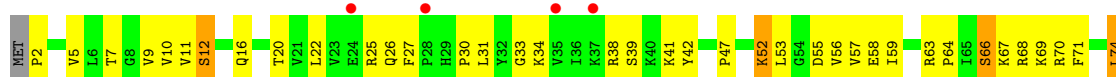


- Molecule 17: 30S ribosomal protein S17

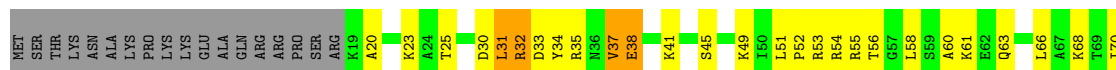




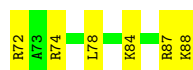
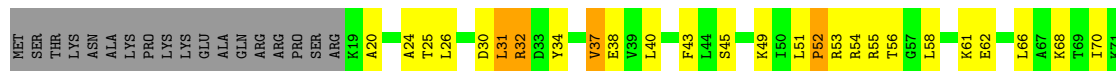
- Molecule 17: 30S ribosomal protein S17



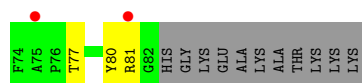
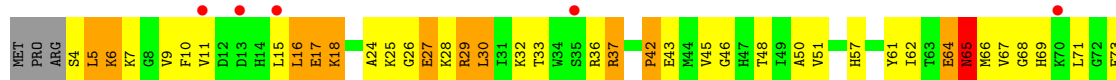
- Molecule 18: 30S ribosomal protein S18



- Molecule 18: 30S ribosomal protein S18



- Molecule 19: 30S ribosomal protein S19

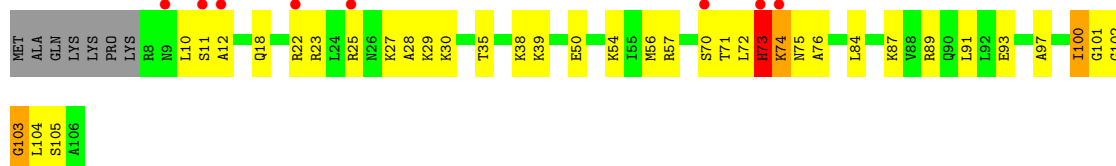


- Molecule 19: 30S ribosomal protein S19

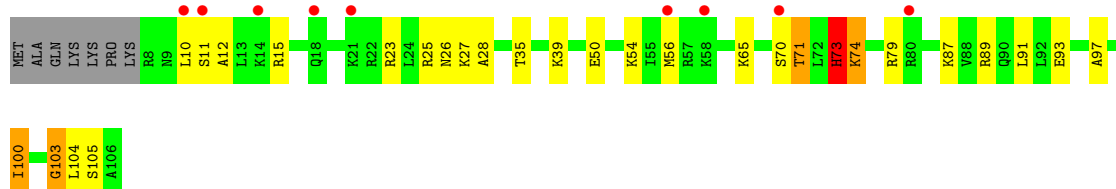




- Molecule 20: 30S ribosomal protein S20



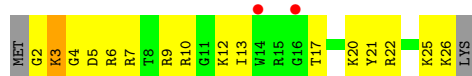
- Molecule 20: 30S ribosomal protein S20



- Molecule 21: 30S ribosomal protein Thx



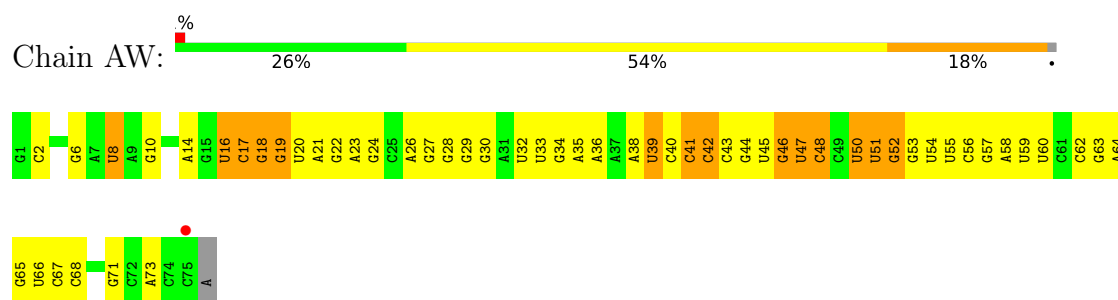
- Molecule 21: 30S ribosomal protein Thx



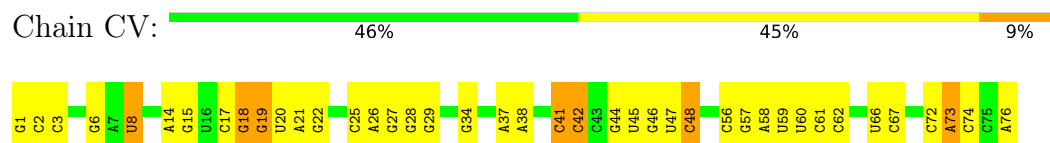
- Molecule 22: E-site tRNA PHE OR P-site tRNA PHE (unmodified bases)



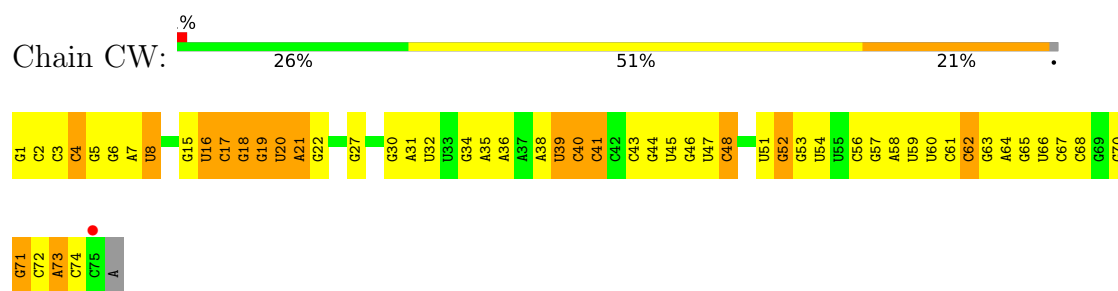
- Molecule 22: E-site tRNA PHE OR P-site tRNA PHE (unmodified bases)



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



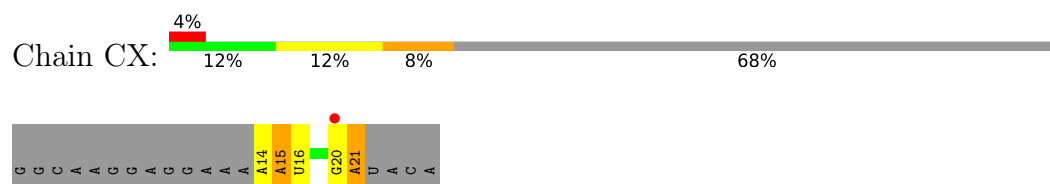
- Molecule 22: E-site tRNA PHE OR P-site tRNA PHE (unmodified bases)



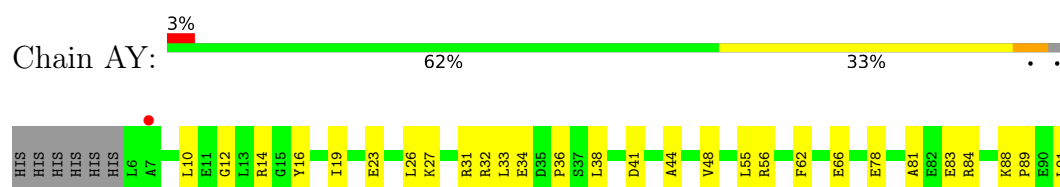
- Molecule 23: mRNA

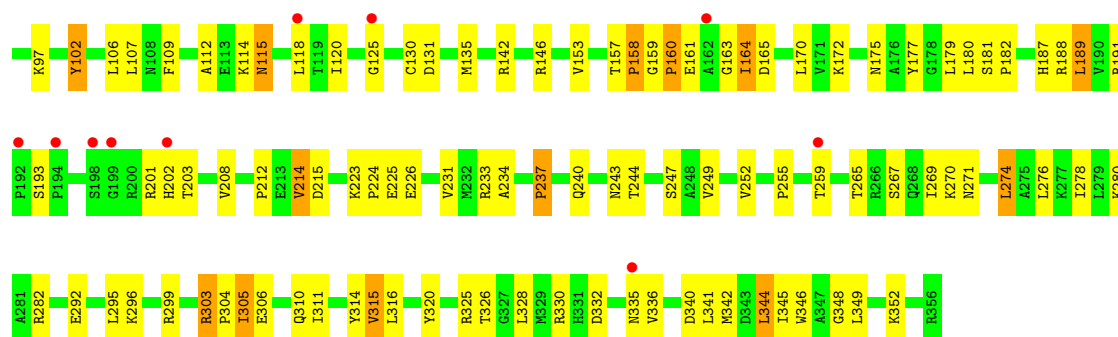


- Molecule 23: mRNA

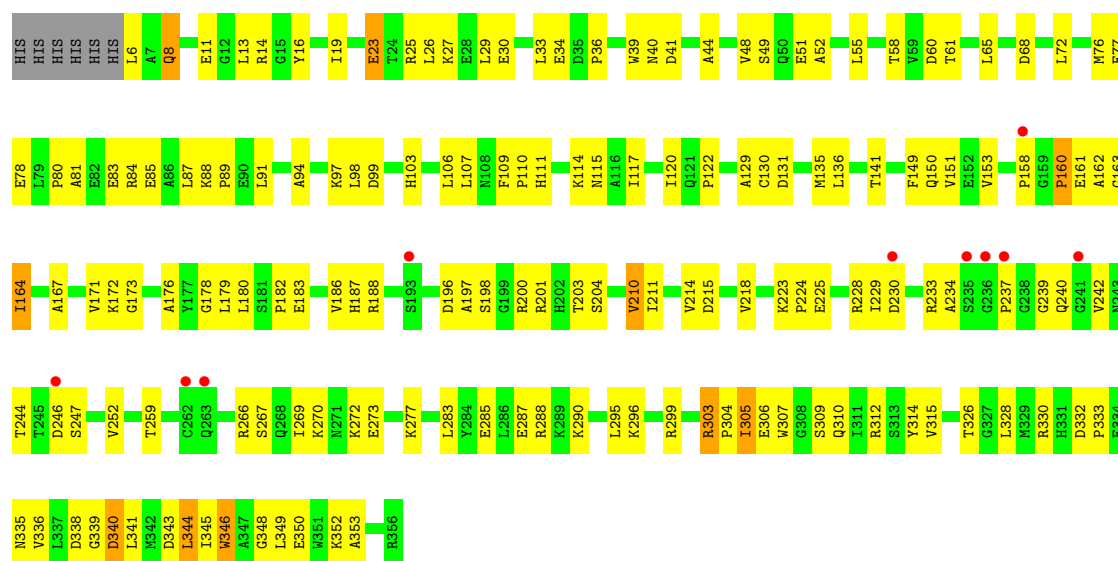


- Molecule 24: Peptide chain release factor 2

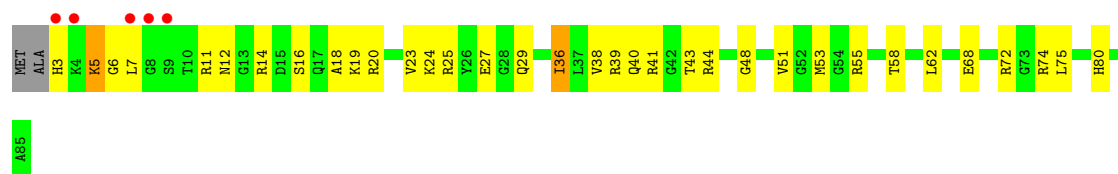




• Molecule 24: Peptide chain release factor 2



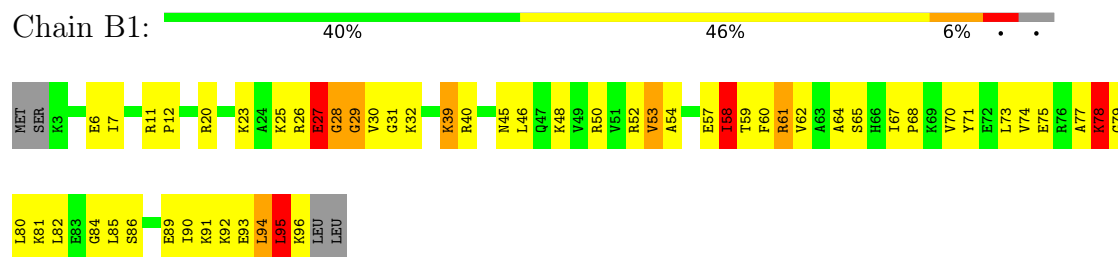
• Molecule 25: 50S ribosomal protein L27



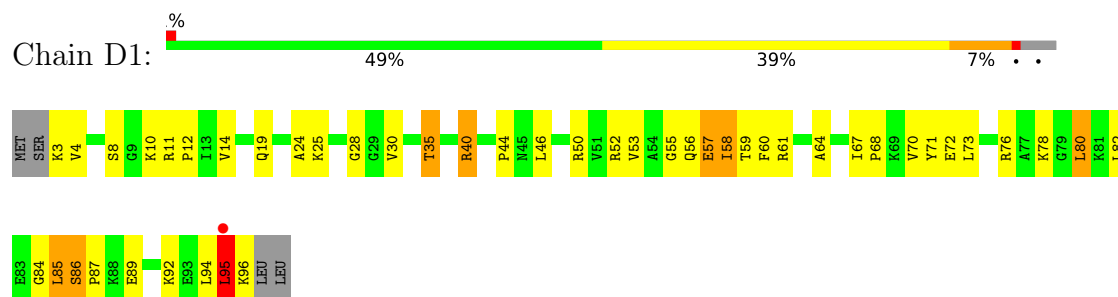
• Molecule 25: 50S ribosomal protein L27



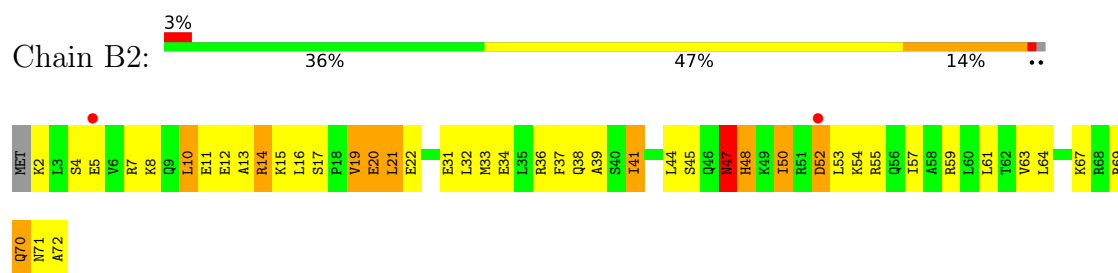
• Molecule 26: 50S ribosomal protein L28



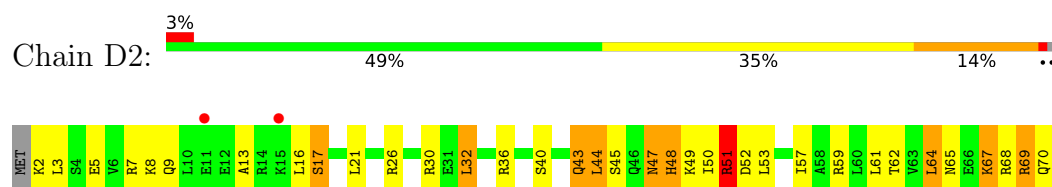
- Molecule 26: 50S ribosomal protein L28



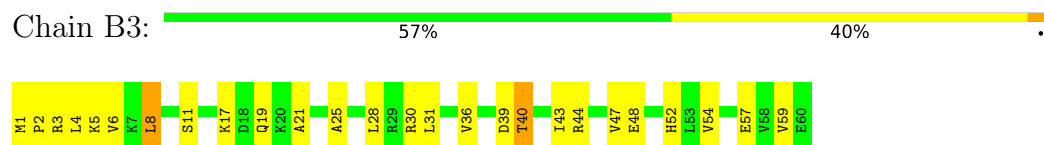
- Molecule 27: 50S ribosomal protein L29



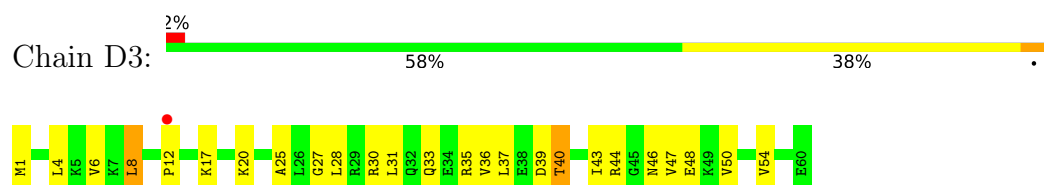
- Molecule 27: 50S ribosomal protein L29



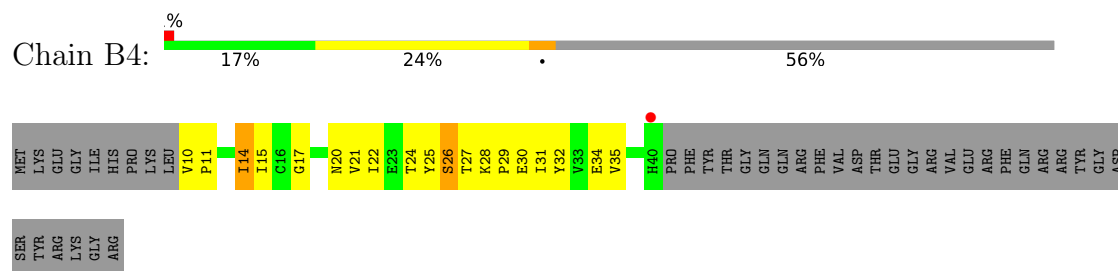
- Molecule 28: 50S ribosomal protein L30



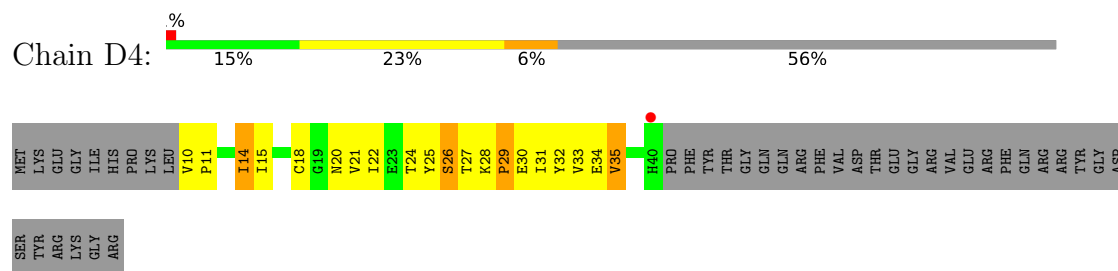
- Molecule 28: 50S ribosomal protein L30



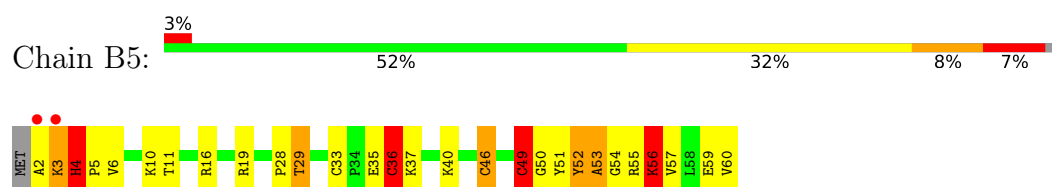
- Molecule 29: 50S ribosomal protein L31



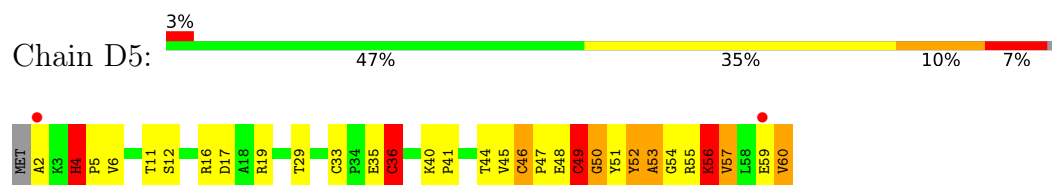
- Molecule 29: 50S ribosomal protein L31



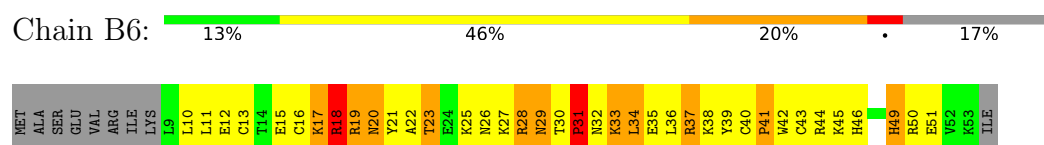
- Molecule 30: 50S ribosomal protein L32



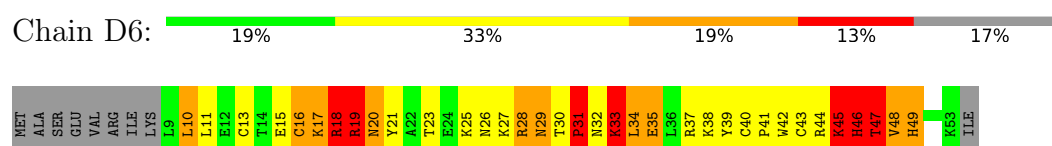
- Molecule 30: 50S ribosomal protein L32



- Molecule 31: 50S ribosomal protein L33



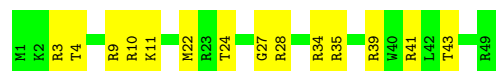
- Molecule 31: 50S ribosomal protein L33



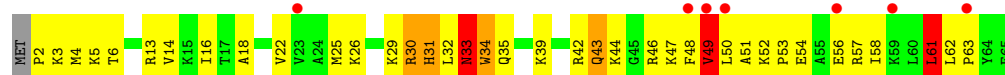
- Molecule 32: 50S ribosomal protein L34



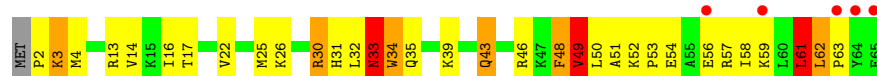
- Molecule 32: 50S ribosomal protein L34



- Molecule 33: 50S ribosomal protein L35



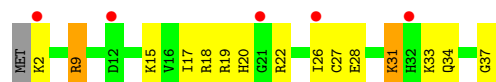
- Molecule 33: 50S ribosomal protein L35



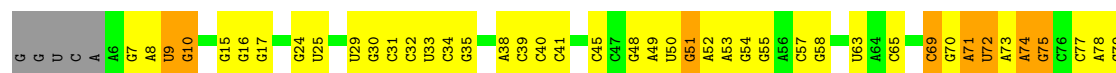
- Molecule 34: 50S ribosomal protein L36



- Molecule 34: 50S ribosomal protein L36

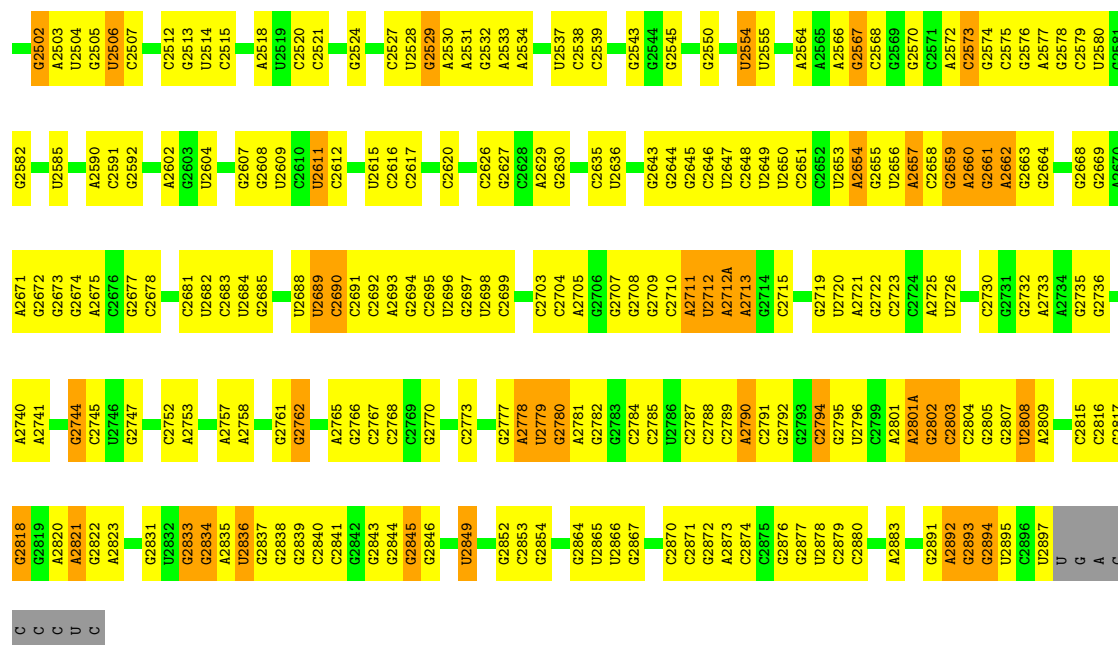


- Molecule 35: 23S rRNA



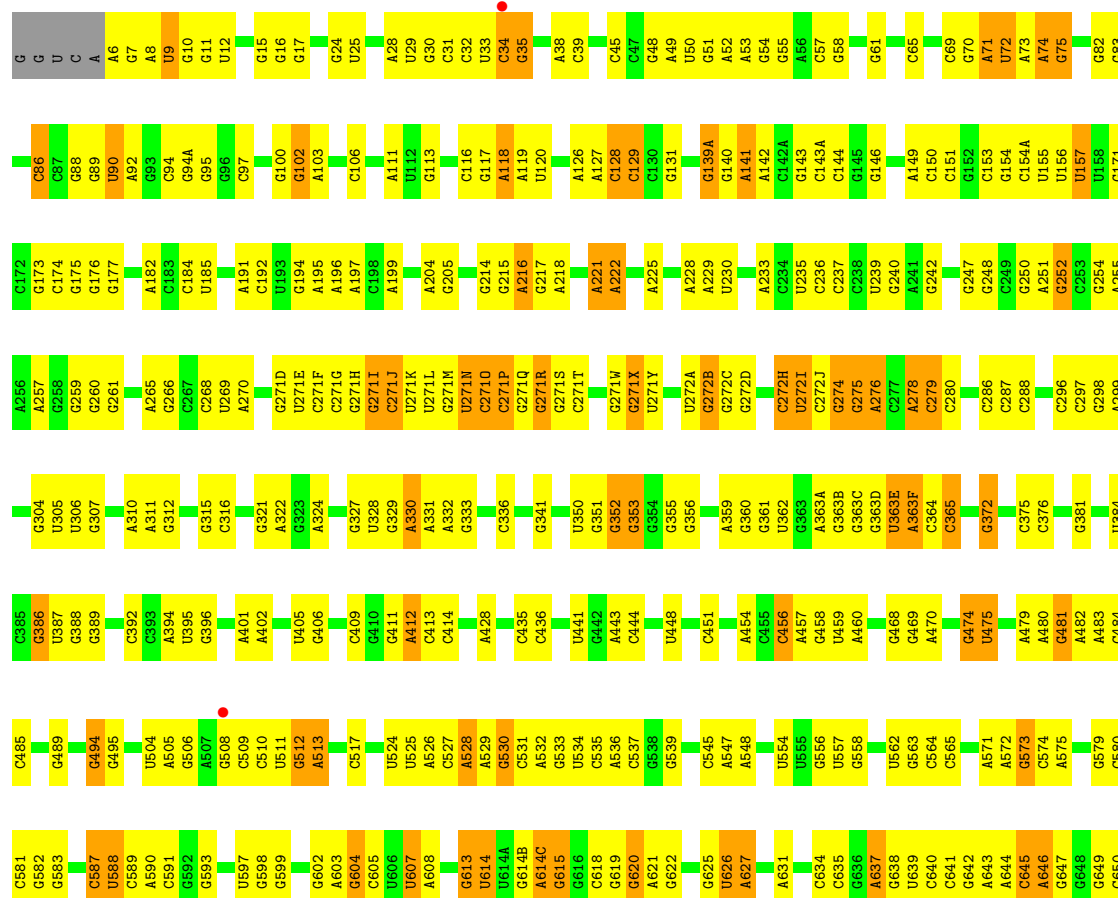
C1181	G1099	G1034	U958	A887	U811	G710	C645	G573	U373	G295	G252	C172	G82
A1182	U1105	U1035	A959	C888	C812	G715	A646	C574	A479	G298	A257	C174	G88
G1183	G1106	G1036	C961	C889	U813	A716	A840	A575	A481	G299	G258	C175	G89
G1184	G1107	G1037	G962	A890	C814	G717	G649	G579	A482	A300	G259	G177	U90
G1185	U1108	G1038	U963	C892	C817	G721	G648	C580	A483	G304	G260	A181	A92
G1187	G1109	G1039	C964	C894	G818	A722	G850	C581	A484	U305	G261	A182	G93
U1188	G1110	G1040	C965	U895	A819	G723	G851	G582	C494	G306	G266	C183	C94
A1189	A1111	C1041	G966	A896	A820	U724	A853	G583	U504	G307	U269	C184	G96
G1190	G1112	G1042	C967	C898	U822	G725	G654	G586	A505	A310	A270	U185	C97
G1191	U1113	G1043	G968	C899	G823	G726	G654B	U588	G508	A311	G271C	G189	G100
G1195	G1114	G1044	U969	A899	A824	G729	G654C	C589	C509	G315	G271D	A190	G102
G1196	G1115	A1045	C970	A900	G830	G730	G654E	A590	C510	C316	U271E	A191	A103
U1198	C1116	A1046	C971	A901	G831	U747	G654F	U584	G512	G321	G271F	A195	G109
U1199	G1119	G1047	G972	C902	U827	U747	A654J	G598	G513	A322	G271G	A196	G110
U1204	G1122	A1048	A973	C903	U828	A752	C854K	G602	C515	G323	G271H	A197	C116
U1205	G1123	G1051	G974	C904	A829	G733	G654L	G603	C516	A324	G271I	C198	G117
G1206	C1124	A1050	C975	U905	G830	C754	G654M	G604	C517	G325	U271J	A199	G118
G1207	G1125	G1052	G975A	G906	C837	C755	G654N	C605	G518	G326	U271K	C203	A119
C1208	U1129	G1053	A980	A909	U833	G760	G654O	U606	G520	U328	G271L	A204	U120
G1209	G1130	A1054	A983	A910	C834	A761	C854P	U607	G521	G329	G271M	G205	A126
U1210	G1131	G1055	G987	A911	A835	G762	G654R	A608	C526	A331	G271N	C208	A127
G1212	G1135	G1056	A988	C912	G836	A764	G654S	A609	A527	G332	G271O	C209	C128
G1217	G1136	G1057	A989	C913	C837	C755	G654T	G610	A528	G333	G271P	C210	C129
U1220	U1139	G1060	G989	C914	C838	G768	A854U	C611	A529	C336	G271Q	C211	C130
C1221	G1140	U1061	C991	A915	U839	A782	A855	G612	G530	A340	G271R	A211	G131
G1223	U1141	G1062	C992	A917	C840	G780	G657	U614	C531	G341	G271S	A212	G132
G1226	U1142	G1063	G993	A918	C846	A784	U614A	U614B	A532	G349	G271T	A213	C133
G1227	A1143	G1064	C995	U922	G848	G776	A614C	A614C	G533	G350	G271U	G143	G139A
G1236	G1149	G1065	A996	C923	A849	G786	G615	G620	C534	G351	U272A	A218	G140
G1239	G1150	G1066	C998	A926	U852	G787	G660	A621	C535	G352	G272B	A222	A141
G1243	G1151	A1070	U999	G931	G855	U779	C671	G622	C545	G353	G272C	A221	C142A
G1244	G1152	G1071	A1000	G932	C856	A780	C672	U626	C547	G356	G272D	A222	C143A
G1245	C1153	G1072	A1001	A933	C857	A782	C673	A627	A548	A359	G272E	A225	G145
G1246	G1154	A1073	G1007	G934	U858	G786	G674	G628	C549	G360	G272F	G226	G146
A1246	A1155	G1074	C1008	C935	G859	A784	A676	G629	C551	G361	U272G	A227	U147
A1247	C1158	G1075	A1009	U945	U871	C790	A677	G630	G556	U362	C272J	A228	C148
G1250	U1159	C1076	A1010	G946	A872	G792	C678	G631	U557	G363	G274	A229	C149
G1253	C1166	U1081	U1019	G947	C876	A793	G886	A632	G558	A363A	G275	U230	C150
G1256	G1169	G1087	A1020	U948	U877	C796	G890	A633	C561	G363B	A276	A233	C151
G1262	G1170	U1088	A1021	C949	A878	C796	G891	C634	C562	G363C	G277	A234	G152
U1263	G1171	G1089	U1023	G950	G881	A802	C692	C635	U562	G363D	A278	U235	C153
G1264	A1175	U1094	G1025	G952	G882	G805	C693	G636	G563	U363E	C279	G242	U154
A1265	G1176	A1095	U1026	C954	G883	C806	C693	A637	U569	A363F	C280	G247	C155A
G1266	A1177	U1096	A1027	C955	C884	U807	C708	G638	G570	C364	G281	U156	U155
G1270	C1178	A1097	A1028	G956	C885	G807	A571	U639	G571	C365	C291	G248	U157
C1270	G1270	A1098	G1030	A957	C886		U709	C641	A572	G372	C292	C249	G171





• Molecule 35: 23S rRNA

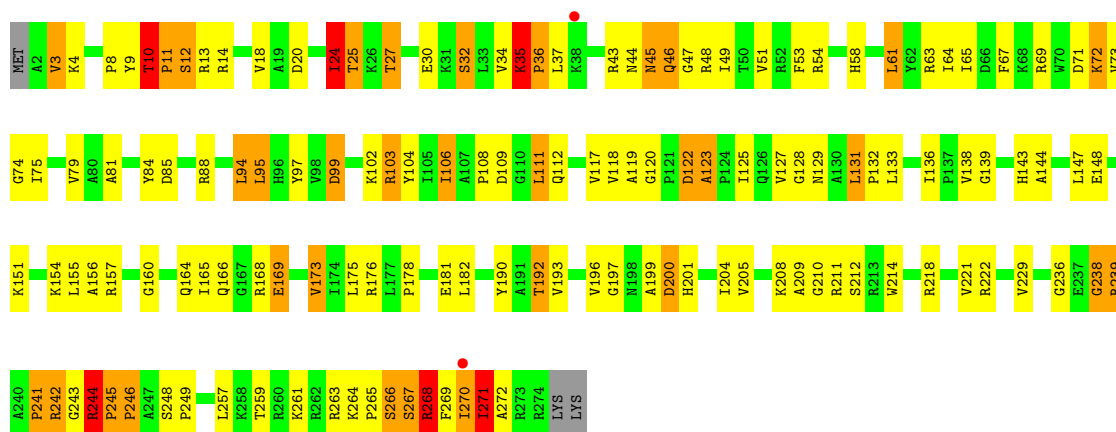
Chain DA:



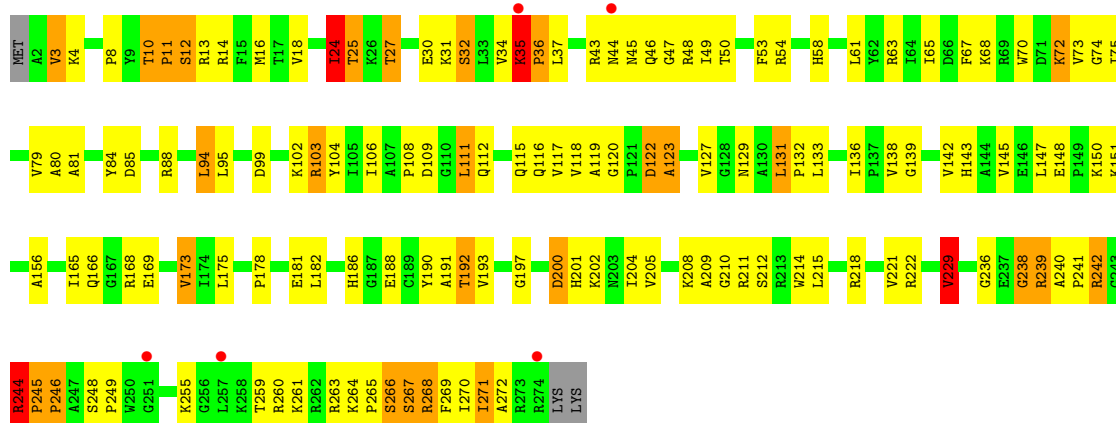




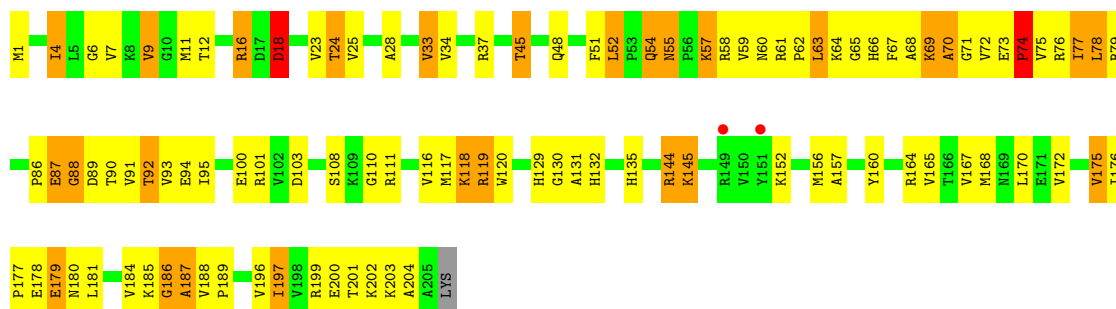




• Molecule 38: 50S ribosomal protein L2

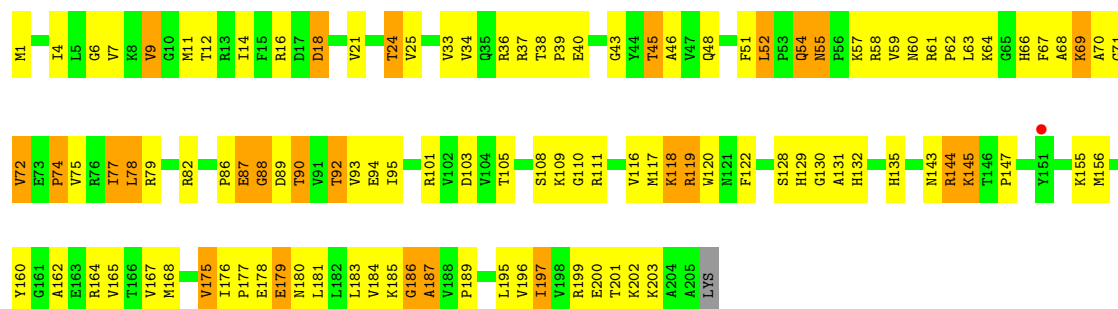


• Molecule 39: 50S ribosomal protein L3



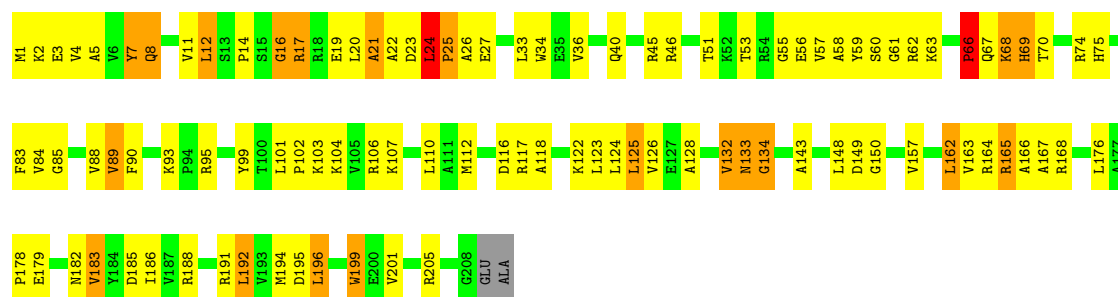
• Molecule 39: 50S ribosomal protein L3





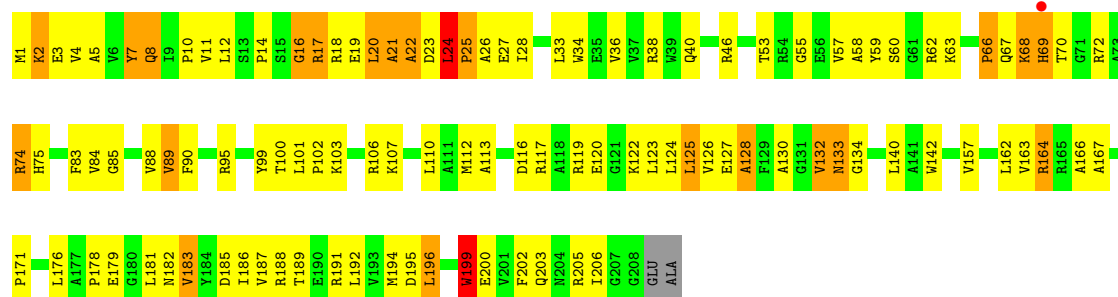
• Molecule 40: 50S ribosomal protein L4

Chain BF: 50% 38% 10% ..



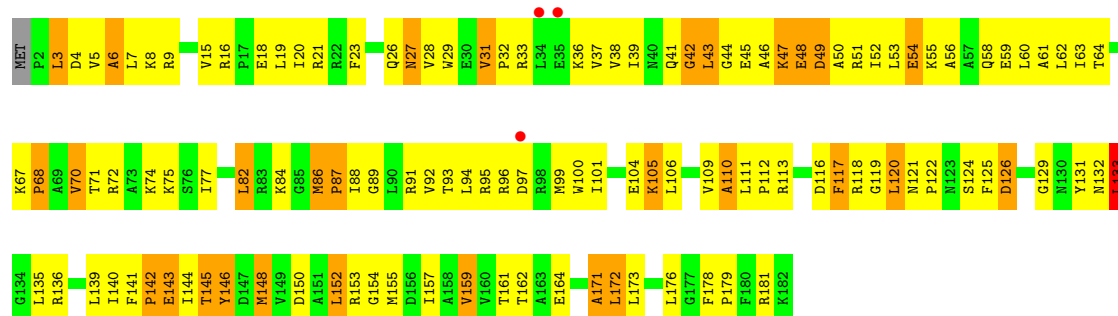
• Molecule 40: 50S ribosomal protein L4

Chain DF: 47% 41% 10% ..

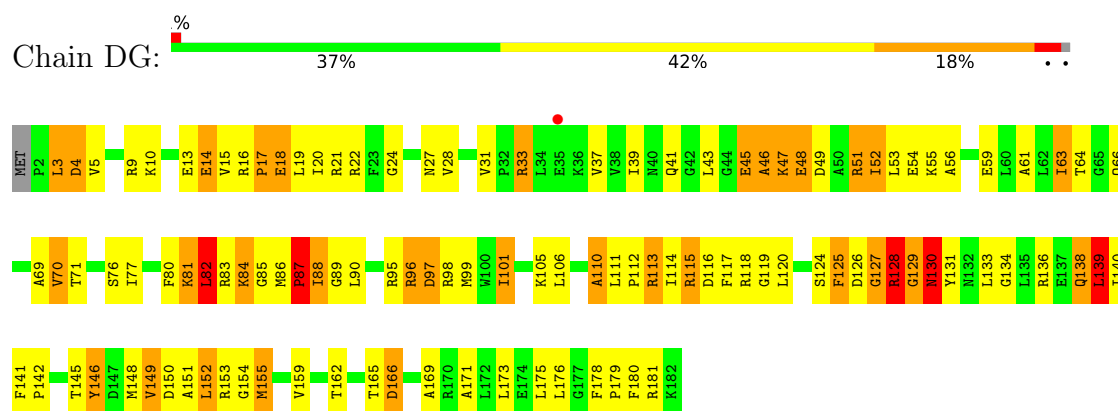


• Molecule 41: 50S ribosomal protein L5

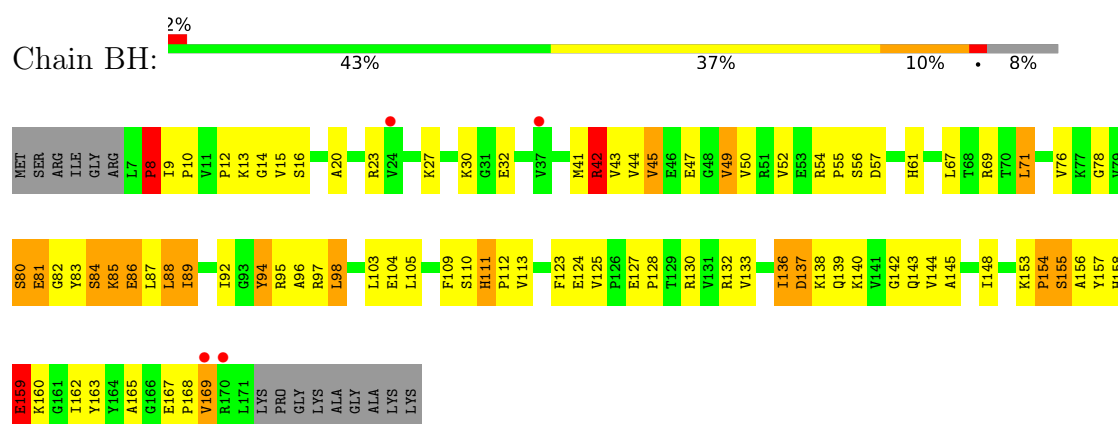
Chain BG: 2% 32% 51% 16% ..



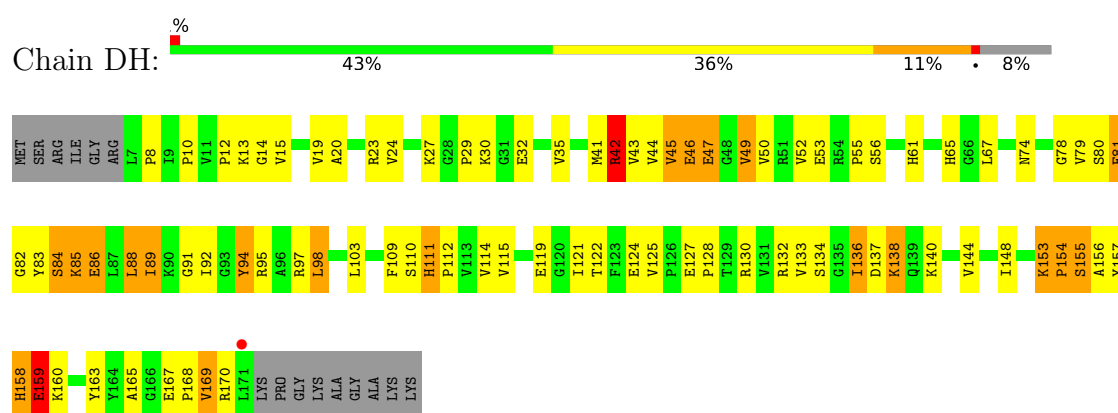
- Molecule 41: 50S ribosomal protein L5



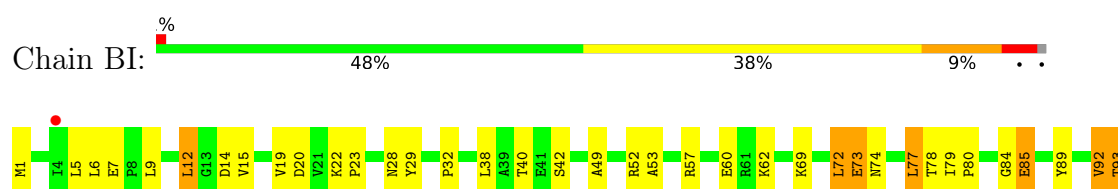
- Molecule 42: 50S ribosomal protein L6



- Molecule 42: 50S ribosomal protein L6



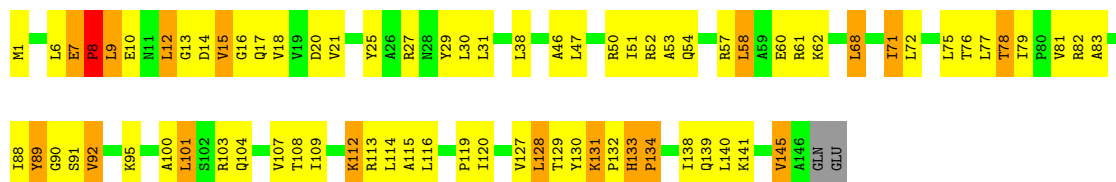
- Molecule 43: 50S ribosomal protein L9





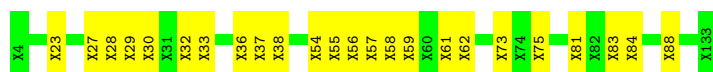
- Molecule 43: 50S ribosomal protein L9

Chain DI: 47% 40% 11% ..



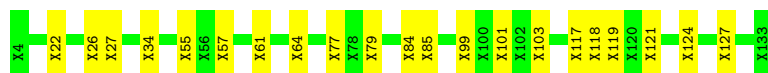
- Molecule 44: 50S ribosomal protein L10

Chain BJ: 82% 18%



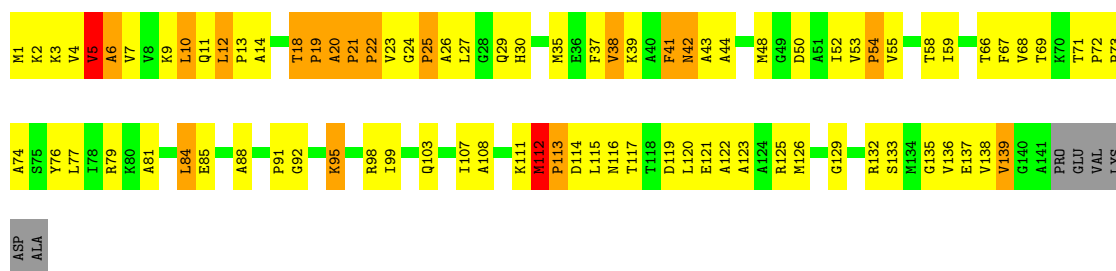
- Molecule 44: 50S ribosomal protein L10

Chain DJ: 84% 16%



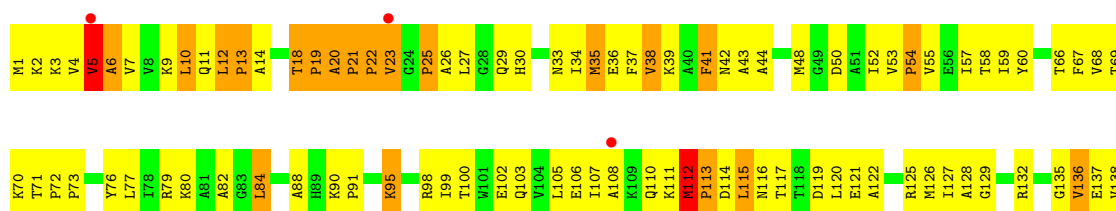
- Molecule 45: 50S ribosomal protein L11

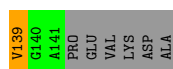
Chain BK: 37% 46% 12% ..



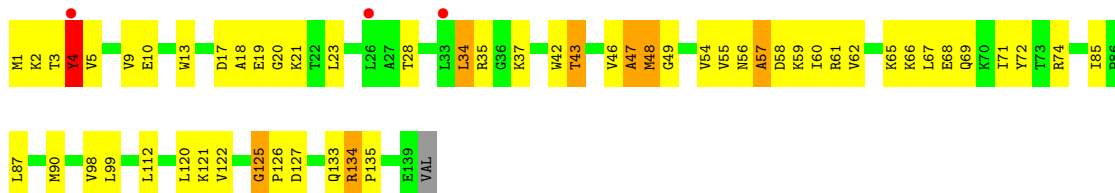
- Molecule 45: 50S ribosomal protein L11

Chain DK: 2% 31% 49% 14% ..

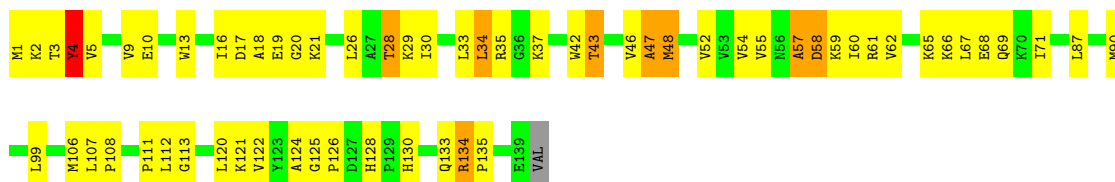




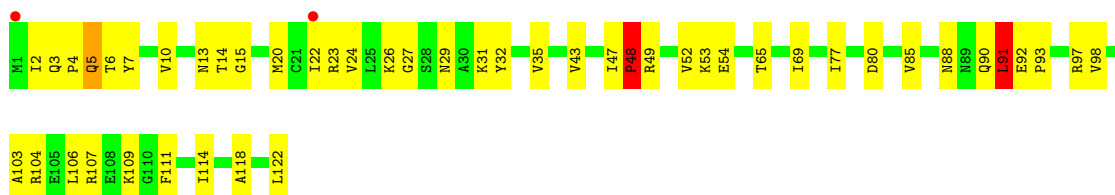
- Molecule 46: 50S ribosomal protein L13



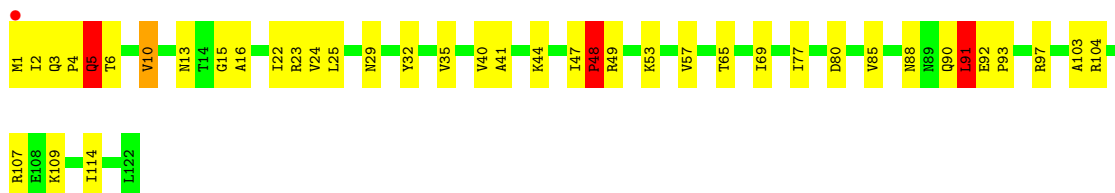
- Molecule 46: 50S ribosomal protein L13



- Molecule 47: 50S ribosomal protein L14

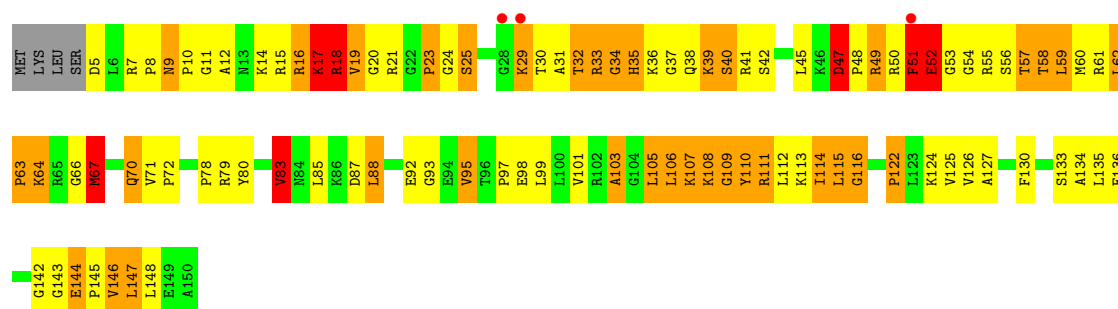


- Molecule 47: 50S ribosomal protein L14

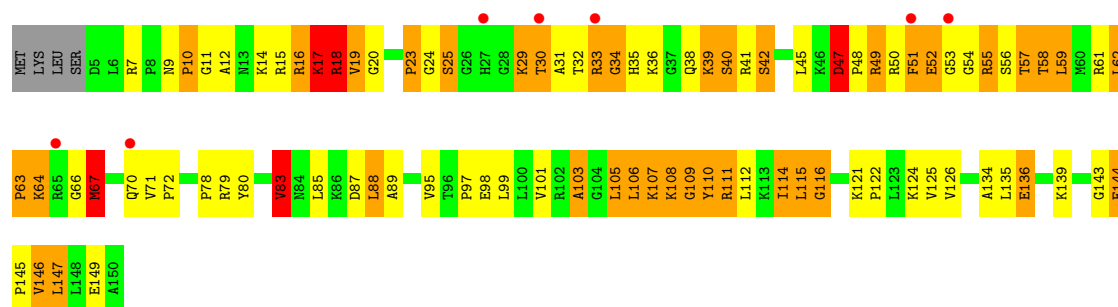


- Molecule 48: 50S ribosomal protein L15

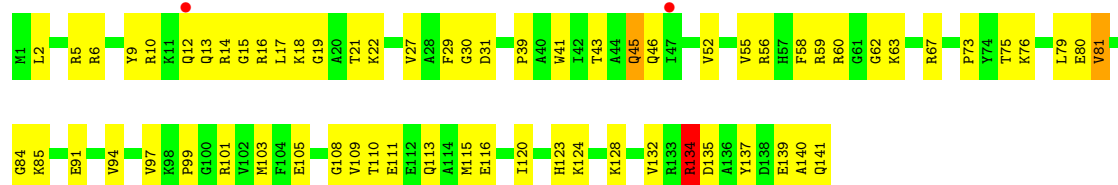




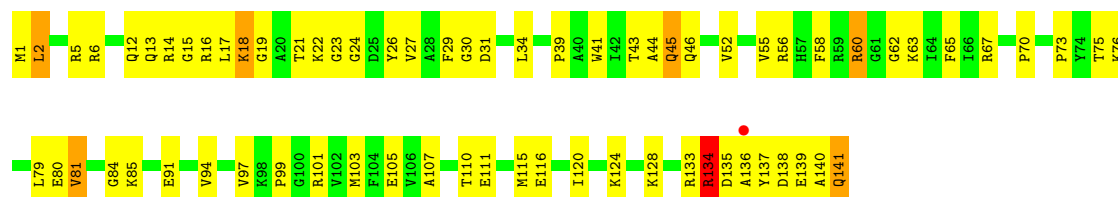
• Molecule 48: 50S ribosomal protein L15



• Molecule 49: 50S ribosomal protein L16

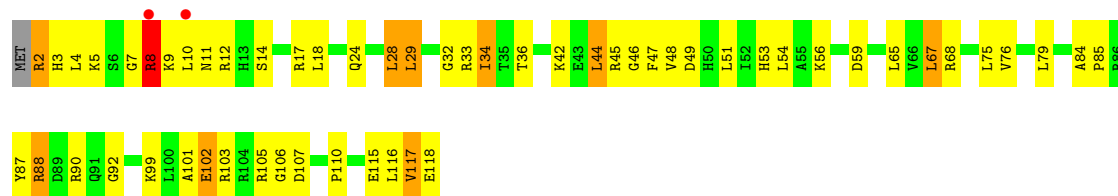


• Molecule 49: 50S ribosomal protein L16

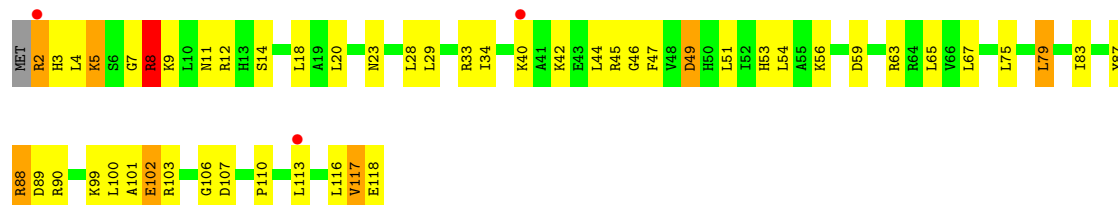


• Molecule 50: 50S ribosomal protein L17

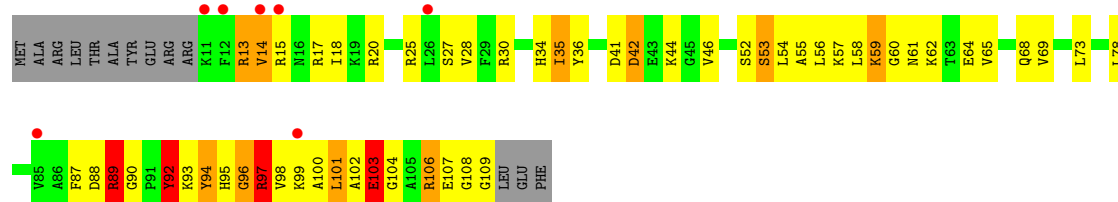




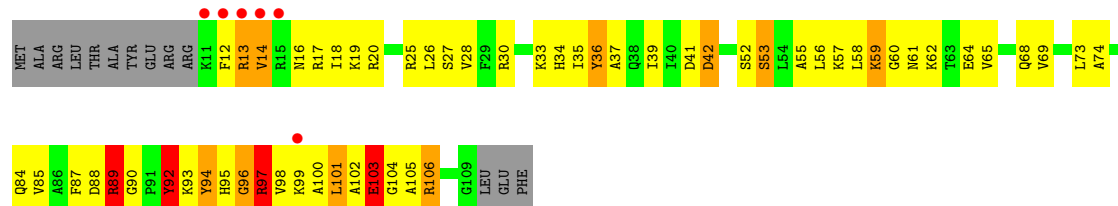
• Molecule 50: 50S ribosomal protein L17



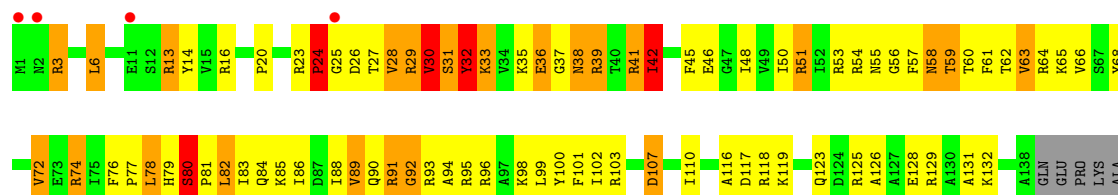
• Molecule 51: 50S ribosomal protein L18



• Molecule 51: 50S ribosomal protein L18



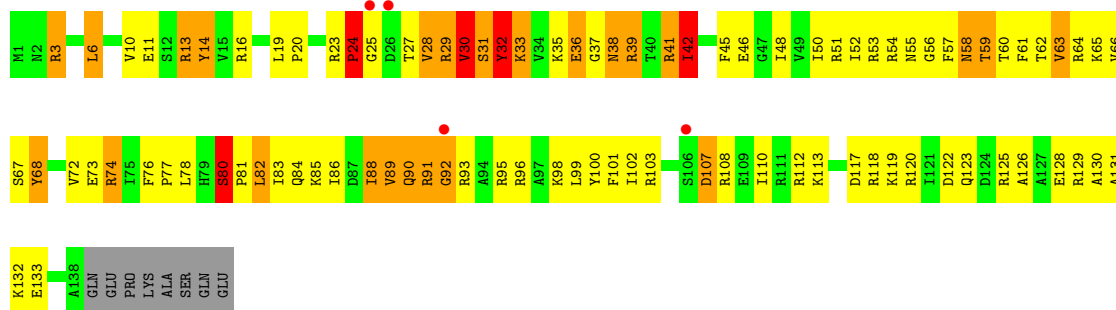
• Molecule 52: 50S ribosomal protein L19



SER
GLN
GLU

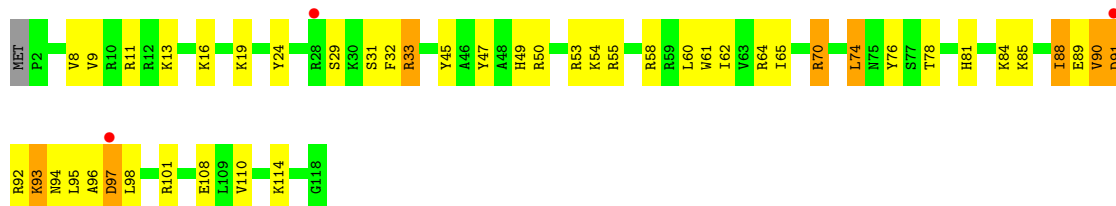
• Molecule 52: 50S ribosomal protein L19

Chain DT: 3% 30% 45% 16% 5%



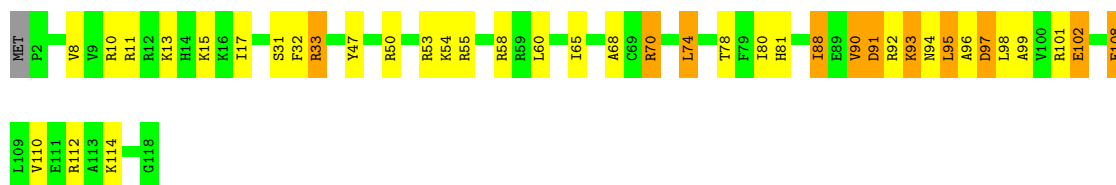
• Molecule 53: 50S ribosomal protein L20

Chain BU: 3% 60% 32% 7%



• Molecule 53: 50S ribosomal protein L20

Chain DU: 65% 25% 9%

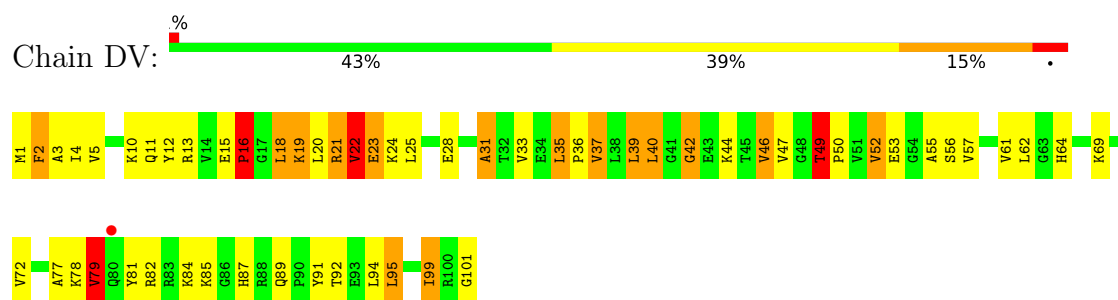


• Molecule 54: 50S ribosomal protein L21

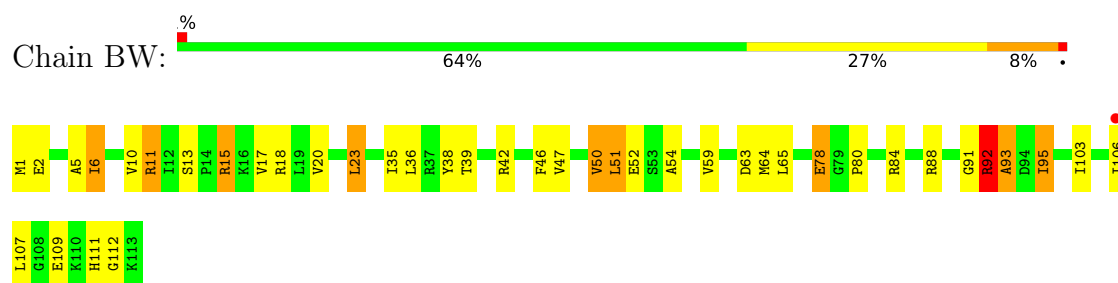
Chain BV: 2% 47% 33% 17%



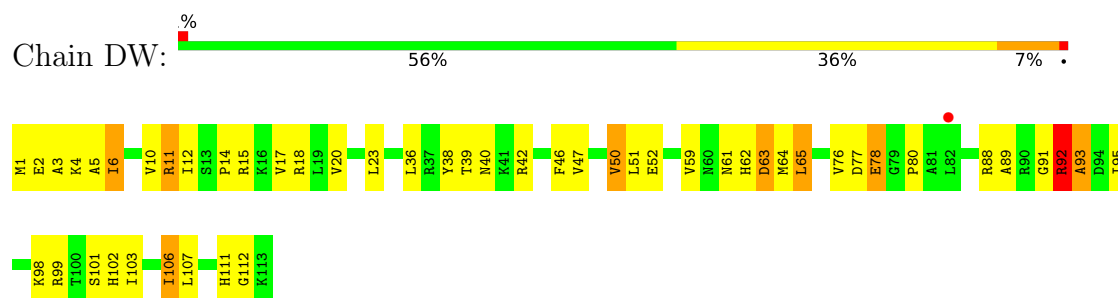
• Molecule 54: 50S ribosomal protein L21



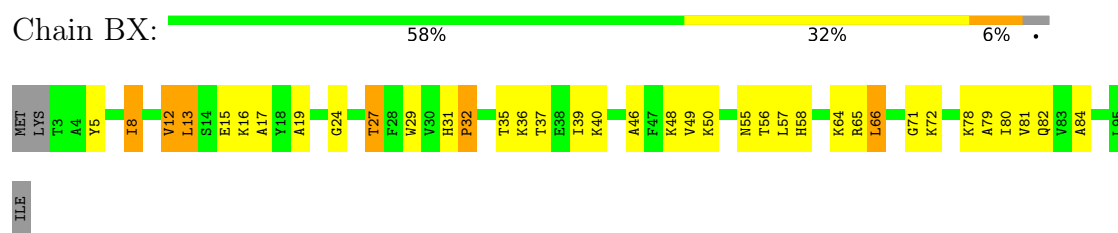
- Molecule 55: 50S ribosomal protein L22



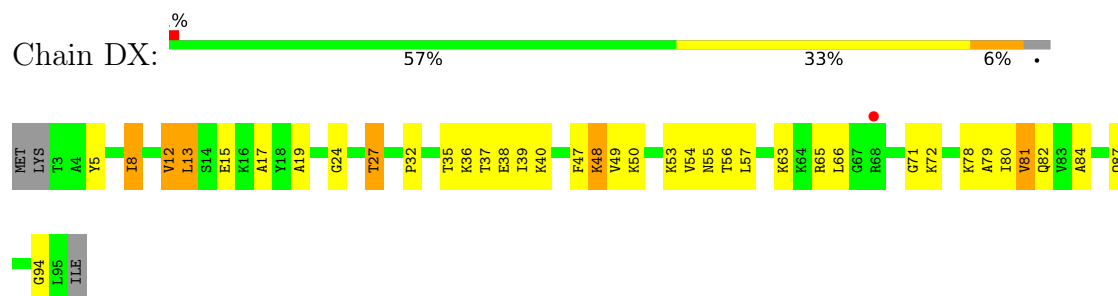
- Molecule 55: 50S ribosomal protein L22



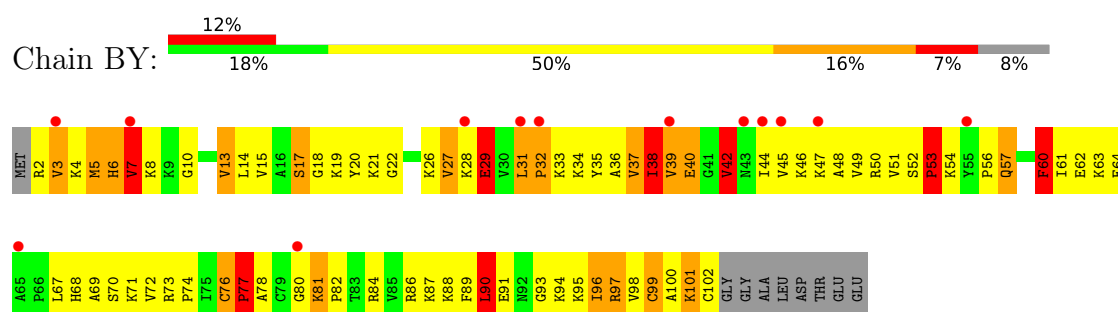
- Molecule 56: 50S ribosomal protein L23



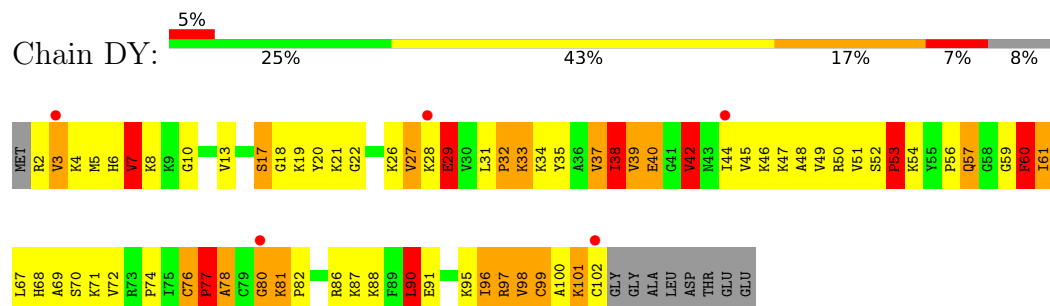
- Molecule 56: 50S ribosomal protein L23



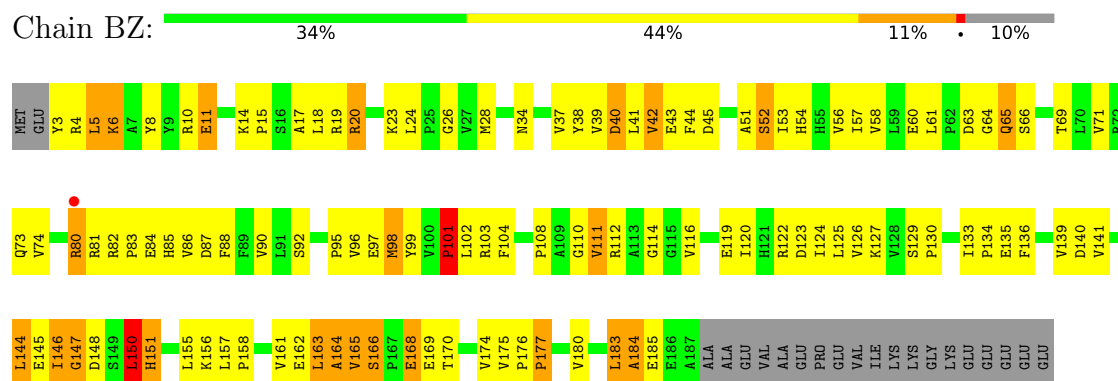
- Molecule 57: 50S ribosomal protein L24



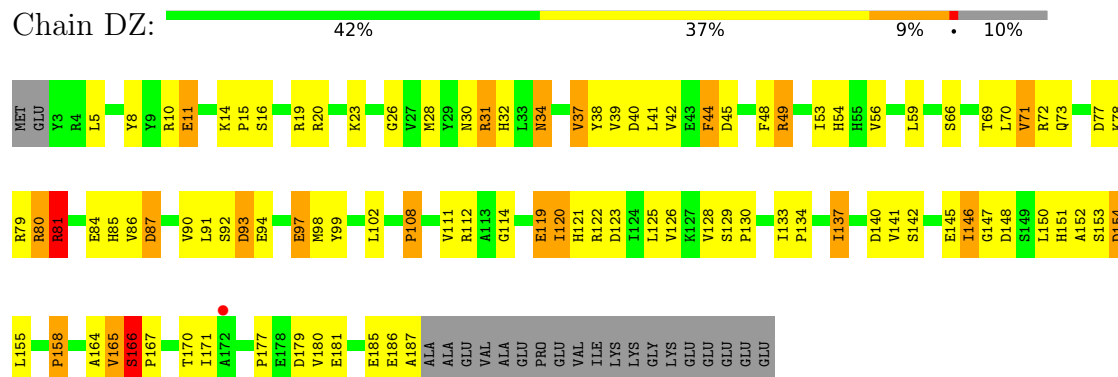
• Molecule 57: 50S ribosomal protein L24



• 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, α , β , γ	211.02Å 452.53Å 623.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.98 – 3.20 48.98 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.98-3.20) 100.0 (48.98-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.16 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.223 , 0.247 0.224 , 0.248	Depositor DCC
R_{free} test set	48519 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	128.7	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 106.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.25$, $\langle L^2 \rangle = 0.12$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	304459	wwPDB-VP
Average B, all atoms (Å ²)	160.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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, MG, MEQ

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	0.19	0/36190	0.42	0/56486
1	CA	0.19	0/36190	0.42	0/56486
2	AB	0.28	0/1936	0.86	1/2611 (0.0%)
2	CB	0.27	0/1936	0.83	0/2611
3	AC	0.26	0/1637	0.80	0/2207
3	CC	0.26	0/1637	0.79	0/2207
4	AD	0.25	0/1733	0.83	0/2318
4	CD	0.28	0/1733	0.83	1/2318 (0.0%)
5	AE	0.25	0/1163	0.76	0/1566
5	CE	0.24	0/1163	0.75	0/1566
6	AF	0.28	0/856	0.83	0/1154
6	CF	0.29	0/856	0.86	0/1154
7	AG	0.23	0/1276	0.79	0/1709
7	CG	0.25	0/1276	0.83	0/1709
8	AH	0.25	0/1136	0.78	0/1527
8	CH	0.23	0/1136	0.77	0/1527
9	AI	0.25	0/1028	0.87	0/1375
9	CI	0.26	0/1028	0.88	0/1375
10	AJ	0.25	0/808	0.80	0/1087
10	CJ	0.29	0/808	0.81	0/1087
11	AK	0.22	0/900	0.72	0/1213
11	CK	0.22	0/900	0.75	0/1213
12	AL	0.27	0/987	0.83	1/1322 (0.1%)
12	CL	0.29	0/987	0.84	1/1322 (0.1%)
13	AM	0.28	0/996	0.87	0/1328
13	CM	0.28	0/996	0.86	0/1328
14	AN	0.24	0/501	0.72	0/664
14	CN	0.25	0/501	0.73	0/664
15	AO	0.27	0/745	0.70	0/992
15	CO	0.23	0/745	0.70	0/992
16	AP	0.23	0/717	0.73	0/965
16	CP	0.24	0/717	0.74	0/965

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.22	0/837	0.78	0/1119
17	CQ	0.22	0/837	0.75	0/1119
18	AR	0.25	0/579	0.81	0/768
18	CR	0.25	0/579	0.83	0/768
19	AS	0.28	0/643	0.87	0/867
19	CS	0.26	0/643	0.84	1/867 (0.1%)
20	AT	0.24	0/765	0.74	0/1007
20	CT	0.23	0/765	0.70	0/1007
21	AU	0.21	0/213	0.87	0/279
21	CU	0.23	0/213	0.68	0/279
22	AV	0.22	0/1809	0.43	0/2819
22	AW	0.25	0/1784	0.47	0/2780
22	CV	0.22	0/1809	0.42	0/2819
22	CW	0.22	0/1784	0.47	0/2780
23	AX	0.27	0/185	0.64	0/286
23	CX	0.28	0/185	0.67	0/286
24	AY	0.25	0/2839	0.62	0/3833
24	CY	0.26	0/2839	0.66	0/3833
25	B0	0.25	0/666	0.74	0/885
25	D0	0.23	0/666	0.70	0/885
26	B1	0.28	0/739	0.90	2/983 (0.2%)
26	D1	0.33	0/739	0.80	0/983
27	B2	0.26	0/600	0.85	1/793 (0.1%)
27	D2	0.29	0/600	0.92	0/793
28	B3	0.32	0/473	0.79	0/636
28	D3	0.23	0/473	0.70	0/636
29	B4	0.29	0/229	0.89	0/311
29	D4	0.29	0/229	0.83	0/311
30	B5	0.38	0/473	1.15	3/639 (0.5%)
30	D5	0.35	0/473	1.06	1/639 (0.2%)
31	B6	0.49	0/387	1.13	0/517
31	D6	0.53	0/388	1.32	5/520 (1.0%)
32	B7	0.20	0/427	0.74	0/563
32	D7	0.20	0/427	0.74	0/563
33	B8	0.30	0/516	0.95	0/681
33	D8	0.29	0/516	0.94	0/681
34	B9	0.27	0/302	0.70	0/397
34	D9	0.28	0/302	0.73	0/397
35	BA	0.21	3/69972 (0.0%)	0.45	1/109237 (0.0%)
35	DA	0.22	1/69972 (0.0%)	0.46	3/109237 (0.0%)
36	BB	0.20	0/2853	0.42	0/4451
36	DB	0.20	0/2853	0.41	0/4451
37	BC	0.23	0/956	0.80	0/1288

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	DC	0.23	0/956	0.78	0/1288
38	BD	0.27	0/2170	0.88	1/2926 (0.0%)
38	DD	0.28	0/2170	0.89	2/2926 (0.1%)
39	BE	0.34	0/1597	0.92	1/2155 (0.0%)
39	DE	0.30	0/1597	0.94	1/2155 (0.0%)
40	BF	0.30	0/1659	0.87	0/2246
40	DF	0.31	0/1659	0.90	3/2246 (0.1%)
41	BG	0.27	0/1498	0.91	2/2013 (0.1%)
41	DG	0.32	0/1499	0.97	4/2016 (0.2%)
42	BH	0.28	0/1271	0.96	2/1720 (0.1%)
42	DH	0.30	0/1271	1.01	3/1720 (0.2%)
43	BI	0.31	0/1147	0.93	0/1553
43	DI	0.30	0/1147	0.94	0/1553
45	BK	0.28	0/1057	0.94	0/1432
45	DK	0.31	0/1057	0.98	2/1432 (0.1%)
46	BN	0.26	0/1132	0.85	0/1527
46	DN	0.26	0/1132	0.81	0/1527
47	BO	0.24	0/943	0.75	0/1269
47	DO	0.25	0/943	0.72	0/1269
48	BP	0.35	0/1131	1.25	9/1504 (0.6%)
48	DP	0.36	0/1131	1.29	13/1504 (0.9%)
49	BQ	0.26	0/1143	0.81	0/1527
49	DQ	0.26	0/1143	0.82	0/1527
50	BR	0.27	0/974	0.77	0/1302
50	DR	0.29	0/974	0.84	1/1302 (0.1%)
51	BS	0.31	0/779	0.93	0/1038
51	DS	0.33	0/779	0.93	0/1038
52	BT	0.31	0/1156	1.00	5/1544 (0.3%)
52	DT	0.33	0/1156	1.03	5/1544 (0.3%)
53	BU	0.27	0/975	0.80	1/1297 (0.1%)
53	DU	0.30	0/975	0.85	2/1297 (0.2%)
54	BV	0.29	0/790	0.84	0/1057
54	DV	0.31	0/790	0.87	0/1057
55	BW	0.37	1/907 (0.1%)	0.80	0/1216
55	DW	0.28	0/907	0.74	0/1216
56	BX	0.27	0/740	0.84	0/995
56	DX	0.26	0/740	0.85	0/995
57	BY	0.48	1/789 (0.1%)	1.08	4/1053 (0.4%)
57	DY	0.36	0/789	1.07	1/1053 (0.1%)
58	BZ	0.28	0/1500	0.88	0/2037
58	DZ	0.29	0/1500	0.86	0/2037
All	All	0.23	6/328430 (0.0%)	0.59	83/490154 (0.0%)

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 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	BY	7	VAL	CB-CG2	6.68	1.74	1.52
35	BA	764	A	O4'-C1'	-6.49	1.32	1.42
35	DA	859	G	C5'-C4'	6.47	1.61	1.51
35	BA	1131	G	C3'-C2'	5.55	1.61	1.52
35	BA	1131	G	C1'-N9	5.49	1.55	1.47

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	DH	10	PRO	N-CA-CB	8.74	111.49	103.19
38	DD	244	ARG	C-N-CD	-7.86	103.32	120.60
38	BD	244	ARG	C-N-CD	-7.70	103.65	120.60
42	BH	8	PRO	N-CA-CB	7.45	111.08	103.25
52	DT	29	ARG	CA-C-N	7.34	135.18	121.97

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	850	0
1	CA	32329	0	16318	863	0
2	AB	1901	0	1951	126	0
2	CB	1901	0	1951	116	0
3	AC	1613	0	1677	89	0
3	CC	1613	0	1677	91	0
4	AD	1703	0	1763	113	0
4	CD	1703	0	1763	105	0
5	AE	1147	0	1207	53	0
5	CE	1147	0	1207	52	0
6	AF	843	0	857	52	0
6	CF	843	0	857	57	0
7	AG	1257	0	1296	45	0
7	CG	1257	0	1296	54	0
8	AH	1116	0	1177	52	0
8	CH	1116	0	1177	56	0
9	AI	1011	0	1042	80	0
9	CI	1011	0	1042	63	0
10	AJ	795	0	840	63	0
10	CJ	795	0	840	67	0
11	AK	885	0	904	39	0
11	CK	885	0	904	35	0
12	AL	971	0	1057	56	0
12	CL	971	0	1057	59	0
13	AM	988	0	1057	93	0
13	CM	988	0	1057	73	0
14	AN	492	0	530	24	0
14	CN	492	0	529	27	0
15	AO	734	0	771	28	0
15	CO	734	0	771	25	0
16	AP	701	0	720	42	0
16	CP	701	0	720	45	0
17	AQ	824	0	891	35	0
17	CQ	824	0	891	33	0
18	AR	574	0	644	33	0
18	CR	574	0	644	29	0
19	AS	630	0	652	33	0
19	CS	630	0	652	35	0
20	AT	763	0	861	27	0
20	CT	763	0	861	24	0
21	AU	209	0	221	15	0
21	CU	209	0	221	15	0
22	AV	1619	0	822	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	AW	1597	0	811	63	0
22	CV	1619	0	822	30	0
22	CW	1597	0	811	60	0
23	AX	166	0	87	3	0
23	CX	166	0	87	9	0
24	AY	2802	0	2818	113	0
24	CY	2802	0	2818	144	0
25	B0	657	0	683	36	0
25	D0	657	0	683	34	0
26	B1	732	0	808	38	0
26	D1	732	0	808	37	0
27	B2	598	0	653	46	0
27	D2	598	0	653	27	0
28	B3	468	0	523	20	0
28	D3	468	0	523	19	0
29	B4	226	0	229	18	0
29	D4	226	0	229	19	0
30	B5	459	0	477	26	0
30	D5	459	0	477	29	0
31	B6	381	0	390	46	0
31	D6	381	0	391	52	0
32	B7	419	0	467	13	0
32	D7	419	0	467	10	0
33	B8	508	0	576	43	0
33	D8	508	0	576	44	0
34	B9	299	0	323	15	0
34	D9	299	0	324	14	0
35	BA	62474	0	31495	1340	0
35	DA	62474	0	31497	1267	0
36	BB	2551	0	1295	55	0
36	DB	2551	0	1295	56	0
37	BC	937	0	957	65	0
37	DC	937	0	957	62	0
38	BD	2120	0	2197	121	0
38	DD	2120	0	2197	115	0
39	BE	1564	0	1629	81	0
39	DE	1564	0	1629	90	0
40	BF	1624	0	1677	86	0
40	DF	1624	0	1677	89	0
41	BG	1474	0	1534	123	0
41	DG	1474	0	1535	116	0
42	BH	1248	0	1289	60	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	DH	1248	0	1289	65	0
43	BI	1132	0	1218	47	0
43	DI	1132	0	1218	62	0
44	BJ	651	0	155	14	0
44	DJ	651	0	157	12	0
45	BK	1038	0	1089	77	0
45	DK	1038	0	1089	99	0
46	BN	1105	0	1180	49	0
46	DN	1105	0	1180	65	0
47	BO	933	0	996	42	0
47	DO	933	0	996	37	0
48	BP	1114	0	1187	135	0
48	DP	1114	0	1187	123	0
49	BQ	1122	0	1179	66	0
49	DQ	1122	0	1179	68	0
50	BR	960	0	1021	51	0
50	DR	960	0	1021	44	0
51	BS	771	0	832	55	0
51	DS	771	0	832	63	0
52	BT	1142	0	1202	88	0
52	DT	1142	0	1202	104	0
53	BU	958	0	1015	54	0
53	DU	958	0	1015	52	0
54	BV	779	0	852	49	0
54	DV	779	0	852	61	0
55	BW	896	0	953	29	0
55	DW	896	0	953	30	0
56	BX	726	0	778	31	0
56	DX	726	0	778	29	0
57	BY	776	0	870	90	0
57	DY	776	0	870	79	0
58	BZ	1468	0	1492	110	0
58	DZ	1468	0	1492	76	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

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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	208396	9411	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 19.

The worst 5 of 9411 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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	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	7
5	CE	149/162 (92%)	117 (78%)	22 (15%)	10 (7%)	1	7
6	AF	99/101 (98%)	71 (72%)	21 (21%)	7 (7%)	1	6
6	CF	99/101 (98%)	73 (74%)	19 (19%)	7 (7%)	1	6
7	AG	153/156 (98%)	116 (76%)	29 (19%)	8 (5%)	1	12
7	CG	153/156 (98%)	118 (77%)	27 (18%)	8 (5%)	1	12
8	AH	136/138 (99%)	106 (78%)	23 (17%)	7 (5%)	1	13
8	CH	136/138 (99%)	106 (78%)	23 (17%)	7 (5%)	1	13
9	AI	123/128 (96%)	86 (70%)	27 (22%)	10 (8%)	1	4
9	CI	123/128 (96%)	86 (70%)	26 (21%)	11 (9%)	0	3
10	AJ	97/105 (92%)	69 (71%)	23 (24%)	5 (5%)	1	12
10	CJ	97/105 (92%)	72 (74%)	20 (21%)	5 (5%)	1	12
11	AK	117/129 (91%)	87 (74%)	26 (22%)	4 (3%)	3	20
11	CK	117/129 (91%)	87 (74%)	26 (22%)	4 (3%)	3	20
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	0
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	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	CN	58/61 (95%)	41 (71%)	11 (19%)	6 (10%)	0	2
15	AO	86/89 (97%)	68 (79%)	16 (19%)	2 (2%)	5	29
15	CO	86/89 (97%)	67 (78%)	17 (20%)	2 (2%)	5	29
16	AP	82/88 (93%)	58 (71%)	17 (21%)	7 (8%)	0	3
16	CP	82/88 (93%)	58 (71%)	16 (20%)	8 (10%)	0	2
17	AQ	98/105 (93%)	75 (76%)	14 (14%)	9 (9%)	0	3
17	CQ	98/105 (93%)	76 (78%)	12 (12%)	10 (10%)	0	2
18	AR	68/88 (77%)	45 (66%)	16 (24%)	7 (10%)	0	2
18	CR	68/88 (77%)	43 (63%)	19 (28%)	6 (9%)	0	3
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	0
20	AT	97/106 (92%)	64 (66%)	25 (26%)	8 (8%)	0	4
20	CT	97/106 (92%)	63 (65%)	26 (27%)	8 (8%)	0	4
21	AU	23/27 (85%)	15 (65%)	6 (26%)	2 (9%)	0	3
21	CU	23/27 (85%)	16 (70%)	6 (26%)	1 (4%)	2	16
24	AY	348/357 (98%)	303 (87%)	37 (11%)	8 (2%)	5	29
24	CY	348/357 (98%)	297 (85%)	40 (12%)	11 (3%)	3	21
25	B0	81/85 (95%)	69 (85%)	11 (14%)	1 (1%)	10	42
25	D0	81/85 (95%)	69 (85%)	11 (14%)	1 (1%)	10	42
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	2
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	2
29	D4	29/71 (41%)	16 (55%)	10 (34%)	3 (10%)	0	2
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

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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%)	3	24
34	D9	34/37 (92%)	31 (91%)	2 (6%)	1 (3%)	3	24
37	BC	116/229 (51%)	89 (77%)	18 (16%)	9 (8%)	1	5
37	DC	116/229 (51%)	88 (76%)	20 (17%)	8 (7%)	1	7
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	2
39	BE	203/206 (98%)	147 (72%)	32 (16%)	24 (12%)	0	1
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	1
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	0
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	0
45	DK	139/147 (95%)	81 (58%)	36 (26%)	22 (16%)	0	0
46	BN	137/140 (98%)	106 (77%)	25 (18%)	6 (4%)	2	15
46	DN	137/140 (98%)	104 (76%)	26 (19%)	7 (5%)	1	13
47	BO	120/122 (98%)	101 (84%)	14 (12%)	5 (4%)	2	16
47	DO	120/122 (98%)	101 (84%)	15 (12%)	4 (3%)	3	21
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%)	1	13
49	DQ	139/141 (99%)	110 (79%)	22 (16%)	7 (5%)	1	13
50	BR	115/118 (98%)	93 (81%)	14 (12%)	8 (7%)	1	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	DR	115/118 (98%)	93 (81%)	15 (13%)	7 (6%)	1	9
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%)	1	12
53	DU	115/118 (98%)	97 (84%)	11 (10%)	7 (6%)	1	9
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	8
55	DW	111/113 (98%)	94 (85%)	9 (8%)	8 (7%)	1	6
56	BX	91/96 (95%)	74 (81%)	10 (11%)	7 (8%)	1	5
56	DX	91/96 (95%)	75 (82%)	8 (9%)	8 (9%)	0	3
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	2
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 ⓘ

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%)	191 (95%)	11 (5%)	20	53
2	CB	202/220 (92%)	191 (95%)	11 (5%)	20	53
3	AC	160/188 (85%)	153 (96%)	7 (4%)	25	59
3	CC	160/188 (85%)	154 (96%)	6 (4%)	29	62
4	AD	180/181 (99%)	165 (92%)	15 (8%)	10	38
4	CD	180/181 (99%)	164 (91%)	16 (9%)	9	34
5	AE	115/123 (94%)	114 (99%)	1 (1%)	70	81
5	CE	115/123 (94%)	114 (99%)	1 (1%)	70	81
6	AF	90/90 (100%)	88 (98%)	2 (2%)	45	71
6	CF	90/90 (100%)	88 (98%)	2 (2%)	45	71
7	AG	126/127 (99%)	123 (98%)	3 (2%)	43	70
7	CG	126/127 (99%)	123 (98%)	3 (2%)	43	70
8	AH	119/119 (100%)	114 (96%)	5 (4%)	26	60
8	CH	119/119 (100%)	114 (96%)	5 (4%)	26	60
9	AI	98/99 (99%)	90 (92%)	8 (8%)	10	39
9	CI	98/99 (99%)	90 (92%)	8 (8%)	10	39
10	AJ	88/92 (96%)	85 (97%)	3 (3%)	32	64
10	CJ	88/92 (96%)	83 (94%)	5 (6%)	18	51
11	AK	90/99 (91%)	87 (97%)	3 (3%)	33	65
11	CK	90/99 (91%)	87 (97%)	3 (3%)	33	65
12	AL	104/109 (95%)	91 (88%)	13 (12%)	4	21
12	CL	104/109 (95%)	91 (88%)	13 (12%)	4	21
13	AM	99/101 (98%)	94 (95%)	5 (5%)	21	54
13	CM	99/101 (98%)	95 (96%)	4 (4%)	28	61
14	AN	49/50 (98%)	45 (92%)	4 (8%)	10	39
14	CN	49/50 (98%)	45 (92%)	4 (8%)	10	39
15	AO	79/80 (99%)	76 (96%)	3 (4%)	29	62
15	CO	79/80 (99%)	76 (96%)	3 (4%)	29	62
16	AP	72/74 (97%)	70 (97%)	2 (3%)	38	68
16	CP	72/74 (97%)	70 (97%)	2 (3%)	38	68
17	AQ	94/97 (97%)	91 (97%)	3 (3%)	34	65
17	CQ	94/97 (97%)	91 (97%)	3 (3%)	34	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	AR	61/77 (79%)	59 (97%)	2 (3%)	33	65
18	CR	61/77 (79%)	59 (97%)	2 (3%)	33	65
19	AS	69/80 (86%)	61 (88%)	8 (12%)	5	24
19	CS	69/80 (86%)	61 (88%)	8 (12%)	5	24
20	AT	76/82 (93%)	71 (93%)	5 (7%)	15	47
20	CT	76/82 (93%)	72 (95%)	4 (5%)	20	53
21	AU	19/22 (86%)	19 (100%)	0	100	100
21	CU	19/22 (86%)	19 (100%)	0	100	100
24	AY	297/303 (98%)	286 (96%)	11 (4%)	30	63
24	CY	297/303 (98%)	291 (98%)	6 (2%)	48	72
25	B0	66/67 (98%)	63 (96%)	3 (4%)	24	58
25	D0	66/67 (98%)	63 (96%)	3 (4%)	24	58
26	B1	78/83 (94%)	69 (88%)	9 (12%)	5	24
26	D1	78/83 (94%)	73 (94%)	5 (6%)	16	48
27	B2	66/67 (98%)	63 (96%)	3 (4%)	24	58
27	D2	66/67 (98%)	57 (86%)	9 (14%)	3	18
28	B3	51/52 (98%)	49 (96%)	2 (4%)	28	62
28	D3	51/52 (98%)	49 (96%)	2 (4%)	28	62
29	B4	27/63 (43%)	25 (93%)	2 (7%)	13	43
29	D4	27/63 (43%)	25 (93%)	2 (7%)	13	43
30	B5	51/52 (98%)	43 (84%)	8 (16%)	2	13
30	D5	51/52 (98%)	43 (84%)	8 (16%)	2	13
31	B6	43/52 (83%)	36 (84%)	7 (16%)	2	12
31	D6	43/52 (83%)	35 (81%)	8 (19%)	1	9
32	B7	41/42 (98%)	40 (98%)	1 (2%)	43	70
32	D7	41/42 (98%)	40 (98%)	1 (2%)	43	70
33	B8	53/55 (96%)	47 (89%)	6 (11%)	5	24
33	D8	53/55 (96%)	47 (89%)	6 (11%)	5	24
34	B9	33/34 (97%)	32 (97%)	1 (3%)	36	66
34	D9	33/34 (97%)	31 (94%)	2 (6%)	17	49
37	BC	99/181 (55%)	97 (98%)	2 (2%)	48	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	DC	99/181 (55%)	97 (98%)	2 (2%)	48	72
38	BD	214/218 (98%)	188 (88%)	26 (12%)	5	22
38	DD	214/218 (98%)	190 (89%)	24 (11%)	6	25
39	BE	165/166 (99%)	142 (86%)	23 (14%)	3	17
39	DE	165/166 (99%)	142 (86%)	23 (14%)	3	17
40	BF	165/166 (99%)	151 (92%)	14 (8%)	10	37
40	DF	165/166 (99%)	149 (90%)	16 (10%)	8	32
41	BG	155/156 (99%)	145 (94%)	10 (6%)	15	47
41	DG	155/156 (99%)	137 (88%)	18 (12%)	5	24
42	BH	132/148 (89%)	122 (92%)	10 (8%)	12	42
42	DH	132/148 (89%)	122 (92%)	10 (8%)	12	42
43	BI	122/124 (98%)	108 (88%)	14 (12%)	5	24
43	DI	122/124 (98%)	107 (88%)	15 (12%)	4	22
45	BK	106/111 (96%)	97 (92%)	9 (8%)	10	37
45	DK	106/111 (96%)	98 (92%)	8 (8%)	12	42
46	BN	117/119 (98%)	110 (94%)	7 (6%)	17	50
46	DN	117/119 (98%)	110 (94%)	7 (6%)	17	50
47	BO	100/100 (100%)	95 (95%)	5 (5%)	22	55
47	DO	100/100 (100%)	94 (94%)	6 (6%)	17	50
48	BP	112/116 (97%)	96 (86%)	16 (14%)	3	16
48	DP	112/116 (97%)	96 (86%)	16 (14%)	3	16
49	BQ	111/111 (100%)	103 (93%)	8 (7%)	13	44
49	DQ	111/111 (100%)	102 (92%)	9 (8%)	11	39
50	BR	100/101 (99%)	88 (88%)	12 (12%)	5	23
50	DR	100/101 (99%)	87 (87%)	13 (13%)	4	20
51	BS	77/88 (88%)	68 (88%)	9 (12%)	5	23
51	DS	77/88 (88%)	67 (87%)	10 (13%)	4	20
52	BT	120/127 (94%)	101 (84%)	19 (16%)	2	13
52	DT	120/127 (94%)	102 (85%)	18 (15%)	3	15
53	BU	92/94 (98%)	86 (94%)	6 (6%)	15	47
53	DU	92/94 (98%)	86 (94%)	6 (6%)	15	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	BV	82/82 (100%)	66 (80%)	16 (20%)	1	8
54	DV	82/82 (100%)	67 (82%)	15 (18%)	2	9
55	BW	91/92 (99%)	79 (87%)	12 (13%)	4	19
55	DW	91/92 (99%)	78 (86%)	13 (14%)	3	16
56	BX	74/78 (95%)	69 (93%)	5 (7%)	14	46
56	DX	74/78 (95%)	68 (92%)	6 (8%)	11	39
57	BY	84/91 (92%)	69 (82%)	15 (18%)	2	9
57	DY	84/91 (92%)	68 (81%)	16 (19%)	1	9
58	BZ	162/179 (90%)	152 (94%)	10 (6%)	16	49
58	DZ	162/179 (90%)	143 (88%)	19 (12%)	5	23
All	All	10552/11256 (94%)	9723 (92%)	829 (8%)	11	40

5 of 829 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	CK	125	PHE
38	DD	117	VAL
57	DY	38	ILE
12	CL	110	VAL
11	CK	103	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 124 such sidechains are listed below:

Mol	Chain	Res	Type
54	BV	80	GLN
41	DG	79	ASN
7	CG	86	GLN
41	DG	40	ASN
49	DQ	12	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	233 (15%)	31 (2%)
1	CA	1503/1522 (98%)	240 (15%)	32 (2%)
22	AV	75/76 (98%)	22 (29%)	0

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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%)	3 (42%)	1 (14%)
35	BA	2900/2915 (99%)	576 (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%)	1759 (18%)	141 (1%)

5 of 1759 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	1.38	2 (25%)	5,10,12	1.79	2 (40%)
24	MEQ	AY	240	24	8,9,10	1.40	2 (25%)	5,10,12	1.80	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	2.49	1.45	1.34
24	CY	240	MEQ	CD-NE2	2.47	1.45	1.34
24	CY	240	MEQ	OE1-CD	-2.22	1.18	1.23
24	AY	240	MEQ	OE1-CD	-2.20	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	3.08	120.71	116.39
24	CY	240	MEQ	CG-CD-NE2	2.83	120.36	116.39
24	CY	240	MEQ	CB-CG-CD	-2.52	107.45	113.06
24	AY	240	MEQ	CB-CG-CD	-2.06	108.47	113.06

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 oligosaccharides 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, 95th 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 ²)	Q<0.9
1	AA	1504/1522 (98%)	-0.83	1 (0%) 92 89	101, 160, 266, 374	0
1	CA	1504/1522 (98%)	-0.81	0 100 100	99, 164, 261, 390	0
2	AB	235/256 (91%)	-0.12	3 (1%) 75 55	171, 220, 260, 279	0
2	CB	235/256 (91%)	-0.20	3 (1%) 75 55	135, 195, 239, 253	0
3	AC	207/239 (86%)	-0.30	3 (1%) 73 54	160, 205, 242, 281	0
3	CC	207/239 (86%)	-0.27	5 (2%) 59 40	146, 179, 215, 234	0
4	AD	208/209 (99%)	-0.04	3 (1%) 73 54	122, 157, 189, 209	0
4	CD	208/209 (99%)	0.25	15 (7%) 21 14	141, 181, 208, 229	0
5	AE	151/162 (93%)	-0.22	1 (0%) 84 69	129, 168, 201, 221	0
5	CE	151/162 (93%)	-0.45	0 100 100	120, 152, 184, 213	0
6	AF	101/101 (100%)	-0.30	0 100 100	157, 189, 218, 247	0
6	CF	101/101 (100%)	-0.41	0 100 100	128, 162, 192, 226	0
7	AG	155/156 (99%)	-0.27	1 (0%) 85 73	166, 199, 235, 255	0
7	CG	155/156 (99%)	-0.29	1 (0%) 85 73	136, 188, 223, 253	0
8	AH	138/138 (100%)	0.03	1 (0%) 84 69	143, 170, 199, 216	0
8	CH	138/138 (100%)	0.01	3 (2%) 62 42	136, 162, 186, 202	0
9	AI	127/128 (99%)	0.28	10 (7%) 18 12	172, 227, 248, 264	0
9	CI	127/128 (99%)	0.06	4 (3%) 51 32	145, 202, 241, 246	0
10	AJ	99/105 (94%)	0.17	0 100 100	174, 216, 246, 256	0
10	CJ	99/105 (94%)	0.18	1 (1%) 79 63	164, 201, 235, 250	0
11	AK	119/129 (92%)	-0.26	3 (2%) 58 39	135, 176, 211, 255	0
11	CK	119/129 (92%)	-0.12	3 (2%) 58 39	130, 159, 197, 249	0
12	AL	125/132 (94%)	-0.06	1 (0%) 82 67	112, 136, 173, 203	0
12	CL	125/132 (94%)	-0.02	2 (1%) 70 51	118, 140, 180, 220	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
13	AM	125/126 (99%)	0.12	7 (5%)	30	19	173, 220, 245, 273	0
13	CM	125/126 (99%)	0.11	6 (4%)	35	22	151, 197, 224, 244	0
14	AN	60/61 (98%)	0.40	3 (5%)	34	22	179, 202, 223, 232	0
14	CN	60/61 (98%)	0.40	2 (3%)	49	30	146, 177, 200, 208	0
15	AO	88/89 (98%)	-0.15	0	100	100	132, 161, 202, 213	0
15	CO	88/89 (98%)	0.04	2 (2%)	61	41	120, 151, 187, 202	0
16	AP	84/88 (95%)	-0.12	3 (3%)	46	28	123, 143, 182, 198	0
16	CP	84/88 (95%)	0.72	10 (11%)	9	6	154, 185, 231, 243	0
17	AQ	100/105 (95%)	-0.16	2 (2%)	65	45	123, 150, 178, 188	0
17	CQ	100/105 (95%)	-0.03	4 (4%)	42	26	121, 152, 181, 200	0
18	AR	70/88 (79%)	-0.32	0	100	100	162, 190, 227, 235	0
18	CR	70/88 (79%)	-0.39	0	100	100	120, 161, 192, 205	0
19	AS	79/93 (84%)	0.29	7 (8%)	15	10	180, 225, 257, 264	0
19	CS	79/93 (84%)	0.17	1 (1%)	75	55	152, 200, 248, 260	0
20	AT	99/106 (93%)	0.26	8 (8%)	18	11	112, 149, 188, 211	0
20	CT	99/106 (93%)	0.44	9 (9%)	15	9	133, 171, 215, 243	0
21	AU	25/27 (92%)	1.25	4 (16%)	5	3	187, 213, 239, 242	0
21	CU	25/27 (92%)	0.54	2 (8%)	18	12	156, 181, 195, 199	0
22	AV	76/76 (100%)	-0.85	0	100	100	152, 210, 242, 302	0
22	AW	75/76 (98%)	-0.34	1 (1%)	75	55	323, 391, 436, 444	0
22	CV	76/76 (100%)	-0.95	0	100	100	141, 191, 230, 296	0
22	CW	75/76 (98%)	-0.35	1 (1%)	75	55	342, 398, 492, 499	0
23	AX	8/25 (32%)	0.86	2 (25%)	2	2	93, 149, 231, 248	0
23	CX	8/25 (32%)	0.55	1 (12%)	8	6	91, 140, 225, 232	0
24	AY	350/357 (98%)	-0.20	11 (3%)	51	32	154, 199, 282, 305	0
24	CY	350/357 (98%)	-0.12	10 (2%)	53	35	149, 202, 279, 297	0
25	B0	83/85 (97%)	0.31	5 (6%)	27	17	114, 138, 194, 242	0
25	D0	83/85 (97%)	-0.02	5 (6%)	27	17	104, 125, 189, 229	0
26	B1	94/98 (95%)	-0.10	0	100	100	94, 124, 167, 203	0
26	D1	94/98 (95%)	-0.06	1 (1%)	78	61	88, 120, 172, 191	0
27	B2	71/72 (98%)	-0.00	2 (2%)	55	35	132, 166, 193, 229	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
27	D2	71/72 (98%)	-0.13	2 (2%) 55 35	87, 125, 166, 194	0
28	B3	60/60 (100%)	0.26	0 100 100	113, 142, 177, 204	0
28	D3	60/60 (100%)	-0.14	1 (1%) 69 49	106, 122, 158, 204	0
29	B4	31/71 (43%)	-0.26	1 (3%) 50 31	200, 226, 244, 255	0
29	D4	31/71 (43%)	-0.55	1 (3%) 50 31	173, 195, 213, 223	0
30	B5	59/60 (98%)	0.01	2 (3%) 48 30	102, 134, 247, 283	0
30	D5	59/60 (98%)	-0.19	2 (3%) 48 30	85, 122, 245, 254	0
31	B6	45/54 (83%)	-0.01	0 100 100	199, 239, 256, 271	0
31	D6	45/54 (83%)	0.11	0 100 100	206, 233, 253, 260	0
32	B7	49/49 (100%)	-0.02	4 (8%) 17 11	90, 105, 164, 187	0
32	D7	49/49 (100%)	-0.25	0 100 100	70, 90, 135, 203	0
33	B8	64/65 (98%)	0.81	7 (10%) 10 7	95, 125, 170, 193	0
33	D8	64/65 (98%)	0.60	5 (7%) 19 12	100, 121, 164, 195	0
34	B9	36/37 (97%)	1.01	3 (8%) 17 11	147, 185, 220, 226	0
34	D9	36/37 (97%)	1.22	5 (13%) 6 5	140, 159, 201, 218	0
35	BA	2901/2915 (99%)	-0.94	2 (0%) 92 89	84, 127, 274, 441	0
35	DA	2901/2915 (99%)	-0.96	2 (0%) 92 89	74, 114, 282, 427	0
36	BB	119/122 (97%)	-0.77	0 100 100	134, 193, 232, 248	0
36	DB	119/122 (97%)	-0.95	0 100 100	122, 159, 190, 222	0
37	BC	120/229 (52%)	0.18	7 (5%) 29 18	214, 309, 343, 358	0
37	DC	120/229 (52%)	0.01	2 (1%) 69 49	227, 322, 369, 374	0
38	BD	273/276 (98%)	-0.13	2 (0%) 84 69	80, 117, 153, 183	0
38	DD	273/276 (98%)	-0.25	5 (1%) 67 48	78, 106, 143, 194	0
39	BE	205/206 (99%)	-0.07	2 (0%) 79 63	88, 126, 179, 217	0
39	DE	205/206 (99%)	-0.09	1 (0%) 87 76	84, 126, 183, 224	0
40	BF	208/210 (99%)	-0.18	0 100 100	88, 134, 196, 257	0
40	DF	208/210 (99%)	-0.28	1 (0%) 87 76	71, 118, 193, 245	0
41	BG	181/182 (99%)	-0.17	3 (1%) 69 49	157, 199, 231, 260	0
41	DG	181/182 (99%)	-0.34	1 (0%) 85 73	133, 165, 214, 276	0
42	BH	165/180 (91%)	-0.12	4 (2%) 59 40	146, 198, 246, 270	0
42	DH	165/180 (91%)	-0.26	1 (0%) 85 73	98, 145, 186, 222	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
43	BI	146/148 (98%)	-0.28	1 (0%) 84 69	117, 175, 202, 218	0
43	DI	146/148 (98%)	-0.50	0 100 100	119, 157, 195, 216	0
44	BJ	0/130	-	-	-	-
44	DJ	0/130	-	-	-	-
45	BK	141/147 (95%)	-0.08	0 100 100	224, 266, 287, 294	0
45	DK	141/147 (95%)	-0.03	3 (2%) 63 43	233, 278, 303, 327	0
46	BN	139/140 (99%)	-0.01	3 (2%) 62 42	106, 144, 181, 204	0
46	DN	139/140 (99%)	-0.05	0 100 100	95, 123, 166, 192	0
47	BO	122/122 (100%)	-0.26	2 (1%) 70 51	88, 118, 144, 157	0
47	DO	122/122 (100%)	-0.29	1 (0%) 82 67	89, 119, 150, 168	0
48	BP	146/150 (97%)	0.16	3 (2%) 63 43	85, 148, 190, 235	0
48	DP	146/150 (97%)	0.30	7 (4%) 35 22	82, 134, 170, 225	0
49	BQ	141/141 (100%)	-0.15	2 (1%) 73 54	113, 141, 176, 223	0
49	DQ	141/141 (100%)	-0.16	1 (0%) 84 69	91, 127, 164, 214	0
50	BR	117/118 (99%)	-0.01	2 (1%) 69 49	98, 125, 162, 200	0
50	DR	117/118 (99%)	0.08	3 (2%) 57 37	95, 123, 158, 187	0
51	BS	99/112 (88%)	0.35	7 (7%) 22 14	131, 183, 209, 216	0
51	DS	99/112 (88%)	0.14	6 (6%) 27 17	122, 163, 196, 216	0
52	BT	138/146 (94%)	0.01	4 (2%) 53 35	91, 137, 214, 284	0
52	DT	138/146 (94%)	0.03	4 (2%) 53 35	106, 145, 229, 264	0
53	BU	117/118 (99%)	0.23	3 (2%) 57 37	100, 138, 184, 207	0
53	DU	117/118 (99%)	-0.14	0 100 100	79, 112, 163, 196	0
54	BV	101/101 (100%)	-0.16	2 (1%) 65 45	96, 159, 197, 229	0
54	DV	101/101 (100%)	-0.33	1 (0%) 79 63	90, 141, 180, 211	0
55	BW	113/113 (100%)	-0.03	1 (0%) 81 64	94, 122, 155, 225	0
55	DW	113/113 (100%)	-0.41	1 (0%) 81 64	81, 106, 145, 264	0
56	BX	93/96 (96%)	0.03	0 100 100	111, 142, 163, 204	0
56	DX	93/96 (96%)	-0.07	1 (1%) 78 61	84, 113, 145, 172	0
57	BY	101/110 (91%)	0.72	13 (12%) 7 6	122, 163, 211, 239	0
57	DY	101/110 (91%)	0.22	5 (4%) 34 22	101, 137, 193, 221	0
58	BZ	185/206 (89%)	-0.31	1 (0%) 87 76	146, 176, 218, 239	0
58	DZ	185/206 (89%)	-0.43	1 (0%) 87 76	117, 165, 209, 235	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	22142/23326 (94%)	-0.41	317 (1%) 73 54	70, 153, 269, 499	0

The worst 5 of 317 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	CK	129	SER	14.4
53	BU	91	ASP	7.8
13	CM	123	ALA	5.3
2	AB	70	PHE	5.2
48	DP	51	PHE	5.0

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, 95th 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 ²)	Q<0.9
24	MEQ	CY	240	10/11	0.90	0.28	149,152,186,247	0
24	MEQ	AY	240	10/11	0.93	0.22	143,154,163,163	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 95th 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 ²)	Q<0.9
59	MG	BA	3105	1/1	0.69	0.24	85,85,85,85	0
59	MG	BA	3145	1/1	0.69	0.14	114,114,114,114	0
59	MG	CA	1617	1/1	0.70	0.20	125,125,125,125	0
60	ZN	B9	101	1/1	0.70	0.21	205,205,205,205	1
59	MG	DA	3213	1/1	0.72	0.19	101,101,101,101	0
59	MG	DA	3137	1/1	0.74	0.26	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	DA	3073	1/1	0.75	0.17	129,129,129,129	0
59	MG	BA	3144	1/1	0.76	0.26	91,91,91,91	0
59	MG	DA	3203	1/1	0.76	0.17	93,93,93,93	0
59	MG	BA	3125	1/1	0.77	0.25	100,100,100,100	0
59	MG	BA	3179	1/1	0.77	0.21	104,104,104,104	0
59	MG	BQ	201	1/1	0.77	0.17	104,104,104,104	0
59	MG	BB	202	1/1	0.78	0.26	95,95,95,95	0
59	MG	BA	3081	1/1	0.78	0.21	107,107,107,107	0
59	MG	DA	3219	1/1	0.79	0.16	115,115,115,115	0
59	MG	AA	1618	1/1	0.79	0.23	94,94,94,94	0
59	MG	BA	3165	1/1	0.80	0.14	111,111,111,111	0
59	MG	DA	3033	1/1	0.80	0.27	77,77,77,77	0
59	MG	AA	1622	1/1	0.80	0.23	96,96,96,96	0
59	MG	CA	1615	1/1	0.80	0.23	98,98,98,98	0
59	MG	DA	3111	1/1	0.81	0.23	80,80,80,80	0
59	MG	BA	3079	1/1	0.81	0.22	83,83,83,83	0
59	MG	DA	3133	1/1	0.82	0.17	91,91,91,91	0
59	MG	DA	3104	1/1	0.82	0.26	82,82,82,82	0
59	MG	DA	3220	1/1	0.82	0.25	99,99,99,99	0
59	MG	BF	301	1/1	0.82	0.16	120,120,120,120	0
59	MG	DA	3202	1/1	0.83	0.21	97,97,97,97	0
59	MG	AA	1628	1/1	0.83	0.23	99,99,99,99	0
59	MG	DA	3080	1/1	0.83	0.25	68,68,68,68	0
59	MG	BA	3114	1/1	0.84	0.11	110,110,110,110	0
59	MG	BA	3152	1/1	0.84	0.20	91,91,91,91	0
59	MG	DA	3141	1/1	0.84	0.18	67,67,67,67	0
59	MG	DA	3190	1/1	0.84	0.15	91,91,91,91	0
59	MG	DA	3120	1/1	0.84	0.21	83,83,83,83	0
59	MG	BA	3117	1/1	0.85	0.14	100,100,100,100	0
59	MG	DA	3192	1/1	0.85	0.21	86,86,86,86	0
59	MG	DA	3195	1/1	0.85	0.21	100,100,100,100	0
59	MG	DA	3124	1/1	0.85	0.19	97,97,97,97	0
59	MG	BA	3088	1/1	0.85	0.17	83,83,83,83	0
59	MG	DA	3207	1/1	0.85	0.14	104,104,104,104	0
59	MG	BA	3148	1/1	0.85	0.21	90,90,90,90	0
59	MG	BA	3138	1/1	0.85	0.17	93,93,93,93	0
59	MG	DA	3179	1/1	0.85	0.15	93,93,93,93	0
59	MG	DA	3180	1/1	0.85	0.14	86,86,86,86	0
59	MG	BA	3120	1/1	0.86	0.09	81,81,81,81	0
59	MG	CA	1603	1/1	0.86	0.19	89,89,89,89	0
59	MG	DA	3114	1/1	0.86	0.17	107,107,107,107	0
59	MG	CA	1621	1/1	0.86	0.13	136,136,136,136	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	DA	3164	1/1	0.86	0.14	91,91,91,91	0
59	MG	DA	3176	1/1	0.86	0.29	87,87,87,87	0
59	MG	AA	1627	1/1	0.87	0.14	90,90,90,90	0
59	MG	CA	1626	1/1	0.87	0.22	97,97,97,97	0
59	MG	BA	3159	1/1	0.87	0.21	81,81,81,81	0
59	MG	DA	3046	1/1	0.87	0.30	74,74,74,74	0
59	MG	AA	1614	1/1	0.87	0.17	105,105,105,105	0
59	MG	DA	3148	1/1	0.87	0.12	87,87,87,87	0
59	MG	AA	1624	1/1	0.87	0.10	110,110,110,110	0
59	MG	BA	3106	1/1	0.87	0.27	90,90,90,90	0
59	MG	CA	1619	1/1	0.87	0.22	87,87,87,87	0
59	MG	CA	1620	1/1	0.87	0.09	121,121,121,121	0
59	MG	BA	3003	1/1	0.88	0.26	62,62,62,62	0
59	MG	DA	3191	1/1	0.88	0.16	83,83,83,83	0
59	MG	BA	3027	1/1	0.88	0.17	76,76,76,76	0
59	MG	BA	3164	1/1	0.88	0.21	84,84,84,84	0
59	MG	BA	3045	1/1	0.88	0.24	63,63,63,63	0
59	MG	BA	3169	1/1	0.88	0.12	94,94,94,94	0
59	MG	CA	1618	1/1	0.88	0.12	105,105,105,105	0
59	MG	BA	3174	1/1	0.88	0.18	87,87,87,87	0
59	MG	AA	1603	1/1	0.88	0.10	102,102,102,102	0
59	MG	BA	3151	1/1	0.88	0.15	87,87,87,87	0
59	MG	DA	3182	1/1	0.88	0.24	80,80,80,80	0
59	MG	CA	1606	1/1	0.89	0.20	75,75,75,75	0
59	MG	BA	3072	1/1	0.89	0.18	80,80,80,80	0
59	MG	DA	3102	1/1	0.89	0.20	77,77,77,77	0
59	MG	BA	3075	1/1	0.89	0.19	78,78,78,78	0
59	MG	AA	1607	1/1	0.89	0.20	83,83,83,83	0
59	MG	BA	3044	1/1	0.89	0.18	81,81,81,81	0
59	MG	AA	1623	1/1	0.89	0.25	83,83,83,83	0
59	MG	BA	3047	1/1	0.89	0.23	72,72,72,72	0
59	MG	CA	1623	1/1	0.89	0.14	151,151,151,151	0
59	MG	CA	1625	1/1	0.89	0.14	110,110,110,110	0
59	MG	DA	3204	1/1	0.89	0.25	85,85,85,85	0
59	MG	BA	3053	1/1	0.89	0.29	71,71,71,71	0
59	MG	DA	3142	1/1	0.89	0.12	84,84,84,84	0
59	MG	BA	3054	1/1	0.89	0.18	74,74,74,74	0
59	MG	DA	3157	1/1	0.89	0.12	80,80,80,80	0
59	MG	DB	202	1/1	0.89	0.12	101,101,101,101	0
59	MG	DW	201	1/1	0.89	0.19	70,70,70,70	0
59	MG	BA	3061	1/1	0.89	0.22	74,74,74,74	0
59	MG	DA	3147	1/1	0.90	0.27	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	BA	3034	1/1	0.90	0.24	75,75,75,75	0
59	MG	AA	1629	1/1	0.90	0.09	120,120,120,120	0
59	MG	DA	3163	1/1	0.90	0.20	84,84,84,84	0
59	MG	BA	3178	1/1	0.90	0.11	96,96,96,96	0
59	MG	DA	3205	1/1	0.90	0.10	86,86,86,86	0
59	MG	DA	3171	1/1	0.90	0.13	104,104,104,104	0
59	MG	AA	1602	1/1	0.90	0.13	87,87,87,87	0
59	MG	DA	3218	1/1	0.90	0.06	82,82,82,82	0
59	MG	DA	3127	1/1	0.90	0.22	78,78,78,78	0
59	MG	BA	3093	1/1	0.90	0.07	110,110,110,110	0
59	MG	BA	3046	1/1	0.90	0.16	77,77,77,77	0
59	MG	BA	3143	1/1	0.90	0.22	86,86,86,86	0
59	MG	AA	1626	1/1	0.90	0.15	132,132,132,132	0
59	MG	BA	3141	1/1	0.91	0.11	72,72,72,72	0
59	MG	BA	3098	1/1	0.91	0.14	66,66,66,66	0
59	MG	DA	3178	1/1	0.91	0.13	79,79,79,79	0
59	MG	BA	3055	1/1	0.91	0.17	85,85,85,85	0
59	MG	BA	3031	1/1	0.91	0.20	82,82,82,82	0
59	MG	DA	3088	1/1	0.91	0.13	75,75,75,75	0
59	MG	BA	3146	1/1	0.91	0.16	104,104,104,104	0
59	MG	BA	3147	1/1	0.91	0.09	70,70,70,70	0
59	MG	BA	3086	1/1	0.91	0.15	69,69,69,69	0
59	MG	BA	3116	1/1	0.91	0.22	75,75,75,75	0
59	MG	CA	1609	1/1	0.91	0.10	110,110,110,110	0
59	MG	BA	3087	1/1	0.91	0.14	74,74,74,74	0
59	MG	BA	3153	1/1	0.91	0.17	98,98,98,98	0
59	MG	BA	3154	1/1	0.91	0.29	92,92,92,92	0
59	MG	AA	1619	1/1	0.91	0.18	90,90,90,90	0
59	MG	BA	3162	1/1	0.91	0.13	79,79,79,79	0
59	MG	BA	3092	1/1	0.91	0.11	80,80,80,80	0
59	MG	CA	1622	1/1	0.91	0.11	104,104,104,104	0
59	MG	BA	3126	1/1	0.91	0.10	108,108,108,108	0
59	MG	CA	1624	1/1	0.91	0.16	91,91,91,91	0
59	MG	BA	3036	1/1	0.91	0.20	76,76,76,76	0
59	MG	BA	3172	1/1	0.91	0.17	78,78,78,78	0
59	MG	DA	3086	1/1	0.92	0.18	65,65,65,65	0
59	MG	BA	3121	1/1	0.92	0.14	65,65,65,65	0
59	MG	BA	3168	1/1	0.92	0.13	78,78,78,78	0
59	MG	BA	3024	1/1	0.92	0.18	50,50,50,50	0
59	MG	BA	3171	1/1	0.92	0.18	91,91,91,91	0
59	MG	BA	3150	1/1	0.92	0.08	94,94,94,94	0
59	MG	DA	3183	1/1	0.92	0.16	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	DA	3189	1/1	0.92	0.14	75,75,75,75	0
59	MG	BA	3080	1/1	0.92	0.20	77,77,77,77	0
59	MG	AA	1630	1/1	0.92	0.26	86,86,86,86	0
59	MG	BA	3082	1/1	0.92	0.25	75,75,75,75	0
59	MG	DA	3131	1/1	0.92	0.38	91,91,91,91	0
59	MG	DA	3197	1/1	0.92	0.09	84,84,84,84	0
59	MG	DA	3198	1/1	0.92	0.18	85,85,85,85	0
59	MG	BB	201	1/1	0.92	0.13	85,85,85,85	0
59	MG	BA	3068	1/1	0.92	0.16	76,76,76,76	0
59	MG	BA	3155	1/1	0.92	0.19	93,93,93,93	0
59	MG	DA	3007	1/1	0.92	0.23	53,53,53,53	0
59	MG	DA	3146	1/1	0.92	0.19	92,92,92,92	0
59	MG	BA	3069	1/1	0.92	0.17	72,72,72,72	0
59	MG	DA	3037	1/1	0.92	0.22	58,58,58,58	0
59	MG	DA	3156	1/1	0.92	0.10	59,59,59,59	0
59	MG	BA	3160	1/1	0.92	0.23	98,98,98,98	0
59	MG	BA	3030	1/1	0.92	0.29	62,62,62,62	0
59	MG	AA	1612	1/1	0.92	0.27	75,75,75,75	0
59	MG	DA	3170	1/1	0.92	0.21	80,80,80,80	0
59	MG	BA	3032	1/1	0.93	0.13	69,69,69,69	0
59	MG	BA	3033	1/1	0.93	0.16	65,65,65,65	0
59	MG	BA	3131	1/1	0.93	0.17	76,76,76,76	0
59	MG	DA	3061	1/1	0.93	0.13	50,50,50,50	0
59	MG	BA	3001	1/1	0.93	0.25	56,56,56,56	0
59	MG	DA	3172	1/1	0.93	0.09	66,66,66,66	0
59	MG	DA	3174	1/1	0.93	0.14	77,77,77,77	0
59	MG	DA	3076	1/1	0.93	0.15	73,73,73,73	0
59	MG	DA	3078	1/1	0.93	0.13	90,90,90,90	0
59	MG	CA	1605	1/1	0.93	0.12	94,94,94,94	0
59	MG	AA	1615	1/1	0.93	0.18	87,87,87,87	0
59	MG	DA	3181	1/1	0.93	0.09	82,82,82,82	0
59	MG	BA	3163	1/1	0.93	0.19	104,104,104,104	0
59	MG	CA	1613	1/1	0.93	0.24	80,80,80,80	0
59	MG	DA	3186	1/1	0.93	0.12	93,93,93,93	0
59	MG	BA	3103	1/1	0.93	0.15	88,88,88,88	0
59	MG	BA	3009	1/1	0.93	0.21	46,46,46,46	0
59	MG	BA	3020	1/1	0.93	0.15	69,69,69,69	0
59	MG	BA	3111	1/1	0.93	0.15	71,71,71,71	0
59	MG	BA	3112	1/1	0.93	0.29	84,84,84,84	0
59	MG	DA	3125	1/1	0.93	0.25	80,80,80,80	0
59	MG	AA	1621	1/1	0.93	0.21	81,81,81,81	0
59	MG	DA	3129	1/1	0.93	0.25	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	BA	3173	1/1	0.93	0.11	84,84,84,84	0
59	MG	AA	1616	1/1	0.93	0.14	77,77,77,77	0
59	MG	DA	3135	1/1	0.93	0.11	56,56,56,56	0
59	MG	BA	3176	1/1	0.93	0.10	98,98,98,98	0
59	MG	DA	3212	1/1	0.93	0.37	92,92,92,92	0
59	MG	DA	3139	1/1	0.93	0.17	90,90,90,90	0
59	MG	BA	3029	1/1	0.93	0.26	59,59,59,59	0
59	MG	AA	1617	1/1	0.93	0.14	73,73,73,73	0
59	MG	D5	102	1/1	0.93	0.16	82,82,82,82	0
59	MG	DA	3003	1/1	0.93	0.24	53,53,53,53	0
59	MG	AA	1609	1/1	0.93	0.33	83,83,83,83	0
59	MG	DA	3013	1/1	0.93	0.23	46,46,46,46	0
59	MG	DA	3122	1/1	0.94	0.12	56,56,56,56	0
59	MG	BA	3059	1/1	0.94	0.20	66,66,66,66	0
59	MG	DA	3011	1/1	0.94	0.17	67,67,67,67	0
59	MG	BA	3102	1/1	0.94	0.14	78,78,78,78	0
59	MG	DA	3019	1/1	0.94	0.18	66,66,66,66	0
59	MG	DA	3023	1/1	0.94	0.16	51,51,51,51	0
59	MG	DA	3187	1/1	0.94	0.12	92,92,92,92	0
59	MG	DA	3188	1/1	0.94	0.12	87,87,87,87	0
59	MG	CA	1614	1/1	0.94	0.20	81,81,81,81	0
59	MG	AA	1605	1/1	0.94	0.19	76,76,76,76	0
59	MG	BA	3022	1/1	0.94	0.11	68,68,68,68	0
59	MG	DA	3054	1/1	0.94	0.14	68,68,68,68	0
59	MG	BA	3016	1/1	0.94	0.19	69,69,69,69	0
59	MG	BA	3158	1/1	0.94	0.15	89,89,89,89	0
59	MG	BA	3108	1/1	0.94	0.16	67,67,67,67	0
59	MG	BA	3084	1/1	0.94	0.16	87,87,87,87	0
59	MG	BA	3070	1/1	0.94	0.12	87,87,87,87	0
59	MG	BA	3056	1/1	0.94	0.18	76,76,76,76	0
59	MG	BA	3115	1/1	0.94	0.17	90,90,90,90	0
59	MG	DA	3092	1/1	0.94	0.14	70,70,70,70	0
59	MG	DA	3210	1/1	0.94	0.20	77,77,77,77	0
59	MG	BT	201	1/1	0.94	0.24	108,108,108,108	0
59	MG	DA	3168	1/1	0.94	0.06	72,72,72,72	0
59	MG	DA	3103	1/1	0.94	0.14	59,59,59,59	0
59	MG	BA	3073	1/1	0.94	0.17	91,91,91,91	0
59	MG	BA	3057	1/1	0.94	0.11	61,61,61,61	0
59	MG	DA	3002	1/1	0.94	0.23	58,58,58,58	0
59	MG	DA	3119	1/1	0.94	0.08	85,85,85,85	0
59	MG	BA	3078	1/1	0.94	0.13	65,65,65,65	0
60	ZN	D9	101	1/1	0.94	0.17	223,223,223,223	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	DA	3126	1/1	0.95	0.14	71,71,71,71	0
59	MG	BA	3123	1/1	0.95	0.09	105,105,105,105	0
59	MG	BA	3091	1/1	0.95	0.19	71,71,71,71	0
59	MG	BA	3166	1/1	0.95	0.13	80,80,80,80	0
59	MG	BA	3049	1/1	0.95	0.15	63,63,63,63	0
59	MG	BA	3051	1/1	0.95	0.15	75,75,75,75	0
59	MG	DA	3136	1/1	0.95	0.22	71,71,71,71	0
59	MG	BA	3170	1/1	0.95	0.11	77,77,77,77	0
59	MG	DA	3138	1/1	0.95	0.12	64,64,64,64	0
59	MG	BA	3133	1/1	0.95	0.12	83,83,83,83	0
59	MG	BA	3136	1/1	0.95	0.12	67,67,67,67	0
59	MG	BA	3094	1/1	0.95	0.09	62,62,62,62	0
59	MG	DA	3143	1/1	0.95	0.15	72,72,72,72	0
59	MG	BA	3139	1/1	0.95	0.07	61,61,61,61	0
59	MG	BA	3097	1/1	0.95	0.11	69,69,69,69	0
59	MG	BA	3177	1/1	0.95	0.20	80,80,80,80	0
59	MG	DA	3150	1/1	0.95	0.09	100,100,100,100	0
59	MG	DA	3151	1/1	0.95	0.09	70,70,70,70	0
59	MG	BA	3052	1/1	0.95	0.12	62,62,62,62	0
59	MG	DA	3029	1/1	0.95	0.14	63,63,63,63	0
59	MG	DA	3032	1/1	0.95	0.21	57,57,57,57	0
59	MG	BA	3101	1/1	0.95	0.09	86,86,86,86	0
59	MG	BA	3012	1/1	0.95	0.27	72,72,72,72	0
59	MG	BA	3074	1/1	0.95	0.16	69,69,69,69	0
59	MG	DA	3049	1/1	0.95	0.16	64,64,64,64	0
59	MG	DA	3053	1/1	0.95	0.14	72,72,72,72	0
59	MG	BD	301	1/1	0.95	0.15	71,71,71,71	0
59	MG	DA	3175	1/1	0.95	0.08	60,60,60,60	0
59	MG	DA	3056	1/1	0.95	0.11	54,54,54,54	0
59	MG	DA	3177	1/1	0.95	0.10	86,86,86,86	0
59	MG	DA	3058	1/1	0.95	0.11	54,54,54,54	0
59	MG	AA	1601	1/1	0.95	0.16	69,69,69,69	0
59	MG	DA	3064	1/1	0.95	0.15	48,48,48,48	0
59	MG	DA	3065	1/1	0.95	0.08	79,79,79,79	0
59	MG	BA	3077	1/1	0.95	0.14	93,93,93,93	0
59	MG	DA	3074	1/1	0.95	0.15	61,61,61,61	0
59	MG	DA	3075	1/1	0.95	0.16	74,74,74,74	0
59	MG	BA	3037	1/1	0.95	0.18	98,98,98,98	0
59	MG	BA	3110	1/1	0.95	0.19	75,75,75,75	0
59	MG	DA	3079	1/1	0.95	0.15	66,66,66,66	0
59	MG	BA	3042	1/1	0.95	0.14	66,66,66,66	0
59	MG	DA	3081	1/1	0.95	0.07	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	BA	3018	1/1	0.95	0.19	52,52,52,52	0
59	MG	AA	1613	1/1	0.95	0.12	117,117,117,117	0
59	MG	DA	3196	1/1	0.95	0.20	69,69,69,69	0
59	MG	DA	3089	1/1	0.95	0.10	67,67,67,67	0
59	MG	CA	1610	1/1	0.95	0.10	71,71,71,71	0
59	MG	DA	3201	1/1	0.95	0.13	82,82,82,82	0
59	MG	DA	3094	1/1	0.95	0.22	64,64,64,64	0
59	MG	CA	1611	1/1	0.95	0.14	72,72,72,72	0
59	MG	CA	1612	1/1	0.95	0.18	77,77,77,77	0
59	MG	BA	3060	1/1	0.95	0.17	76,76,76,76	0
59	MG	DA	3108	1/1	0.95	0.18	69,69,69,69	0
59	MG	DA	3109	1/1	0.95	0.10	80,80,80,80	0
59	MG	BA	3157	1/1	0.95	0.11	107,107,107,107	0
59	MG	AA	1620	1/1	0.95	0.20	69,69,69,69	0
59	MG	DA	3116	1/1	0.95	0.21	71,71,71,71	0
59	MG	BA	3063	1/1	0.95	0.16	74,74,74,74	0
59	MG	BA	3066	1/1	0.95	0.15	75,75,75,75	0
59	MG	BA	3161	1/1	0.95	0.07	80,80,80,80	0
59	MG	DD	301	1/1	0.95	0.20	53,53,53,53	0
59	MG	DP	201	1/1	0.95	0.07	57,57,57,57	0
59	MG	DA	3123	1/1	0.95	0.13	77,77,77,77	0
59	MG	BA	3011	1/1	0.95	0.14	58,58,58,58	0
59	MG	BA	3122	1/1	0.95	0.17	67,67,67,67	0
59	MG	BA	3038	1/1	0.96	0.13	63,63,63,63	0
59	MG	DA	3085	1/1	0.96	0.13	52,52,52,52	0
59	MG	DA	3159	1/1	0.96	0.11	89,89,89,89	0
59	MG	DA	3161	1/1	0.96	0.06	58,58,58,58	0
59	MG	DA	3162	1/1	0.96	0.05	70,70,70,70	0
59	MG	BA	3076	1/1	0.96	0.12	68,68,68,68	0
59	MG	DA	3087	1/1	0.96	0.12	73,73,73,73	0
59	MG	DA	3165	1/1	0.96	0.12	60,60,60,60	0
59	MG	BA	3167	1/1	0.96	0.12	79,79,79,79	0
59	MG	DA	3016	1/1	0.96	0.17	58,58,58,58	0
59	MG	BA	3039	1/1	0.96	0.17	60,60,60,60	0
59	MG	BA	3062	1/1	0.96	0.12	70,70,70,70	0
59	MG	DA	3096	1/1	0.96	0.27	62,62,62,62	0
59	MG	DA	3099	1/1	0.96	0.18	71,71,71,71	0
59	MG	DA	3101	1/1	0.96	0.14	71,71,71,71	0
59	MG	DA	3028	1/1	0.96	0.11	51,51,51,51	0
59	MG	BA	3096	1/1	0.96	0.08	76,76,76,76	0
59	MG	BA	3041	1/1	0.96	0.15	63,63,63,63	0
59	MG	AA	1606	1/1	0.96	0.12	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	DA	3036	1/1	0.96	0.17	40,40,40,40	0
59	MG	DA	3110	1/1	0.96	0.10	77,77,77,77	0
59	MG	BA	3100	1/1	0.96	0.08	102,102,102,102	0
59	MG	DA	3184	1/1	0.96	0.17	85,85,85,85	0
59	MG	DA	3113	1/1	0.96	0.20	74,74,74,74	0
59	MG	DA	3042	1/1	0.96	0.08	45,45,45,45	0
59	MG	DA	3044	1/1	0.96	0.20	56,56,56,56	0
59	MG	AA	1611	1/1	0.96	0.19	69,69,69,69	0
59	MG	DA	3047	1/1	0.96	0.10	63,63,63,63	0
59	MG	BA	3175	1/1	0.96	0.07	69,69,69,69	0
59	MG	BA	3019	1/1	0.96	0.14	64,64,64,64	0
59	MG	BA	3083	1/1	0.96	0.14	64,64,64,64	0
59	MG	BA	3104	1/1	0.96	0.13	80,80,80,80	0
59	MG	DA	3057	1/1	0.96	0.15	52,52,52,52	0
59	MG	BA	3132	1/1	0.96	0.08	71,71,71,71	0
59	MG	DA	3199	1/1	0.96	0.07	81,81,81,81	0
59	MG	DA	3200	1/1	0.96	0.11	79,79,79,79	0
59	MG	DA	3059	1/1	0.96	0.14	66,66,66,66	0
59	MG	DA	3060	1/1	0.96	0.15	57,57,57,57	0
59	MG	BA	3180	1/1	0.96	0.07	99,99,99,99	0
59	MG	DA	3063	1/1	0.96	0.17	54,54,54,54	0
59	MG	BA	3007	1/1	0.96	0.33	54,54,54,54	0
59	MG	DA	3206	1/1	0.96	0.10	67,67,67,67	0
59	MG	BA	3085	1/1	0.96	0.09	76,76,76,76	0
59	MG	DA	3208	1/1	0.96	0.12	87,87,87,87	0
59	MG	DA	3069	1/1	0.96	0.14	71,71,71,71	0
59	MG	DA	3070	1/1	0.96	0.12	71,71,71,71	0
59	MG	DA	3072	1/1	0.96	0.17	61,61,61,61	0
59	MG	BA	3015	1/1	0.96	0.20	59,59,59,59	0
59	MG	BA	3109	1/1	0.96	0.11	74,74,74,74	0
59	MG	D5	101	1/1	0.96	0.07	78,78,78,78	0
59	MG	DB	201	1/1	0.96	0.15	78,78,78,78	0
59	MG	BA	3058	1/1	0.96	0.15	66,66,66,66	0
59	MG	BA	3048	1/1	0.96	0.18	54,54,54,54	0
59	MG	DD	302	1/1	0.96	0.12	54,54,54,54	0
59	MG	DA	3149	1/1	0.96	0.17	59,59,59,59	0
59	MG	CA	1602	1/1	0.96	0.13	64,64,64,64	0
59	MG	DA	3004	1/1	0.96	0.16	52,52,52,52	0
59	MG	DA	3154	1/1	0.96	0.09	80,80,80,80	0
59	MG	AA	1625	1/1	0.97	0.19	78,78,78,78	0
59	MG	BA	3026	1/1	0.97	0.14	58,58,58,58	0
59	MG	BA	3050	1/1	0.97	0.07	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	DA	3105	1/1	0.97	0.12	60,60,60,60	0
59	MG	DA	3173	1/1	0.97	0.07	102,102,102,102	0
59	MG	BA	3134	1/1	0.97	0.08	86,86,86,86	0
59	MG	DA	3052	1/1	0.97	0.16	51,51,51,51	0
59	MG	BA	3135	1/1	0.97	0.08	71,71,71,71	0
59	MG	AA	1604	1/1	0.97	0.22	76,76,76,76	0
59	MG	DA	3112	1/1	0.97	0.17	75,75,75,75	0
59	MG	BA	3137	1/1	0.97	0.08	80,80,80,80	0
59	MG	BA	3113	1/1	0.97	0.08	74,74,74,74	0
59	MG	BA	3065	1/1	0.97	0.15	74,74,74,74	0
59	MG	BA	3004	1/1	0.97	0.08	49,49,49,49	0
59	MG	BA	3142	1/1	0.97	0.15	74,74,74,74	0
59	MG	BA	3005	1/1	0.97	0.16	59,59,59,59	0
59	MG	DA	3185	1/1	0.97	0.18	76,76,76,76	0
59	MG	DA	3062	1/1	0.97	0.13	51,51,51,51	0
59	MG	DA	3010	1/1	0.97	0.15	47,47,47,47	0
59	MG	AA	1610	1/1	0.97	0.17	64,64,64,64	0
59	MG	BA	3119	1/1	0.97	0.14	80,80,80,80	0
59	MG	DA	3067	1/1	0.97	0.11	57,57,57,57	0
59	MG	DA	3014	1/1	0.97	0.19	61,61,61,61	0
59	MG	DA	3015	1/1	0.97	0.19	51,51,51,51	0
59	MG	DA	3193	1/1	0.97	0.06	96,96,96,96	0
59	MG	DA	3194	1/1	0.97	0.11	67,67,67,67	0
59	MG	BA	3043	1/1	0.97	0.10	67,67,67,67	0
59	MG	DA	3134	1/1	0.97	0.09	64,64,64,64	0
59	MG	BA	3071	1/1	0.97	0.08	84,84,84,84	0
59	MG	DA	3021	1/1	0.97	0.15	56,56,56,56	0
59	MG	BA	3008	1/1	0.97	0.21	58,58,58,58	0
59	MG	DA	3024	1/1	0.97	0.20	53,53,53,53	0
59	MG	DA	3025	1/1	0.97	0.17	44,44,44,44	0
59	MG	DA	3140	1/1	0.97	0.09	69,69,69,69	0
59	MG	BA	3149	1/1	0.97	0.09	84,84,84,84	0
59	MG	B5	101	1/1	0.97	0.05	73,73,73,73	0
59	MG	DA	3030	1/1	0.97	0.14	42,42,42,42	0
59	MG	DA	3082	1/1	0.97	0.06	73,73,73,73	0
59	MG	DA	3084	1/1	0.97	0.09	56,56,56,56	0
59	MG	CA	1616	1/1	0.97	0.07	98,98,98,98	0
59	MG	BA	3124	1/1	0.97	0.07	90,90,90,90	0
59	MG	DA	3211	1/1	0.97	0.07	80,80,80,80	0
59	MG	DA	3034	1/1	0.97	0.14	47,47,47,47	0
59	MG	DA	3035	1/1	0.97	0.12	50,50,50,50	0
59	MG	DA	3215	1/1	0.97	0.12	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	DA	3153	1/1	0.97	0.21	66,66,66,66	0
59	MG	BA	3010	1/1	0.97	0.23	54,54,54,54	0
59	MG	BA	3035	1/1	0.97	0.18	51,51,51,51	0
59	MG	DA	3221	1/1	0.97	0.10	92,92,92,92	0
59	MG	DA	3093	1/1	0.97	0.14	74,74,74,74	0
59	MG	DA	3038	1/1	0.97	0.14	62,62,62,62	0
59	MG	DA	3040	1/1	0.97	0.22	63,63,63,63	0
59	MG	DA	3097	1/1	0.97	0.10	77,77,77,77	0
59	MG	DA	3098	1/1	0.97	0.24	60,60,60,60	0
59	MG	DA	3041	1/1	0.97	0.10	44,44,44,44	0
59	MG	BA	3130	1/1	0.97	0.21	63,63,63,63	0
59	MG	DA	3167	1/1	0.97	0.10	58,58,58,58	0
59	MG	BA	3095	1/1	0.98	0.11	69,69,69,69	0
59	MG	DA	3169	1/1	0.98	0.06	62,62,62,62	0
59	MG	DA	3022	1/1	0.98	0.08	40,40,40,40	0
59	MG	BA	3017	1/1	0.98	0.21	59,59,59,59	0
59	MG	BA	3067	1/1	0.98	0.05	67,67,67,67	0
59	MG	BE	301	1/1	0.98	0.17	73,73,73,73	0
59	MG	DA	3066	1/1	0.98	0.07	58,58,58,58	0
59	MG	DA	3027	1/1	0.98	0.34	57,57,57,57	0
59	MG	DA	3115	1/1	0.98	0.07	55,55,55,55	0
59	MG	DA	3068	1/1	0.98	0.13	56,56,56,56	0
59	MG	DA	3117	1/1	0.98	0.08	53,53,53,53	0
59	MG	DA	3118	1/1	0.98	0.09	67,67,67,67	0
59	MG	BA	3127	1/1	0.98	0.03	63,63,63,63	0
59	MG	BA	3129	1/1	0.98	0.03	69,69,69,69	0
59	MG	DA	3121	1/1	0.98	0.10	50,50,50,50	0
59	MG	DA	3071	1/1	0.98	0.06	66,66,66,66	0
59	MG	BA	3021	1/1	0.98	0.12	66,66,66,66	0
59	MG	CA	1601	1/1	0.98	0.17	78,78,78,78	0
59	MG	BA	3099	1/1	0.98	0.09	67,67,67,67	0
59	MG	BA	3028	1/1	0.98	0.17	56,56,56,56	0
59	MG	CA	1604	1/1	0.98	0.20	58,58,58,58	0
59	MG	DA	3128	1/1	0.98	0.13	72,72,72,72	0
59	MG	DA	3077	1/1	0.98	0.11	70,70,70,70	0
59	MG	AA	1608	1/1	0.98	0.08	90,90,90,90	0
59	MG	DA	3132	1/1	0.98	0.27	72,72,72,72	0
59	MG	BA	3089	1/1	0.98	0.13	60,60,60,60	0
59	MG	BA	3090	1/1	0.98	0.15	60,60,60,60	0
59	MG	DA	3039	1/1	0.98	0.12	60,60,60,60	0
59	MG	DA	3006	1/1	0.98	0.12	51,51,51,51	0
59	MG	DA	3083	1/1	0.98	0.12	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	BA	3118	1/1	0.98	0.06	80,80,80,80	0
59	MG	DA	3008	1/1	0.98	0.12	61,61,61,61	0
59	MG	DA	3043	1/1	0.98	0.19	53,53,53,53	0
59	MG	DA	3009	1/1	0.98	0.12	45,45,45,45	0
59	MG	BA	3023	1/1	0.98	0.14	45,45,45,45	0
59	MG	BA	3156	1/1	0.98	0.10	62,62,62,62	0
59	MG	DA	3144	1/1	0.98	0.06	70,70,70,70	0
59	MG	DA	3090	1/1	0.98	0.20	47,47,47,47	0
59	MG	DA	3091	1/1	0.98	0.12	56,56,56,56	0
59	MG	DA	3048	1/1	0.98	0.24	51,51,51,51	0
59	MG	DA	3012	1/1	0.98	0.24	60,60,60,60	0
59	MG	DA	3209	1/1	0.98	0.07	64,64,64,64	0
59	MG	DA	3051	1/1	0.98	0.11	60,60,60,60	0
59	MG	DA	3095	1/1	0.98	0.09	59,59,59,59	0
59	MG	DA	3152	1/1	0.98	0.11	61,61,61,61	0
59	MG	BA	3013	1/1	0.98	0.09	62,62,62,62	0
59	MG	DA	3214	1/1	0.98	0.07	80,80,80,80	0
59	MG	BA	3025	1/1	0.98	0.07	73,73,73,73	0
59	MG	DA	3217	1/1	0.98	0.14	56,56,56,56	0
59	MG	BA	3140	1/1	0.98	0.08	85,85,85,85	0
59	MG	DA	3055	1/1	0.98	0.17	62,62,62,62	0
59	MG	DA	3158	1/1	0.98	0.10	71,71,71,71	0
59	MG	DA	3100	1/1	0.98	0.04	57,57,57,57	0
59	MG	DA	3160	1/1	0.98	0.07	85,85,85,85	0
59	MG	BA	3107	1/1	0.98	0.13	91,91,91,91	0
59	MG	DA	3017	1/1	0.98	0.16	45,45,45,45	0
59	MG	DA	3018	1/1	0.98	0.12	56,56,56,56	0
59	MG	BA	3040	1/1	0.98	0.09	55,55,55,55	0
59	MG	DU	201	1/1	0.98	0.12	62,62,62,62	0
59	MG	DA	3020	1/1	0.98	0.16	35,35,35,35	0
60	ZN	AD	301	1/1	0.98	0.19	117,117,117,117	0
60	ZN	AN	101	1/1	0.98	0.06	165,165,165,165	0
59	MG	DA	3166	1/1	0.98	0.11	55,55,55,55	0
59	MG	DA	3107	1/1	0.98	0.06	66,66,66,66	0
59	MG	DA	3050	1/1	0.99	0.09	49,49,49,49	0
59	MG	DA	3216	1/1	0.99	0.04	62,62,62,62	0
59	MG	BA	3128	1/1	0.99	0.07	83,83,83,83	0
59	MG	CA	1607	1/1	0.99	0.19	55,55,55,55	0
59	MG	DA	3001	1/1	0.99	0.19	36,36,36,36	0
59	MG	DA	3106	1/1	0.99	0.09	43,43,43,43	0
59	MG	CA	1608	1/1	0.99	0.24	78,78,78,78	0
59	MG	DA	3031	1/1	0.99	0.13	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	BA	3064	1/1	0.99	0.13	51,51,51,51	0
59	MG	DA	3155	1/1	0.99	0.08	59,59,59,59	0
59	MG	BA	3002	1/1	0.99	0.24	50,50,50,50	0
59	MG	DA	3045	1/1	0.99	0.17	43,43,43,43	0
59	MG	DA	3005	1/1	0.99	0.21	44,44,44,44	0
59	MG	BA	3014	1/1	0.99	0.21	50,50,50,50	0
59	MG	BA	3006	1/1	0.99	0.20	41,41,41,41	0
59	MG	DA	3026	1/1	0.99	0.08	44,44,44,44	0
59	MG	DA	3145	1/1	0.99	0.03	58,58,58,58	0
60	ZN	CD	301	1/1	0.99	0.17	107,107,107,107	0
60	ZN	CN	101	1/1	0.99	0.04	170,170,170,170	0
59	MG	DA	3130	1/1	0.99	0.12	63,63,63,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.