



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:50 PM GMT

PDB ID : 4V6D
Title : Crystal structure of the E. coli 70S ribosome in an intermediate state of ratcheting
Authors : Zhang, W.; Dunkle, J.A.; Cate, J.H.D.
Deposited on : 2009-06-27
Resolution : 3.81 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

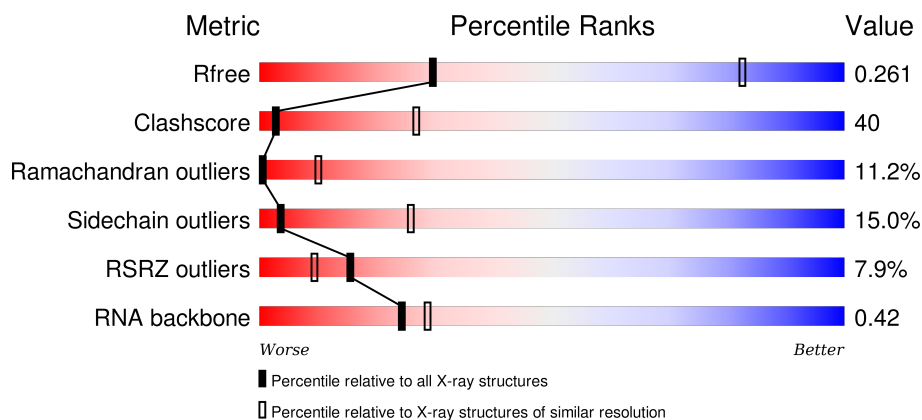
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.81 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}	91344	1324 (4.14-3.50)
Clashscore	102246	1028 (4.12-3.52)
Ramachandran outliers	100387	1404 (4.14-3.50)
Sidechain outliers	100360	1399 (4.14-3.50)
RSRZ outliers	91569	1332 (4.14-3.50)
RNA backbone	2183	1071 (4.84-2.80)

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

Mol	Chain	Length	Quality of chain
1	AB	241	<div> <div>44%</div> <div> <div>17%</div> <div>55%</div> <div>15%</div> <div>•</div> <div>10%</div> </div> </div>
1	CB	241	<div> <div>20%</div> <div>20%</div> <div>56%</div> <div>13%</div> <div>•</div> <div>10%</div> </div>
2	AC	233	<div> <div>2%</div> <div>33%</div> <div>44%</div> <div>10%</div> <div>•</div> <div>12%</div> </div>
2	CC	233	<div> <div>%</div> <div>32%</div> <div>45%</div> <div>11%</div> <div>•</div> <div>12%</div> </div>

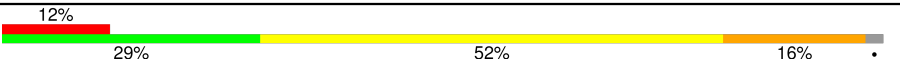
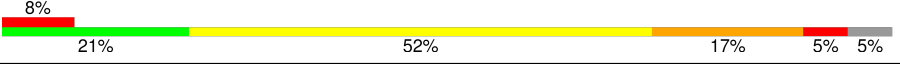

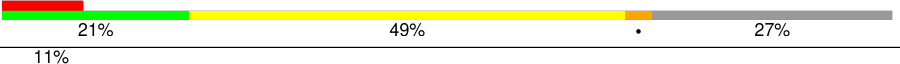
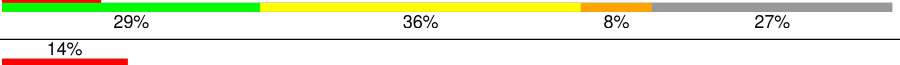

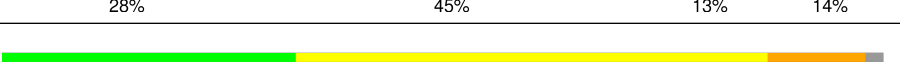

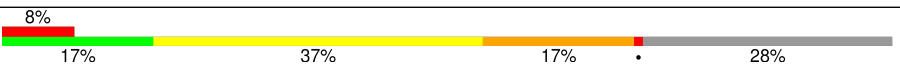

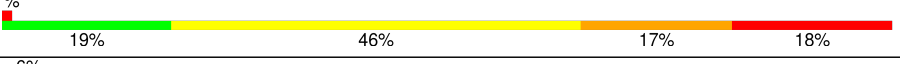
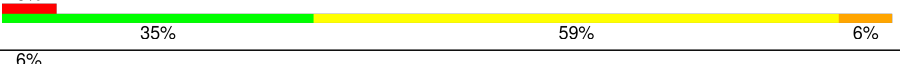



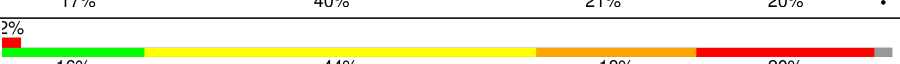
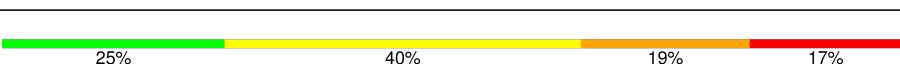
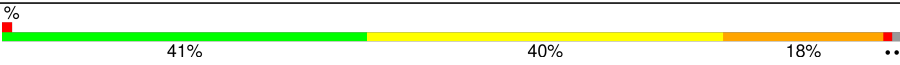
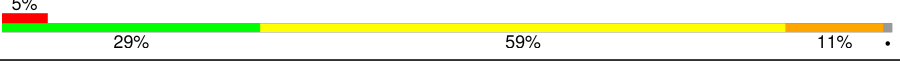
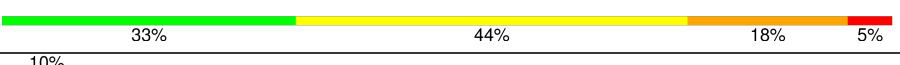





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Mol	Chain	Length	Quality of chain
3	AD	206	
3	CD	206	
4	AE	167	
4	CE	167	
5	AF	135	
5	CF	135	
6	AG	179	
6	CG	179	
7	AH	130	
7	CH	130	
8	AI	130	
8	CI	130	
9	AJ	103	
9	CJ	103	
10	AK	129	
10	CK	129	
11	AL	124	
11	CL	124	
12	AM	118	
12	CM	118	
13	AN	101	
13	CN	101	
14	AO	89	
14	CO	89	
15	AP	82	

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Mol	Chain	Length	Quality of chain
15	CP	82	
16	AQ	84	
16	CQ	84	
17	AR	75	
17	CR	75	
18	AS	92	
18	CS	92	
19	AT	87	
19	CT	87	
20	AU	71	
20	CU	71	
21	AA	1533	
22	AV	17	
22	CV	17	
23	AW	6	
23	CW	6	
24	BA	2903	
24	DA	2903	
25	BB	118	
26	BC	273	
26	DC	273	
27	BD	209	
27	DD	209	
28	BE	201	
28	DE	201	

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Mol	Chain	Length	Quality of chain
29	BF	179	
29	DF	179	
30	BG	177	
30	DG	177	
31	BH	149	
31	DH	149	
32	BI	142	
32	DI	142	
33	BJ	142	
33	DJ	142	
34	BK	123	
34	DK	123	
35	BL	144	
35	DL	144	
36	BM	136	
36	DM	136	
37	BN	127	
37	DN	127	
38	BO	117	
38	DO	117	
39	BP	115	
39	DP	115	
40	BQ	118	
40	DQ	118	
41	BR	103	


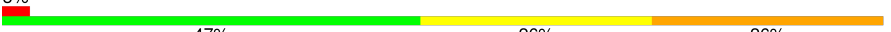

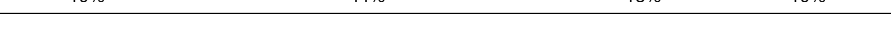
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Mol	Chain	Length	Quality of chain
41	DR	103	
42	BS	110	
42	DS	110	
43	BT	100	
43	DT	100	
44	BU	104	
44	DU	104	
45	BV	94	
45	DV	94	
46	BW	85	
46	DW	85	
47	BX	78	
47	DX	78	
48	BY	63	
48	DY	63	
49	BZ	59	
49	DZ	59	
50	B0	57	
50	D0	57	
51	B1	55	
51	D1	55	
52	B2	46	
52	D2	46	
53	B3	65	
53	D3	65	

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Mol	Chain	Length	Quality of chain
54	B4	38	
54	D4	38	
55	CA	1530	
56	DB	117	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	AA	1607	-	-	-	X
57	MG	AA	1629	-	-	-	X
57	MG	AA	1631	-	-	-	X
57	MG	AA	1641	-	-	-	X
57	MG	AA	1642	-	-	-	X
57	MG	BA	3002	-	-	-	X
57	MG	BA	3005	-	-	-	X
57	MG	BA	3028	-	-	-	X
57	MG	BA	3037	-	-	-	X
57	MG	BA	3041	-	-	-	X
57	MG	BA	3058	-	-	-	X
57	MG	BA	3071	-	-	-	X
57	MG	BA	3072	-	-	-	X
57	MG	BA	3104	-	-	-	X
57	MG	BA	3105	-	-	-	X
57	MG	BA	3109	-	-	-	X
57	MG	BA	3118	-	-	-	X
57	MG	BA	3124	-	-	-	X
57	MG	BA	3132	-	-	-	X
57	MG	BA	3136	-	-	-	X
57	MG	CA	1617	-	-	-	X
57	MG	CA	1625	-	-	-	X
57	MG	CA	1628	-	-	-	X
57	MG	CA	1629	-	-	-	X
57	MG	CA	1637	-	-	-	X
57	MG	CA	1639	-	-	-	X
57	MG	DA	3002	-	-	-	X
57	MG	DA	3041	-	-	-	X
57	MG	DA	3054	-	-	-	X
57	MG	DA	3062	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	DA	3071	-	-	-	X
57	MG	DA	3077	-	-	-	X
57	MG	DA	3101	-	-	-	X
57	MG	DA	3109	-	-	-	X
57	MG	DA	3134	-	-	-	X

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 285420 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 protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AB	218	Total	C	N	O	S	0	0	0
			1704	1081	305	311	7			
1	CB	218	Total	C	N	O	S	0	0	0
			1704	1081	305	311	7			

- Molecule 2 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AC	206	Total	C	N	O	S	0	0	0
			1624	1028	305	288	3			
2	CC	206	Total	C	N	O	S	0	0	0
			1624	1028	305	288	3			

- Molecule 3 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			
3	CD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AE	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			
4	CE	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			

- Molecule 5 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			
5	CF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			

- Molecule 6 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AG	151	Total	C	N	O	S	0	0	0
			1181	735	227	215	4			
6	CG	150	Total	C	N	O	S	0	0	0
			1174	730	226	214	4			

- Molecule 7 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			
7	CH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			

- Molecule 8 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			
8	CI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			

- Molecule 9 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AJ	98	Total	C	N	O	S	0	0	0
			786	493	150	142	1			
9	CJ	98	Total	C	N	O	S	0	0	0
			786	493	150	142	1			

- Molecule 10 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			

- Molecule 11 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			
11	CL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AM	114	Total	C	N	O	S	0	0	0
			883	546	178	156	3			
12	CM	113	Total	C	N	O	S	0	0	0
			876	541	177	155	3			

- Molecule 13 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			
13	CN	95	Total	C	N	O	S	0	0	0
			769	480	159	127	3			

- Molecule 14 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			
14	CO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			

- Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			
15	CP	80	Total	C	N	O	S	0	0	0
			638	400	126	111	1			

- Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AQ	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			
16	CQ	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			

- Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	AR	55	Total	C	N	O	0	0	0
			455	288	86	81			
17	CR	55	Total	C	N	O	0	0	0
			455	288	86	81			

- Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AS	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			
18	CS	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			

- Molecule 19 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			
19	CT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			

- Molecule 20 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AU	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			
20	CU	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			

- Molecule 21 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AA	1533	Total	C	N	O	P	0	0	0
			32895	14671	6036	10655	1533			

- Molecule 22 is a RNA chain called P-site tRNA ASL fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	17	Total	C	N	O	P	0	0	0
			360	161	64	118	17			
22	CV	17	Total	C	N	O	P	0	0	0
			360	161	64	118	17			

- Molecule 23 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	6	Total	C	N	O	P	0	0	0
			125	56	18	45	6			
23	CW	6	Total	C	N	O	P	0	0	0
			125	56	18	45	6			

- Molecule 24 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	BA	2854	Total	C	N	O	P	0	0	0
			61274	27334	11279	19807	2854			
24	DA	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			

- Molecule 25 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			

- Molecule 26 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			
26	DC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			

- Molecule 27 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			
27	DD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			

- Molecule 28 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			
28	DE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			

- Molecule 29 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BF	177	Total	C	N	O	S	0	0	0
			1410	899	249	256	6			
29	DF	178	Total	C	N	O	S	0	0	0
			1420	905	251	258	6			

- Molecule 30 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			
30	DG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			

- Molecule 31 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BH	149	Total	C	N	O	S	0	0	0
			1111	699	197	214	1			
31	DH	149	Total	C	N	O	S	0	0	0
			1111	699	197	214	1			

- Molecule 32 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	DI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			

- Molecule 33 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BJ	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			
33	DJ	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			

- Molecule 34 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BK	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			
34	DK	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			

- Molecule 35 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BL	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			
35	DL	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			

- Molecule 36 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BM	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			
36	DM	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			

- Molecule 37 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BN	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			
37	DN	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			

- Molecule 38 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
38	BO	116	Total	C	N	O	0	0	0
			892	552	178	162			
38	DO	116	Total	C	N	O	0	0	0
			892	552	178	162			

- Molecule 39 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BP	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			
39	DP	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			

- Molecule 40 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	BQ	117	Total	C	N	O	0	0	0
			947	604	192	151			
40	DQ	117	Total	C	N	O	0	0	0
			947	604	192	151			

- Molecule 41 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BR	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			
41	DR	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			

- Molecule 42 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BS	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			
42	DS	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			

- Molecule 43 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BT	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			
43	DT	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			

- Molecule 44 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BU	102	Total	C	N	O	S	0	0	0
			779	492	146	141				
44	DU	102	Total	C	N	O	S	0	0	0
			779	492	146	141				

- Molecule 45 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BV	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			
45	DV	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			

- Molecule 46 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BW	79	Total	C	N	O	S	0	0	0
			596	367	120	108	1			
46	DW	79	Total	C	N	O	S	0	0	0
			596	367	120	108	1			

- Molecule 47 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BX	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			
47	DX	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			

- Molecule 48 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BY	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	DY	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			

- Molecule 49 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BZ	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			
49	DZ	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			
50	D0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			

- Molecule 51 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
51	B1	50	Total	C	N	O	0	0	0
			409	263	75	71			
51	D1	50	Total	C	N	O	0	0	0
			409	263	75	71			

- Molecule 52 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			
52	D2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

- Molecule 53 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			
53	D3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

- Molecule 54 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			
54	D4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

- Molecule 55 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	CA	1530	Total	C	N	O	P	0	0	0
			32831	14642	6024	10635	1530			

- Molecule 56 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	DB	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	BB	4	Total	Mg	0	0
			4	4		
57	BA	136	Total	Mg	0	0
			136	136		
57	CA	42	Total	Mg	0	0
			42	42		
57	DJ	1	Total	Mg	0	0
			1	1		
57	BD	1	Total	Mg	0	0
			1	1		
57	AA	43	Total	Mg	0	0
			43	43		
57	DA	134	Total	Mg	0	0
			134	134		
57	DC	1	Total	Mg	0	0
			1	1		
57	DB	1	Total	Mg	0	0
			1	1		

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	B4	1	Total Zn 1 1	0	0
58	D4	1	Total Zn 1 1	0	0

- Molecule 59 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	AE	1	Total O 1 1	0	0
59	AL	3	Total O 3 3	0	0
59	AN	5	Total O 5 5	0	0
59	AT	3	Total O 3 3	0	0
59	AU	1	Total O 1 1	0	0
59	AA	195	Total O 195 195	0	0
59	BA	615	Total O 615 615	0	0
59	BB	19	Total O 19 19	0	0
59	BC	7	Total O 7 7	0	0
59	BD	2	Total O 2 2	0	0
59	BE	1	Total O 1 1	0	0
59	BL	4	Total O 4 4	0	0
59	BN	2	Total O 2 2	0	0
59	BQ	1	Total O 1 1	0	0
59	BT	1	Total O 1 1	0	0
59	BV	1	Total O 1 1	0	0
59	B2	2	Total O 2 2	0	0
59	B3	3	Total O 3 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	B4	2	Total 2	O 2	0	0
59	CE	3	Total 3	O 3	0	0
59	CI	1	Total 1	O 1	0	0
59	CL	1	Total 1	O 1	0	0
59	CN	2	Total 2	O 2	0	0
59	CT	2	Total 2	O 2	0	0
59	CU	2	Total 2	O 2	0	0
59	CA	196	Total 196	O 196	0	0
59	DC	14	Total 14	O 14	0	0
59	DD	4	Total 4	O 4	0	0
59	DE	2	Total 2	O 2	0	0
59	DJ	3	Total 3	O 3	0	0
59	DL	5	Total 5	O 5	0	0
59	DN	2	Total 2	O 2	0	0
59	DT	2	Total 2	O 2	0	0
59	DU	1	Total 1	O 1	0	0
59	DV	1	Total 1	O 1	0	0
59	D2	1	Total 1	O 1	0	0
59	D3	1	Total 1	O 1	0	0
59	D4	5	Total 5	O 5	0	0
59	DA	598	Total 598	O 598	0	0

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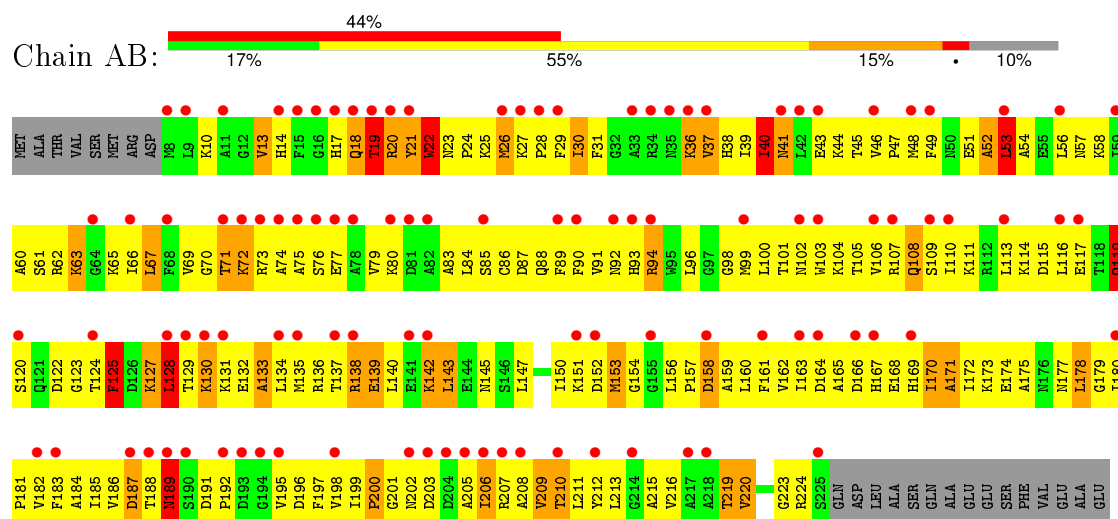
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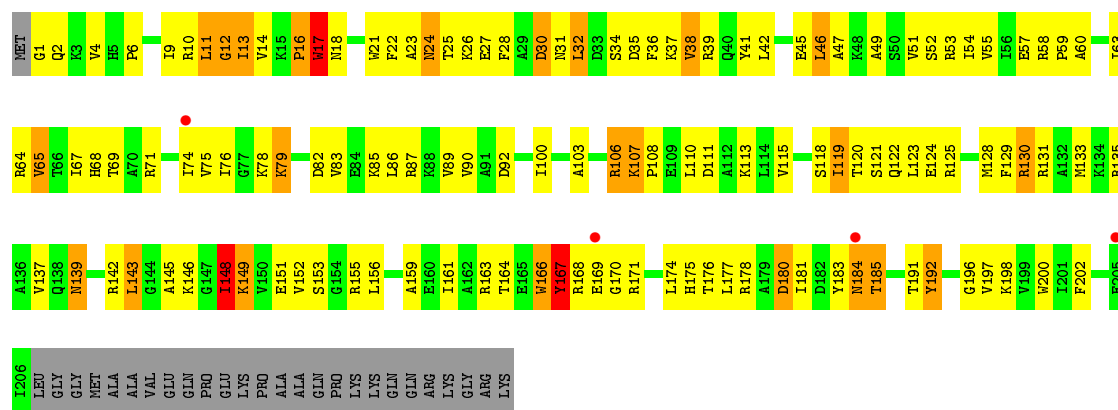
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	DB	4	Total	O	0	0
			4	4		

3 Residue-property plots

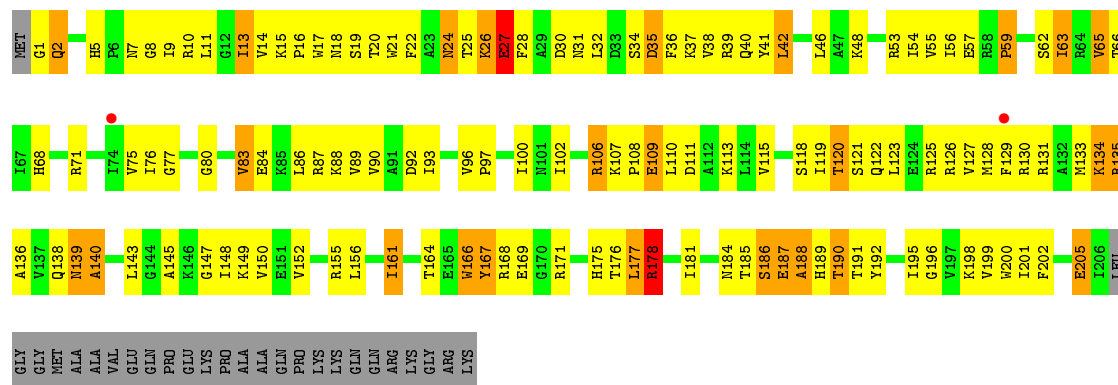
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: 30S ribosomal protein S2

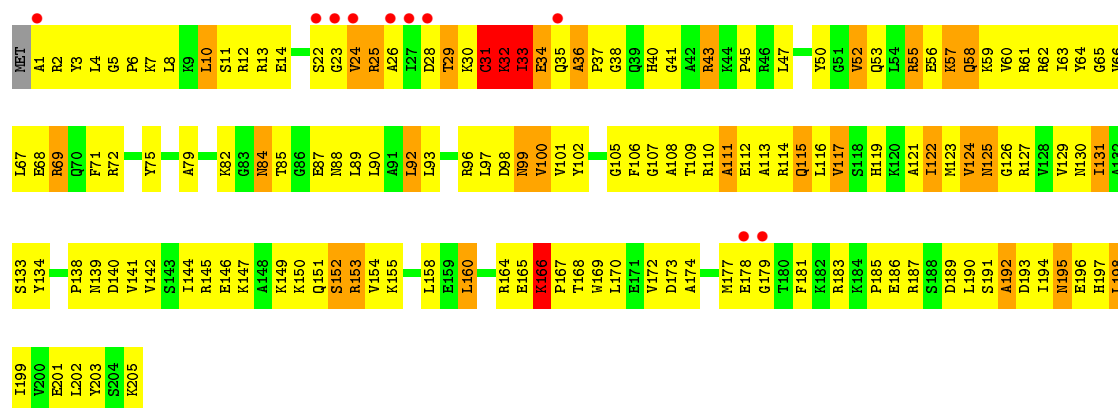




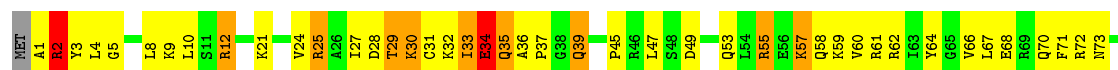
• Molecule 2: 30S ribosomal protein S3

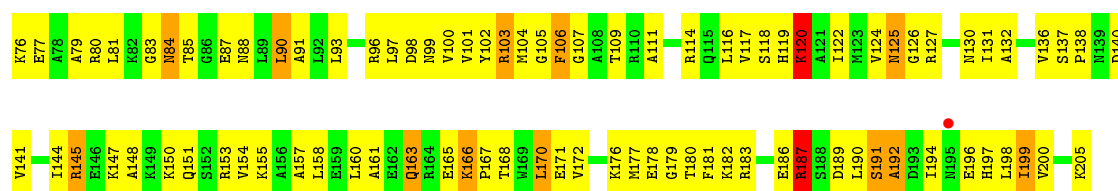


• Molecule 3: 30S ribosomal protein S4

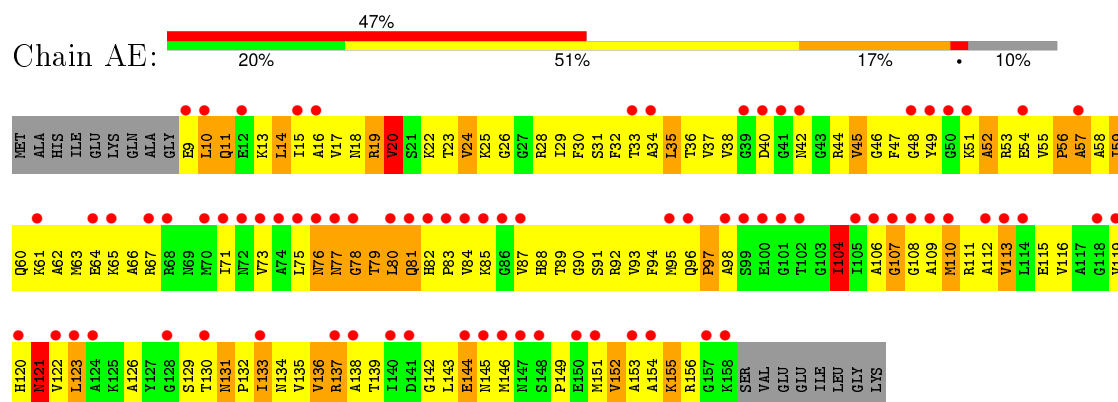


• Molecule 3: 30S ribosomal protein S4

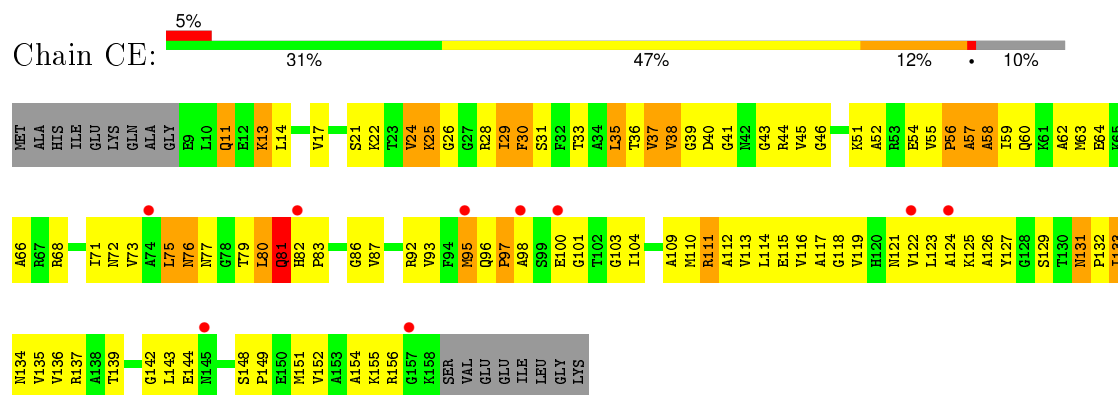




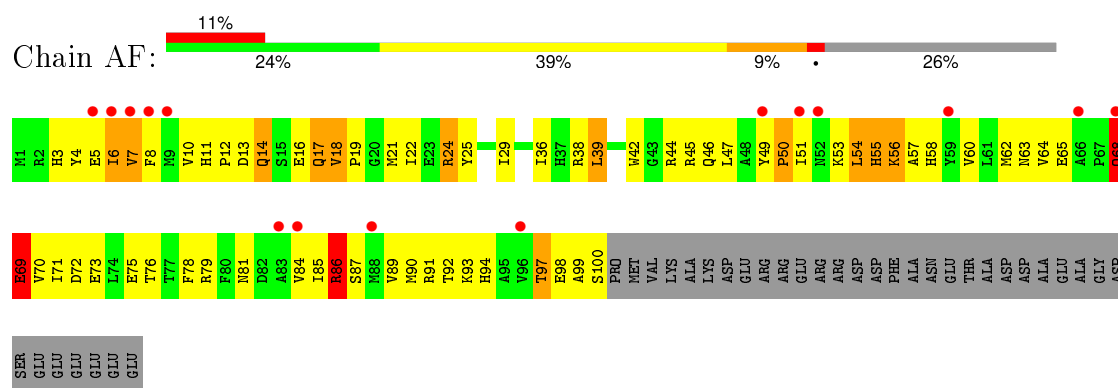
• Molecule 4: 30S ribosomal protein S5



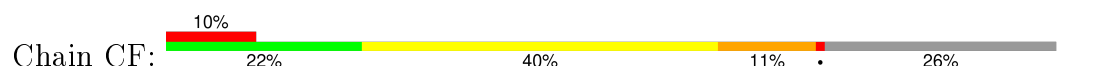
• Molecule 4: 30S ribosomal protein S5

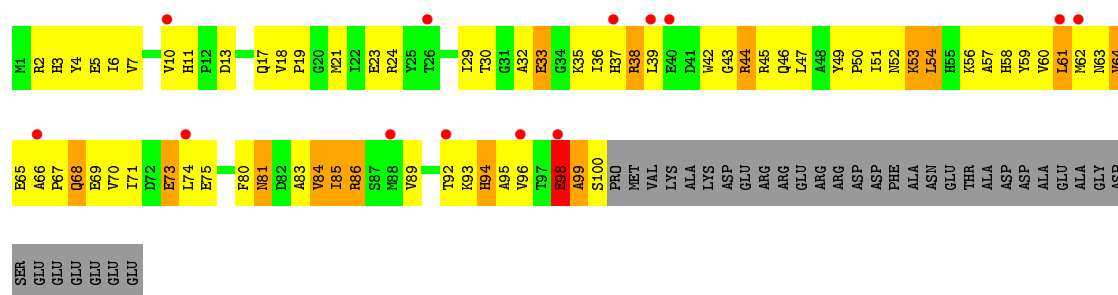


• Molecule 5: 30S ribosomal protein S6

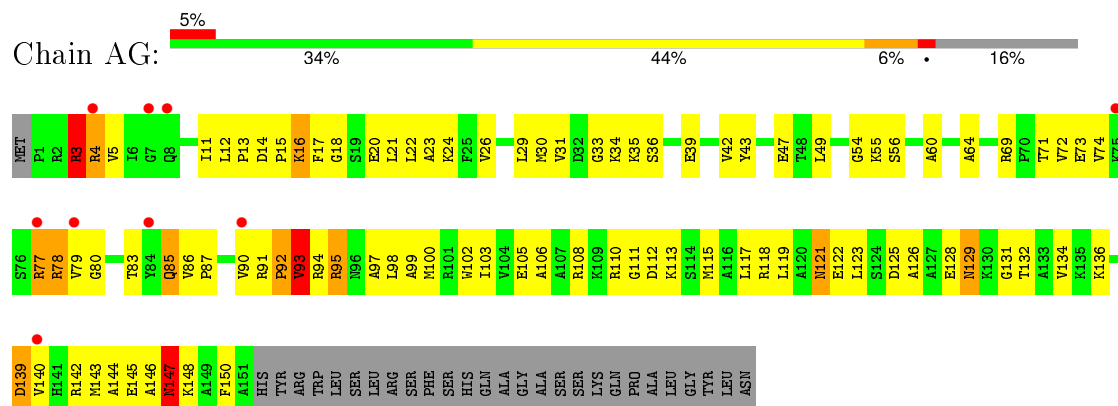


• Molecule 5: 30S ribosomal protein S6

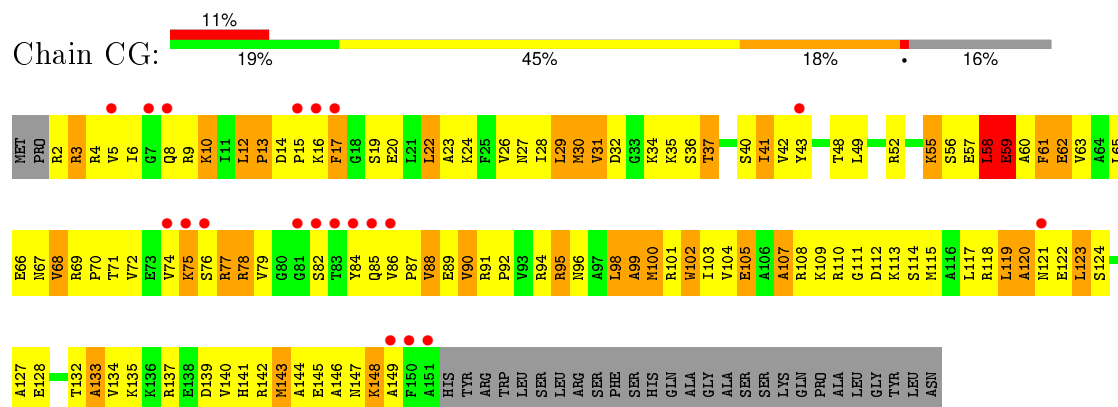




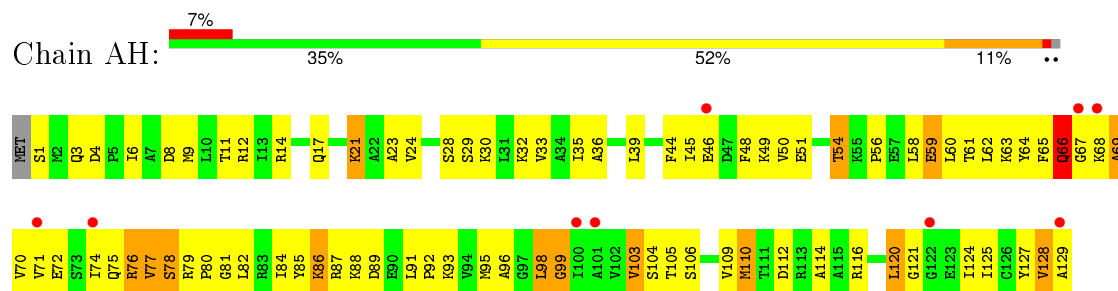
• Molecule 6: 30S ribosomal protein S7



• Molecule 6: 30S ribosomal protein S7

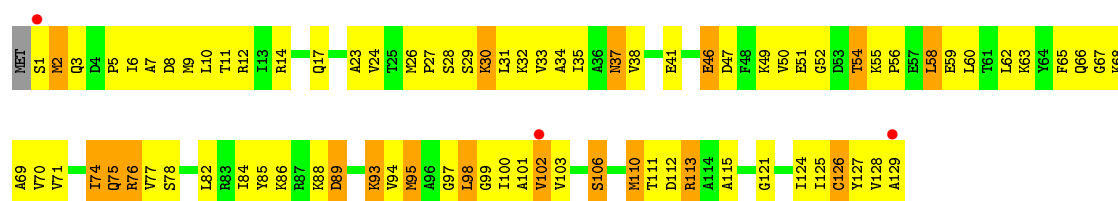


• Molecule 7: 30S ribosomal protein S8

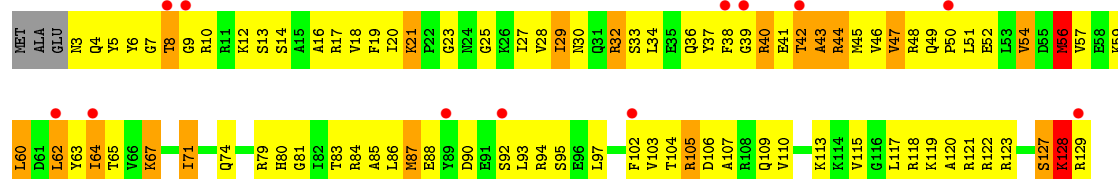


• Molecule 7: 30S ribosomal protein S8

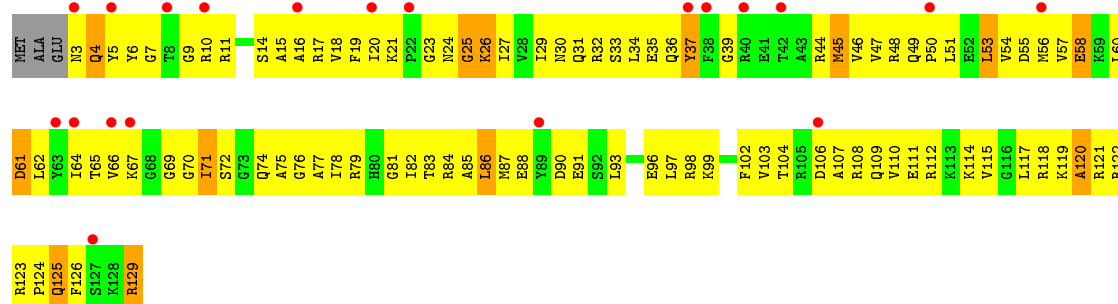




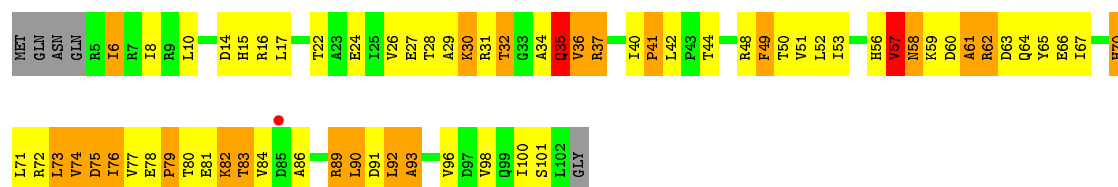
• Molecule 8: 30S ribosomal protein S9



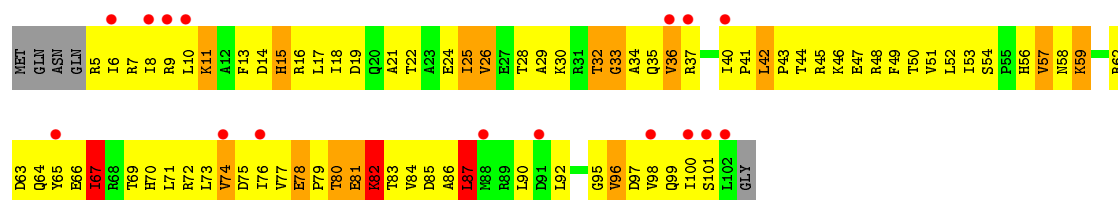
• Molecule 8: 30S ribosomal protein S9



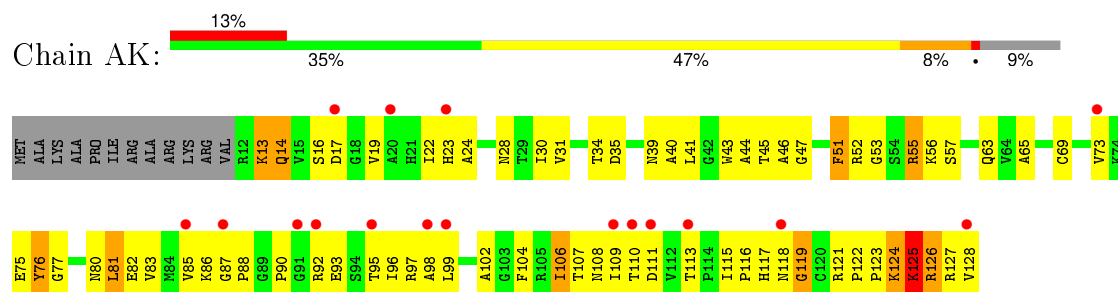
• Molecule 9: 30S ribosomal protein S10



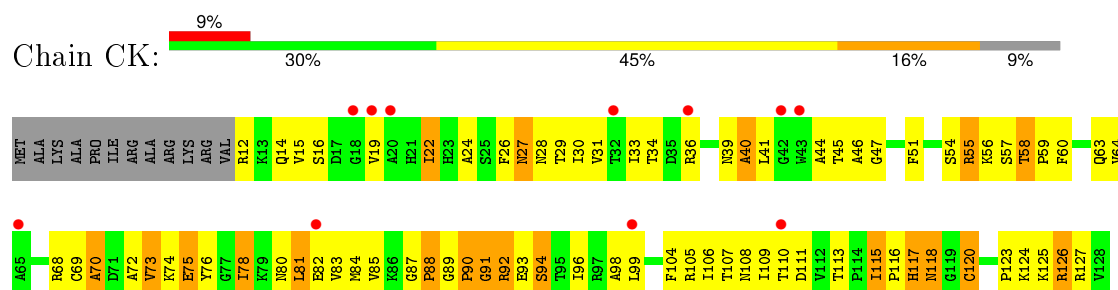
• Molecule 9: 30S ribosomal protein S10



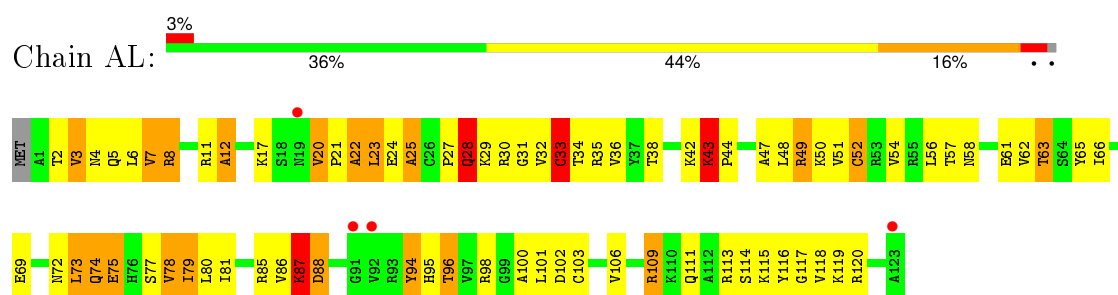
- Molecule 10: 30S ribosomal protein S11



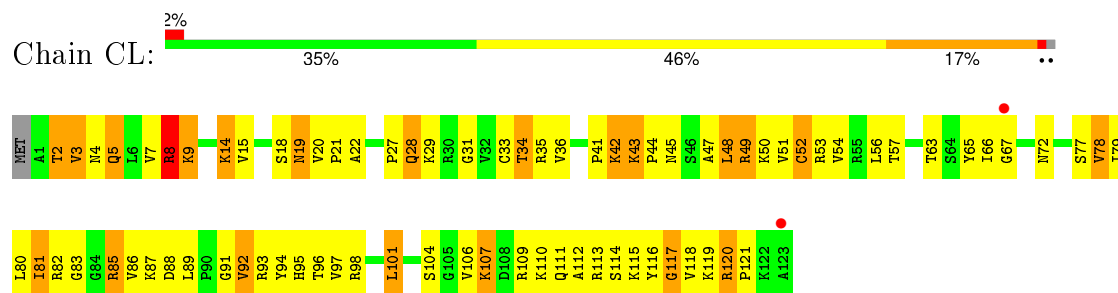
- Molecule 10: 30S ribosomal protein S11



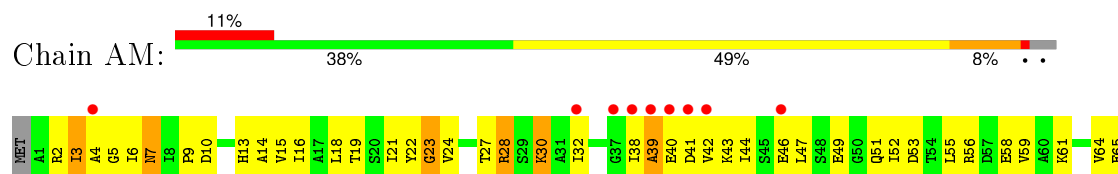
- Molecule 11: 30S ribosomal protein S12

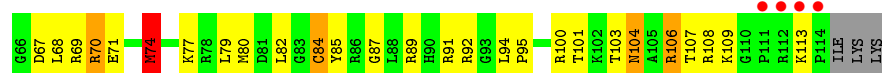


- Molecule 11: 30S ribosomal protein S12

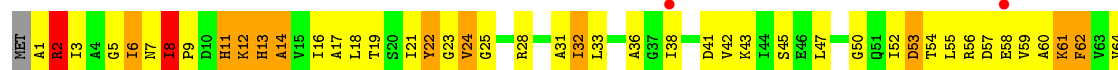


- Molecule 12: 30S ribosomal protein S13





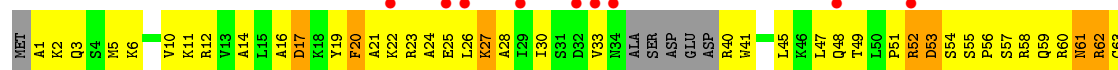
- Molecule 12: 30S ribosomal protein S13



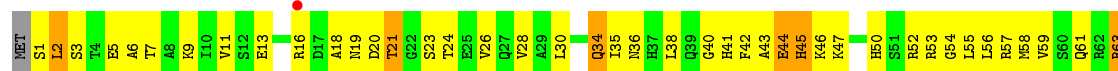
- Molecule 13: 30S ribosomal protein S14



- Molecule 13: 30S ribosomal protein S14

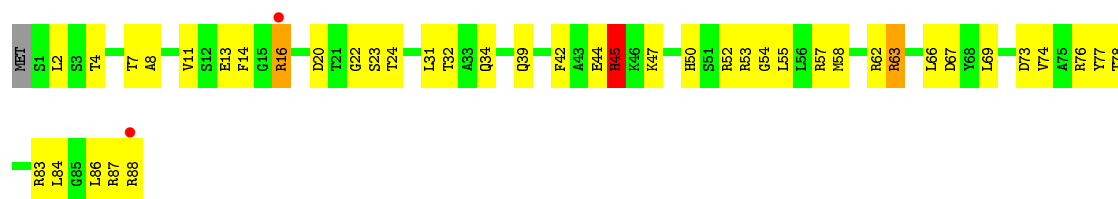


- Molecule 14: 30S ribosomal protein S15

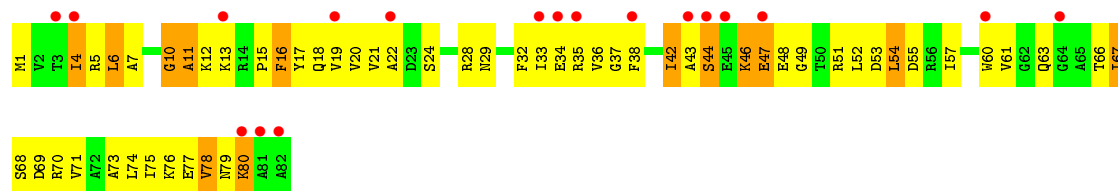


- Molecule 14: 30S ribosomal protein S15





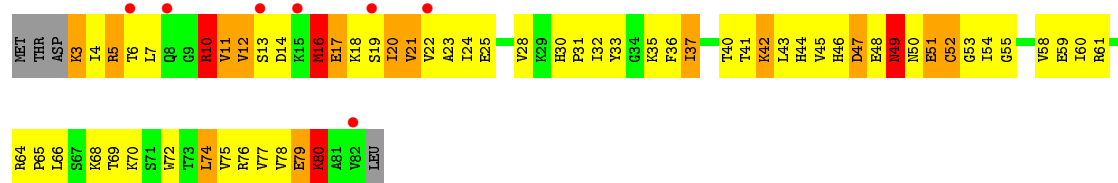
- Molecule 15: 30S ribosomal protein S16



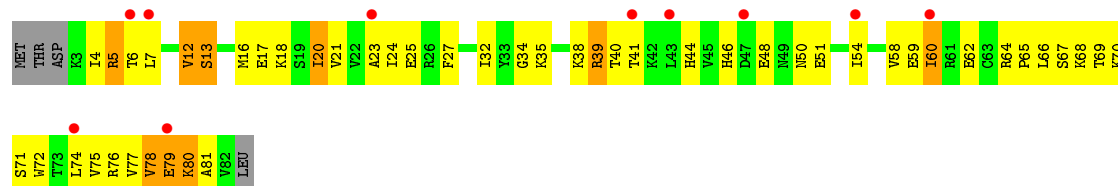
- Molecule 15: 30S ribosomal protein S16



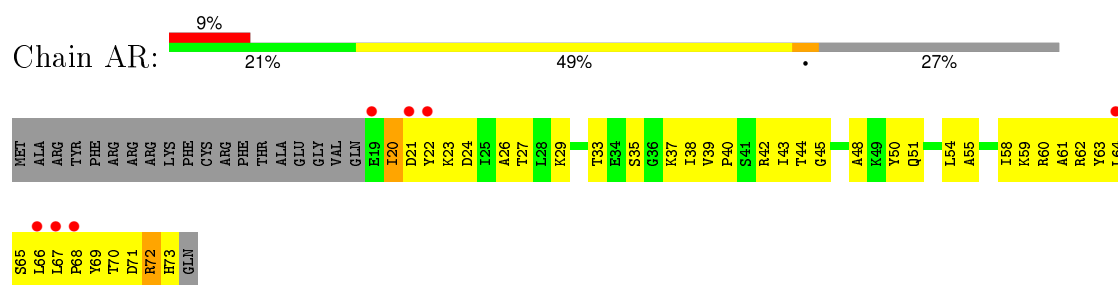
- Molecule 16: 30S ribosomal protein S17



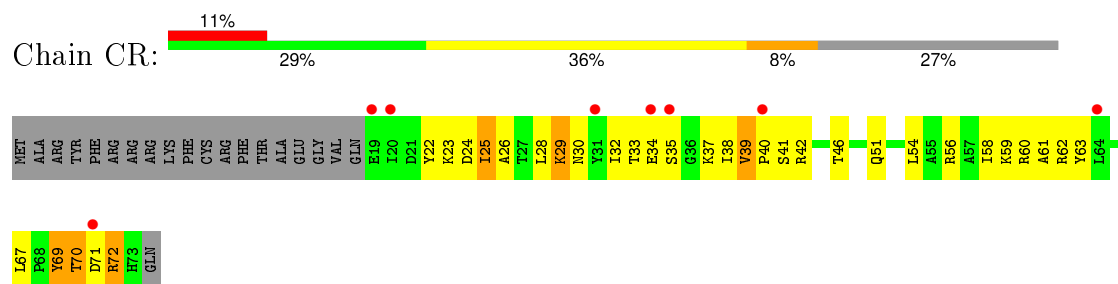
- Molecule 16: 30S ribosomal protein S17



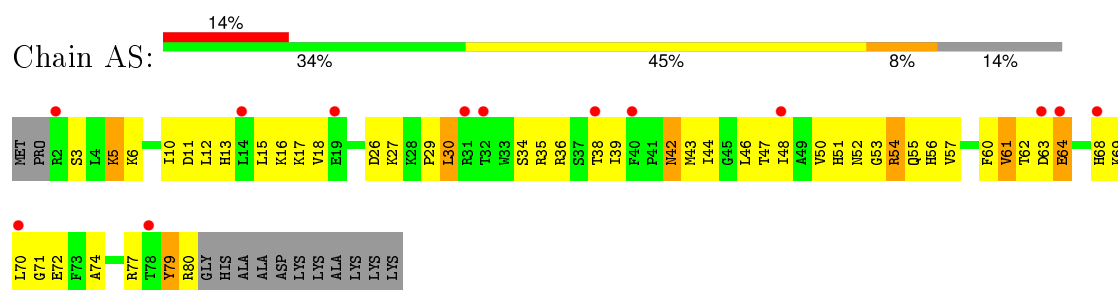
- Molecule 17: 30S ribosomal protein S18



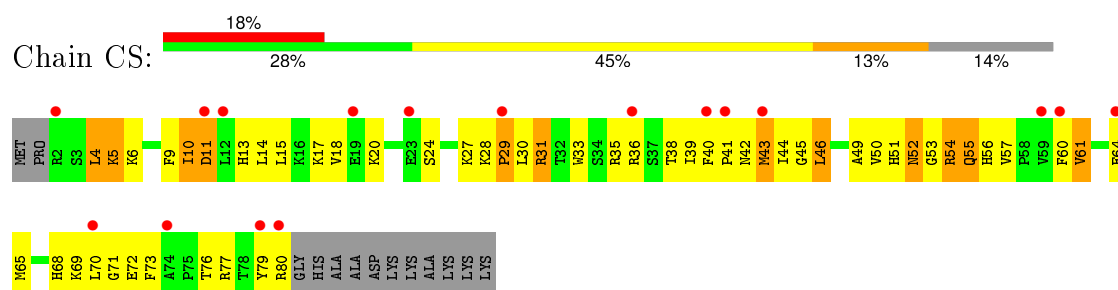
- Molecule 17: 30S ribosomal protein S18



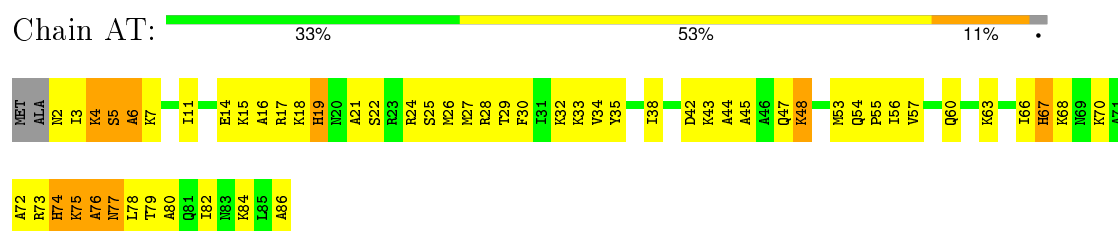
- Molecule 18: 30S ribosomal protein S19



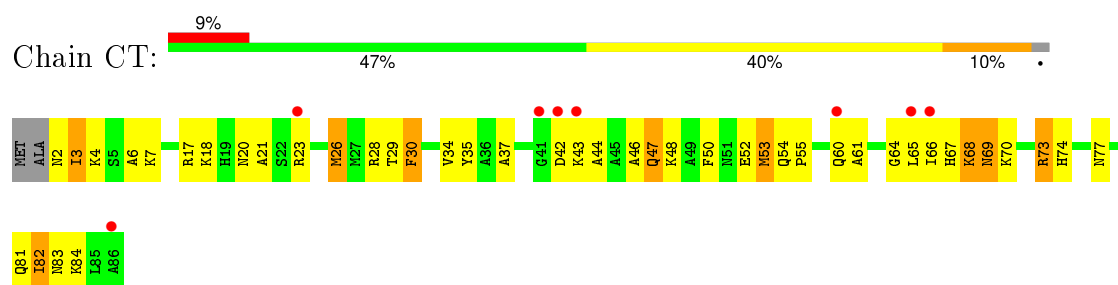
- Molecule 18: 30S ribosomal protein S19



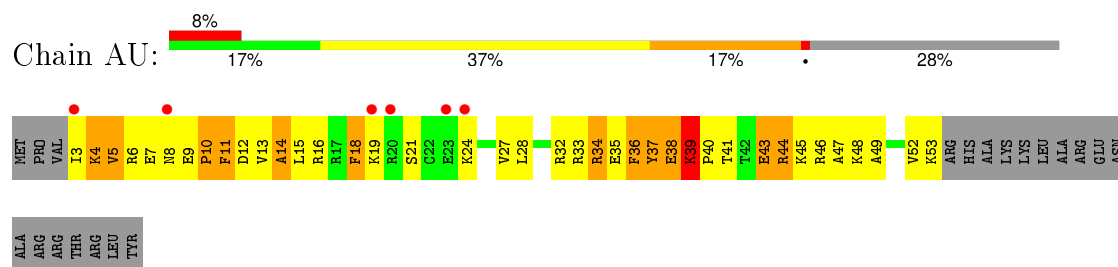
- Molecule 19: 30S ribosomal protein S20



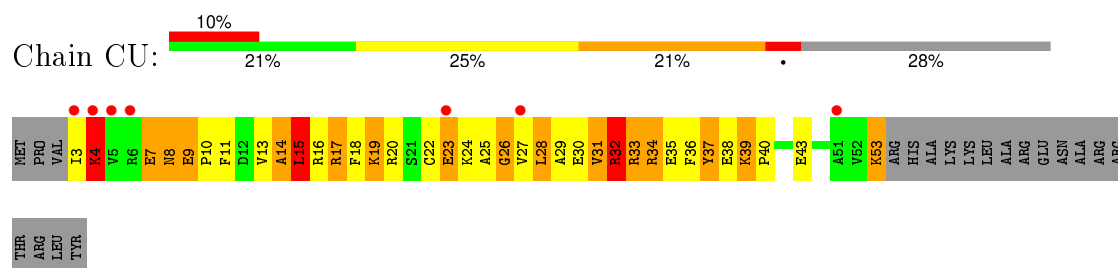
- Molecule 19: 30S ribosomal protein S20



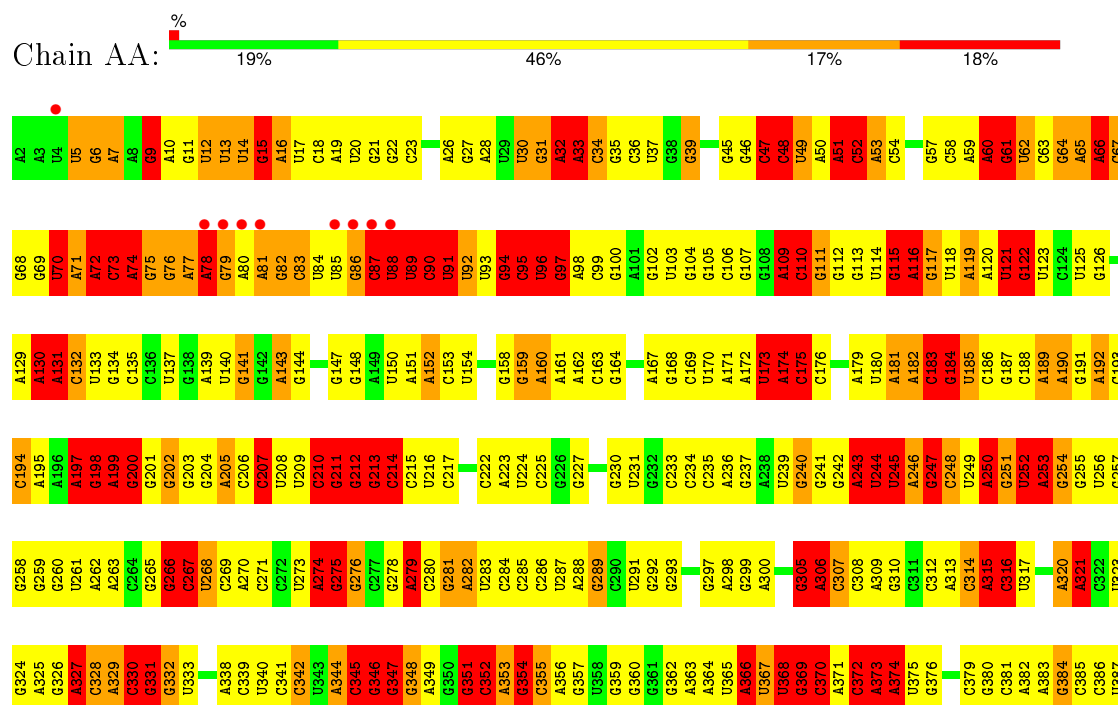
• Molecule 20: 30S ribosomal protein S21



• Molecule 20: 30S ribosomal protein S21



• Molecule 21: 16S rRNA



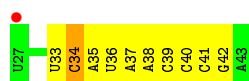
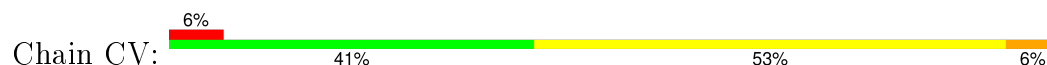
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G1379	G1316	A1251	G1187	G1127	G1057	C995	G928	A864	A718	A653	G654	G587	C525	U463	A389
U1380	C1317	A1252	A1188	C1128	U1060	A996	G929	A865	C719	A955	A655	U589	C526	U464	U390
U1381	A1129	G1253	U1189	C1129	G1061	U997	C930	A866	A790	A656	U657	U590	G527	A465	G391
C1382	A1319	A1254	A1190	A1130	U1062	C998	C931	C866	G791	G721	C558	U591	G530	U467	A392
C1383	G1320	G1255	G1191	G1131	G1063	C999	C934	G867	A792	G722	G58	U592	G531	U468	C393
G1384	U1321	A1256	C1182	C1132	C1064	A1000	A935	C868	U793	U723	U662	C593	U531	C469	G394
G1385	C1322	A1257	U1193	G1133	G1065	C1001	A936	C869	A794	G724	A663	U594	A532	C470	C395
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G1387	C1259	A1196	A1197	U1135	C1066	A1003	A937	U871	C796	G726	A665	A596	U534	U471	U472
C1388	G1260	A1197	A1136	A1004	U1067	A1004	A938	A872	C797	G727	A666	A597	A535	U472	C400
C1389	A1261	G1198	G1137	G1068	C1068	A1005	G939	A873	U798	A728	G667	U598	C536	U473	G404
U1390	U1199	G1138	C1138	A1006	U1070	A1006	C940	G874	G731	G732	G668	C599	G537	U474	G405
U1391	C1200	G1139	C1200	U1007	U1071	U1007	G941	U875	G803	G733	G669	A600	A539	U475	G406
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U1392	U1265	C1141	U1072	U1010	U1073	A946	A846	G877	G735	G736	G671	A602	G541	U477	A408
G1331	C1265	G1142	A1073	U1013	G1074	U947	G947	A878	C810	G739	A673	G604	G544	U478	A411
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A1339	A1275	U1211	U1083	G1020	A1082	U957	U957	A889	G818	G748	C580	C614	U552	U486	G419
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C1341	G1277	A1152	G1084	A1022	U1084	A958	U958	C890	U820	G749	A554	G616	A554	U488	G421
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U1350	A1286	C1162	U1093	G1032	U1093	C967	C967	A901	U829	A759	A564	C625	U562	U497	G430
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U1353	A1289	U1165	C1096	A1035	C1096	A971	A971	U904	A832	U762	A567	G628	C565	A503	C436
G1354	U1290	G1166	C1097	A1036	C1097	A972	A972	U905	A833	C763	A568	G629	C566	U437	U437
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U1356	U1224	A1168	C1100	C1038	C1100	A974	A974	A907	U835	C765	A570	U632	C568	U439	U439
U1357	A1225	C1169	A1101	G1039	C1101	A975	A975	C910	G836	A766	A571	U633	C569	U440	A436
U1358	C1226	U1170	A1102	U1040	U1102	A976	A976	U911	U837	A767	A572	U634	C570	A441	A437
U1359	G1227	A1171	C1103	U1041	C1103	A977	A977	C912	G838	A768	A573	U635	C571	A442	U438
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U1361	C1229	U1173	A1105	G1043	G1105	C979	C979	A914	C840	C770	A575	U637	C573	A444	G449
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U1367	G1235	A1180	U1116	U1049	U1116	A985	A985	A920	A846	A776	A581	U643	C579	A450	G455
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U1371	A1239	U1183	C1120	U1053	C1053	A989	A989	A924	C858	A780	A585	U647	C583	A454	A457
U1372	C1240	G1184	U1121	C1054	C1054	U990	U990	C925	G859	A781	A586	U648	C584	A455	A458
U1373	U1241	U1185	U1122	U1055	C1055	U991	U991	G926	A860	A782	A587	U649	C585	A456	A459
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U1375	U1243	U1186	U1124	C1057	C1057	U993	U993	G928	A862	A784	A589	U651	C587	A458	A461
U1376	C1244	C1249	U1125	U1058	A1058	U994	U994	G929	A863	A785	A590	U652	C588	A459	A462
U1377	U1245	U1187	U1126	C1059	C1059	U995	U995	G930	A864	A786	A591	U653	C589	A460	A463
U1378	G1246	C1249	U1127	U1060	C1060	U996	U996	G931	A865	A787	A592	U654	C590	A461	A464
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U1380	C1248	U1189	U1129	U1062	C1062	U998	U998	G933	A867	A789	A594	U656	C592	A463	A466
U1381	U1249	U1190	U1130	U1063	C1063	U999	U999	G934	A868	A790	A595	U657	C593	A464	A467
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U1383	A1251	A1192	U1132	U1065	C1065	C1001	A936	C936	A792	G722	A597	U659	C595	A466	A469
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U1385	U1322	A1257	U1193	U1067	C1067	C1002	A938	A871	G724	G724	A599	U661	C597	A468	C471
G1386	G1258	U1258	U1194	U1068	C1068	A1003	A939	A872	G725	G725	A600	U662	C598	A469	C472
G1387	C1259	A1196	A1197	U1069	C1069	A1004	A940	A873	G726	G726	A601	U663	C599	A470	C473
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G1389	A1261	G1198	G1137	U1071	U1071	A1006	G942	U875	G728	G728	A603	U665	C601	A472	G405
U1390	U1199	G1138	C1138	U1072	U1072	U1007	G943	C876	G729	G729	A604	U666	C602	A473	G406
A1329	C1200	G1139	C1200	U1073	U1073	U1008	G944	U876	G730	G730	A605	U667	C603	A474	G407
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U1393	C1265	G1142	A1073	U1076	U1076	U1011	A946	C879	G733	G733	A608	U670	C606	A477	U407
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C1398	G1272	C1147	U1078	A1018	U1081	U1016	A951	C884	G738	G738	A613	U675	C611	A482	A414
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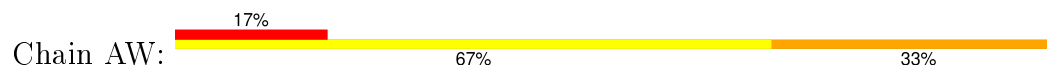
• Molecule 22: P-site tRNA ASL fragment



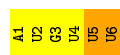
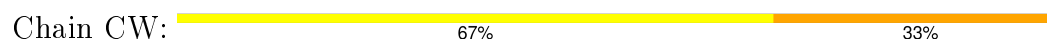
• Molecule 22: P-site tRNA ASL fragment



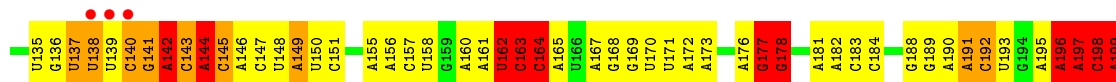
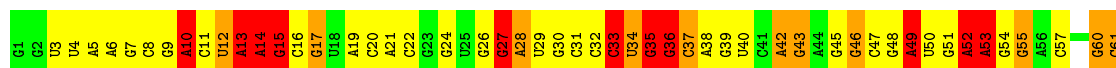
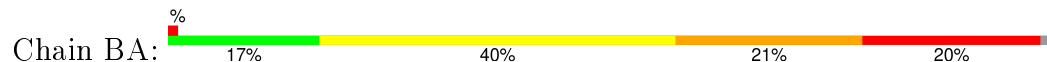
• Molecule 23: messenger RNA



• Molecule 23: messenger RNA

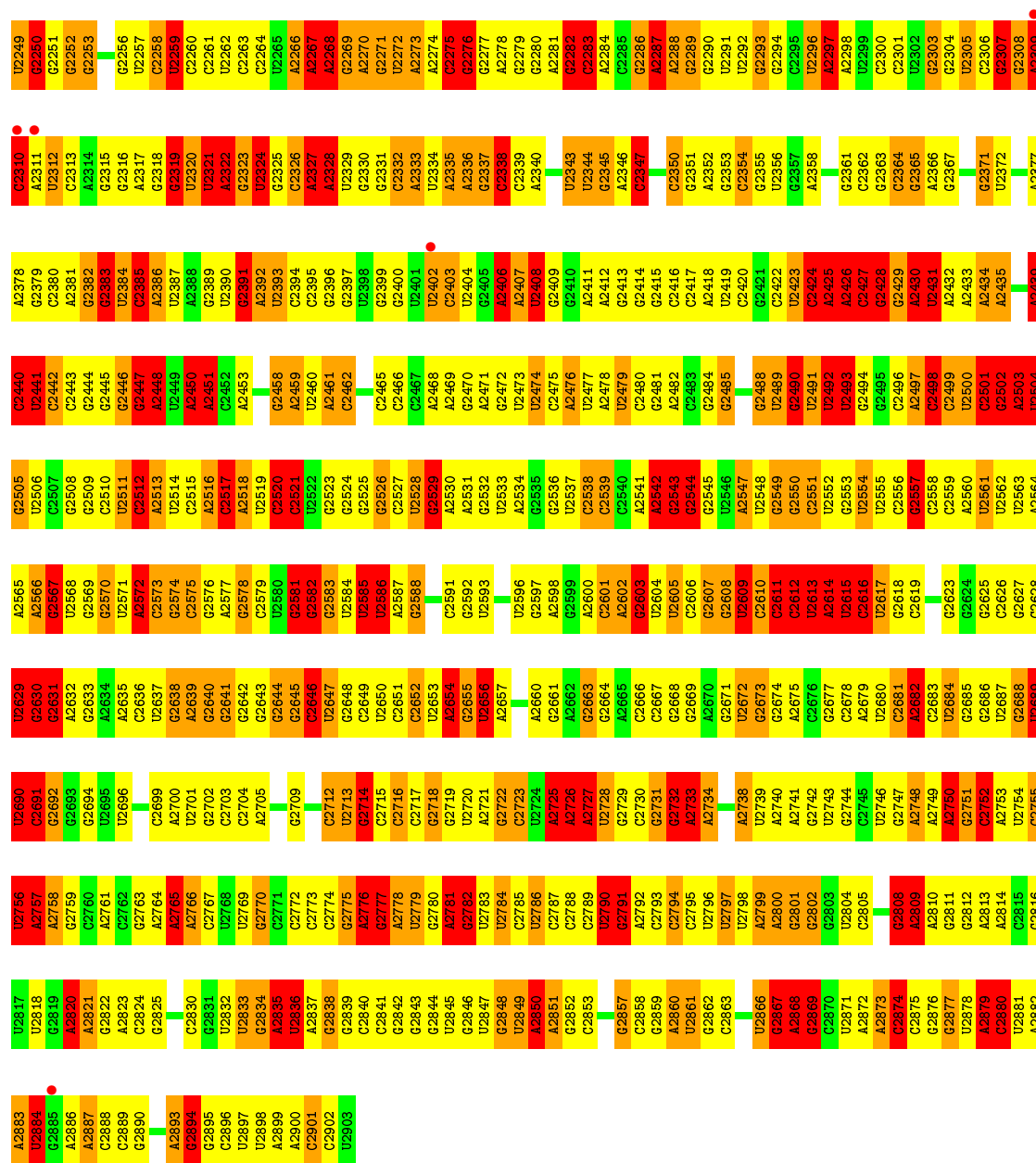


• Molecule 24: 23S rRNA

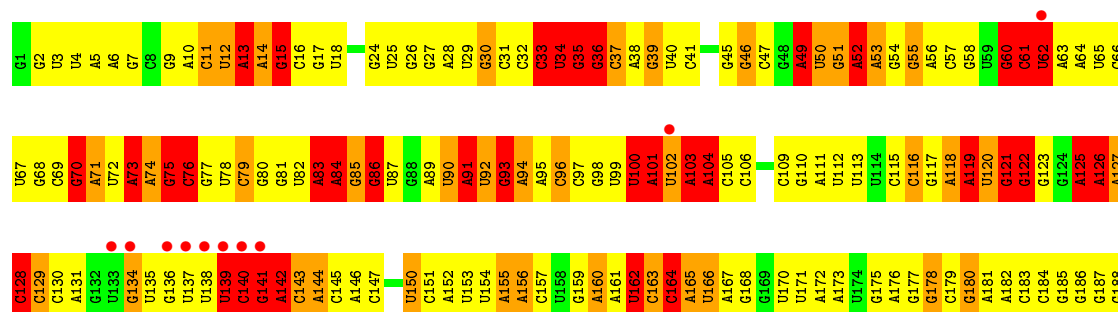
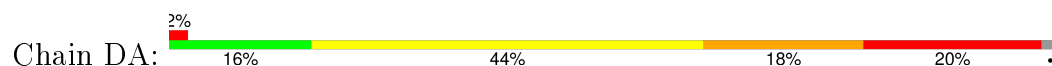


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G962	G963	G964	G965	G966	G967	G968	G969	G970	G971	G972	G973	G974	G975	G976	G977	G978	G979	G980	G981	G982	G983	G984	G985	G986	G987	G988	G989	G990	G991	G992	G993	G994	G995	G996	G997	G998	G999	G1000	G1001	G1002	G1003	G1004	G1005	G1006	G1007	G1008	G1009	G1010	G1011	G1012	G1013	G1014	U1015	U1016	U1017	U1018	U1019	U1020	U1021	U1022	U1023	U1024																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
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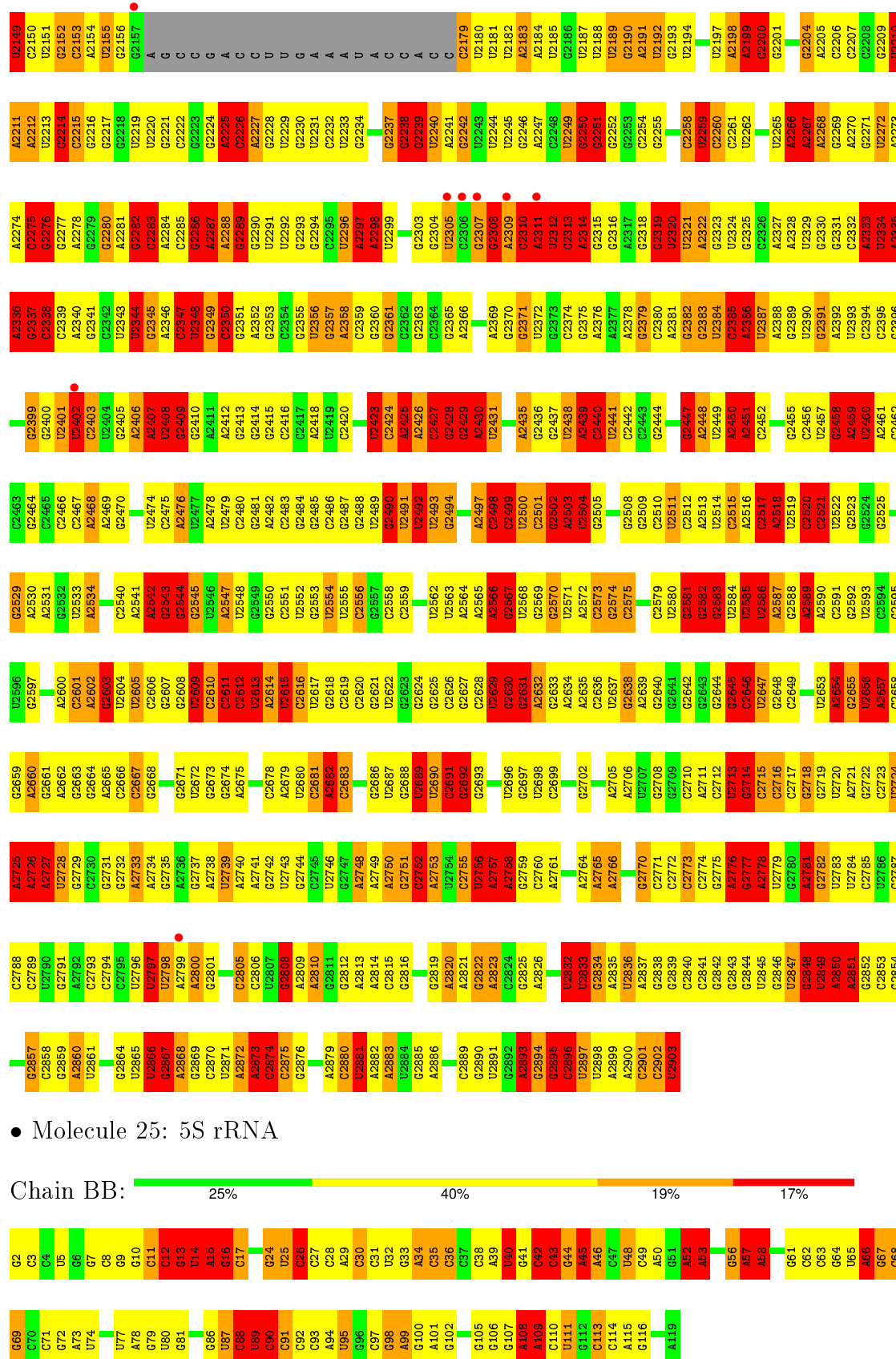


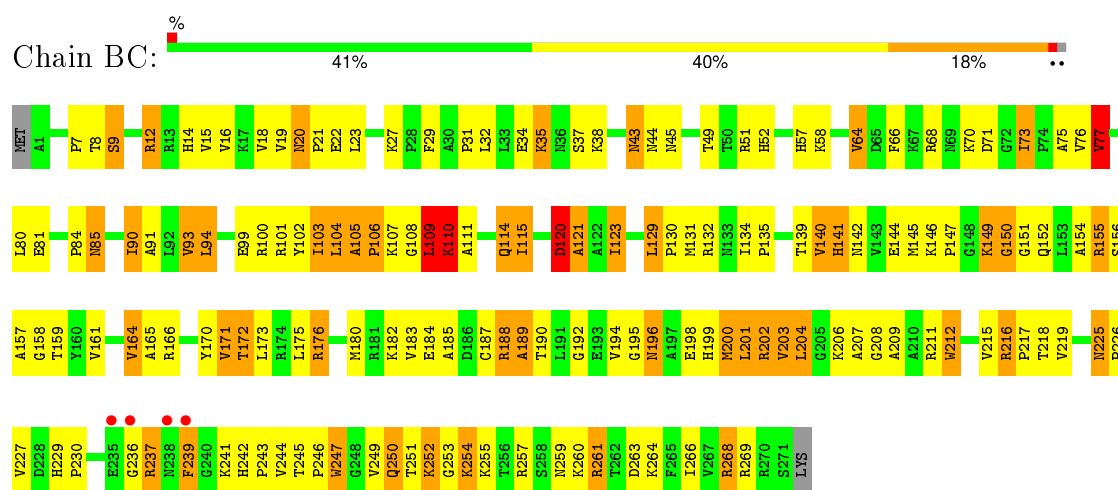
Molecule 24: 23S rRNA



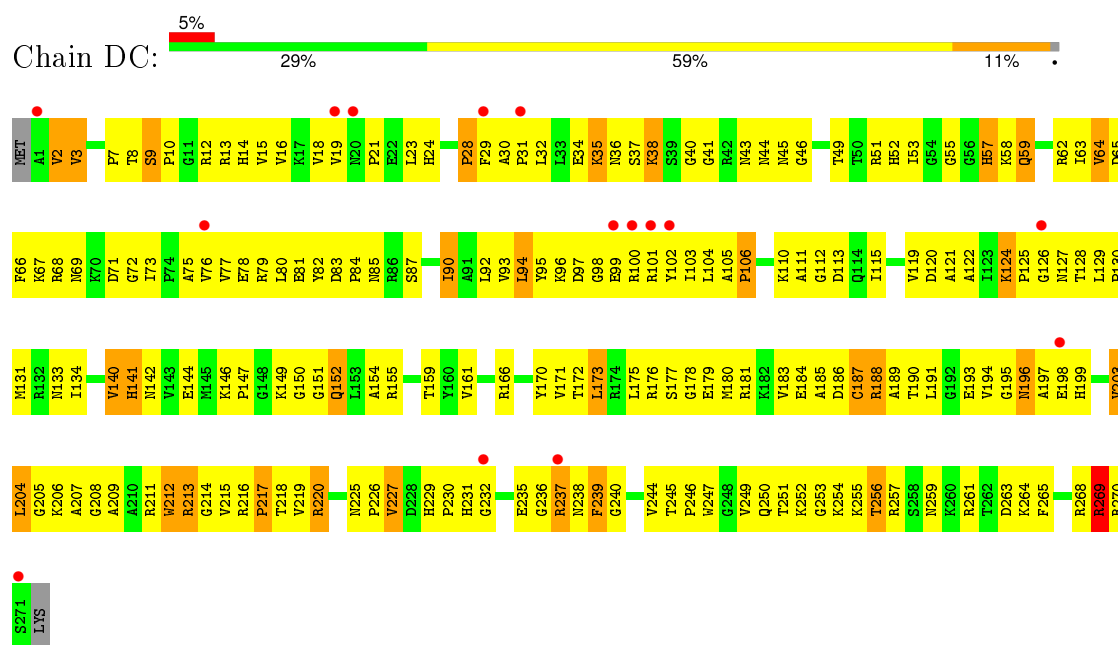
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G1139	A1077	G1016	G955	C	G823	A761	G696	G630	U567	A502	A251	G377	G316	A251	A191
C1140	U1078	U1017	G956	A	U824	U762	G697	A631	U568	A503	A439	G378	G317	C192	C192
U1141	C1079	U1018	C957	U	A825	G763	A699	A632	U569	A504	C253	G379	C318	C253	U193
A1142	A1080	U1019	U958	C	U826	A764	G700	A633	G570	A505	U441	G380	G319	G254	G194
A1143	U1081	A1020	A959	C	U827	G765	G700	C634	U571	G506	G442	C381	A320	A255	A195
A1144	U1082	G1021	A960	C	U828	U766	G701	C635	A572	G507	A443	A382	U321	A196	A196
C1145	U1083	A1022	A961	C	A829	U767	G701	C636	U573	A508	A444	C383	U322	G259	A197
C1146	U1084	G1023	G962	A	G830	U768	G704	A637	A574	C509	C445	G386	C323	G260	C198
U1149	A1085	U1024	G963	C	G831	U769	A705	G638	A575	C510	G446	G387	A324	A199	A199
C1150	U1086	G1025	C964	U	U832	U773	A706	U639	U576	U511	A447	U387	G325	A262	U200
C1151	A1088	G1026	C965	U	A833	G774	G707	C640	G577	G512	U448	G388	G326	G263	C201
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G1154	G1091	U1030	C968	C	G836	G777	G711	U645	U580	A515	U451	U391	U329	G266	A204
A1155	U970	G1031	G969	C	U839	G778	A715	G646	C581	G518	G452	U392	A330	G205	G205
A1156	U1092	A1032	U971	G	G840	G779	A716	G647	C582	U519	A453	U393	A331	C269	U206
U1093	G1093	C1033	G971	G	G841	U780	A717	G648	G583	U520	A454	U394	A332	A270	A207
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A1095	G973	G1035	C973	C	G843	A782	C719	U652	G585	U522	A457	U397	G334	A272	C209
A1096	G974	U1036	C908	C	A844	A783	U720	U653	A586	G524	C458	U398	C335	G273	C210
U1097	A975	G1037	A909	C	U845	A784	U721	A654	C587	U525	U459	U399	C336	C274	C211
A1098	G976	G1038	A910	C	U846	G785	A722	A655	U588	A526	A460	U400	C337	C275	G212
G1099	G977	A1039	A911	C	U847	G786	G723	G656	U589	C527	C461	G401	G338	U276	G213
C1100	G978	A1040	C912	C	G848	C787	G724	U657	A590	G528	G462	A402	U339	G277	G214
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G1102	C1042	U1042	C914	C	U850	G789	A726	U659	A592	G530	A464	U404	A341	A279	A216
A1103	C1043	C1043	C915	C	C851	U790	G726	G659	U593	G531	U466	U405	A342	U280	A217
C1104	A983	U1044	U929	C	U852	A791	A727	C660	U594	C532	G465	U406	C343	C281	A218
U1045	A984	G1045	C930	C	C853	C791	G728	A661	C595	A532	A466	G406	A344	A282	A219
C985	C985	A1046	U919	C	G854	A792	G729	G662	G600	G533	C467	G407	A345	G283	G220
C986	C986	U1047	A920	C	G855	A793	A730	U663	G601	U534	G468	U408	A346	U284	A221
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A988	C922	U1049	C922	C	G857	C795	G732	U665	G603	G536	G477	U410	A348	U286	A223
A989	G923	A1050	G923	C	G858	C796	G733	U666	A604	G537	A472	G411	U349	G287	U224
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C992	A925	C1052	A925	C	U860	G798	A735	U668	G606	G539	G474	C413	C351	U289	A226
C993	G926	C1053	G926	C	A861	G799	G736	U669	U606	C540	C475	C414	A352	U292	A227
G994	A928	G1055	A928	C	G862	A800	U737	A670	U607	A541	G476	A415	C353	U293	C228
C995	U929	G1056	U929	C	A863	G801	A738	C672	A608	G544	A478	U416	A354	A294	C229
A996	A996	A1057	C930	C	G864	A802	G739	C673	A609	U545	A479	C417	U355	G293	G230
G997	U931	U1058	U931	C	C965	U803	A741	A675	C610	U546	A480	C418	G356	G295	A231
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G1002	G1002	C1063	G1002	C	U871	G809	U746	G682	G616	C550	C484	A424	A363	A300	C236
U1003	A941	U1064	A941	C	U872	U810	U747	U683	A617	G553	C485	G424	G364	G301	C237
U1004	G942	U1065	G942	C	C873	U811	G748	G684	G618	U554	G489	C426	U365	G302	C238
C1005	A943	U1066	A943	C	G874	C812	A749	G685	G619	G555	C490	U427	U366	U304	C239
C1006	C944	U1067	A944	C	U875	U813	A750	U686	G620	U558	G491	A428	C367	C305	C240
C1007	U1007	G1068	A945	C	C876	C814	A751	C687	A621	U559	A492	A429	A368	G242	A241
A1008	C946	A1069	C946	C	A877	C815	A752	U688	G622	G560	G493	A430	U369	G308	U243
A1009	A947	U1070	A947	C	A878	C816	A753	A689	G623	C561	G494	U431	U370	A244	A244
A1010	C948	G1071	C948	C	G	C817	U754	G690	C624	G562	A497	A432	A371	A309	G245
U1011	G949	C1072	G949	C	G	G818	U755	G691	G625	U563	A498	C433	G372	A310	G246
U1012	C1012	U1012	U1012	C	G	A819	A756	C692	A626	A563	G499	U434	U373	C247	C247
C1013	G952	G1074	G952	C	G	A820	G757	A693	A627	C564	U499	C435	A374	G313	G248

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A2090	G1959	G1960	G2027	G1959	G1896	C1830	U1769	G1702	C1639	C1575	G1514	G1452	G1389	A1328	U1264	C1200
G2093	G1961	C1832	U2028	C1832	G1897	G1831	C1771	C1706	A1640	C1576	A1515	A1453	U1390	C1329	A1265	U1201
A2030	C1962	C1833	G2029	C1833	G1898	C1832	G1772	G1707	A1641	C1577	A1516	G1454	U1391	C1330	G1266	G1202
A2031	C1963	A1899	A2030	U1834	A1900	G1833	A1773	G1708	G1642	U1578	G1517	G1455	A1392	G1331	U1267	U1203
G2032	G1964	A1901	G2032	G1835	A1901	G1834	C1774	U1709	G1643	A1579	C1518	G1456	A1393	G1332	A1268	A1204
A2033	C1965	A1902	A2033	C1836	G1902	G1835	C1775	U1710	C1644	A1580	G1519	U1457	U1394	G1333	A1269	A1205
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A2037	A1969	G1906	A2037	U1840	G1906	U1714	U1779	U1714	G1649	A1585	G1524	C1462	U1398	G1337	G1273	U1209
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C2045	A1977	U1916	C2045	G1849	U1916	G1722	A1787	U1722	U1657	C1592	A1532	A1469	U1406	C1345	G1281	U1219
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G2047	U1979	A1918	G2047	A1853	A1918	G1724	U1789	G1724	G1661	A1596	U1534	G1473	G1408	A1347	U1283	G1221
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G2057	U1929	U1930	G2057	U1864	U1930	G1739	C1800	G1739	A1670	C1605	G1543	U1489	G1426	C1362	G1233	U1234
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G2060	G1933	G1933	G2060	G1868	G1933	G1736	A1803	U1736	G1673	A1609	A1548	U1489	G1429	G1364	G1238	G1237
A2061	C1934	A1934	A2061	C1869	G1934	G1737	C1804	G1737	C1674	A1608	A1549	U1489	G1430	A1302	G1239	U1240
G2062	G1935	G1935	G2062	G1870	G1935	G1740	A1805	G1740	A1677	C1612	A1551	U1489	G1431	A1303	U1241	A1242
C2063	A1936	A1936	C2063	C1871	A1936	U1747	G1806	U1747	G1684	G1619	C1557	U1490	G1432	G1365	G1297	C1233
G2064	U1937	A1937	G2064	G1872	U1937	U1748	G1807	U1748	G1685	G1620	C1558	U1491	G1433	A1304	U1298	U1234
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G2068	A1941	C1941	G2068	A1876	C1941	A1745	G1811	A1745	G1682	C1617	C1556	A1494	G1437	G1371	U1312	G1248
A2069	C1942	C1942	A2069	A1877	C1942	U1746	U1812	U1746	U1683	A1618	C1557	U1495	U1375	G1372	U1249	U1250
U2070	U1943	U1943	U2070	G1878	U1943	U1747	G1813	U1747	G1684	G1619	C1558	U1497	G1438	G1373	C1314	C1251
C2071	G1944	G1944	C2071	U1880	G1944	U1750	A1815	G1750	C1686	C1624	U1560	U1498	U1439	G1374	G1315	G1252
A2072	U1945	A1945	A2072	C1881	U1945	U1751	C1816	U1751	G1687	C1625	C1561	C1499	G1437	G1375	U1316	A1253
G2073	U1946	U1946	G2073	G1884	U1946	G1752	G1817	G1752	U1688	G1626	U1562	G1500	U1438	G1376	G1317	U1254
U2074	A2014	A2014	U2074	U1885	A2014	G1753	A1819	G1753	A1689	G1627	C1563	G1501	U1440	G1377	U1318	U1255
G2075	U2016	U2016	G2075	U1886	U2016	U1756	U1820	U1756	U1690	G1628	C1564	A1504	G1441	U1378	G1319	G1256
U2076	U2017	U2017	U2076	A1887	U2017	A1757	U1821	A1757	U1693	G1631	C1565	A1505	U1442	G1380	C1320	U1257
A2077	G1948	G1948	A2077	C1888	G1948	U1758	A1822	U1758	G1694	G1632	G1567	U1506	U1443	G1381	G1321	U1258
G2078	U1951	U1951	G2078	A1889	U1951	G1759	A1823	G1759	G1695	A1633	U1568	C1507	G1444	G1382	A1322	G1259
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U2080	G1953	G1953	U2080	G1891	G1953	C1761	U1825	C1761	G1697	A1634	A1570	A1509	C1446	A1384	G1324	G1261
A2081	C1954	C1954	A2081	G1892	C1954	U1762	G1826	U1762	A1698	A1635	A1571	G1510	G1448	A1385	C1325	U1262
C2082	U1955	U1955	C2082	C1893	U1955	G1763	G1827	G1763	G1699	U1636	A1572	G1511	G1449	C1386	C1326	G1263
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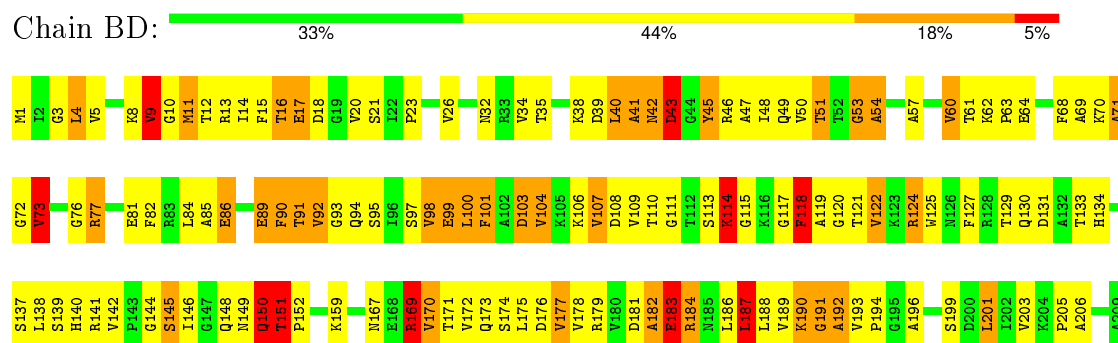




• Molecule 26: 50S ribosomal protein L2

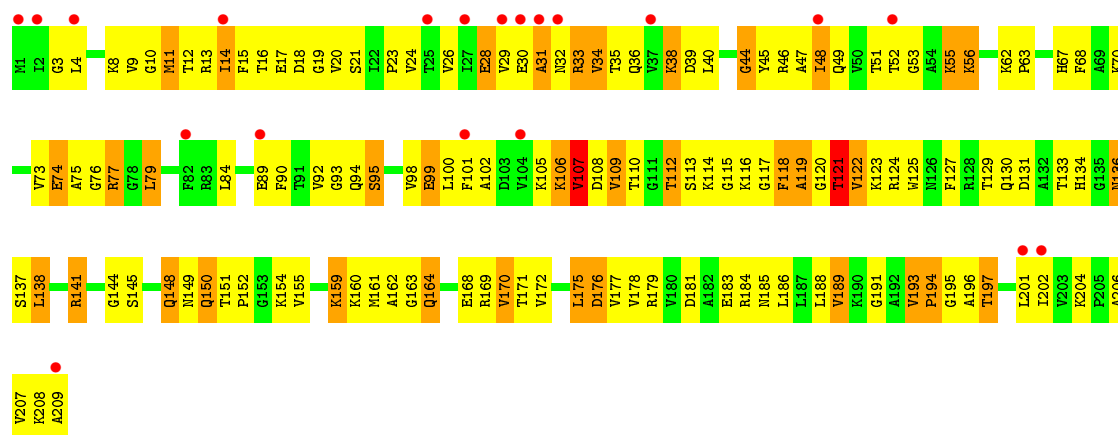


• Molecule 27: 50S ribosomal protein L3

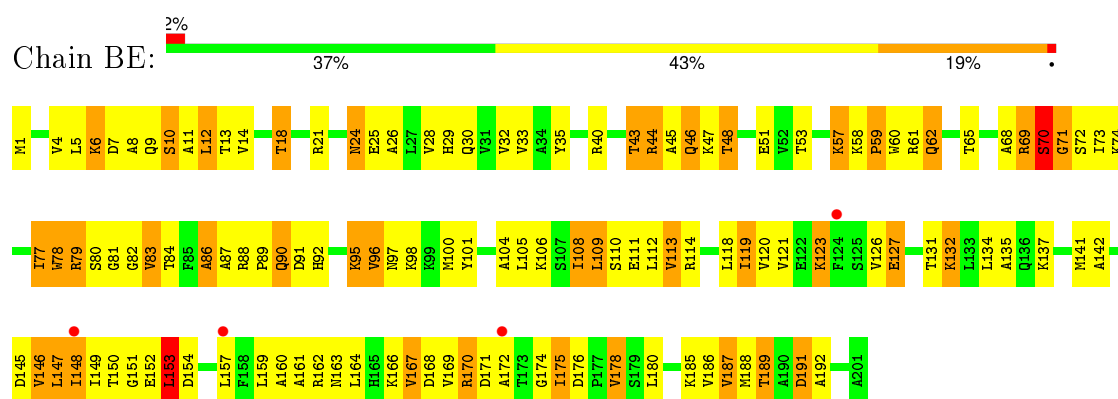


• Molecule 27: 50S ribosomal protein L3

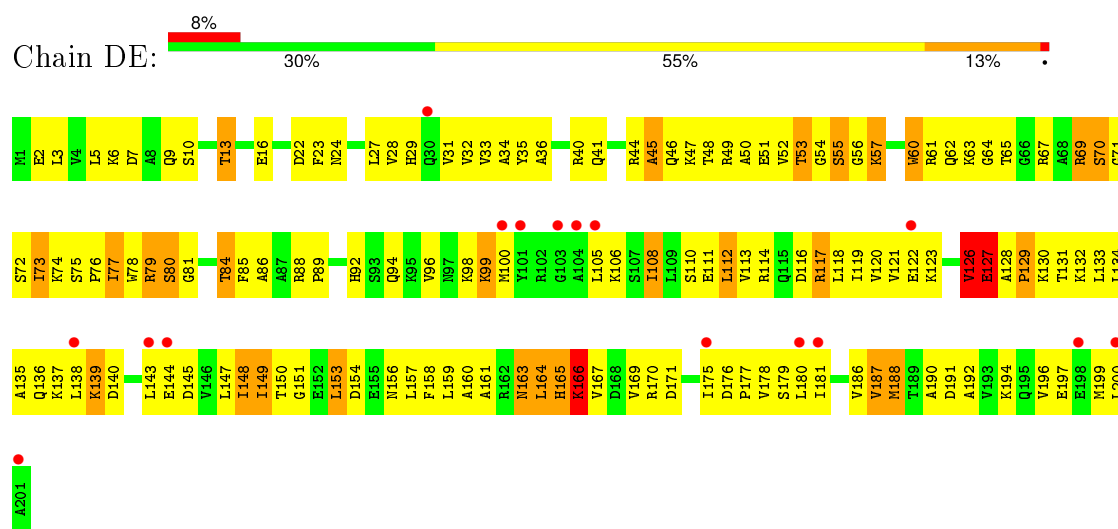




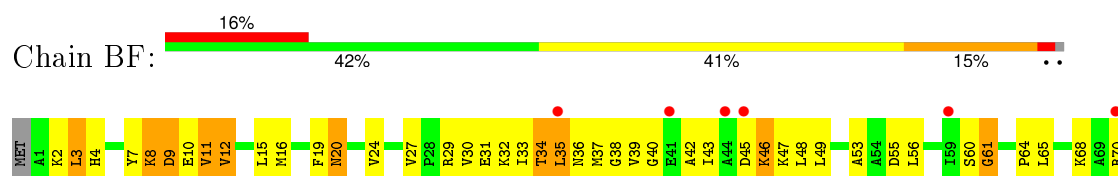
• Molecule 28: 50S ribosomal protein L4

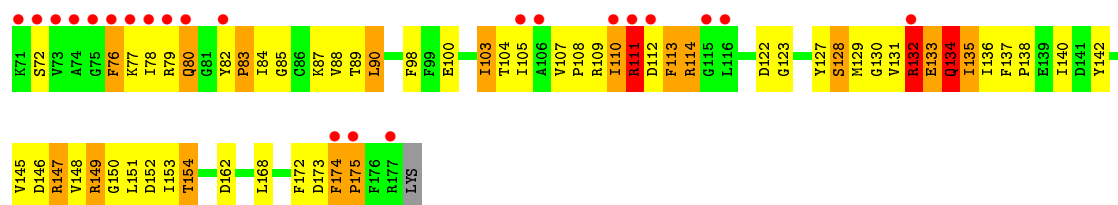


• Molecule 28: 50S ribosomal protein L4

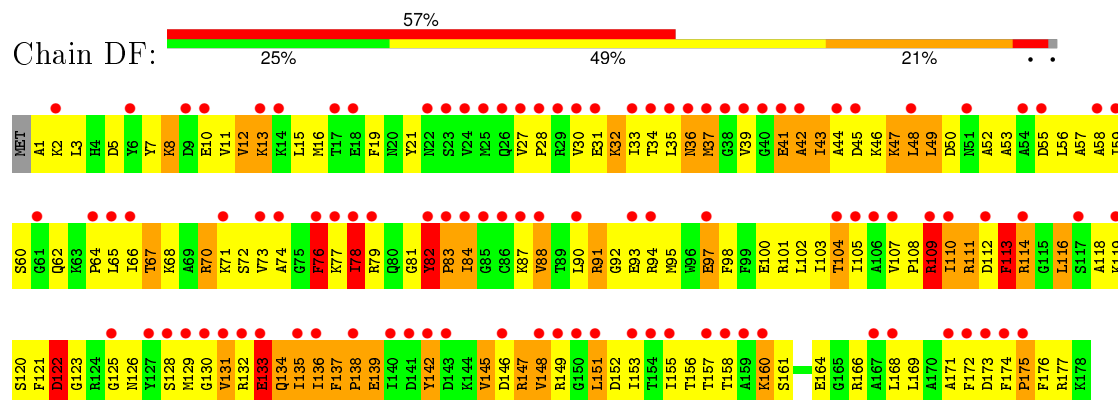


• Molecule 29: 50S ribosomal protein L5

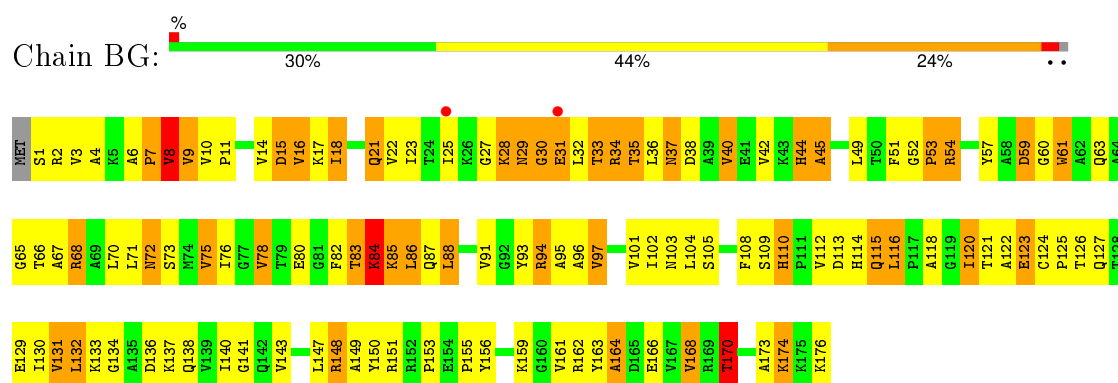




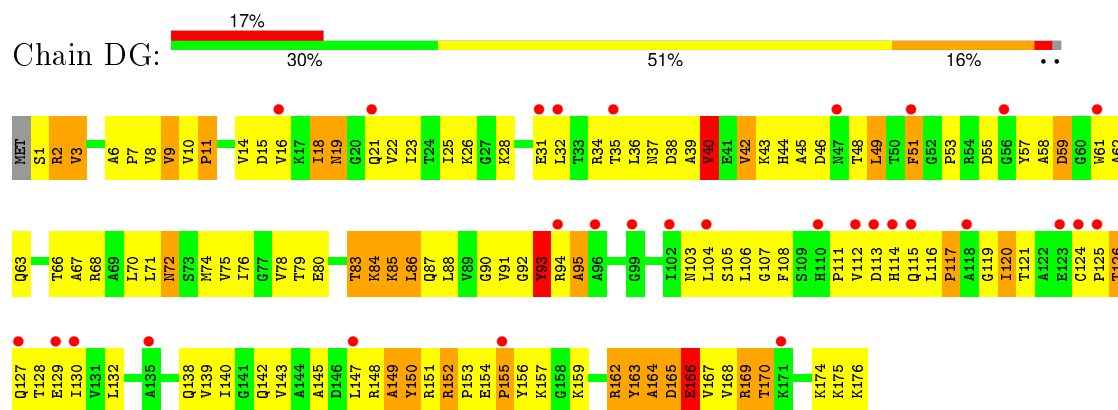
• Molecule 29: 50S ribosomal protein L5



• Molecule 30: 50S ribosomal protein L6

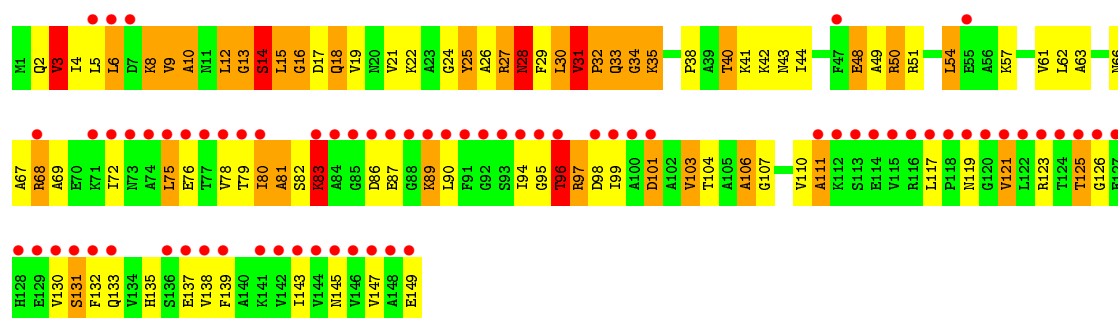


• Molecule 30: 50S ribosomal protein L6

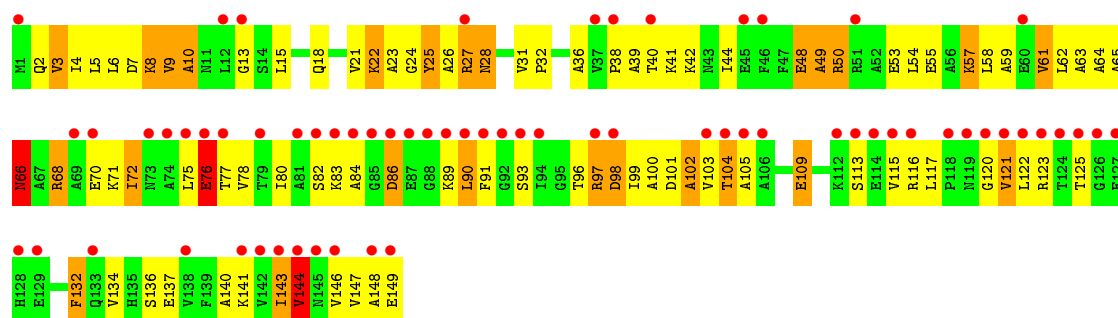


• Molecule 31: 50S ribosomal protein L9

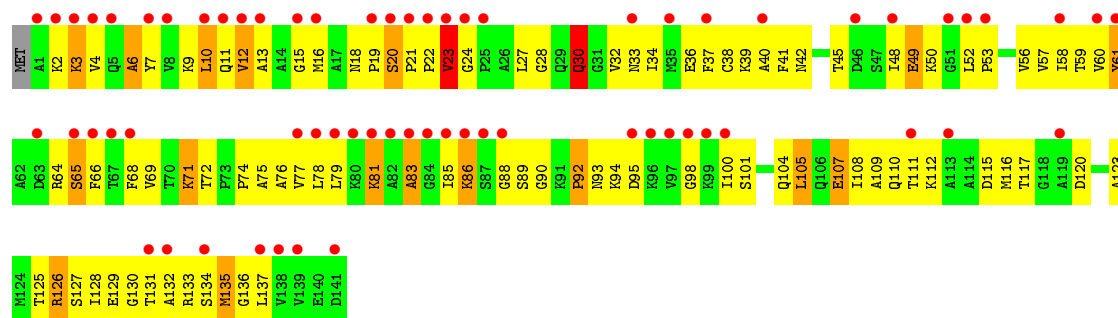




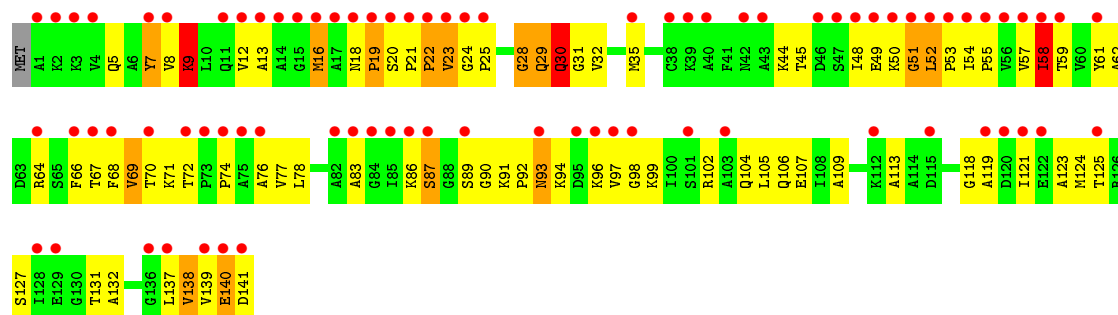
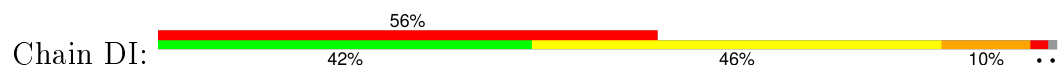
- Molecule 31: 50S ribosomal protein L9



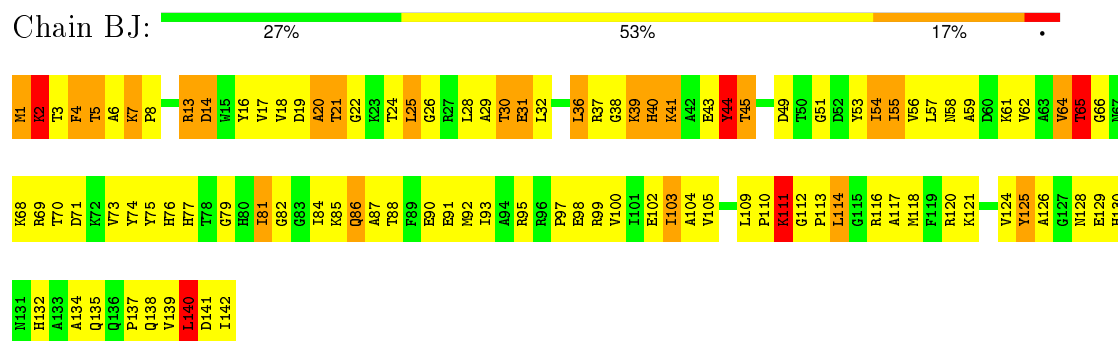
- Molecule 32: 50S ribosomal protein L11



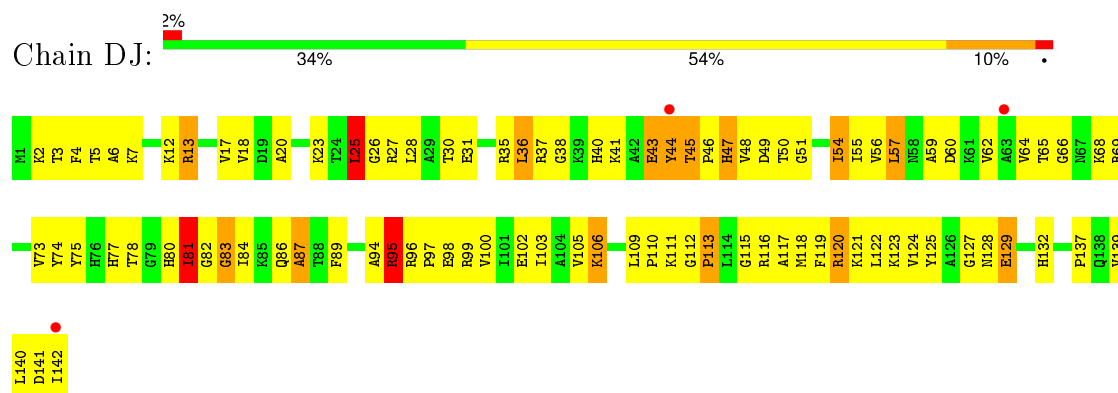
- Molecule 32: 50S ribosomal protein L11



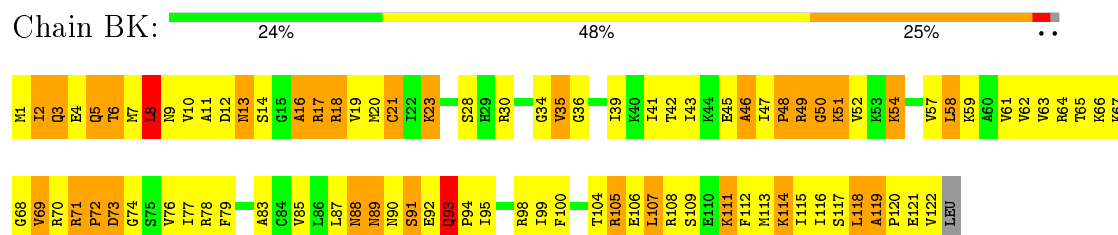
- Molecule 33: 50S ribosomal protein L13



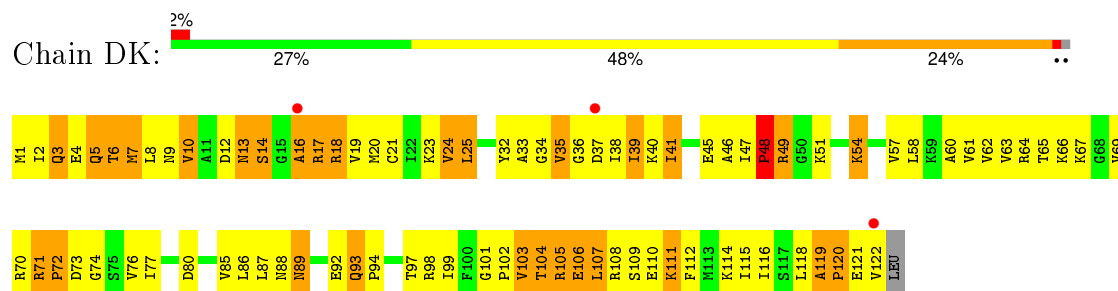
- Molecule 33: 50S ribosomal protein L13



- Molecule 34: 50S ribosomal protein L14

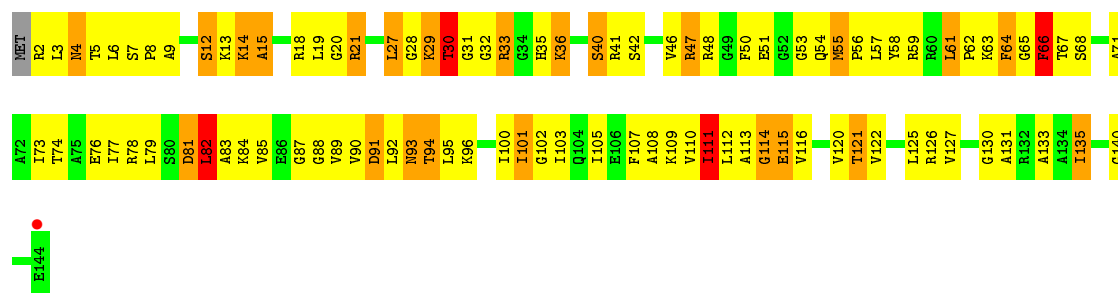


- Molecule 34: 50S ribosomal protein L14

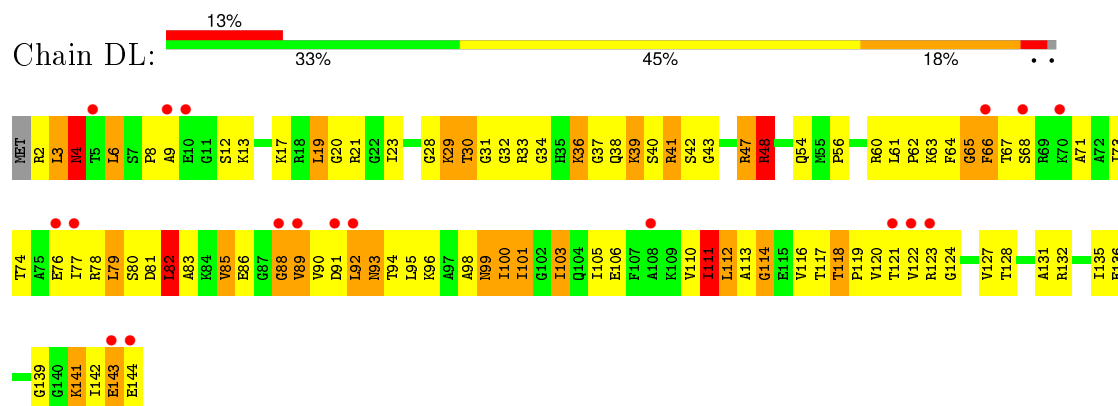


- Molecule 35: 50S ribosomal protein L15

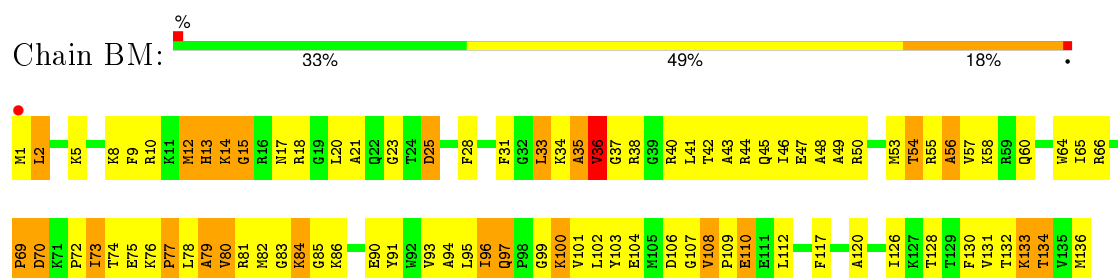




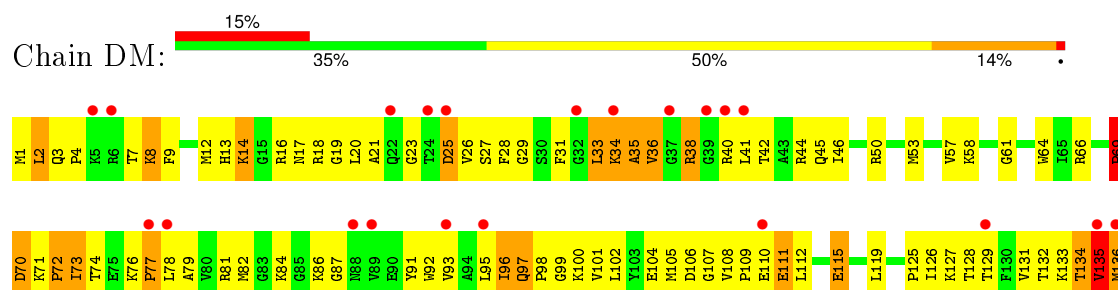
- Molecule 35: 50S ribosomal protein L15



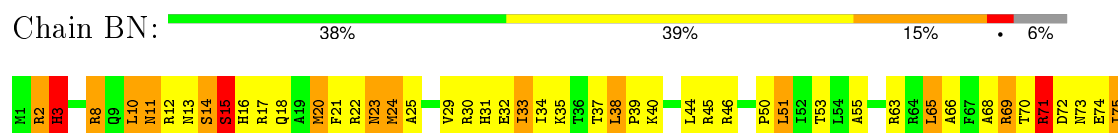
- Molecule 36: 50S ribosomal protein L16



- Molecule 36: 50S ribosomal protein L16

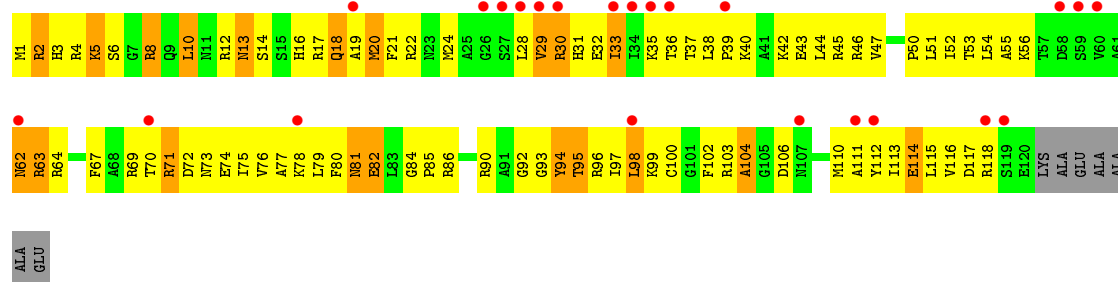


- Molecule 37: 50S ribosomal protein L17

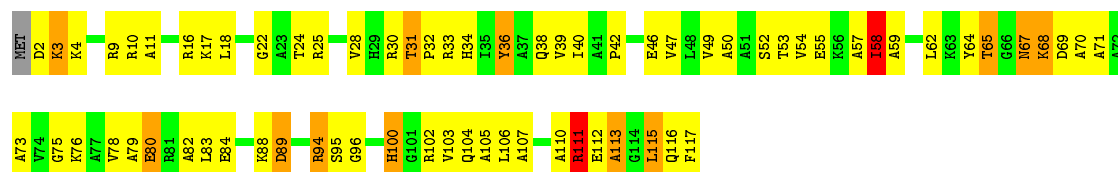




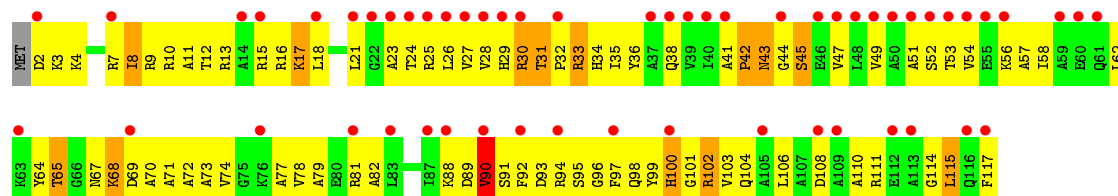
• Molecule 37: 50S ribosomal protein L17



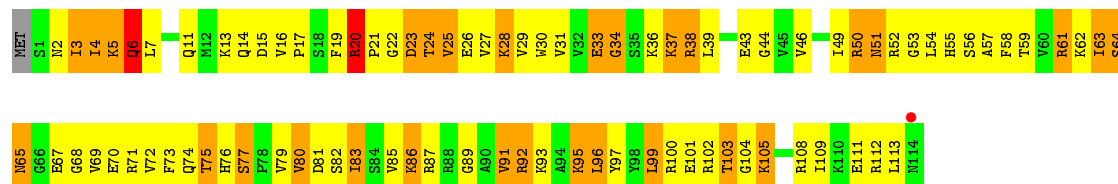
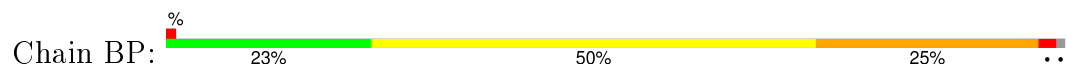
• Molecule 38: 50S ribosomal protein L18



• Molecule 38: 50S ribosomal protein L18

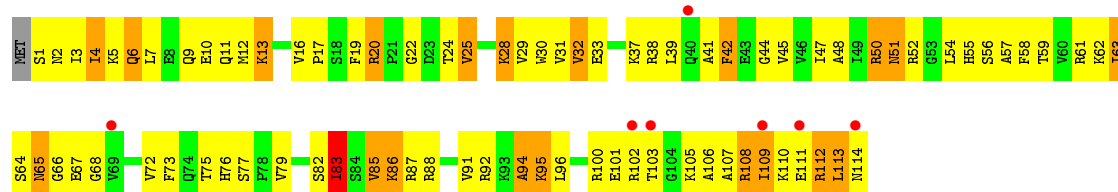


• Molecule 39: 50S ribosomal protein L19



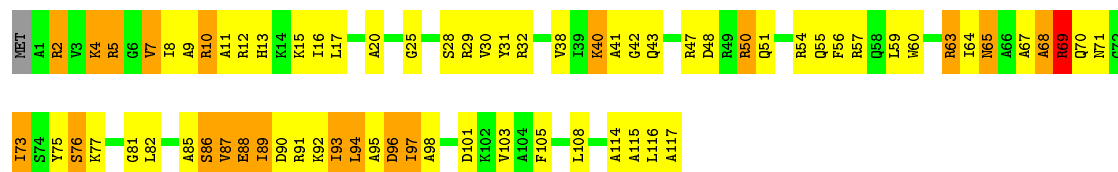
• Molecule 39: 50S ribosomal protein L19





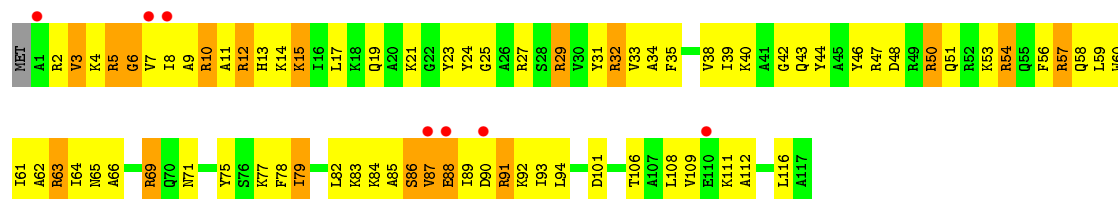
- Molecule 40: 50S ribosomal protein L20

Chain BQ: 39% 42% 17% ..



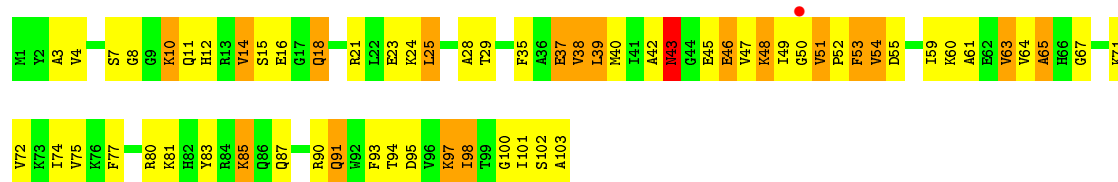
- Molecule 40: 50S ribosomal protein L20

Chain DQ: 6% 34% 50% 15% .



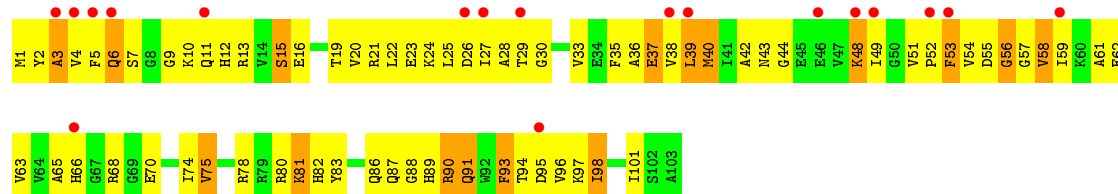
- Molecule 41: 50S ribosomal protein L21

Chain BR: 39% 43% 17% .

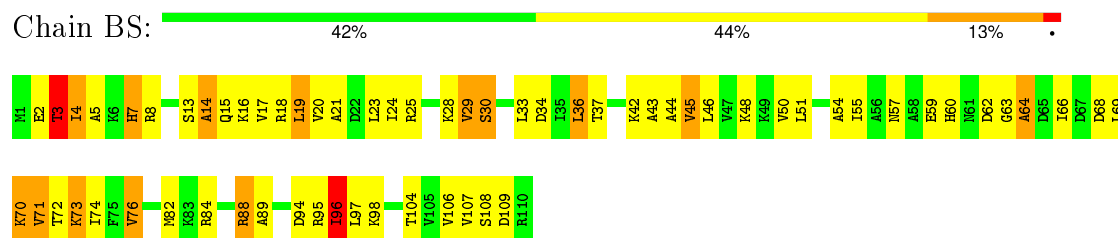


- Molecule 41: 50S ribosomal protein L21

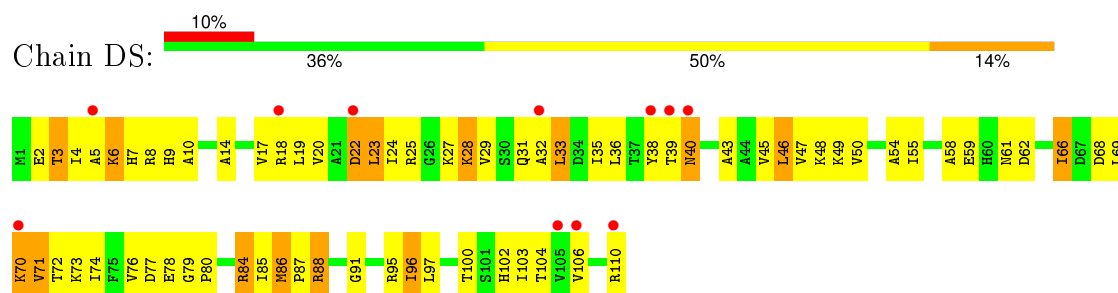
Chain DR: 17% 28% 56% 16%



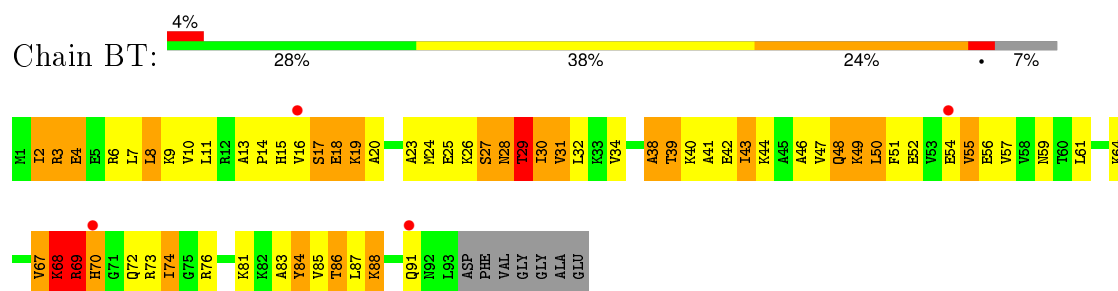
- Molecule 42: 50S ribosomal protein L22



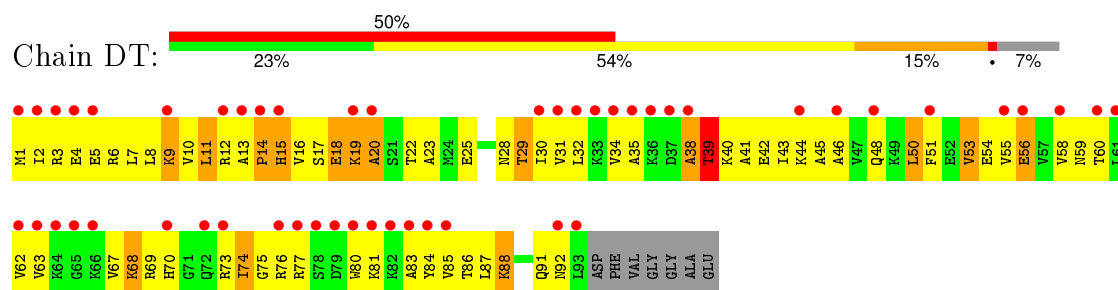
• Molecule 42: 50S ribosomal protein L22



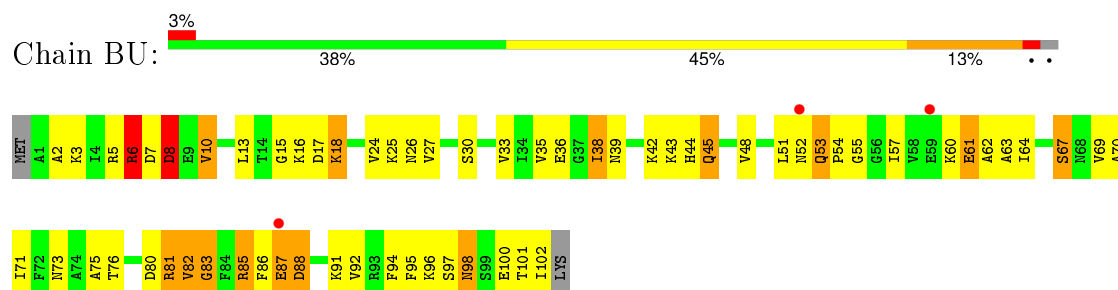
• Molecule 43: 50S ribosomal protein L23



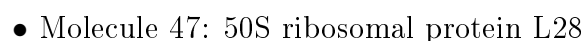
• Molecule 43: 50S ribosomal protein L23

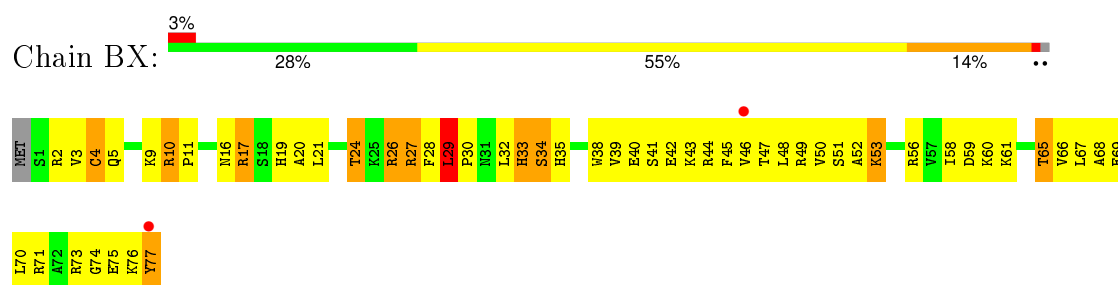


• Molecule 44: 50S ribosomal protein L24

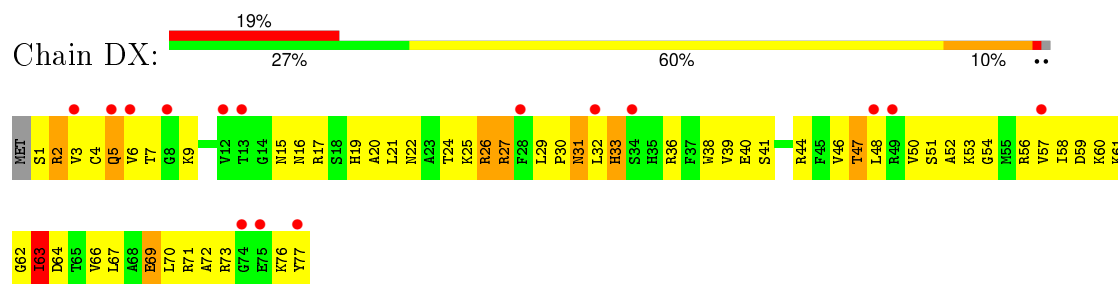


• Molecule 44: 50S ribosomal protein L24

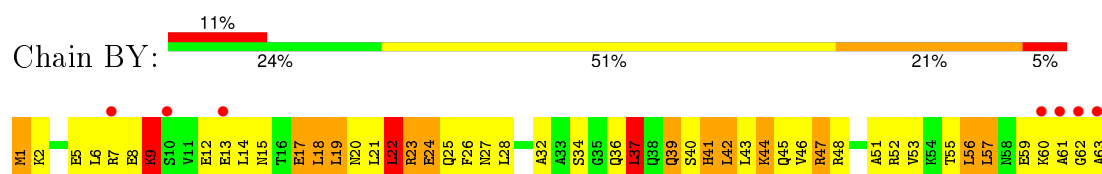




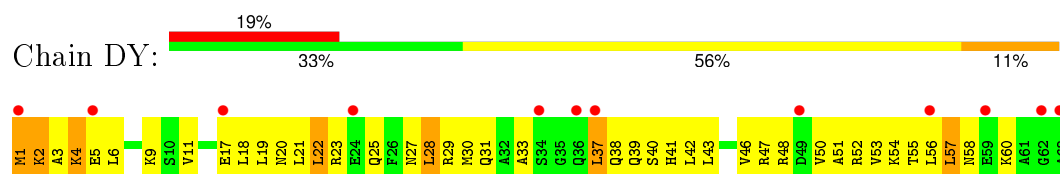
- Molecule 47: 50S ribosomal protein L28



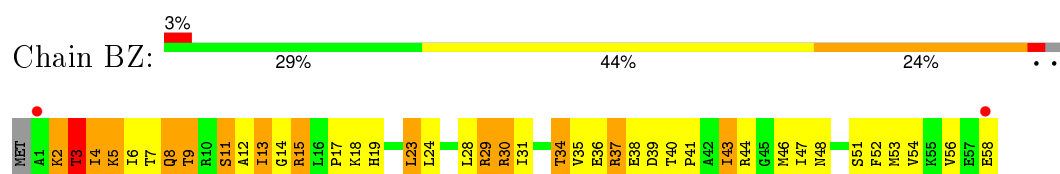
- Molecule 48: 50S ribosomal protein L29



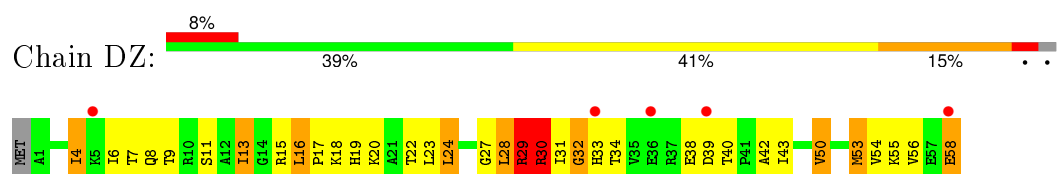
- Molecule 48: 50S ribosomal protein L29



- Molecule 49: 50S ribosomal protein L30

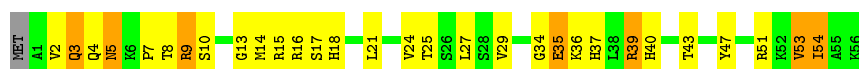


- Molecule 49: 50S ribosomal protein L30

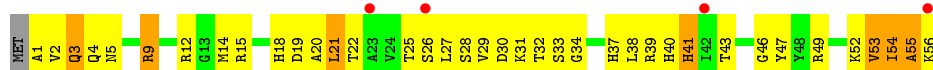


- Molecule 50: 50S ribosomal protein L32

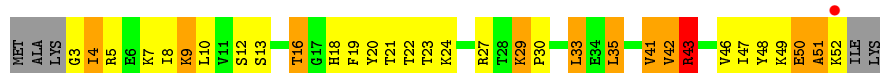




- Molecule 50: 50S ribosomal protein L32



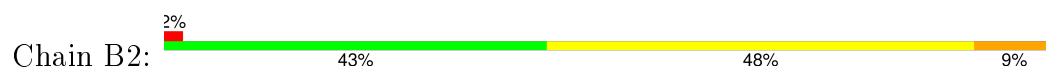
- Molecule 51: 50S ribosomal protein L33



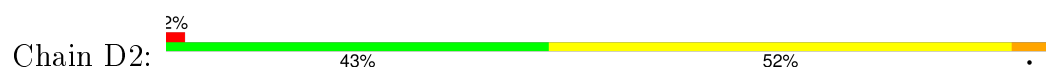
- Molecule 51: 50S ribosomal protein L33



- Molecule 52: 50S ribosomal protein L34



- Molecule 52: 50S ribosomal protein L34

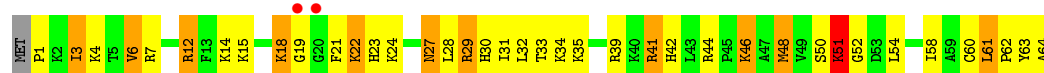


- Molecule 53: 50S ribosomal protein L35



- Molecule 53: 50S ribosomal protein L35

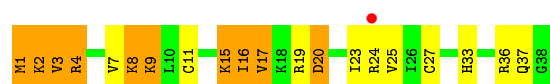




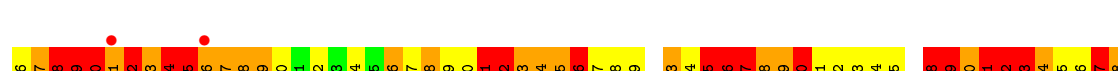
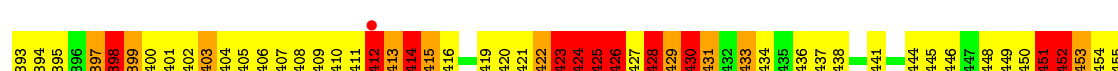
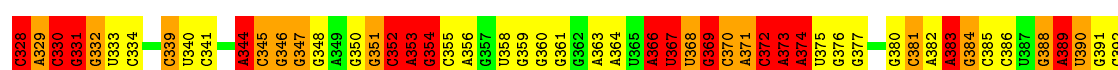
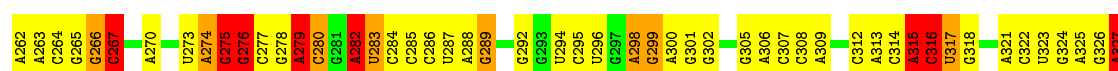
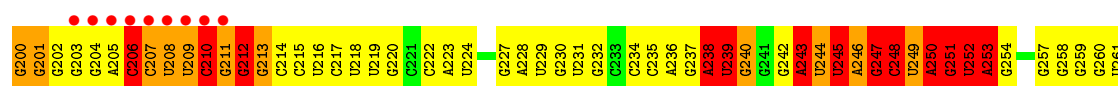
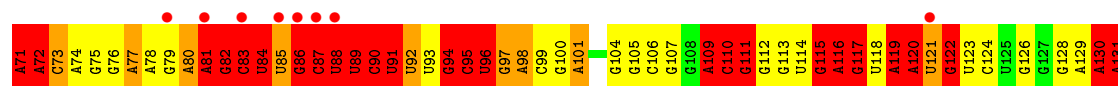
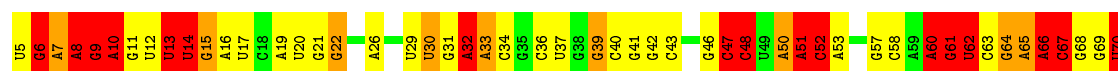
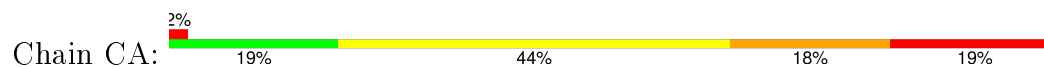
- Molecule 54: 50S ribosomal protein L36



- Molecule 54: 50S ribosomal protein L36



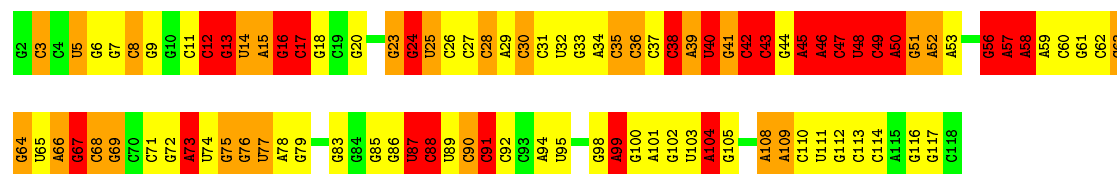
- Molecule 55: 16S rRNA



U1495	C1496	G1497	A1498	A1499	A1500	C1501	G1492	A1503	C1504	G1495	A1506	A1507	A1508	C1509	G1510	G1511	U1512	C1520	C1521	U1522	G1523		G1526	U1527	U1528	A1456	G1457	C1529	G1530	A1531	U1532	C1533	A1534	C1466	C1467	A1468		G1473	A1474	G1475		C1479	A1480	U1481	G1482	A1483		G1487	G1488	G1489	G1490	G1491	A1418		A1492	A1493	G1494																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
U1424	U1425		A1428	A1429	A1430	A1431	G1432	A1433	A1434	G1435	U1436	A1437	G1438	G1439	U1440	A1441	G1442		C1443	U1444	U1445	A1446	A1447	C1448	C1449	U1450	U1451	C1452	G1453	G1454	C1389	A1390	A1396	C1397	A1398	C1399	C1400		G1473	A1474	G1475		C1479	A1480	U1481	G1482	A1483		G1487	G1488	G1489	G1490	G1491	A1418		A1492	A1493	G1494																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
U1354	G1355	A1356	A1357	U1358	A1359	C1360	G1361	A1362	C1363	U1364	G1365	A1366	C1367	U1368	C1369	G1370	G1371		C1372	G1373	U1374	A1375	A1376	A1377	C1378	U1379	U1380	U1381	C1382		C1389	A1390	A1396	C1397	A1398	C1399	C1400		G1473	A1474	G1475		C1479	A1480	U1481	G1482	A1483		G1487	G1488	G1489	G1490	G1491	A1418		A1492	A1493	G1494																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
G1294	U1295	C1296	G1297	U1298	A1299	G1300	U1301	C1302	C1303	G1304	G1305	A1306	U1307	U1308	C1309	G1310	A1311	G1312	U1313	A1314	U1315	G1316	G1317	A1318	U1319	C1320	U1321	C1322	G1323	A1324	C1325	U1326	G1327	U1328	A1329	U1330	G1331	A1332	A1333	G1334	U1335	C1336	G1337	C1338	G1339	A1340	U1341	C1342	G1343	C1344	U1345	A1346	G1347	U1348	A1349	A1350	U1351	C1352	G1353																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
U1232	G1233	U1234	U1235	A1236	U1237	A1238	A1239	U1240	G1241	G1242	C1243	C1244	C1245	U1246	U1247	A1248	G1249	A1250	U1251	A1252	U1253	G1254	U1255	A1256	U1257	C1258	U1259	C1260	A1261		C1265	G1266	U1267	C1268	A1269	U1270	C1271	G1272	C1273	A1274	A1275	G1276	C1277	G1278	G1279	A1280	C1281	U1282	C1283	U1284	C1285	A1286	U1287	A1288	U1289	A1290	U1291	A1292	C1293	G1294																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
G1156	A1157	U1158	A1159	A1160	C1161	A1162	A1163	G1164		G1178	A1179	A1180	G1181	U1182	U1183	G1184	G1185	U1186	G1187	U1188	U1189	G1190	A1191	C1192	U1193	U1194	C1195	A1196	A1197	U1198	U1199	C1200	A1201	U1202	C1203		G1206		U1211	U1212	A1213	C1214	G1215	A1216	G1217	G1218	A1219	C1220	G1221	G1222	U1223	C1224	A1225	C1226	A1227	U1228	U1229	A1230		U1234	A1235	U1236	U1237	A1238	U1239	A1240	U1241	U1242	U1243	U1244	U1245	U1246	U1247	U1248	U1249	U1250	U1251	U1252	U1253	U1254	U1255	U1256	U1257	U1258	U1259	U1260	U1261	U1262	U1263	U1264	U1265	U1266	U1267	U1268	U1269	U1270	U1271	U1272	U1273	U1274	U1275	U1276	U1277	U1278	U1279	U1280	U1281	U1282	U1283	U1284	U1285	U1286	U1287	U1288	U1289	U1290	U1291	U1292	U1293	U1294	U1295	U1296	U1297	U1298	U1299	U1300	U1301	U1302	U1303	U1304	U1305	U1306	U1307	U1308	U1309	U1310	U1311	U1312	U1313	U1314	U1315	U1316	U1317	U1318	U1319	U1320	U1321	U1322	U1323	U1324	U1325	U1326	U1327	U1328	U1329	U1330	U1331	U1332	U1333	U1334	U1335	U1336	U1337	U1338	U1339	U1340	U1341	U1342	U1343	U1344	U1345	U1346	U1347	U1348	U1349	U1350	U1351	U1352	U1353	U1354	U1355	U1356	U1357	U1358	U1359	U1360	U1361	U1362	U1363	U1364	U1365	U1366	U1367	U1368	U1369	U1370	U1371	U1372	U1373	U1374	U1375	U1376	U1377	U1378	U1379	U1380	U1381	U1382	U1383	U1384	U1385	U1386	U1387	U1388	U1389	U1390	U1391	U1392	U1393	U1394	U1395	U1396	U1397	U1398	U1399	U1400	U1401	U1402	U1403	U1404	U1405	U1406	U1407	U1408	U1409	U1410	U1411	U1412	U1413	U1414	U1415	U1416	U1417	U1418	U1419	U1420	U1421	U1422	U1423	U1424	U1425	U1426	U1427	U1428	U1429	U1430	U1431	U1432	U1433	U1434	U1435	U1436	U1437	U1438	U1439	U1440	U1441	U1442	U1443	U1444	U1445	U1446	U1447	U1448	U1449	U1450	U1451	U1452	U1453	U1454	U1455	U1456	U1457	U1458	U1459	U1460	U1461	U1462	U1463	U1464	U1465	U1466	U1467	U1468	U1469	U1470	U1471	U1472	U1473	U1474	U1475	U1476	U1477	U1478	U1479	U1480	U1481	U1482	U1483	U1484	U1485	U1486	U1487	U1488	U1489	U1490	U1491	U1492	U1493	U1494	U1495	U1496	U1497	U1498	U1499	U1500	U1501	U1502	U1503	U1504	U1505	U1506	U1507	U1508	U1509	U1510	U1511	U1512	U1513	U1514	U1515	U1516	U1517	U1518	U1519	U1520	U1521	U1522	U1523	U1524	U1525	U1526	U1527	U1528	U1529	U1530	U1531	U1532	U1533	U1534	U1535	U1536	U1537	U1538	U1539	U1540	U1541	U1542	U1543	U1544	U1545	U1546	U1547	U1548	U1549	U1550	U1551	U1552	U1553	U1554	U1555	U1556	U1557	U1558	U1559	U1560	U1561	U1562	U1563	U1564	U1565	U1566	U1567	U1568	U1569	U1570	U1571	U1572	U1573	U1574	U1575	U1576	U1577	U1578	U1579	U1580	U1581	U1582	U1583	U1584	U1585	U1586	U1587	U1588	U1589	U1590	U1591	U1592	U1593	U1594	U1595	U1596	U1597	U1598	U1599	U1600	U1601	U1602	U1603	U1604	U1605	U1606	U1607	U1608	U1609	U1610	U1611	U1612	U1613	U1614	U1615	U1616	U1617	U1618	U1619	U1620	U1621	U1622	U1623	U1624	U1625	U1626	U1627	U1628	U1629	U1630	U1631	U1632	U1633	U1634	U1635	U1636	U1637	U1638	U1639	U1640	U1641	U1642	U1643	U1644	U1645	U1646	U1647	U1648	U1649	U1650	U1651	U1652	U1653	U1654	U1655	U1656	U1657	U1658	U1659	U1660	U1661	U1662	U1663	U1664	U1665	U1666	U1667	U1668	U1669	U1670	U1671	U1672	U1673	U1674	U1675	U1676	U1677	U1678	U1679	U1680	U1681	U1682	U1683	U1684	U1685	U1686	U1687	U1688	U1689	U1690	U1691	U1692	U1693	U1694	U1695	U1696	U1697	U1698	U1699	U1700	U1701	U1702	U1703	U1704	U1705	U1706	U1707	U1708	U1709	U1710	U1711	U1712	U1713	U1714	U1715	U1716	U1717	U1718	U1719	U1720	U1721	U1722	U1723	U1724	U1725	U1726	U1727	U1728	U1729	U1730	U1731	U1732	U1733	U1734	U1735	U1736	U1737	U1738	U1739	U1740	U1741	U1742	U1743	U1744	U1745	U1746	U1747	U1748	U1749	U1750	U1751	U1752	U1753	U1754	U1755	U1756	U1757	U1758	U1759	U1760	U1761	U1762	U1763	U1764	U1765	U1766	U1767	U1768	U1769	U1770	U1771	U1772	U1773	U1774	U1775	U1776	U1777	U1778	U1779	U1780	U1781	U1782	U1783	U1784	U1785	U1786	U1787	U1788	U1789	U1790	U1791	U1792	U1793	U1794	U1795	U1796	U1797	U1798	U1799	U1800	U1801	U1802	U1803	U1804	U1805	U1806	U1807	U1808	U1809	U1810	U1811	U1812	U1813	U1814	U1815	U1816	U1817	U1818	U1819	U1820	U1821	U1822	U1823	U1824	U1825	U1826	U1827	U1828	U1829	U1830	U1831	U1832	U1833	U1834	U1835	U1836	U1837	U1838	U1839	U1840	U1841	U1842	U1843	U1844	U1845	U1846	U1847	U1848	U1849	U1850	U1851	U1852	U1853	U1854	U1855	U1856	U1857	U1858	U1859	U1860	U1861	U1862	U1863	U1864	U1865	U1866	U1867	U1868	U1869	U1870	U1871	U1872	U1873	U1874	U1875	U1876	U1877	U1878	U1879	U1880	U1881	U1882	U1883	U1884	U1885	U1886	U1887	U1888	U1889	U1890	U1891	U1892	U1893	U1894	U1895	U1896	U1897	U1898	U1899	U1900	U1901	U1902	U1903	U1904	U1905	U1906	U1907	U1908	U1909	U1910	U1911	U1912	U1913	U1914	U1915	U1916	U1917	U1918	U1919	U1920	U1921	U1922	U1923	U1924	U1925	U1926	U1927	U1928	U1929	U1930	U1931	U1932	U1933	U1934	U1935	U1936	U1937	U1938	U1939	U1940	U1941	U1942	U1943	U1944	U1945	U1946	U1947	U1948	U1949	U1950	U1951	U1952	U1953	U1954	U1955	U1956	U1957	U1958	U1959	U1960	U1961	U1962	U1963	U1964	U1965	U1966	U1967	U1968	U1969	U1970	U1971	U1972	U1973	U1974	U1975	U1976	U1977	U1978	U1979	U1980	U1981	U1982	U1983	U1984	U1985	U1986	U1987	U1988	U1989	U1990	U1991	U1992	U1993	U1994	U1995	U1996	U1997	U1998	U1999	U2000	U2001	U2002	U2003	U2004	U2005	U2006	U2007	U2008	U2009	U2010	U2011	U2012	U2013	U2014	U2015	U2016	U2017	U2018	U2019	U2020	U2021	U2022	U2023	U2024	U2025	U2026	U2027	U2028	U2029	U2030	U2031	U2032	U2033	U2034	U2035	U2036	U2037	U2038	U2039	U2040	U2041	U2042	U2043	U2044	U2045	U2046	U2047	U2048	U2049	U2050	U2051	U2052	U2053	U2054	U2055	U2056	U2057	U2058	U2059	U2060	U2061	U2062	U2063	U2064	U2065	U2066	U2067	U2068	U2069	U2070	U2071	U2072	U2073	U2074	U2075	U2076	U2077	U2078	U2079	U2080	U2081	U2082	U2083	U2084	U2085	U2086	U2087	U2088	U2089	U2090	U2091	U2092	U2093	U2094	U2095	U2096	U2097	U2098	U2099	U2100	U2101	U2102	U2103	U2104	U2105	U2106	U2107	U2108	U2109	U2110	U2111	U2112	U2113	U2114	U2115	U2116	U2117	U2118	U2119	U2120	U2121	U2122	U2123	U2124	U2125	U2126	U2127	U2128	U2129	U2130	U2131	U2132	U2133	U2134	U2135	U2136	U2137	U2138	U2139	U2140	U2141	U2142	U2143	U2144	U2145	U2146	U2147

• Molecule 56: 5S rRNA

Frequency	Percentage
Daily	17%
Often	39%
Sometimes	22%
Never	21%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.72Å 435.07Å 628.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	75.71 – 3.81 75.71 – 3.81	Depositor EDS
% Data completeness (in resolution range)	78.6 (75.71-3.81) 78.7 (75.71-3.81)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 3.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.207 , 0.253 0.217 , 0.261	Depositor DCC
R_{free} test set	8852 reflections (2.02%)	DCC
Wilson B-factor (Å ²)	99.2	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 63.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	1 of 438428 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	285420	wwPDB-VP
Average B, all atoms (Å ²)	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.11% 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, 0.375 respectively for untwinned datasets, and 0.333, 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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AB	0.27	0/1735	0.48	0/2338
1	CB	0.28	0/1735	0.52	0/2338
2	AC	0.28	0/1651	0.50	0/2225
2	CC	0.29	0/1651	0.48	0/2225
3	AD	0.29	0/1665	0.48	0/2227
3	CD	0.36	0/1665	0.53	0/2227
4	AE	0.35	0/1118	0.64	1/1504 (0.1%)
4	CE	0.34	0/1118	0.55	0/1504
5	AF	0.27	0/835	0.49	0/1128
5	CF	0.26	0/835	0.48	0/1128
6	AG	0.26	0/1195	0.45	0/1602
6	CG	0.30	0/1187	0.51	0/1591
7	AH	0.31	0/989	0.49	0/1326
7	CH	0.30	0/989	0.50	0/1326
8	AI	0.26	0/1034	0.46	0/1375
8	CI	0.26	0/1034	0.46	0/1375
9	AJ	0.26	0/796	0.49	0/1077
9	CJ	0.26	0/796	0.50	0/1077
10	AK	0.26	0/893	0.48	0/1205
10	CK	0.30	0/893	0.52	0/1205
11	AL	0.34	0/969	0.60	0/1300
11	CL	0.30	0/969	0.56	0/1300
12	AM	0.27	0/892	0.54	1/1193 (0.1%)
12	CM	0.36	0/884	1.04	4/1181 (0.3%)
13	AN	0.25	0/785	0.45	0/1043
13	CN	0.26	0/780	0.45	0/1036
14	AO	0.25	0/722	0.45	0/964
14	CO	0.26	0/722	0.47	0/964
15	AP	0.30	0/659	0.50	0/884
15	CP	0.30	0/648	0.49	0/870
16	AQ	0.32	0/657	0.57	0/881
16	CQ	0.31	0/657	0.49	0/881

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AR	0.25	0/462	0.46	0/621
17	CR	0.31	0/462	0.49	0/621
18	AS	0.25	0/652	0.44	0/877
18	CS	0.25	0/652	0.46	0/877
19	AT	0.30	0/671	0.51	0/888
19	CT	0.27	0/671	0.46	0/888
20	AU	0.28	0/430	0.53	0/570
20	CU	0.33	0/430	0.57	0/570
21	AA	0.57	0/36834	1.45	646/57462 (1.1%)
22	AV	0.56	0/401	1.20	2/622 (0.3%)
22	CV	0.55	0/401	1.18	1/622 (0.2%)
23	AW	0.76	0/138	1.54	3/212 (1.4%)
23	CW	0.79	0/138	1.93	4/212 (1.9%)
24	BA	0.77	12/68626 (0.0%)	1.70	1788/107056 (1.7%)
24	DA	0.57	3/68314 (0.0%)	1.49	1376/106569 (1.3%)
25	BB	0.71	0/2828	1.59	62/4410 (1.4%)
26	BC	0.47	0/2121	0.73	1/2852 (0.0%)
26	DC	0.35	0/2121	0.58	0/2852
27	BD	0.52	0/1586	0.81	1/2134 (0.0%)
27	DD	0.32	0/1586	0.60	0/2134
28	BE	0.45	0/1571	0.67	0/2113
28	DE	0.33	0/1571	0.53	0/2113
29	BF	0.44	1/1434 (0.1%)	0.62	1/1926 (0.1%)
29	DF	0.45	3/1444 (0.2%)	0.79	5/1937 (0.3%)
30	BG	0.38	0/1343	0.64	0/1816
30	DG	0.28	0/1343	0.50	0/1816
31	BH	0.48	1/1122 (0.1%)	0.62	1/1515 (0.1%)
31	DH	0.39	0/1122	0.54	0/1515
32	BI	0.24	0/1046	0.50	0/1410
32	DI	0.24	0/1046	0.44	0/1410
33	BJ	0.56	0/1152	0.77	1/1551 (0.1%)
33	DJ	0.37	0/1152	0.62	0/1551
34	BK	0.53	0/947	0.82	1/1268 (0.1%)
34	DK	0.35	0/947	0.61	0/1268
35	BL	0.47	0/1054	0.76	1/1403 (0.1%)
35	DL	0.34	0/1054	0.58	0/1403
36	BM	0.50	0/1093	0.70	0/1460
36	DM	0.45	0/1093	0.63	0/1460
37	BN	0.48	0/973	0.73	1/1301 (0.1%)
37	DN	0.32	0/973	0.56	0/1301
38	BO	0.41	0/902	0.61	0/1209
38	DO	0.44	0/902	0.71	2/1209 (0.2%)
39	BP	0.48	0/929	0.74	0/1242

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	DP	0.33	0/929	0.52	0/1242
40	BQ	0.58	0/960	0.74	0/1278
40	DQ	0.36	0/960	0.54	0/1278
41	BR	0.57	0/829	0.77	0/1107
41	DR	0.38	0/829	0.58	0/1107
42	BS	0.54	0/864	0.78	0/1156
42	DS	0.30	0/864	0.56	0/1156
43	BT	0.44	0/744	0.67	0/994
43	DT	0.27	0/744	0.51	0/994
44	BU	0.42	0/787	0.71	1/1051 (0.1%)
44	DU	0.35	0/787	0.56	1/1051 (0.1%)
45	BV	0.47	0/766	0.68	0/1025
45	DV	0.68	3/766 (0.4%)	0.81	3/1025 (0.3%)
46	BW	0.54	0/603	0.84	0/797
46	DW	0.34	0/603	0.55	0/797
47	BX	0.41	0/635	0.68	1/848 (0.1%)
47	DX	0.32	0/635	0.55	0/848
48	BY	0.42	0/510	0.67	0/677
48	DY	0.28	0/510	0.49	0/677
49	BZ	0.47	0/453	0.73	0/605
49	DZ	0.32	0/453	0.58	0/605
50	B0	0.40	0/450	0.70	0/599
50	D0	0.31	0/450	0.55	0/599
51	B1	0.40	0/416	0.59	0/554
51	D1	0.31	0/416	0.49	0/554
52	B2	0.48	0/380	0.80	0/498
52	D2	0.31	0/380	0.53	0/498
53	B3	0.46	0/513	0.67	0/676
53	D3	0.36	0/513	0.57	0/676
54	B4	0.50	0/303	0.80	0/397
54	D4	0.41	0/303	0.60	0/397
55	CA	0.55	1/36762 (0.0%)	1.45	694/57350 (1.2%)
56	DB	0.68	4/2803 (0.1%)	1.79	112/4371 (2.6%)
All	All	0.57	28/307815 (0.0%)	1.37	4715/460233 (1.0%)

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
27	BD	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
29	DF	0	1
36	DM	0	1
All	All	0	4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BA	1142	A	N9-C4	-11.34	1.31	1.37
45	DV	31	TYR	CE1-CZ	10.97	1.52	1.38
24	DA	1060	U	C2-N3	7.54	1.43	1.37
24	BA	1142	A	C8-N7	7.36	1.36	1.31
24	BA	2857	G	N3-C4	7.16	1.40	1.35

The worst 5 of 4715 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	CM	2	ARG	NE-CZ-NH1	-22.49	109.06	120.30
24	BA	2447	G	C6-N1-C2	-18.42	114.05	125.10
12	CM	2	ARG	NE-CZ-NH2	17.95	129.28	120.30
24	BA	1330	C	N1-C1'-C2'	-17.28	91.53	114.00
56	DB	104	A	C8-N9-C4	-16.28	99.29	105.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	BD	10	GLY	Peptide
27	BD	9	VAL	Peptide
29	DF	78	ILE	Peptide
36	DM	135	VAL	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AB	1704	0	1732	269	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CB	1704	0	1732	208	0
2	AC	1624	0	1699	139	0
2	CC	1624	0	1699	159	0
3	AD	1643	0	1710	172	0
3	CD	1643	0	1710	143	0
4	AE	1105	0	1148	242	0
4	CE	1105	0	1148	122	0
5	AF	817	0	808	78	0
5	CF	817	0	808	79	0
6	AG	1181	0	1240	98	0
6	CG	1174	0	1230	151	0
7	AH	979	0	1034	118	0
7	CH	979	0	1034	95	0
8	AI	1022	0	1070	116	0
8	CI	1022	0	1070	141	0
9	AJ	786	0	828	77	0
9	CJ	786	0	828	124	0
10	AK	877	0	887	85	0
10	CK	877	0	887	99	0
11	AL	955	0	1019	96	0
11	CL	955	0	1019	102	0
12	AM	883	0	944	71	0
12	CM	876	0	937	137	0
13	AN	774	0	827	80	0
13	CN	769	0	822	89	0
14	AO	714	0	737	54	0
14	CO	714	0	737	40	0
15	AP	649	0	666	55	0
15	CP	638	0	656	65	0
16	AQ	648	0	691	82	0
16	CQ	648	0	691	47	0
17	AR	455	0	478	42	0
17	CR	455	0	478	40	0
18	AS	637	0	665	51	0
18	CS	637	0	665	78	0
19	AT	665	0	714	59	0
19	CT	665	0	714	47	0
20	AU	425	0	449	68	0
20	CU	425	0	449	76	0
21	AA	32895	0	16553	1701	0
22	AV	360	0	185	10	0
22	CV	360	0	185	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	AW	125	0	63	4	0
23	CW	125	0	63	6	0
24	BA	61274	0	30819	3143	0
24	DA	60995	0	30677	3530	0
25	BB	2529	0	1281	108	0
26	BC	2082	0	2157	200	0
26	DC	2082	0	2157	211	0
27	BD	1565	0	1616	189	0
27	DD	1565	0	1616	165	0
28	BE	1552	0	1619	150	0
28	DE	1552	0	1619	167	0
29	BF	1410	0	1447	123	0
29	DF	1420	0	1460	197	0
30	BG	1323	0	1374	163	0
30	DG	1323	0	1374	147	0
31	BH	1111	0	1148	109	0
31	DH	1111	0	1148	106	0
32	BI	1032	0	1088	110	0
32	DI	1032	0	1088	67	0
33	BJ	1129	0	1162	158	0
33	DJ	1129	0	1162	118	0
34	BK	938	0	1012	113	0
34	DK	938	0	1012	112	0
35	BL	1045	0	1117	123	0
35	DL	1045	0	1117	142	0
36	BM	1074	0	1157	111	0
36	DM	1074	0	1157	109	0
37	BN	960	0	1000	99	0
37	DN	960	0	1000	115	0
38	BO	892	0	923	67	0
38	DO	892	0	923	155	0
39	BP	917	0	965	134	0
39	DP	917	0	965	106	0
40	BQ	947	0	1022	130	0
40	DQ	947	0	1022	129	0
41	BR	816	0	839	88	0
41	DR	816	0	839	97	0
42	BS	857	0	922	69	0
42	DS	857	0	922	69	0
43	BT	738	0	807	108	0
43	DT	738	0	807	93	0
44	BU	779	0	834	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	DU	779	0	834	107	0
45	BV	753	0	780	53	0
45	DV	753	0	780	118	0
46	BW	596	0	610	179	0
46	DW	596	0	610	120	0
47	BX	625	0	655	69	0
47	DX	625	0	655	73	0
48	BY	509	0	543	67	0
48	DY	509	0	543	62	0
49	BZ	449	0	491	46	0
49	DZ	449	0	491	38	0
50	B0	444	0	461	32	0
50	D0	444	0	461	52	0
51	B1	409	0	440	37	0
51	D1	409	0	440	33	0
52	B2	377	0	418	32	0
52	D2	377	0	418	33	0
53	B3	504	0	574	46	0
53	D3	504	0	574	50	0
54	B4	302	0	340	32	0
54	D4	302	0	340	24	0
55	CA	32831	0	16521	1808	0
56	DB	2507	0	1270	203	0
57	AA	43	0	0	0	0
57	BA	136	0	0	0	0
57	BB	4	0	0	0	0
57	BD	1	0	0	0	0
57	CA	42	0	0	0	0
57	DA	134	0	0	0	0
57	DB	1	0	0	0	0
57	DC	1	0	0	0	0
57	DJ	1	0	0	0	0
58	B4	1	0	0	0	0
58	D4	1	0	0	0	0
59	AA	195	0	0	7	0
59	AE	1	0	0	0	0
59	AL	3	0	0	1	0
59	AN	5	0	0	0	0
59	AT	3	0	0	0	0
59	AU	1	0	0	0	0
59	B2	2	0	0	0	0
59	B3	3	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	B4	2	0	0	0	0
59	BA	615	0	0	31	0
59	BB	19	0	0	0	0
59	BC	7	0	0	1	0
59	BD	2	0	0	3	0
59	BE	1	0	0	1	0
59	BL	4	0	0	1	0
59	BN	2	0	0	0	0
59	BQ	1	0	0	0	0
59	BT	1	0	0	1	0
59	BV	1	0	0	1	0
59	CA	196	0	0	4	0
59	CE	3	0	0	1	0
59	CI	1	0	0	0	0
59	CL	1	0	0	0	0
59	CN	2	0	0	0	0
59	CT	2	0	0	0	0
59	CU	2	0	0	0	0
59	D2	1	0	0	0	0
59	D3	1	0	0	0	0
59	D4	5	0	0	0	0
59	DA	598	0	0	14	0
59	DB	4	0	0	0	0
59	DC	14	0	0	2	0
59	DD	4	0	0	0	0
59	DE	2	0	0	0	0
59	DJ	3	0	0	0	0
59	DL	5	0	0	0	0
59	DN	2	0	0	0	0
59	DT	2	0	0	0	0
59	DU	1	0	0	0	0
59	DV	1	0	0	0	0
All	All	285420	0	191332	18973	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 40.

The worst 5 of 18973 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)
24:DA:1439:A:C2	24:DA:1552:A:C6	2.21	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:DA:1439:A:N1	24:DA:1552:A:C5	2.03	1.26
24:DA:1439:A:C2	24:DA:1552:A:C5	2.25	1.25
38:DO:100:HIS:CE1	56:DB:48:U:O2'	1.89	1.25
38:DO:30:ARG:HB2	38:DO:30:ARG:NH1	1.53	1.21

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AB	216/241 (90%)	128 (59%)	60 (28%)	28 (13%)	0	7
1	CB	216/241 (90%)	145 (67%)	49 (23%)	22 (10%)	1	12
2	AC	204/233 (88%)	139 (68%)	51 (25%)	14 (7%)	1	23
2	CC	204/233 (88%)	146 (72%)	41 (20%)	17 (8%)	1	17
3	AD	203/206 (98%)	126 (62%)	52 (26%)	25 (12%)	0	8
3	CD	203/206 (98%)	141 (70%)	40 (20%)	22 (11%)	0	11
4	AE	148/167 (89%)	100 (68%)	31 (21%)	17 (12%)	0	9
4	CE	148/167 (89%)	98 (66%)	37 (25%)	13 (9%)	1	16
5	AF	98/135 (73%)	62 (63%)	25 (26%)	11 (11%)	0	10
5	CF	98/135 (73%)	65 (66%)	21 (21%)	12 (12%)	0	8
6	AG	149/179 (83%)	109 (73%)	29 (20%)	11 (7%)	1	21
6	CG	148/179 (83%)	80 (54%)	44 (30%)	24 (16%)	0	5
7	AH	127/130 (98%)	97 (76%)	22 (17%)	8 (6%)	2	26
7	CH	127/130 (98%)	96 (76%)	24 (19%)	7 (6%)	2	29
8	AI	125/130 (96%)	80 (64%)	34 (27%)	11 (9%)	1	16
8	CI	125/130 (96%)	86 (69%)	33 (26%)	6 (5%)	3	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	AJ	96/103 (93%)	69 (72%)	12 (12%)	15 (16%)	0	5
9	CJ	96/103 (93%)	61 (64%)	20 (21%)	15 (16%)	0	5
10	AK	115/129 (89%)	86 (75%)	22 (19%)	7 (6%)	2	26
10	CK	115/129 (89%)	74 (64%)	31 (27%)	10 (9%)	1	16
11	AL	121/124 (98%)	80 (66%)	24 (20%)	17 (14%)	0	6
11	CL	121/124 (98%)	86 (71%)	25 (21%)	10 (8%)	1	17
12	AM	112/118 (95%)	87 (78%)	16 (14%)	9 (8%)	1	19
12	CM	111/118 (94%)	65 (59%)	30 (27%)	16 (14%)	0	6
13	AN	92/101 (91%)	58 (63%)	25 (27%)	9 (10%)	1	14
13	CN	91/101 (90%)	59 (65%)	24 (26%)	8 (9%)	1	16
14	AO	86/89 (97%)	64 (74%)	17 (20%)	5 (6%)	2	28
14	CO	86/89 (97%)	72 (84%)	13 (15%)	1 (1%)	16	63
15	AP	80/82 (98%)	54 (68%)	15 (19%)	11 (14%)	0	6
15	CP	78/82 (95%)	56 (72%)	14 (18%)	8 (10%)	1	12
16	AQ	78/84 (93%)	48 (62%)	21 (27%)	9 (12%)	0	9
16	CQ	78/84 (93%)	59 (76%)	13 (17%)	6 (8%)	1	20
17	AR	53/75 (71%)	40 (76%)	11 (21%)	2 (4%)	4	39
17	CR	53/75 (71%)	44 (83%)	6 (11%)	3 (6%)	2	28
18	AS	77/92 (84%)	67 (87%)	6 (8%)	4 (5%)	2	30
18	CS	77/92 (84%)	54 (70%)	19 (25%)	4 (5%)	2	30
19	AT	83/87 (95%)	55 (66%)	21 (25%)	7 (8%)	1	17
19	CT	83/87 (95%)	59 (71%)	21 (25%)	3 (4%)	4	41
20	AU	49/71 (69%)	22 (45%)	18 (37%)	9 (18%)	0	3
20	CU	49/71 (69%)	20 (41%)	17 (35%)	12 (24%)	0	1
26	BC	269/273 (98%)	184 (68%)	59 (22%)	26 (10%)	1	14
26	DC	269/273 (98%)	181 (67%)	60 (22%)	28 (10%)	1	12
27	BD	207/209 (99%)	141 (68%)	32 (16%)	34 (16%)	0	5
27	DD	207/209 (99%)	132 (64%)	45 (22%)	30 (14%)	0	5
28	BE	199/201 (99%)	151 (76%)	24 (12%)	24 (12%)	0	8
28	DE	199/201 (99%)	130 (65%)	43 (22%)	26 (13%)	0	7
29	BF	175/179 (98%)	133 (76%)	25 (14%)	17 (10%)	1	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	DF	176/179 (98%)	97 (55%)	45 (26%)	34 (19%)	0	3
30	BG	174/177 (98%)	112 (64%)	35 (20%)	27 (16%)	0	5
30	DG	174/177 (98%)	105 (60%)	41 (24%)	28 (16%)	0	5
31	BH	147/149 (99%)	62 (42%)	54 (37%)	31 (21%)	0	2
31	DH	147/149 (99%)	76 (52%)	50 (34%)	21 (14%)	0	6
32	BI	139/142 (98%)	84 (60%)	44 (32%)	11 (8%)	1	19
32	DI	139/142 (98%)	81 (58%)	39 (28%)	19 (14%)	0	6
33	BJ	140/142 (99%)	106 (76%)	20 (14%)	14 (10%)	1	13
33	DJ	140/142 (99%)	95 (68%)	33 (24%)	12 (9%)	1	17
34	BK	120/123 (98%)	84 (70%)	18 (15%)	18 (15%)	0	5
34	DK	120/123 (98%)	80 (67%)	21 (18%)	19 (16%)	0	5
35	BL	141/144 (98%)	101 (72%)	28 (20%)	12 (8%)	1	17
35	DL	141/144 (98%)	83 (59%)	37 (26%)	21 (15%)	0	5
36	BM	134/136 (98%)	94 (70%)	25 (19%)	15 (11%)	0	10
36	DM	134/136 (98%)	92 (69%)	25 (19%)	17 (13%)	0	7
37	BN	118/127 (93%)	87 (74%)	21 (18%)	10 (8%)	1	17
37	DN	118/127 (93%)	71 (60%)	35 (30%)	12 (10%)	1	12
38	BO	114/117 (97%)	79 (69%)	26 (23%)	9 (8%)	1	19
38	DO	114/117 (97%)	76 (67%)	29 (25%)	9 (8%)	1	19
39	BP	112/115 (97%)	71 (63%)	22 (20%)	19 (17%)	0	4
39	DP	112/115 (97%)	67 (60%)	28 (25%)	17 (15%)	0	5
40	BQ	115/118 (98%)	88 (76%)	18 (16%)	9 (8%)	1	19
40	DQ	115/118 (98%)	79 (69%)	26 (23%)	10 (9%)	1	16
41	BR	101/103 (98%)	79 (78%)	14 (14%)	8 (8%)	1	19
41	DR	101/103 (98%)	72 (71%)	19 (19%)	10 (10%)	1	13
42	BS	108/110 (98%)	76 (70%)	27 (25%)	5 (5%)	3	33
42	DS	108/110 (98%)	81 (75%)	18 (17%)	9 (8%)	1	17
43	BT	91/100 (91%)	53 (58%)	23 (25%)	15 (16%)	0	4
43	DT	91/100 (91%)	48 (53%)	28 (31%)	15 (16%)	0	4
44	BU	100/104 (96%)	71 (71%)	13 (13%)	16 (16%)	0	5
44	DU	100/104 (96%)	51 (51%)	28 (28%)	21 (21%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	BV	92/94 (98%)	75 (82%)	15 (16%)	2 (2%)	8	52
45	DV	92/94 (98%)	59 (64%)	26 (28%)	7 (8%)	1	20
46	BW	77/85 (91%)	29 (38%)	22 (29%)	26 (34%)	0	0
46	DW	77/85 (91%)	32 (42%)	27 (35%)	18 (23%)	0	1
47	BX	75/78 (96%)	59 (79%)	13 (17%)	3 (4%)	4	37
47	DX	75/78 (96%)	48 (64%)	21 (28%)	6 (8%)	1	19
48	BY	61/63 (97%)	36 (59%)	17 (28%)	8 (13%)	0	7
48	DY	61/63 (97%)	44 (72%)	12 (20%)	5 (8%)	1	18
49	BZ	56/59 (95%)	39 (70%)	13 (23%)	4 (7%)	1	22
49	DZ	56/59 (95%)	31 (55%)	18 (32%)	7 (12%)	0	8
50	B0	54/57 (95%)	39 (72%)	9 (17%)	6 (11%)	0	10
50	D0	54/57 (95%)	40 (74%)	8 (15%)	6 (11%)	0	10
51	B1	48/55 (87%)	37 (77%)	7 (15%)	4 (8%)	1	17
51	D1	48/55 (87%)	35 (73%)	9 (19%)	4 (8%)	1	17
52	B2	44/46 (96%)	35 (80%)	8 (18%)	1 (2%)	8	51
52	D2	44/46 (96%)	32 (73%)	7 (16%)	5 (11%)	0	9
53	B3	62/65 (95%)	49 (79%)	11 (18%)	2 (3%)	5	44
53	D3	62/65 (95%)	39 (63%)	17 (27%)	6 (10%)	1	14
54	B4	36/38 (95%)	29 (81%)	4 (11%)	3 (8%)	1	17
54	D4	36/38 (95%)	22 (61%)	9 (25%)	5 (14%)	0	6
All	All	11238/11970 (94%)	7499 (67%)	2485 (22%)	1254 (11%)	0	10

5 of 1254 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AB	20	ARG
1	AB	22	TRP
1	AB	40	ILE
1	AB	71	THR
1	AB	72	LYS

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	
1	AB	180/199 (90%)	147 (82%)	33 (18%)	2	15
1	CB	180/199 (90%)	157 (87%)	23 (13%)	5	32
2	AC	170/190 (90%)	148 (87%)	22 (13%)	5	32
2	CC	170/190 (90%)	153 (90%)	17 (10%)	9	43
3	AD	172/173 (99%)	144 (84%)	28 (16%)	3	21
3	CD	172/173 (99%)	146 (85%)	26 (15%)	3	25
4	AE	113/126 (90%)	90 (80%)	23 (20%)	1	11
4	CE	113/126 (90%)	97 (86%)	16 (14%)	4	29
5	AF	87/116 (75%)	77 (88%)	10 (12%)	7	37
5	CF	87/116 (75%)	78 (90%)	9 (10%)	9	42
6	AG	124/147 (84%)	116 (94%)	8 (6%)	21	62
6	CG	123/147 (84%)	97 (79%)	26 (21%)	1	10
7	AH	104/105 (99%)	92 (88%)	12 (12%)	7	37
7	CH	104/105 (99%)	87 (84%)	17 (16%)	3	21
8	AI	105/107 (98%)	88 (84%)	17 (16%)	3	21
8	CI	105/107 (98%)	91 (87%)	14 (13%)	5	31
9	AJ	86/90 (96%)	72 (84%)	14 (16%)	3	21
9	CJ	86/90 (96%)	74 (86%)	12 (14%)	4	29
10	AK	90/99 (91%)	81 (90%)	9 (10%)	9	43
10	CK	90/99 (91%)	73 (81%)	17 (19%)	2	14
11	AL	103/104 (99%)	85 (82%)	18 (18%)	2	18
11	CL	103/104 (99%)	85 (82%)	18 (18%)	2	18
12	AM	92/96 (96%)	87 (95%)	5 (5%)	27	68
12	CM	91/96 (95%)	75 (82%)	16 (18%)	2	17
13	AN	79/84 (94%)	74 (94%)	5 (6%)	22	63
13	CN	79/84 (94%)	67 (85%)	12 (15%)	3	25
14	AO	76/77 (99%)	69 (91%)	7 (9%)	11	48
14	CO	76/77 (99%)	71 (93%)	5 (7%)	21	62
15	AP	65/65 (100%)	59 (91%)	6 (9%)	11	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	CP	65/65 (100%)	59 (91%)	6 (9%)	11	48
16	AQ	74/78 (95%)	57 (77%)	17 (23%)	1	8
16	CQ	74/78 (95%)	64 (86%)	10 (14%)	5	30
17	AR	48/65 (74%)	47 (98%)	1 (2%)	61	86
17	CR	48/65 (74%)	45 (94%)	3 (6%)	22	63
18	AS	70/79 (89%)	62 (89%)	8 (11%)	7	37
18	CS	70/79 (89%)	59 (84%)	11 (16%)	3	24
19	AT	65/66 (98%)	56 (86%)	9 (14%)	4	30
19	CT	65/66 (98%)	58 (89%)	7 (11%)	8	40
20	AU	44/61 (72%)	36 (82%)	8 (18%)	2	16
20	CU	44/61 (72%)	33 (75%)	11 (25%)	1	6
26	BC	216/218 (99%)	177 (82%)	39 (18%)	2	16
26	DC	216/218 (99%)	191 (88%)	25 (12%)	7	36
27	BD	164/164 (100%)	133 (81%)	31 (19%)	2	14
27	DD	164/164 (100%)	144 (88%)	20 (12%)	6	34
28	BE	165/165 (100%)	128 (78%)	37 (22%)	1	9
28	DE	165/165 (100%)	150 (91%)	15 (9%)	12	48
29	BF	148/150 (99%)	129 (87%)	19 (13%)	5	32
29	DF	149/150 (99%)	121 (81%)	28 (19%)	2	14
30	BG	137/138 (99%)	108 (79%)	29 (21%)	1	10
30	DG	137/138 (99%)	120 (88%)	17 (12%)	6	33
31	BH	114/114 (100%)	98 (86%)	16 (14%)	4	29
31	DH	114/114 (100%)	97 (85%)	17 (15%)	4	26
32	BI	109/110 (99%)	92 (84%)	17 (16%)	3	24
32	DI	109/110 (99%)	102 (94%)	7 (6%)	22	63
33	BJ	116/116 (100%)	91 (78%)	25 (22%)	1	9
33	DJ	116/116 (100%)	105 (90%)	11 (10%)	11	46
34	BK	103/104 (99%)	82 (80%)	21 (20%)	1	11
34	DK	103/104 (99%)	85 (82%)	18 (18%)	2	18
35	BL	102/103 (99%)	77 (76%)	25 (24%)	1	7
35	DL	102/103 (99%)	87 (85%)	15 (15%)	4	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	BM	109/109 (100%)	89 (82%)	20 (18%)	2	15
36	DM	109/109 (100%)	96 (88%)	13 (12%)	6	35
37	BN	100/103 (97%)	78 (78%)	22 (22%)	1	9
37	DN	100/103 (97%)	87 (87%)	13 (13%)	5	32
38	BO	86/87 (99%)	69 (80%)	17 (20%)	1	12
38	DO	86/87 (99%)	76 (88%)	10 (12%)	7	36
39	BP	99/100 (99%)	77 (78%)	22 (22%)	1	9
39	DP	99/100 (99%)	91 (92%)	8 (8%)	15	54
40	BQ	89/90 (99%)	73 (82%)	16 (18%)	2	16
40	DQ	89/90 (99%)	78 (88%)	11 (12%)	6	33
41	BR	84/84 (100%)	68 (81%)	16 (19%)	2	14
41	DR	84/84 (100%)	72 (86%)	12 (14%)	4	28
42	BS	93/93 (100%)	76 (82%)	17 (18%)	2	15
42	DS	93/93 (100%)	80 (86%)	13 (14%)	4	29
43	BT	80/84 (95%)	63 (79%)	17 (21%)	1	10
43	DT	80/84 (95%)	75 (94%)	5 (6%)	22	63
44	BU	83/85 (98%)	73 (88%)	10 (12%)	6	34
44	DU	83/85 (98%)	72 (87%)	11 (13%)	5	31
45	BV	78/78 (100%)	64 (82%)	14 (18%)	2	16
45	DV	78/78 (100%)	65 (83%)	13 (17%)	3	20
46	BW	59/63 (94%)	39 (66%)	20 (34%)	0	2
46	DW	59/63 (94%)	43 (73%)	16 (27%)	0	5
47	BX	67/68 (98%)	56 (84%)	11 (16%)	3	21
47	DX	67/68 (98%)	58 (87%)	9 (13%)	5	30
48	BY	55/55 (100%)	41 (74%)	14 (26%)	1	6
48	DY	55/55 (100%)	51 (93%)	4 (7%)	17	58
49	BZ	48/49 (98%)	34 (71%)	14 (29%)	0	4
49	DZ	48/49 (98%)	39 (81%)	9 (19%)	2	14
50	B0	47/48 (98%)	43 (92%)	4 (8%)	13	52
50	D0	47/48 (98%)	41 (87%)	6 (13%)	5	32
51	B1	45/49 (92%)	35 (78%)	10 (22%)	1	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
51	D1	45/49 (92%)	41 (91%)	4 (9%)	12 50
52	B2	38/38 (100%)	32 (84%)	6 (16%)	3 23
52	D2	38/38 (100%)	34 (90%)	4 (10%)	8 41
53	B3	51/52 (98%)	45 (88%)	6 (12%)	6 35
53	D3	51/52 (98%)	42 (82%)	9 (18%)	2 17
54	B4	34/34 (100%)	29 (85%)	5 (15%)	4 27
54	D4	34/34 (100%)	29 (85%)	5 (15%)	4 27
All	All	9331/9756 (96%)	7927 (85%)	1404 (15%)	3 26

5 of 1404 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
42	BS	29	VAL
1	CB	19	THR
42	DS	22	ASP
43	BT	17	SER
47	BX	24	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 327 such sidechains are listed below:

Mol	Chain	Res	Type
45	BV	51	GLN
3	CD	125	ASN
44	DU	53	GLN
46	BW	49	ASN
1	CB	14	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1532/1533 (99%)	474 (30%)	255 (16%)
22	AV	16/17 (94%)	0	0
22	CV	16/17 (94%)	1 (6%)	0
23	AW	5/6 (83%)	3 (60%)	1 (20%)
23	CW	5/6 (83%)	2 (40%)	1 (20%)
24	BA	2850/2903 (98%)	958 (33%)	492 (17%)
24	DA	2838/2903 (97%)	1000 (35%)	519 (18%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
25	BB	117/118 (99%)	33 (28%)	19 (16%)
55	CA	1530/1530 (100%)	519 (33%)	252 (16%)
56	DB	116/117 (99%)	42 (36%)	18 (15%)
All	All	9025/9150 (98%)	3032 (33%)	1557 (17%)

5 of 3032 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	5	U
21	AA	6	G
21	AA	7	A
21	AA	9	G
21	AA	13	U

5 of 1557 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
24	BA	2609	U
55	CA	500	G
24	DA	2287	A
24	BA	2732	G
55	CA	89	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 365 ligands modelled in this entry, 365 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	AB	218/241 (90%)	2.68	106 (48%) 0 1	206, 268, 283, 298	0
1	CB	218/241 (90%)	0.98	49 (22%) 1 1	146, 174, 199, 216	0
2	AC	206/233 (88%)	0.34	4 (1%) 70 54	106, 135, 169, 198	0
2	CC	206/233 (88%)	0.23	2 (0%) 84 72	111, 140, 177, 195	0
3	AD	205/206 (99%)	0.23	10 (4%) 33 22	102, 139, 185, 204	0
3	CD	205/206 (99%)	-0.24	1 (0%) 91 85	86, 109, 140, 157	0
4	AE	150/167 (89%)	2.98	79 (52%) 0 1	102, 214, 237, 255	0
4	CE	150/167 (89%)	0.46	9 (6%) 25 15	86, 134, 166, 209	0
5	AF	100/135 (74%)	0.66	15 (15%) 3 2	140, 166, 186, 192	0
5	CF	100/135 (74%)	0.74	13 (13%) 5 4	140, 170, 200, 208	0
6	AG	151/179 (84%)	0.50	9 (5%) 25 15	128, 157, 186, 202	0
6	CG	150/179 (83%)	0.51	20 (13%) 4 4	115, 165, 204, 219	0
7	AH	129/130 (99%)	0.49	9 (6%) 19 11	102, 134, 158, 182	0
7	CH	129/130 (99%)	0.25	3 (2%) 64 48	106, 135, 159, 174	0
8	AI	127/130 (97%)	0.49	12 (9%) 11 6	108, 158, 190, 210	0
8	CI	127/130 (97%)	0.75	20 (15%) 3 2	114, 174, 206, 221	0
9	AJ	98/103 (95%)	0.18	1 (1%) 84 72	105, 150, 194, 211	0
9	CJ	98/103 (95%)	0.84	16 (16%) 2 2	113, 165, 210, 220	0
10	AK	117/129 (90%)	0.87	17 (14%) 3 3	100, 149, 183, 200	0
10	CK	117/129 (90%)	0.62	11 (9%) 11 6	89, 133, 167, 192	0
11	AL	123/124 (99%)	0.19	4 (3%) 50 35	75, 95, 132, 157	0
11	CL	123/124 (99%)	0.11	2 (1%) 74 60	83, 101, 132, 151	0
12	AM	114/118 (96%)	0.56	13 (11%) 7 5	122, 182, 213, 232	0
12	CM	113/118 (95%)	0.64	9 (7%) 15 9	133, 193, 225, 235	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AN	96/101 (95%)	0.27	3 (3%) 52 36	111, 142, 184, 210	0
13	CN	95/101 (94%)	0.58	10 (10%) 8 5	117, 149, 199, 207	0
14	AO	88/89 (98%)	0.17	1 (1%) 82 69	105, 133, 163, 199	0
14	CO	88/89 (98%)	0.15	2 (2%) 64 48	113, 141, 174, 197	0
15	AP	82/82 (100%)	0.95	18 (21%) 1 1	95, 127, 165, 208	0
15	CP	80/82 (97%)	0.89	10 (12%) 5 4	98, 122, 156, 189	0
16	AQ	80/84 (95%)	0.76	7 (8%) 12 8	69, 100, 142, 159	0
16	CQ	80/84 (95%)	0.94	10 (12%) 5 4	72, 111, 142, 159	0
17	AR	55/75 (73%)	0.63	7 (12%) 5 4	129, 148, 180, 190	0
17	CR	55/75 (73%)	0.88	8 (14%) 3 3	131, 150, 170, 182	0
18	AS	79/92 (85%)	0.84	13 (16%) 2 2	140, 176, 210, 235	0
18	CS	79/92 (85%)	1.25	17 (21%) 1 1	151, 182, 215, 230	0
19	AT	85/87 (97%)	0.17	0 100 100	89, 121, 149, 180	0
19	CT	85/87 (97%)	0.68	8 (9%) 11 6	115, 153, 185, 206	0
20	AU	51/71 (71%)	0.63	6 (11%) 6 5	98, 145, 201, 208	0
20	CU	51/71 (71%)	0.67	7 (13%) 4 3	104, 139, 173, 193	0
21	AA	1533/1533 (100%)	-0.43	15 (0%) 84 72	65, 123, 208, 301	0
22	AV	17/17 (100%)	-0.11	1 (5%) 26 16	102, 112, 149, 197	0
22	CV	17/17 (100%)	-0.17	1 (5%) 26 16	99, 104, 145, 179	0
23	AW	6/6 (100%)	0.60	1 (16%) 2 2	100, 109, 120, 155	0
23	CW	6/6 (100%)	0.24	0 100 100	98, 105, 123, 130	0
24	BA	2854/2903 (98%)	-0.38	40 (1%) 78 63	36, 66, 188, 342	0
24	DA	2841/2903 (97%)	-0.03	57 (2%) 68 53	79, 132, 236, 340	0
25	BB	118/118 (100%)	-0.59	0 100 100	52, 81, 113, 162	0
26	BC	271/273 (99%)	-0.10	4 (1%) 76 62	44, 80, 122, 159	0
26	DC	271/273 (99%)	0.46	15 (5%) 29 19	89, 133, 164, 189	0
27	BD	209/209 (100%)	-0.12	0 100 100	37, 59, 105, 146	0
27	DD	209/209 (100%)	0.52	20 (9%) 10 6	83, 131, 164, 186	0
28	BE	201/201 (100%)	-0.01	4 (1%) 68 53	38, 84, 131, 164	0
28	DE	201/201 (100%)	0.53	16 (7%) 15 9	95, 171, 212, 250	0
29	BF	177/179 (98%)	1.00	28 (15%) 3 2	90, 148, 201, 218	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
29	DF	178/179 (99%)	2.88	102 (57%) 0 1	250, 278, 301, 305	0
30	BG	176/177 (99%)	0.05	2 (1%) 82 69	66, 91, 135, 160	0
30	DG	176/177 (99%)	1.01	30 (17%) 2 2	120, 148, 177, 204	0
31	BH	149/149 (100%)	3.03	70 (46%) 0 1	89, 262, 290, 299	0
31	DH	149/149 (100%)	2.50	66 (44%) 0 1	156, 244, 279, 286	0
32	BI	141/142 (99%)	2.26	65 (46%) 0 1	237, 306, 364, 376	0
32	DI	141/142 (99%)	2.80	80 (56%) 0 1	277, 331, 367, 378	0
33	BJ	142/142 (100%)	-0.27	0 100 100	41, 57, 102, 157	0
33	DJ	142/142 (100%)	0.22	3 (2%) 67 51	92, 115, 142, 181	0
34	BK	122/123 (99%)	-0.20	0 100 100	41, 56, 110, 177	0
34	DK	122/123 (99%)	0.53	3 (2%) 61 44	93, 115, 144, 173	0
35	BL	143/144 (99%)	-0.19	1 (0%) 89 80	38, 77, 119, 160	0
35	DL	143/144 (99%)	0.72	18 (12%) 5 4	93, 155, 197, 209	0
36	BM	136/136 (100%)	-0.11	1 (0%) 89 80	41, 67, 114, 152	0
36	DM	136/136 (100%)	0.91	21 (15%) 3 2	80, 107, 142, 164	0
37	BN	120/127 (94%)	-0.09	0 100 100	46, 63, 84, 138	0
37	DN	120/127 (94%)	1.10	23 (19%) 2 1	122, 154, 180, 217	0
38	BO	116/117 (99%)	-0.25	0 100 100	73, 84, 124, 149	0
38	DO	116/117 (99%)	2.06	55 (47%) 0 1	165, 197, 217, 225	0
39	BP	114/115 (99%)	-0.18	1 (0%) 85 74	49, 67, 123, 152	0
39	DP	114/115 (99%)	0.48	7 (6%) 25 15	117, 137, 163, 182	0
40	BQ	117/118 (99%)	-0.46	0 100 100	40, 58, 100, 127	0
40	DQ	117/118 (99%)	0.49	7 (5%) 25 15	97, 119, 143, 172	0
41	BR	103/103 (100%)	-0.08	1 (0%) 84 72	39, 70, 116, 158	0
41	DR	103/103 (100%)	0.88	18 (17%) 2 2	96, 133, 157, 164	0
42	BS	110/110 (100%)	-0.34	0 100 100	41, 58, 95, 161	0
42	DS	110/110 (100%)	0.70	11 (10%) 9 6	98, 141, 173, 188	0
43	BT	93/100 (93%)	0.40	4 (4%) 39 25	56, 95, 135, 165	0
43	DT	93/100 (93%)	2.17	50 (53%) 0 1	144, 196, 226, 237	0
44	BU	102/104 (98%)	0.29	3 (2%) 55 38	77, 105, 139, 194	0
44	DU	102/104 (98%)	2.36	57 (55%) 0 1	174, 208, 248, 279	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
45	BV	94/94 (100%)	0.04	0 100 100	60, 81, 115, 143	0
45	DV	94/94 (100%)	1.80	37 (39%) 0 1	125, 188, 226, 239	0
46	BW	79/85 (92%)	0.11	2 (2%) 61 44	50, 75, 131, 168	0
46	DW	79/85 (92%)	1.24	20 (25%) 1 1	88, 134, 164, 184	0
47	BX	77/78 (98%)	-0.24	2 (2%) 59 43	50, 84, 126, 147	0
47	DX	77/78 (98%)	0.94	15 (19%) 1 1	110, 157, 187, 203	0
48	BY	63/63 (100%)	0.25	7 (11%) 7 5	87, 109, 154, 163	0
48	DY	63/63 (100%)	0.93	12 (19%) 2 1	196, 218, 251, 257	0
49	BZ	58/59 (98%)	-0.04	2 (3%) 49 34	49, 63, 106, 145	0
49	DZ	58/59 (98%)	0.52	5 (8%) 13 8	97, 116, 142, 155	0
50	B0	56/57 (98%)	-0.45	0 100 100	40, 63, 119, 143	0
50	D0	56/57 (98%)	0.55	4 (7%) 19 11	93, 152, 190, 202	0
51	B1	50/55 (90%)	0.40	1 (2%) 68 53	63, 91, 117, 156	0
51	D1	50/55 (90%)	1.19	11 (22%) 1 1	113, 142, 173, 179	0
52	B2	46/46 (100%)	-0.27	1 (2%) 65 50	50, 61, 80, 165	0
52	D2	46/46 (100%)	0.22	1 (2%) 65 50	118, 137, 161, 174	0
53	B3	64/65 (98%)	-0.25	0 100 100	45, 63, 98, 133	0
53	D3	64/65 (98%)	0.47	2 (3%) 52 36	105, 123, 146, 174	0
54	B4	38/38 (100%)	-0.14	0 100 100	54, 68, 100, 118	0
54	D4	38/38 (100%)	0.83	1 (2%) 59 43	95, 117, 138, 142	0
55	CA	1530/1530 (100%)	-0.21	28 (1%) 71 56	77, 126, 214, 305	0
56	DB	117/117 (100%)	-0.35	0 100 100	87, 166, 194, 210	0
All	All	20477/21120 (96%)	0.26	1613 (7%) 15 9	36, 125, 246, 378	0

The worst 5 of 1613 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
31	BH	92	GLY	21.6
31	DH	93	SER	21.1
31	DH	92	GLY	21.0
29	DF	129	MET	20.4
31	BH	119	ASN	18.4

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3062	1/1	0.69	1.05	27.92	85,85,85,85	0
57	MG	DA	3134	1/1	0.82	1.43	26.26	126,126,126,126	0
57	MG	DA	3077	1/1	0.92	0.67	22.00	86,86,86,86	0
57	MG	DA	3109	1/1	0.65	0.45	21.47	92,92,92,92	0
57	MG	BA	3037	1/1	0.85	0.36	17.52	42,42,42,42	0
57	MG	BA	3058	1/1	0.83	0.49	16.57	44,44,44,44	0
57	MG	BA	3071	1/1	0.83	0.36	16.11	38,38,38,38	0
57	MG	BA	3041	1/1	0.94	0.26	11.89	43,43,43,43	0
57	MG	CA	1625	1/1	0.85	0.33	11.43	86,86,86,86	0
57	MG	DA	3054	1/1	0.86	0.39	10.03	88,88,88,88	0
57	MG	CA	1629	1/1	0.87	0.51	8.99	111,111,111,111	0
57	MG	BA	3005	1/1	0.87	0.21	8.96	73,73,73,73	0
57	MG	AA	1607	1/1	0.19	0.36	7.70	88,88,88,88	0
57	MG	BA	3136	1/1	0.98	0.44	6.92	47,47,47,47	0
57	MG	BA	3124	1/1	0.82	0.55	6.73	41,41,41,41	0
57	MG	CA	1628	1/1	0.90	0.35	6.15	79,79,79,79	0
57	MG	BA	3002	1/1	0.93	0.32	6.03	47,47,47,47	0
57	MG	BA	3118	1/1	0.96	0.24	5.99	42,42,42,42	0
57	MG	DA	3002	1/1	0.91	0.30	5.38	125,125,125,125	0
57	MG	DA	3071	1/1	0.74	0.60	5.33	94,94,94,94	0
57	MG	BA	3105	1/1	0.95	0.21	5.29	38,38,38,38	0
57	MG	AA	1642	1/1	0.87	0.20	5.27	74,74,74,74	0
57	MG	AA	1631	1/1	0.92	0.27	4.39	98,98,98,98	0
57	MG	DA	3041	1/1	0.70	0.26	3.96	113,113,113,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3072	1/1	0.94	0.22	3.59	38,38,38,38	0
57	MG	BA	3109	1/1	0.95	0.21	3.43	42,42,42,42	0
57	MG	AA	1641	1/1	0.83	0.33	3.43	89,89,89,89	0
57	MG	CA	1637	1/1	0.98	0.31	3.11	83,83,83,83	0
57	MG	AA	1629	1/1	0.90	0.23	2.92	129,129,129,129	0
57	MG	DA	3101	1/1	0.93	0.26	2.77	82,82,82,82	0
57	MG	BA	3104	1/1	0.97	0.19	2.58	38,38,38,38	0
57	MG	CA	1639	1/1	0.84	0.24	2.53	165,165,165,165	0
57	MG	CA	1617	1/1	0.67	0.45	2.06	130,130,130,130	0
57	MG	BA	3028	1/1	0.85	0.21	2.05	39,39,39,39	0
57	MG	CA	1604	1/1	0.91	0.13	2.00	106,106,106,106	0
57	MG	DA	3107	1/1	0.68	0.23	1.98	130,130,130,130	0
57	MG	CA	1613	1/1	0.87	0.24	1.88	79,79,79,79	0
57	MG	CA	1630	1/1	0.90	0.28	1.87	79,79,79,79	0
57	MG	CA	1607	1/1	0.83	0.23	1.78	89,89,89,89	0
57	MG	AA	1604	1/1	0.80	0.12	1.42	126,126,126,126	0
57	MG	DA	3053	1/1	0.90	0.24	1.40	101,101,101,101	0
57	MG	BB	202	1/1	0.94	0.17	1.25	114,114,114,114	0
57	MG	CA	1618	1/1	0.92	0.21	1.15	108,108,108,108	0
57	MG	CA	1641	1/1	0.97	0.18	0.88	91,91,91,91	0
57	MG	BA	3132	1/1	0.94	0.45	0.83	42,42,42,42	0
57	MG	BA	3059	1/1	0.96	0.20	0.82	50,50,50,50	0
57	MG	DA	3003	1/1	0.92	0.23	0.81	94,94,94,94	0
57	MG	DA	3104	1/1	0.93	0.22	0.79	107,107,107,107	0
57	MG	CA	1621	1/1	0.96	0.19	0.68	85,85,85,85	0
57	MG	BA	3130	1/1	0.97	0.17	0.68	49,49,49,49	0
57	MG	DA	3094	1/1	0.90	0.18	0.63	126,126,126,126	0
57	MG	DA	3129	1/1	0.87	0.28	0.46	83,83,83,83	0
57	MG	BA	3038	1/1	0.95	0.17	0.44	42,42,42,42	0
57	MG	BA	3008	1/1	0.99	0.17	0.37	43,43,43,43	0
57	MG	DA	3027	1/1	0.84	0.18	0.35	87,87,87,87	0
57	MG	DA	3025	1/1	0.97	0.19	0.26	105,105,105,105	0
57	MG	BA	3048	1/1	0.94	0.16	0.23	74,74,74,74	0
57	MG	DA	3086	1/1	0.70	0.21	0.16	148,148,148,148	0
57	MG	AA	1613	1/1	0.97	0.15	0.15	74,74,74,74	0
57	MG	BA	3128	1/1	0.96	0.15	0.14	52,52,52,52	0
57	MG	BA	3101	1/1	0.97	0.17	0.12	38,38,38,38	0
57	MG	DA	3050	1/1	0.90	0.20	-0.09	148,148,148,148	0
57	MG	BA	3108	1/1	0.98	0.14	-0.34	40,40,40,40	0
57	MG	BA	3107	1/1	0.89	0.18	-0.43	49,49,49,49	0
57	MG	AA	1625	1/1	0.79	0.15	-0.62	90,90,90,90	0
57	MG	DA	3085	1/1	0.60	0.15	-0.71	190,190,190,190	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	AA	1622	1/1	0.97	0.15	-0.72	85,85,85,85	0
57	MG	DA	3105	1/1	0.96	0.17	-0.77	91,91,91,91	0
57	MG	AA	1611	1/1	0.94	0.15	-0.82	91,91,91,91	0
57	MG	BA	3051	1/1	0.96	0.13	-0.84	39,39,39,39	0
57	MG	DA	3046	1/1	0.92	0.17	-0.86	142,142,142,142	0
57	MG	DA	3019	1/1	0.84	0.13	-0.98	150,150,150,150	0
57	MG	AA	1617	1/1	0.85	0.10	-1.00	123,123,123,123	0
57	MG	DA	3039	1/1	0.98	0.15	-1.03	104,104,104,104	0
57	MG	BA	3114	1/1	0.92	0.13	-1.05	73,73,73,73	0
57	MG	DA	3106	1/1	0.92	0.14	-1.07	92,92,92,92	0
57	MG	DA	3116	1/1	0.85	0.17	-1.08	98,98,98,98	0
58	ZN	B4	101	1/1	0.98	0.11	-1.08	79,79,79,79	0
57	MG	BA	3134	1/1	0.92	0.14	-1.20	38,38,38,38	0
57	MG	CA	1642	1/1	0.86	0.12	-1.26	102,102,102,102	0
57	MG	DA	3125	1/1	0.96	0.16	-1.41	90,90,90,90	0
57	MG	BA	3024	1/1	0.93	0.13	-1.44	42,42,42,42	0
57	MG	DA	3068	1/1	0.80	0.16	-1.46	86,86,86,86	0
57	MG	DA	3070	1/1	0.82	0.14	-1.51	94,94,94,94	0
57	MG	BD	301	1/1	0.95	0.13	-1.56	39,39,39,39	0
58	ZN	D4	101	1/1	0.99	0.04	-1.68	79,79,79,79	0
57	MG	BA	3013	1/1	0.97	0.12	-1.68	38,38,38,38	0
57	MG	CA	1631	1/1	0.94	0.14	-1.68	91,91,91,91	0
57	MG	AA	1606	1/1	0.90	0.12	-1.72	96,96,96,96	0
57	MG	CA	1609	1/1	0.85	0.17	-1.78	96,96,96,96	0
57	MG	BA	3116	1/1	0.96	0.14	-1.83	38,38,38,38	0
57	MG	CA	1634	1/1	0.78	0.11	-1.84	97,97,97,97	0
57	MG	BA	3066	1/1	0.98	0.14	-1.90	43,43,43,43	0
57	MG	CA	1616	1/1	0.78	0.13	-2.03	136,136,136,136	0
57	MG	DA	3044	1/1	0.98	0.14	-2.07	116,116,116,116	0
57	MG	BA	3022	1/1	0.94	0.11	-2.11	38,38,38,38	0
57	MG	DA	3113	1/1	0.93	0.14	-2.15	86,86,86,86	0
57	MG	BA	3110	1/1	0.96	0.10	-2.15	50,50,50,50	0
57	MG	BA	3050	1/1	0.98	0.12	-2.15	40,40,40,40	0
57	MG	BA	3018	1/1	0.96	0.06	-2.19	67,67,67,67	0
57	MG	DA	3098	1/1	0.94	0.15	-2.20	87,87,87,87	0
57	MG	DA	3024	1/1	0.95	0.14	-2.27	90,90,90,90	0
57	MG	CA	1606	1/1	0.68	0.14	-2.29	85,85,85,85	0
57	MG	BA	3063	1/1	0.92	0.11	-2.33	37,37,37,37	0
57	MG	DA	3026	1/1	0.94	0.14	-2.34	88,88,88,88	0
57	MG	BA	3012	1/1	0.96	0.14	-2.34	38,38,38,38	0
57	MG	BA	3120	1/1	0.94	0.12	-2.39	41,41,41,41	0
57	MG	DA	3052	1/1	0.88	0.15	-2.41	118,118,118,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3018	1/1	0.92	0.14	-2.55	106,106,106,106	0
57	MG	DA	3013	1/1	0.93	0.14	-2.62	93,93,93,93	0
57	MG	DA	3081	1/1	0.81	0.14	-2.69	87,87,87,87	0
57	MG	BA	3023	1/1	0.97	0.08	-2.69	41,41,41,41	0
57	MG	DA	3132	1/1	0.93	0.09	-2.70	94,94,94,94	0
57	MG	BA	3040	1/1	0.85	0.15	-2.75	41,41,41,41	0
57	MG	AA	1634	1/1	0.98	0.10	-2.78	102,102,102,102	0
57	MG	AA	1643	1/1	0.95	0.10	-2.95	81,81,81,81	0
57	MG	DA	3074	1/1	0.92	0.11	-3.06	98,98,98,98	0
57	MG	BA	3025	1/1	0.86	0.10	-3.18	41,41,41,41	0
57	MG	BA	3080	1/1	0.88	0.13	-3.24	74,74,74,74	0
57	MG	DA	3102	1/1	0.94	0.11	-3.29	84,84,84,84	0
57	MG	BA	3078	1/1	0.95	0.08	-3.29	86,86,86,86	0
57	MG	DA	3057	1/1	0.83	0.14	-3.30	92,92,92,92	0
57	MG	AA	1616	1/1	0.96	0.10	-3.31	126,126,126,126	0
57	MG	BA	3069	1/1	0.95	0.11	-3.43	52,52,52,52	0
57	MG	BA	3054	1/1	0.97	0.11	-3.49	44,44,44,44	0
57	MG	AA	1609	1/1	0.95	0.12	-3.59	91,91,91,91	0
57	MG	BA	3097	1/1	0.97	0.10	-3.60	49,49,49,49	0
57	MG	BA	3017	1/1	0.99	0.09	-4.69	39,39,39,39	0
57	MG	BA	3036	1/1	0.95	0.07	-6.24	47,47,47,47	0
57	MG	DA	3042	1/1	0.94	0.14	-6.25	101,101,101,101	0
57	MG	DA	3063	1/1	0.97	0.13	-6.98	92,92,92,92	0
57	MG	BA	3129	1/1	0.98	0.08	-8.30	39,39,39,39	0
57	MG	DA	3033	1/1	0.94	0.17	-	94,94,94,94	0
57	MG	DA	3131	1/1	0.69	0.88	-	103,103,103,103	0
57	MG	CA	1612	1/1	0.69	0.33	-	86,86,86,86	0
57	MG	CA	1623	1/1	0.93	0.21	-	89,89,89,89	0
57	MG	DA	3092	1/1	0.96	0.20	-	102,102,102,102	0
57	MG	AA	1618	1/1	0.69	0.17	-	104,104,104,104	0
57	MG	BA	3091	1/1	0.93	0.10	-	69,69,69,69	0
57	MG	DA	3031	1/1	0.85	0.39	-	98,98,98,98	0
57	MG	AA	1630	1/1	0.75	0.13	-	79,79,79,79	0
57	MG	BA	3123	1/1	0.89	0.17	-	63,63,63,63	0
57	MG	DA	3088	1/1	0.68	0.21	-	101,101,101,101	0
57	MG	BA	3031	1/1	0.99	0.14	-	42,42,42,42	0
57	MG	DA	3020	1/1	0.91	0.16	-	153,153,153,153	0
57	MG	BA	3113	1/1	0.96	0.16	-	38,38,38,38	0
57	MG	BA	3061	1/1	0.96	0.50	-	39,39,39,39	0
57	MG	DA	3065	1/1	0.52	1.84	-	84,84,84,84	0
57	MG	BA	3099	1/1	0.90	0.21	-	41,41,41,41	0
57	MG	CA	1602	1/1	0.81	0.39	-	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3072	1/1	0.92	0.13	-	84,84,84,84	0
57	MG	BA	3082	1/1	0.99	0.12	-	38,38,38,38	0
57	MG	CA	1638	1/1	0.79	0.12	-	141,141,141,141	0
57	MG	CA	1608	1/1	0.91	0.22	-	86,86,86,86	0
57	MG	BA	3093	1/1	0.93	0.27	-	84,84,84,84	0
57	MG	BA	3103	1/1	0.98	0.10	-	64,64,64,64	0
57	MG	BA	3126	1/1	0.96	0.25	-	57,57,57,57	0
57	MG	BA	3095	1/1	0.82	0.30	-	75,75,75,75	0
57	MG	DA	3017	1/1	0.82	0.53	-	102,102,102,102	0
57	MG	DA	3112	1/1	0.49	0.70	-	115,115,115,115	0
57	MG	AA	1620	1/1	0.88	0.20	-	144,144,144,144	0
57	MG	DA	3021	1/1	0.82	0.68	-	132,132,132,132	0
57	MG	DA	3061	1/1	0.94	0.43	-	84,84,84,84	0
57	MG	BA	3083	1/1	0.97	0.05	-	43,43,43,43	0
57	MG	BA	3074	1/1	0.98	0.07	-	38,38,38,38	0
57	MG	BA	3046	1/1	0.86	0.17	-	63,63,63,63	0
57	MG	BA	3034	1/1	0.96	0.19	-	40,40,40,40	0
57	MG	DA	3064	1/1	0.79	0.50	-	87,87,87,87	0
57	MG	DA	3082	1/1	0.91	0.29	-	83,83,83,83	0
57	MG	BA	3089	1/1	0.95	0.11	-	50,50,50,50	0
57	MG	DA	3099	1/1	0.71	0.80	-	98,98,98,98	0
57	MG	AA	1603	1/1	0.96	0.12	-	76,76,76,76	0
57	MG	BA	3035	1/1	0.86	0.20	-	55,55,55,55	0
57	MG	DA	3049	1/1	0.88	0.16	-	150,150,150,150	0
57	MG	BA	3042	1/1	0.93	0.14	-	56,56,56,56	0
57	MG	DA	3095	1/1	0.92	0.13	-	159,159,159,159	0
57	MG	CA	1622	1/1	0.77	0.11	-	138,138,138,138	0
57	MG	CA	1610	1/1	0.86	0.10	-	129,129,129,129	0
57	MG	BB	204	1/1	0.93	0.17	-	57,57,57,57	0
57	MG	AA	1628	1/1	0.81	0.33	-	107,107,107,107	0
57	MG	DA	3069	1/1	0.96	0.13	-	86,86,86,86	0
57	MG	BA	3021	1/1	0.97	0.10	-	42,42,42,42	0
57	MG	AA	1612	1/1	0.96	0.12	-	82,82,82,82	0
57	MG	DA	3012	1/1	0.88	0.31	-	96,96,96,96	0
57	MG	DA	3133	1/1	0.63	0.67	-	115,115,115,115	0
57	MG	BA	3122	1/1	0.98	0.18	-	40,40,40,40	0
57	MG	BA	3016	1/1	0.99	0.33	-	39,39,39,39	0
57	MG	BA	3015	1/1	0.82	0.64	-	38,38,38,38	0
57	MG	DA	3010	1/1	0.91	0.13	-	108,108,108,108	0
57	MG	AA	1621	1/1	0.69	0.19	-	67,67,67,67	0
57	MG	BA	3011	1/1	0.94	0.38	-	44,44,44,44	0
57	MG	DA	3090	1/1	0.58	0.34	-	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3016	1/1	0.66	1.17	-	96,96,96,96	0
57	MG	BA	3086	1/1	0.92	0.14	-	43,43,43,43	0
57	MG	DA	3123	1/1	0.97	0.16	-	93,93,93,93	0
57	MG	DA	3130	1/1	0.96	0.66	-	85,85,85,85	0
57	MG	BA	3049	1/1	0.94	0.12	-	45,45,45,45	0
57	MG	AA	1635	1/1	0.89	0.10	-	114,114,114,114	0
57	MG	DA	3029	1/1	0.87	0.29	-	108,108,108,108	0
57	MG	BA	3006	1/1	0.95	0.11	-	88,88,88,88	0
57	MG	DA	3006	1/1	0.84	0.21	-	149,149,149,149	0
57	MG	DA	3056	1/1	0.97	0.17	-	101,101,101,101	0
57	MG	BA	3102	1/1	0.86	0.31	-	40,40,40,40	0
57	MG	BA	3009	1/1	0.95	0.13	-	46,46,46,46	0
57	MG	AA	1619	1/1	0.20	0.84	-	136,136,136,136	0
57	MG	AA	1602	1/1	0.95	0.23	-	79,79,79,79	0
57	MG	BA	3019	1/1	0.92	0.12	-	70,70,70,70	0
57	MG	CA	1635	1/1	0.91	0.09	-	114,114,114,114	0
57	MG	BA	3014	1/1	0.94	0.30	-	38,38,38,38	0
57	MG	DA	3115	1/1	0.89	0.21	-	84,84,84,84	0
57	MG	AA	1636	1/1	0.70	0.38	-	120,120,120,120	0
57	MG	BA	3062	1/1	0.87	0.52	-	38,38,38,38	0
57	MG	BA	3106	1/1	0.95	0.14	-	40,40,40,40	0
57	MG	BA	3039	1/1	0.94	0.11	-	40,40,40,40	0
57	MG	AA	1601	1/1	0.92	0.08	-	111,111,111,111	0
57	MG	DA	3051	1/1	0.92	0.21	-	177,177,177,177	0
57	MG	DA	3014	1/1	0.90	0.35	-	90,90,90,90	0
57	MG	BA	3117	1/1	0.95	0.14	-	56,56,56,56	0
57	MG	DA	3008	1/1	0.90	0.22	-	177,177,177,177	0
57	MG	CA	1627	1/1	0.80	0.24	-	106,106,106,106	0
57	MG	BA	3119	1/1	0.83	0.35	-	52,52,52,52	0
57	MG	BA	3096	1/1	0.96	0.09	-	45,45,45,45	0
57	MG	BA	3077	1/1	0.91	0.31	-	45,45,45,45	0
57	MG	DA	3078	1/1	0.87	0.31	-	79,79,79,79	0
57	MG	BA	3127	1/1	0.96	0.05	-	40,40,40,40	0
57	MG	DA	3100	1/1	0.84	0.55	-	149,149,149,149	0
57	MG	BA	3081	1/1	0.95	0.17	-	40,40,40,40	0
57	MG	BA	3075	1/1	0.86	0.47	-	40,40,40,40	0
57	MG	BA	3004	1/1	0.95	0.25	-	69,69,69,69	0
57	MG	DA	3007	1/1	0.48	0.35	-	192,192,192,192	0
57	MG	BA	3115	1/1	0.78	0.31	-	49,49,49,49	0
57	MG	DA	3047	1/1	0.55	0.20	-	148,148,148,148	0
57	MG	BA	3032	1/1	0.92	0.13	-	40,40,40,40	0
57	MG	DA	3030	1/1	0.96	0.50	-	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DB	201	1/1	0.79	0.31	-	108,108,108,108	0
57	MG	DA	3060	1/1	0.22	0.54	-	96,96,96,96	0
57	MG	CA	1615	1/1	0.83	0.38	-	118,118,118,118	0
57	MG	DA	3022	1/1	0.92	0.21	-	105,105,105,105	0
57	MG	BA	3068	1/1	0.97	0.19	-	52,52,52,52	0
57	MG	DA	3005	1/1	0.81	0.12	-	157,157,157,157	0
57	MG	AA	1626	1/1	0.95	0.23	-	107,107,107,107	0
57	MG	BA	3057	1/1	0.98	0.34	-	42,42,42,42	0
57	MG	BA	3090	1/1	0.90	0.13	-	47,47,47,47	0
57	MG	BA	3052	1/1	0.85	0.13	-	38,38,38,38	0
57	MG	BA	3033	1/1	0.96	0.12	-	40,40,40,40	0
57	MG	DA	3110	1/1	0.34	1.51	-	82,82,82,82	0
57	MG	DA	3004	1/1	0.61	1.93	-	150,150,150,150	0
57	MG	DA	3036	1/1	0.96	0.13	-	84,84,84,84	0
57	MG	BA	3065	1/1	0.94	0.25	-	38,38,38,38	0
57	MG	BA	3030	1/1	0.93	0.45	-	41,41,41,41	0
57	MG	CA	1633	1/1	0.97	0.12	-	101,101,101,101	0
57	MG	BA	3047	1/1	0.93	0.15	-	63,63,63,63	0
57	MG	DA	3119	1/1	0.88	0.16	-	138,138,138,138	0
57	MG	BA	3064	1/1	0.96	0.10	-	38,38,38,38	0
57	MG	BA	3044	1/1	0.88	0.10	-	71,71,71,71	0
57	MG	DA	3009	1/1	0.73	0.20	-	121,121,121,121	0
57	MG	DA	3124	1/1	0.89	0.19	-	133,133,133,133	0
57	MG	CA	1636	1/1	0.89	0.75	-	88,88,88,88	0
57	MG	BB	203	1/1	0.98	0.09	-	57,57,57,57	0
57	MG	BA	3112	1/1	0.84	0.22	-	46,46,46,46	0
57	MG	DA	3028	1/1	0.94	0.95	-	103,103,103,103	0
57	MG	DA	3043	1/1	0.87	0.19	-	107,107,107,107	0
57	MG	AA	1605	1/1	0.95	0.09	-	103,103,103,103	0
57	MG	CA	1619	1/1	0.86	0.83	-	119,119,119,119	0
57	MG	CA	1614	1/1	0.84	0.24	-	114,114,114,114	0
57	MG	DA	3103	1/1	0.93	0.20	-	91,91,91,91	0
57	MG	DA	3127	1/1	0.93	0.22	-	104,104,104,104	0
57	MG	BA	3060	1/1	0.89	0.31	-	39,39,39,39	0
57	MG	DA	3023	1/1	0.88	0.65	-	101,101,101,101	0
57	MG	BA	3067	1/1	0.98	0.09	-	40,40,40,40	0
57	MG	DA	3034	1/1	0.94	0.21	-	89,89,89,89	0
57	MG	CA	1605	1/1	0.95	0.21	-	89,89,89,89	0
57	MG	BA	3100	1/1	0.97	0.09	-	59,59,59,59	0
57	MG	DA	3037	1/1	0.92	0.17	-	83,83,83,83	0
57	MG	DA	3059	1/1	0.78	0.46	-	88,88,88,88	0
57	MG	AA	1610	1/1	0.95	0.16	-	125,125,125,125	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3053	1/1	0.95	0.12	-	41,41,41,41	0
57	MG	BA	3020	1/1	0.98	0.10	-	46,46,46,46	0
57	MG	DA	3108	1/1	0.90	0.26	-	82,82,82,82	0
57	MG	CA	1620	1/1	0.88	0.26	-	93,93,93,93	0
57	MG	DA	3066	1/1	0.84	0.34	-	92,92,92,92	0
57	MG	DA	3084	1/1	0.68	0.15	-	157,157,157,157	0
57	MG	BA	3084	1/1	0.88	0.55	-	49,49,49,49	0
57	MG	DA	3055	1/1	0.98	0.16	-	85,85,85,85	0
57	MG	DA	3126	1/1	0.77	0.48	-	99,99,99,99	0
57	MG	BA	3001	1/1	0.91	0.15	-	45,45,45,45	0
57	MG	DA	3048	1/1	0.86	0.19	-	131,131,131,131	0
57	MG	DA	3114	1/1	0.97	0.08	-	98,98,98,98	0
57	MG	BA	3121	1/1	0.92	0.10	-	45,45,45,45	0
57	MG	DA	3058	1/1	0.92	0.14	-	96,96,96,96	0
57	MG	DA	3075	1/1	0.80	0.11	-	255,255,255,255	0
57	MG	DA	3089	1/1	0.79	0.30	-	110,110,110,110	0
57	MG	BA	3076	1/1	0.94	0.15	-	47,47,47,47	0
57	MG	BA	3045	1/1	0.90	0.25	-	62,62,62,62	0
57	MG	DA	3096	1/1	0.90	0.63	-	120,120,120,120	0
57	MG	AA	1615	1/1	0.95	0.08	-	117,117,117,117	0
57	MG	BA	3131	1/1	0.76	0.75	-	48,48,48,48	0
57	MG	DA	3083	1/1	0.91	0.22	-	121,121,121,121	0
57	MG	BA	3087	1/1	0.97	0.11	-	45,45,45,45	0
57	MG	BA	3094	1/1	0.88	0.12	-	75,75,75,75	0
57	MG	BA	3125	1/1	0.97	0.17	-	40,40,40,40	0
57	MG	BA	3088	1/1	0.95	0.07	-	58,58,58,58	0
57	MG	AA	1623	1/1	0.92	0.21	-	108,108,108,108	0
57	MG	BA	3135	1/1	0.86	0.48	-	43,43,43,43	0
57	MG	AA	1640	1/1	0.89	0.12	-	132,132,132,132	0
57	MG	AA	1639	1/1	0.96	0.06	-	119,119,119,119	0
57	MG	CA	1626	1/1	0.92	0.14	-	110,110,110,110	0
57	MG	AA	1632	1/1	0.89	0.16	-	95,95,95,95	0
57	MG	DA	3117	1/1	0.91	0.15	-	90,90,90,90	0
57	MG	BA	3092	1/1	0.89	0.19	-	108,108,108,108	0
57	MG	DA	3097	1/1	0.86	0.20	-	119,119,119,119	0
57	MG	DA	3015	1/1	0.82	0.23	-	88,88,88,88	0
57	MG	DA	3091	1/1	0.94	0.13	-	93,93,93,93	0
57	MG	BA	3027	1/1	0.98	0.06	-	41,41,41,41	0
57	MG	BA	3085	1/1	0.95	0.53	-	42,42,42,42	0
57	MG	DA	3040	1/1	0.88	0.49	-	102,102,102,102	0
57	MG	AA	1637	1/1	0.81	0.21	-	87,87,87,87	0
57	MG	BA	3056	1/1	0.92	0.34	-	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3079	1/1	0.80	0.09	-	89,89,89,89	0
57	MG	DJ	201	1/1	0.87	0.43	-	101,101,101,101	0
57	MG	AA	1633	1/1	0.96	0.13	-	107,107,107,107	0
57	MG	DA	3067	1/1	0.96	0.16	-	86,86,86,86	0
57	MG	BA	3133	1/1	0.86	0.57	-	53,53,53,53	0
57	MG	CA	1611	1/1	0.96	0.09	-	93,93,93,93	0
57	MG	BA	3026	1/1	0.84	0.36	-	41,41,41,41	0
57	MG	DA	3032	1/1	0.86	0.27	-	87,87,87,87	0
57	MG	DC	301	1/1	0.53	0.38	-	103,103,103,103	0
57	MG	AA	1627	1/1	0.91	0.58	-	109,109,109,109	0
57	MG	BB	201	1/1	0.81	0.57	-	105,105,105,105	0
57	MG	DA	3011	1/1	0.88	0.55	-	110,110,110,110	0
57	MG	DA	3087	1/1	0.96	0.09	-	88,88,88,88	0
57	MG	BA	3029	1/1	0.96	0.10	-	38,38,38,38	0
57	MG	BA	3055	1/1	0.97	0.13	-	44,44,44,44	0
57	MG	DA	3080	1/1	0.94	0.53	-	84,84,84,84	0
57	MG	DA	3093	1/1	0.53	0.52	-	93,93,93,93	0
57	MG	DA	3045	1/1	0.80	0.20	-	141,141,141,141	0
57	MG	BA	3073	1/1	0.98	0.08	-	43,43,43,43	0
57	MG	BA	3111	1/1	0.83	0.15	-	38,38,38,38	0
57	MG	CA	1640	1/1	0.94	0.41	-	87,87,87,87	0
57	MG	DA	3001	1/1	0.95	0.22	-	115,115,115,115	0
57	MG	BA	3007	1/1	0.83	0.22	-	90,90,90,90	0
57	MG	DA	3121	1/1	0.93	0.22	-	97,97,97,97	0
57	MG	BA	3043	1/1	0.97	0.15	-	56,56,56,56	0
57	MG	DA	3073	1/1	0.93	0.28	-	98,98,98,98	0
57	MG	DA	3079	1/1	0.95	0.22	-	90,90,90,90	0
57	MG	DA	3120	1/1	0.85	0.67	-	96,96,96,96	0
57	MG	DA	3038	1/1	0.93	0.17	-	108,108,108,108	0
57	MG	DA	3122	1/1	0.96	0.23	-	142,142,142,142	0
57	MG	BA	3010	1/1	0.95	0.09	-	46,46,46,46	0
57	MG	BA	3070	1/1	0.57	0.19	-	140,140,140,140	0
57	MG	DA	3035	1/1	0.87	0.21	-	88,88,88,88	0
57	MG	DA	3076	1/1	-0.05	1.26	-	109,109,109,109	0
57	MG	DA	3128	1/1	0.72	0.56	-	100,100,100,100	0
57	MG	DA	3111	1/1	0.88	0.21	-	164,164,164,164	0
57	MG	CA	1632	1/1	0.69	0.15	-	125,125,125,125	0
57	MG	AA	1608	1/1	0.96	0.24	-	82,82,82,82	0
57	MG	AA	1614	1/1	0.92	0.24	-	113,113,113,113	0
57	MG	CA	1624	1/1	0.71	0.92	-	79,79,79,79	0
57	MG	CA	1603	1/1	0.77	0.39	-	92,92,92,92	0
57	MG	BA	3003	1/1	0.98	0.07	-	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	AA	1624	1/1	0.75	0.21	-	94,94,94,94	0
57	MG	AA	1638	1/1	0.91	0.14	-	81,81,81,81	0
57	MG	DA	3118	1/1	0.96	0.32	-	99,99,99,99	0
57	MG	CA	1601	1/1	0.80	0.07	-	142,142,142,142	0
57	MG	BA	3098	1/1	0.97	0.64	-	52,52,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.