



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:58 PM GMT

PDB ID : 4V4H  
Title : Crystal structure of the bacterial ribosome from Escherichia coli in complex with the antibiotic kasugamyin at 3.5Å resolution.  
Authors : Schuwirth, B.S.; Vila-Sanjurjo, A.; Cate, J.H.D.  
Deposited on : 2006-08-04  
Resolution : 3.46 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 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

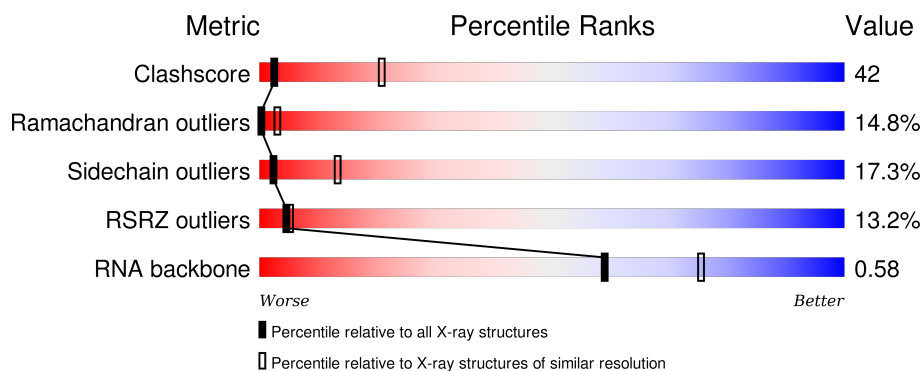
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.46 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1090 (3.56-3.36)
Ramachandran outliers	100387	1057 (3.56-3.36)
Sidechain outliers	100360	1058 (3.56-3.36)
RSRZ outliers	91569	1005 (3.56-3.36)
RNA backbone	2183	1045 (4.10-2.80)

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  $\geq 3$ , 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	AA	1542	<div> <div>2%</div> <div>23% 63% 13%</div> </div>
1	CA	1542	<div> <div>%</div> <div>22% 64% 12%</div> </div>
2	AC	233	<div> <div>12%</div> <div>25% 52% 11% 12%</div> </div>
2	CC	233	<div> <div>5%</div> <div>30% 45% 12% 12%</div> </div>
3	AD	206	<div> <div>22%</div> <div>31% 51% 16%</div> </div>

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Mol	Chain	Length	Quality of chain
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	
15	CP	82	

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Mol	Chain	Length	Quality of chain
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	AB	241	
20	CB	241	
21	AU	71	
21	CU	71	
22	BA	120	
22	DA	120	
23	BB	2904	
23	DB	2904	
24	BV	94	
24	DV	94	
25	BC	273	
25	DC	273	
26	BD	209	
26	DD	209	
27	BE	201	
27	DE	201	
28	BF	179	

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Mol	Chain	Length	Quality of chain
28	DF	179	
29	BG	177	
29	DG	177	
30	BH	149	
30	DH	149	
31	BJ	142	
31	DJ	142	
32	BK	123	
32	DK	123	
33	BL	144	
33	DL	144	
34	BM	136	
34	DM	136	
35	BN	127	
35	DN	127	
36	BO	117	
36	DO	117	
37	BP	115	
37	DP	115	
38	BQ	118	
38	DQ	118	
39	BR	103	
39	DR	103	
40	BS	110	
40	DS	110	

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Mol	Chain	Length	Quality of chain
41	BT	100	
41	DT	100	
42	BU	104	
42	DU	104	
43	BW	85	
43	DW	85	
44	BX	63	
44	DX	63	
45	BY	59	
45	DY	59	
46	BZ	70	
46	DZ	70	
47	B0	57	
47	D0	57	
48	B1	55	
48	D1	55	
49	B2	46	
49	D2	46	
50	B3	65	
50	D3	65	
51	B4	38	
51	D4	38	
52	BI	142	
52	DI	142	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
53	KSG	AA	1601	-	-	-	X
53	KSG	CA	1601	-	-	-	X
54	MG	BB	3086	-	-	-	X
54	MG	BB	3100	-	-	-	X
54	MG	DB	3082	-	-	-	X

## 2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 284160 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S RIBOSOMAL RNA.

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

- 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	150	Total	C	N	O	S	0	0	0
			1174	730	226	214	4			
6	CG	152	Total	C	N	O	S	0	0	0
			1196	745	230	217	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	96	Total	C	N	O	S	0	0	0
			774	483	160	128	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
			716	440	146	129	1			
14	CO	88	Total	C	N	O	S	0	0	0
			716	440	146	129	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	81	Total	C	N	O	S	0	0	0
			657	417	122	115	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	80	Total	C	N	O	S	0	0	0
			644	413	121	108	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 S2.

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

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN S21.

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

- Molecule 22 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	BA	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			
22	DA	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			

- Molecule 23 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	BB	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			
23	DB	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			

- Molecule 24 is a protein called 50S RIBOSOMAL PROTEIN L25.

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

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BC	267	Total	C	N	O	S	0	0	0
			2053	1271	416	359	7			
25	DC	267	Total	C	N	O	S	0	0	0
			2053	1271	416	359	7			

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L3.

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

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

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L4.

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

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BF	178	Total	C	N	O	S	0	0	0
			1420	905	251	258	6			
28	DF	178	Total	C	N	O	S	0	0	0
			1420	905	251	258	6			

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L6.

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

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L9.

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

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BJ	140	Total	C	N	O	S	0	0	0
			1112	704	210	194	4			
31	DJ	140	Total	C	N	O	S	0	0	0
			1112	704	210	194	4			

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BK	121	Total	C	N	O	S	0	0	0
			930	582	179	164	5			
32	DK	121	Total	C	N	O	S	0	0	0
			930	582	179	164	5			

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BL	144	Total	C	N	O	S	0	0	0
			1053	654	207	190	2			
33	DL	144	Total	C	N	O	S	0	0	0
			1053	654	207	190	2			

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L16.

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

- Molecule 35 is a protein called 50S RIBOSOMAL PROTEIN L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BN	127	Total	C	N	O	S	0	0	0
			1008	621	204	178	5			
35	DN	127	Total	C	N	O	S	0	0	0
			1008	621	204	178	5			

- Molecule 36 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BO	117	Total	C	N	O	S	0	0	0
			900	557	179	163	1			
36	DO	117	Total	C	N	O	S	0	0	0
			900	557	179	163	1			

- Molecule 37 is a protein called 50S RIBOSOMAL PROTEIN L19.

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

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L20.

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

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L21.

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

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L22.

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

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BT	99	Total	C	N	O	S	0	0	0
			777	491	145	139	2			
41	DT	99	Total	C	N	O	S	0	0	0
			777	491	145	139	2			

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L24.

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

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

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BW	84	Total	C	N	O	S			
			634	391	129	113	1	0	0	0
43	DW	84	Total	C	N	O	S			
			634	391	129	113	1	0	0	0

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BX	63	Total	C	N	O	S			
			509	313	99	95	2	0	0	0
44	DX	63	Total	C	N	O	S			
			509	313	99	95	2	0	0	0

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BY	58	Total	C	N	O	S			
			449	281	87	79	2	0	0	0
45	DY	58	Total	C	N	O	S			
			449	281	87	79	2	0	0	0

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BZ	70	Total	C	N	O	S			
			549	339	104	100	6	0	0	0
46	DZ	70	Total	C	N	O	S			
			549	339	104	100	6	0	0	0

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L32.

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



- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
48	B1	54	Total	C	N	O	0	0	0
			441	284	81	76			
48	D1	54	Total	C	N	O	0	0	0
			441	284	81	76			

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L34.

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

- Molecule 50 is a protein called 50S RIBOSOMAL PROTEIN L35.

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

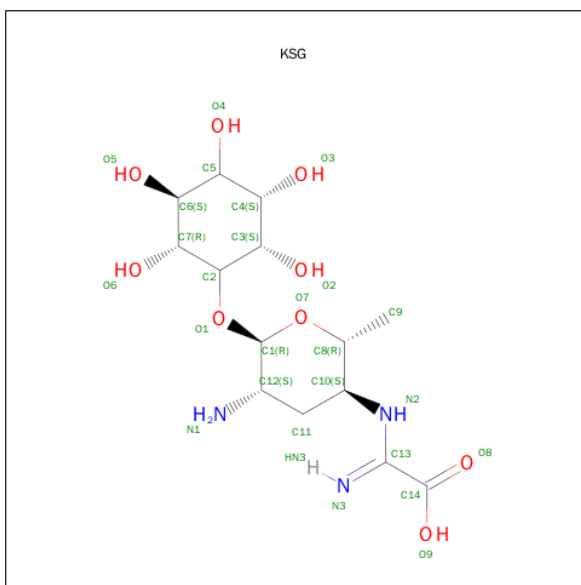
- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L36.

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

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L11.

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

- Molecule 53 is (1S,2R,3S,4R,5S,6S)-2,3,4,5,6-PENTAHYDROXYCYCLOHEXYL 2-AMINO-4-{{[CARBOXY(IMINO)METHYL]AMINO}}-2,3,4,6-TETRADEOXY-ALPHA-D-ARABINO-HEXOPYRANOSIDE (three-letter code: KSG) (formula: C<sub>14</sub>H<sub>25</sub>N<sub>3</sub>O<sub>9</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
53	AA	1	Total	C	N	O	0	0
			26	14	3	9		
53	CA	1	Total	C	N	O	0	0
			26	14	3	9		

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	BB	110	Total	Mg	0	0
			110	110		
54	DE	1	Total	Mg	0	0
			1	1		
54	CA	62	Total	Mg	0	0
			62	62		
54	AA	60	Total	Mg	0	0
			60	60		
54	DN	1	Total	Mg	0	0
			1	1		
54	DB	109	Total	Mg	0	0
			109	109		

- Molecule 55 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	AA	289	Total	O	0	0
			289	289		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	AE	3	Total 3	O 3	0	0
55	AK	2	Total 2	O 2	0	0
55	AN	3	Total 3	O 3	0	0
55	AP	2	Total 2	O 2	0	0
55	AT	1	Total 1	O 1	0	0
55	BB	497	Total 497	O 497	0	0
55	BC	1	Total 1	O 1	0	0
55	BE	5	Total 5	O 5	0	0
55	BH	1	Total 1	O 1	0	0
55	BL	2	Total 2	O 2	0	0
55	BN	1	Total 1	O 1	0	0
55	CA	293	Total 293	O 293	0	0
55	CE	3	Total 3	O 3	0	0
55	CK	1	Total 1	O 1	0	0
55	CL	4	Total 4	O 4	0	0
55	CN	3	Total 3	O 3	0	0
55	CP	1	Total 1	O 1	0	0
55	CT	3	Total 3	O 3	0	0
55	DB	501	Total 501	O 501	0	0
55	DC	1	Total 1	O 1	0	0
55	DD	1	Total 1	O 1	0	0

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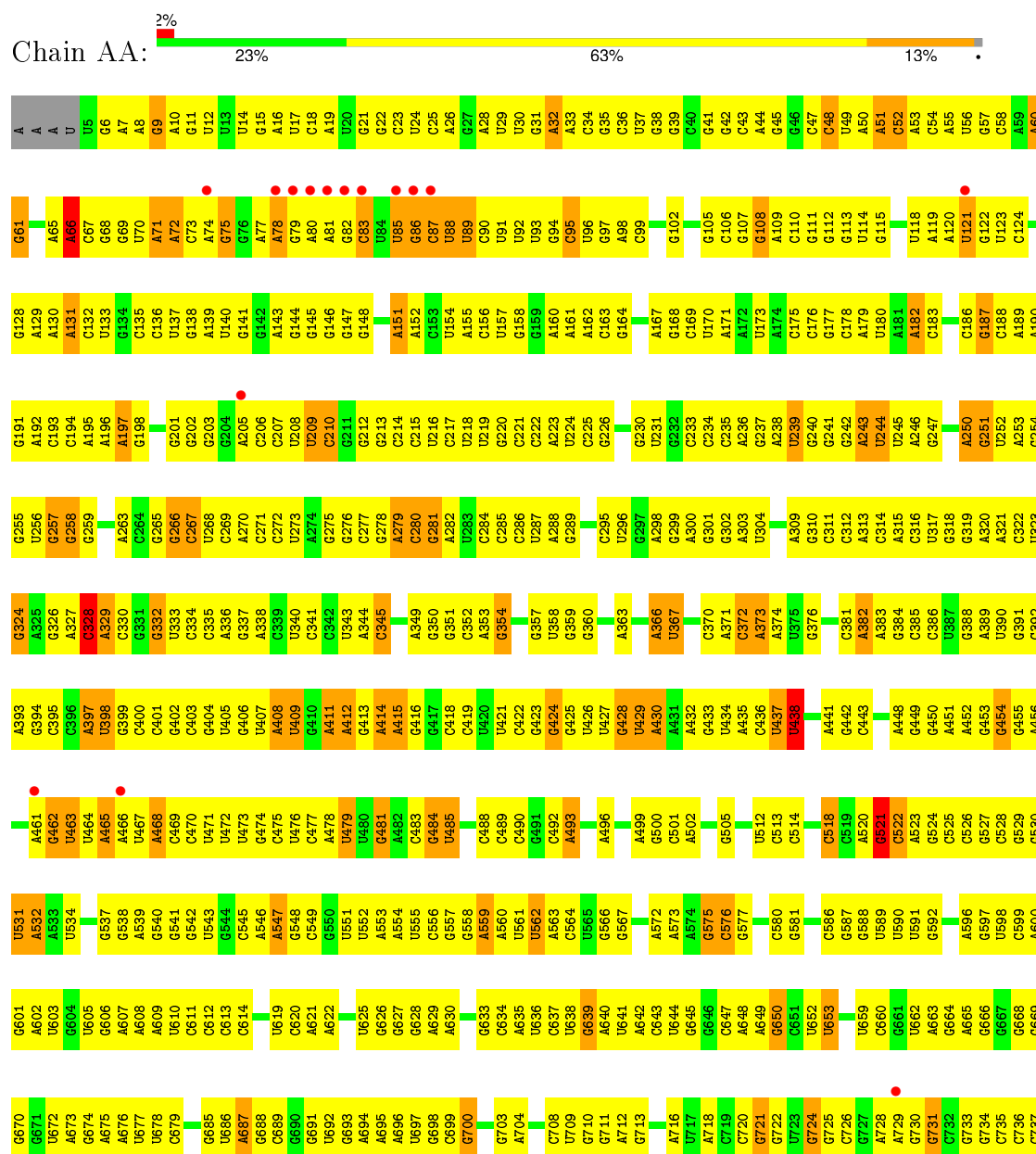
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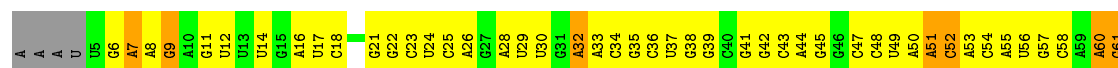
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	DE	3	Total 3	O 3	0	0
55	DL	1	Total 1	O 1	0	0
55	DN	2	Total 2	O 2	0	0
55	DT	1	Total 1	O 1	0	0
55	D2	2	Total 2	O 2	0	0

### 3 Residue-property plots

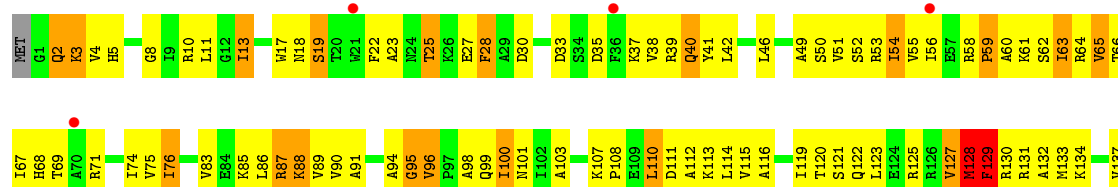
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ( $\text{RSRZ} > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: 16S RIBOSOMAL RNA

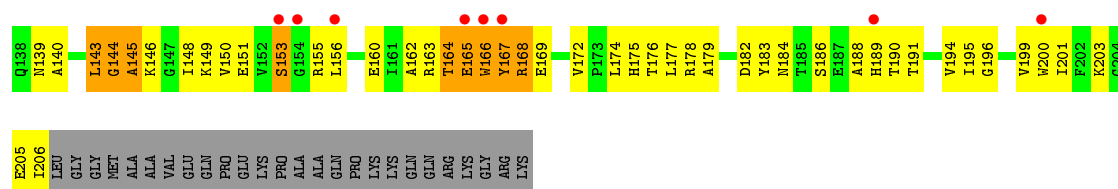




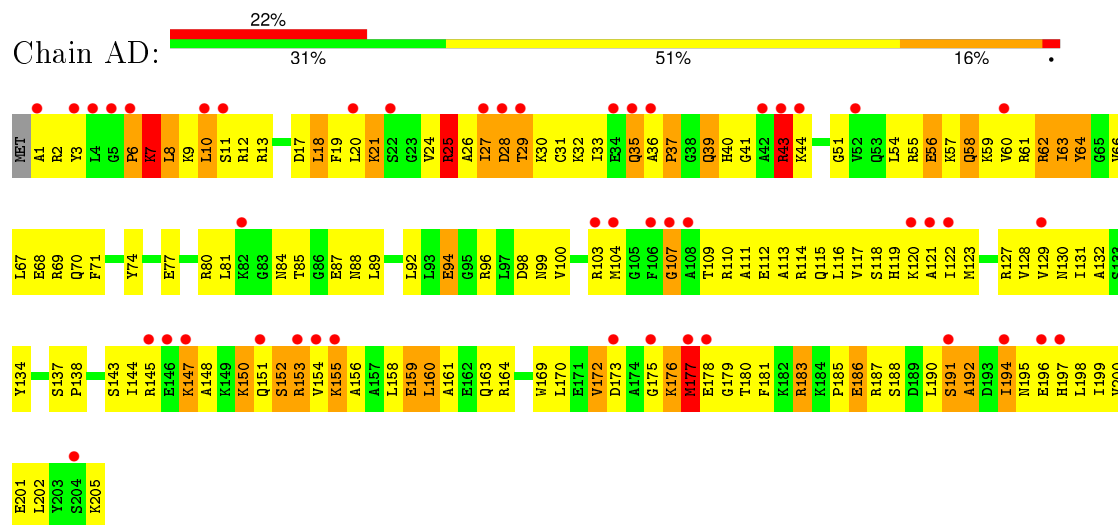
A1067	G1006	G945	U875	C808	C736	G669	U605	G537	U463	A397	A327	G259	C194	A130	G64
G1068	U1007	A946	U876	G809	C737	G669	G606	G538	U464	U396	C328	G260	A195	A131	G65
U1069	U1008	G947	U877	C810	C738	U672	A607	G539	A465	G399	C329	A262	A196	A132	
C1070	U1009	C948	C879	C811	C739	A673	A608	A539	A466	C400	C330	A263	A197	U133	
G1071	U1010	A949	G880	G812	U740	G674	A609	G540	U467	C401	G331	G264	G198	G134	G69
A1012	G1011	U950	G881	U813	G741	A675	U610	G541	A468	C402	G332	G265		G135	U70
U1073	A1012	G951	C882	A814	G742	A676	C611	G542	C469	C403	U333	G266	G202	A171	A71
G1074	G1013	U952	C883	A815	A743	U677	C612	U543	C470	C404	U334	G267	G203	A72	C73
U1075	A1014	G953	A816	G816	G744	U678	C613	G544	U471	U405	C335	U268	G204	U140	A74
G1076	G1015	C954	U884	A817	G745	A679	C614	C545	U472	C406	A336	C269	C306	U141	A75
U1077	A1016	G955	G885	C817	G746	C679		A546	U473	U407	G337	A270	C307	G143	A76
G1078	U1017	U956	G890	A819	A747	U684	G617	A547	C474	A408	A338	C271	U208	A143	A77
U1079	G1018	U957	U885	U820	G748	G685	G618	G548	C475	U409	C339	C272	U209	G144	A78
A1080	A1019		C893	G821	A749	U686	U619	C549	U476	G410	U340	U273	G210	G145	A79
A1081	G1020	A956	G894	U822	A750	A887	C620	G550	C477	A411	C341	A274	G211	A150	A80
U1082	A1021	U960	G895	C823	C751	G688	A621	U551	U478	A412	U342	G275	G212	G146	A81
G1083	U1022	U961	G896	G824	G752	C689	A622	U552	U479	A413	U343	G276	G213	G147	A82
U1084	A1023	C962	G897	A825	A753	G690		A553	U480	A414	A344	G277	G214	G148	
U1085	G1024	G963			C754	G691	U625	A554	A481	A415	C345	G278	C215	A149	C83
U1086	U1025	A964	A900	U828	G755	U692	G626	U555	A482	G416	G346	A279	C216	U150	U84
	G1026	U965	A901	G829		G693	G627	C556	C483	G417		C280	U216	A151	U85
U1091	C1027	G966	G902	G830	G761	A694	G628	G557	G484	C418	A349	G281	C217	A152	G86
A1092	C1028	C967	G903	A831	U762	A695	A629	G558	U485	C419	G350	A282	U218	C153	C87
G1093	U1029	A968	U904	G832	G763	A696	A630	A559		U420	G351	U283	U219	U154	U88
A1094	U1030	A969	G905	G833	C764	U697		A560	C488	U421	C352	C284	G220	A155	U89
U1095	G1031	A906	A906	U834	G765	G698	G633	U561	C489	C422	A353	C285	C221	C156	C90
	U1032		A907	U835		G699	G634	U562	C490	G423	G354	C286	C222	U157	U91
C1096	G1033	C972	A908	U836	A766	G700	A635	A563	G491	G424	G357	A287	A223	G158	U92
C1097	U1034	A974	A909	U837	G768		U636	C564	C492	G425	G358	A288	U224	G159	U93
G1098	A1035	A975	G910	G838	G769	G703	U637	U565	A493	U426	U358	C225	G226	A160	G94
U1099	U1036	G976	U911	C839	C770	G704	U638	G566		U427	G359	C289		A161	C95
A1101	C1037	A977	C912	C840	G771	G705	G639	G567	A496	G428	G360			A162	U96
A1102	U1038	A978	A913	C841	U772	A706	A640			U429		C295	G230	C163	G97
C1103	G1039	C979	A914	U842		U707	U641	A572	A499	A430	U367	C297	U231	G164	A98
G1104	U1040	C980	A915	U843	A777	G708	A642	A573	G500	A431	U368	A298	C232	A167	C99
A1105	G1041	U981	U916	G844	G778	U709	C643	A574	C501	A432	G299	A300	C233	G168	G102
G1106	A1042	U982	G917	A845	G779	G710	U644	G575	A502	G433	A370	A300	C234	C169	
C1107	G1043	A983	A918	G846	A780	G711	G645	C576		U434	A371	C301	C235		
	A1044	C984	A919	G847	A781	A712	G646	G577	G505	A435	C372	G302	A236	U170	G105
	C1045	C985	U920	C948	A782	G713	C647			C436	A373	A303	G237		C106
U1116	U1046	U986	U921	C853	C783	A716	A648	C580	U512	U437	U375	U304	A238	U173	G107
U1117	G1047	G988	A923	U854	G785		G650	G581	C514	U439	G376		G240	C175	A109
C1119	U1049	C990	G924	C857	A786	G719	C651	C586	U518	G440		A309	G241	C176	C110
U1120	G1050	U991	G925	G858	A787	C720	U652	G587	C518	A441	C381	C310	G242	G177	G111
C1121	U1051	U992	G926	G859	U788	G721	U653	G588	G521	G442	A382	C312	A243	C178	G112
U1122	G1052	G993	G927	A860		G722	G656	U589	C522	C443	A383	C313	U244	A179	G113
G1123	A1053	A994	G928	G861	A792	U723	U657	U591	A523	A448	C384	C314	U245	U180	U114
U1124	G1054	C995	G929	C862	A793	G724	G658	G592	G524	C449	C385	A315	A246	A181	G115
U1125	U1055	A996	C930	U863		G725	U659		C525	G450	U386	C316	G247	A182	
U1126	U1056	U997	C931	A864	C797	G726	C660	A596	C526	G451	U387	U317		C183	U118
		C998	G932	A865		G727	G661	G597	G527	A452	G388	G318	A250	A119	A119
C1128	U1060	C999	G933	C866	U801	A728	U662	U598	C528	G453	A389	G319	G251	C186	A120
A1130	U1061	A1000	G934	G867	A802	G729	A663	C599	G529	C454	U390	A320	U252	G187	U121
U1131	U1062	C1001	A935	G868	G803	G730	G664	C600	G530	G455	G391	A321	A253	C188	G122
G1132	G1063	G1002		G869	U804	G731	A665	G801	U531	A456	C392	A322	G254	A189	U123
U1133	U1064	G1003	G940	G805	G805	C732	A666	A602	A532		U323	G324	G255	A190	G124
G1134	C1066	A1005	G941	A872	A807	G733	G667	U603	A533	A461	G394	G325	U256	G191	G128
						G734	G668	G604	U534	G462	C396		G258	C193	A129



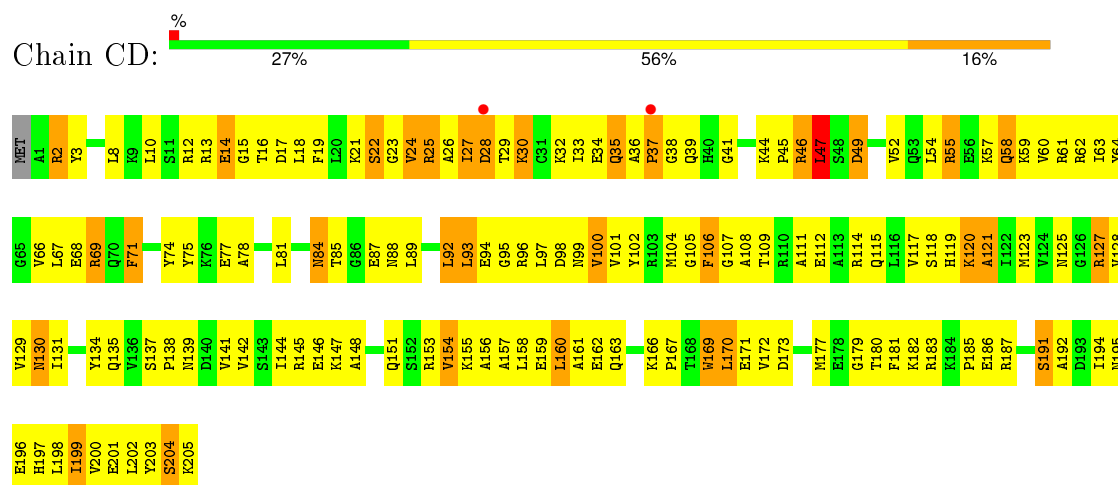




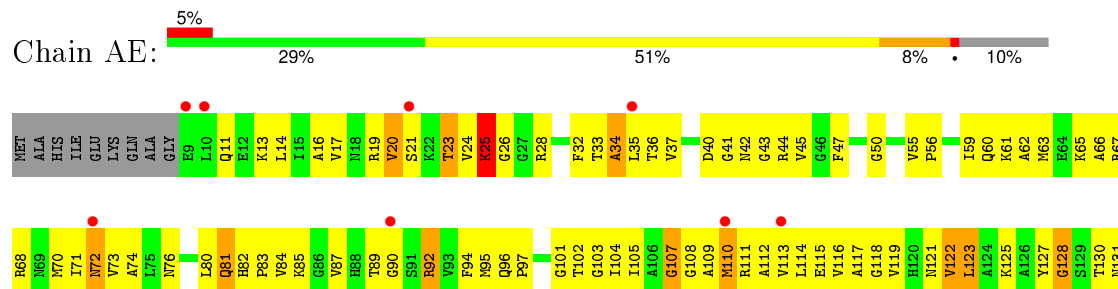
### • Molecule 3: 30S RIBOSOMAL PROTEIN S4

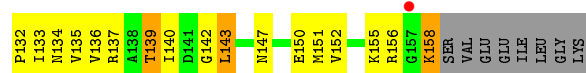


### • Molecule 3: 30S RIBOSOMAL PROTEIN S4

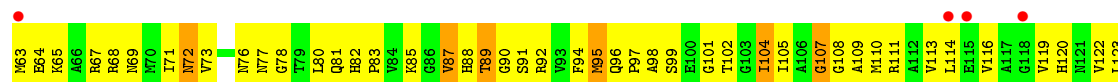


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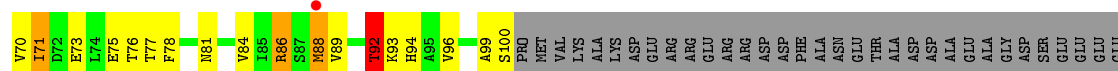
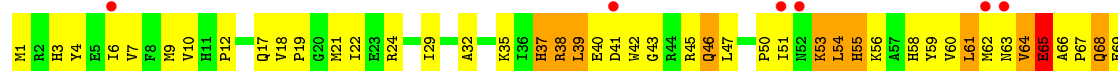




• Molecule 4: 30S RIBOSOMAL PROTEIN S5

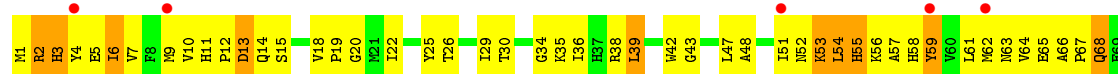
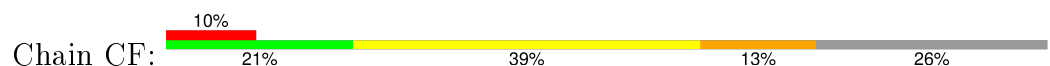


• Molecule 5: 30S RIBOSOMAL PROTEIN S6



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GLU

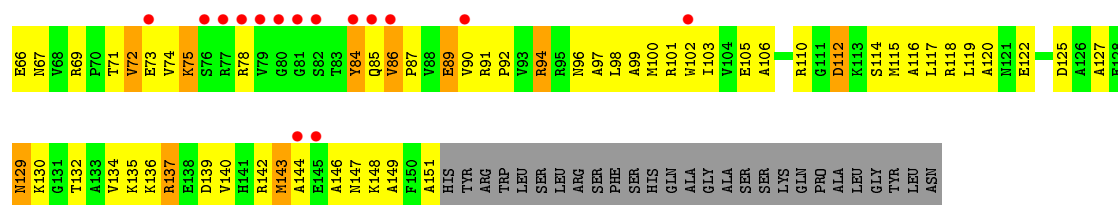
• Molecule 5: 30S RIBOSOMAL PROTEIN S6



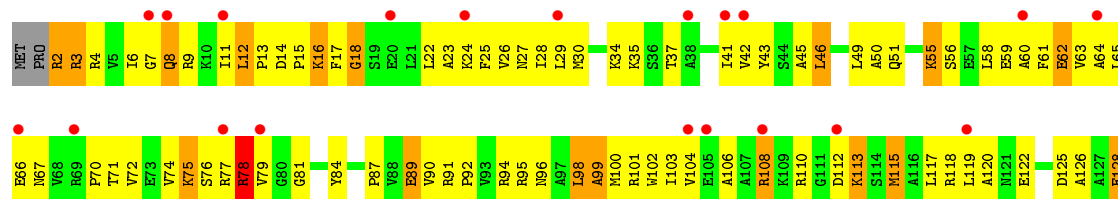
GLU  
GLU  
GLU  
GLU

• Molecule 6: 30S RIBOSOMAL PROTEIN S7

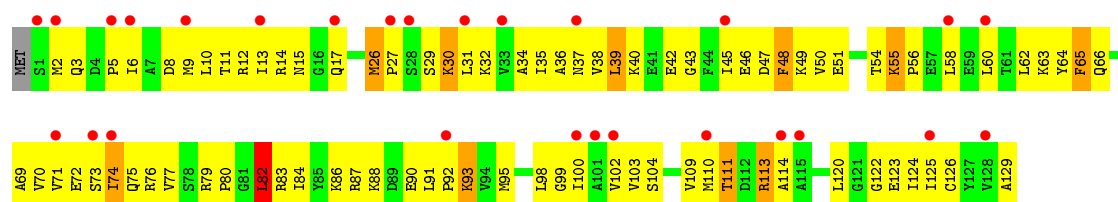




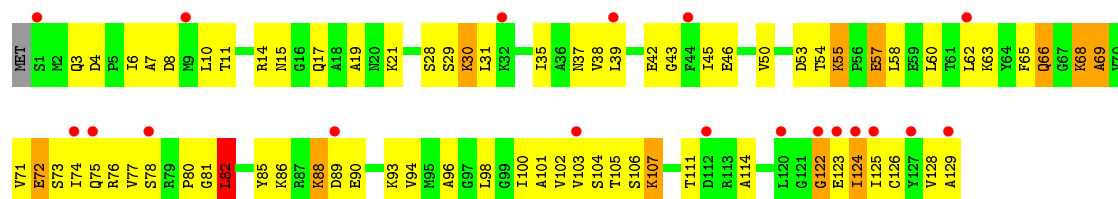
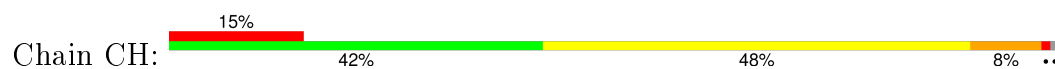
• Molecule 6: 30S RIBOSOMAL PROTEIN S7



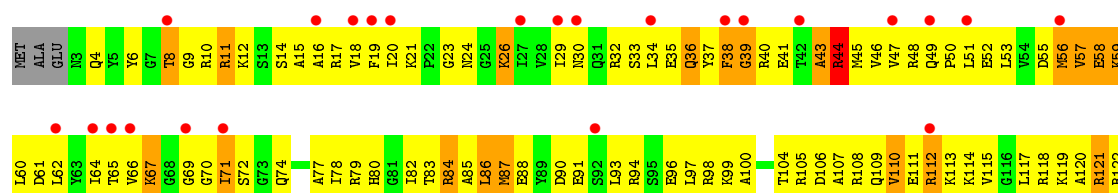
• Molecule 7: 30S RIBOSOMAL PROTEIN S8

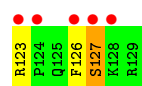


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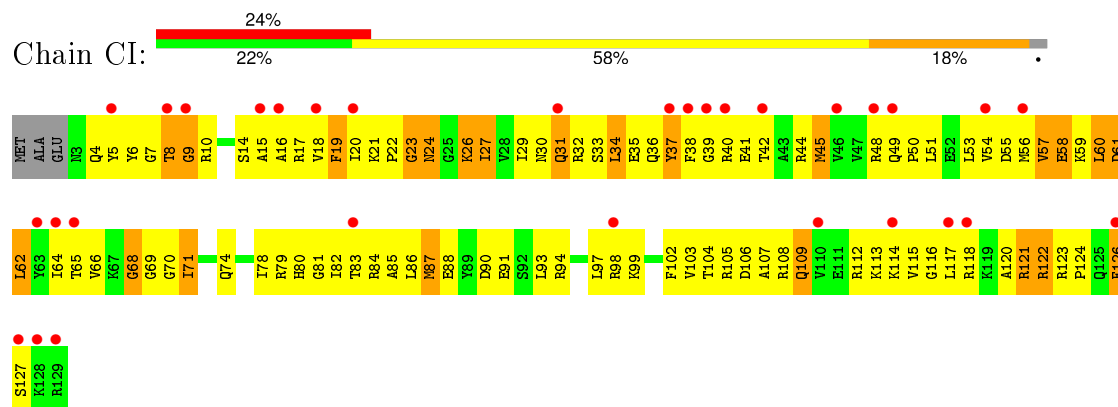


• Molecule 8: 30S RIBOSOMAL PROTEIN S9

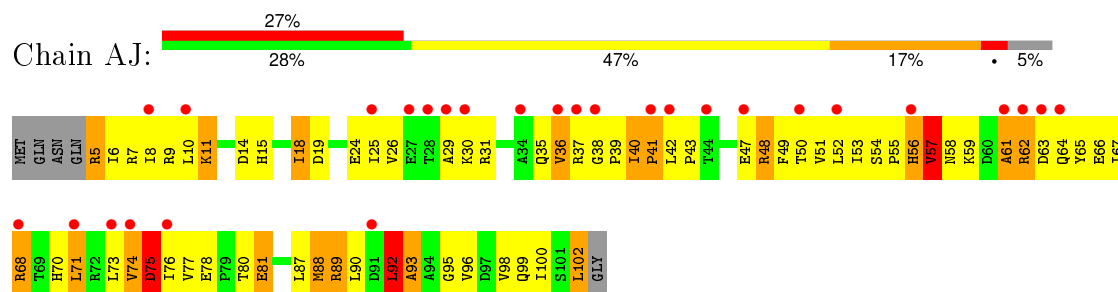




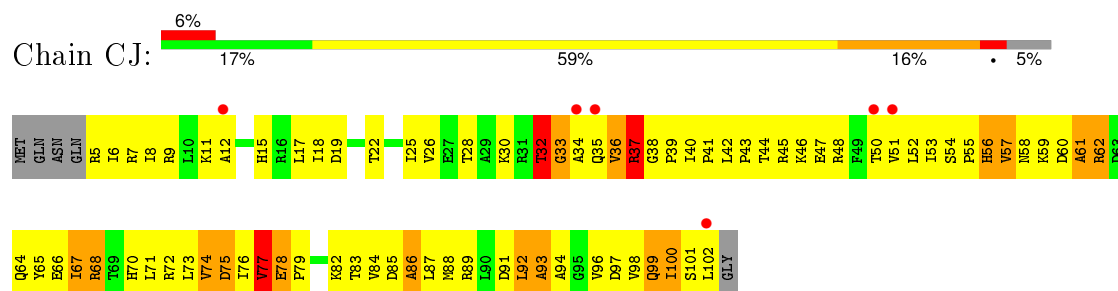
• Molecule 8: 30S RIBOSOMAL PROTEIN S9



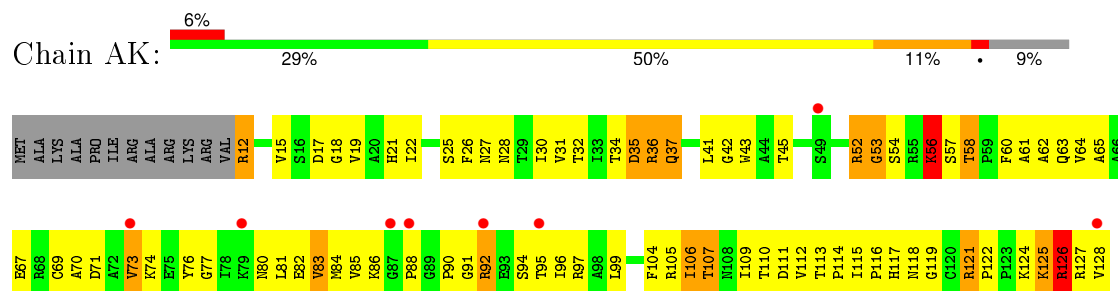
• Molecule 9: 30S RIBOSOMAL PROTEIN S10



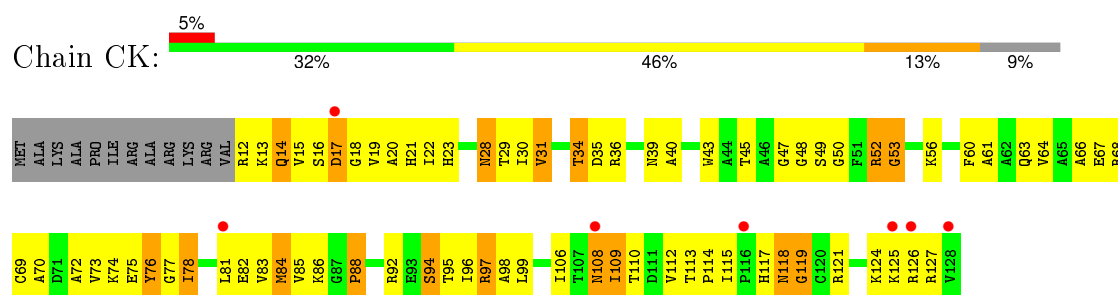
• Molecule 9: 30S RIBOSOMAL PROTEIN S10



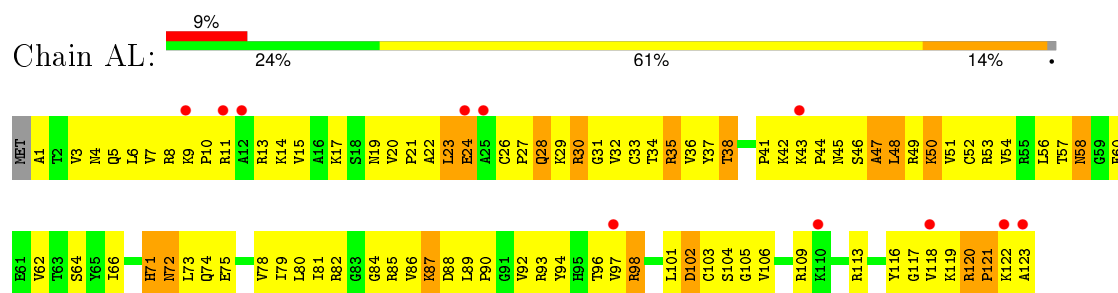
• Molecule 10: 30S RIBOSOMAL PROTEIN S11



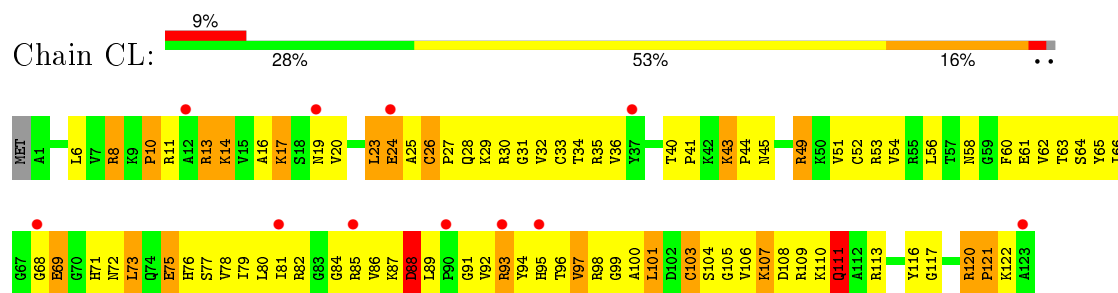
• Molecule 10: 30S RIBOSOMAL PROTEIN S11



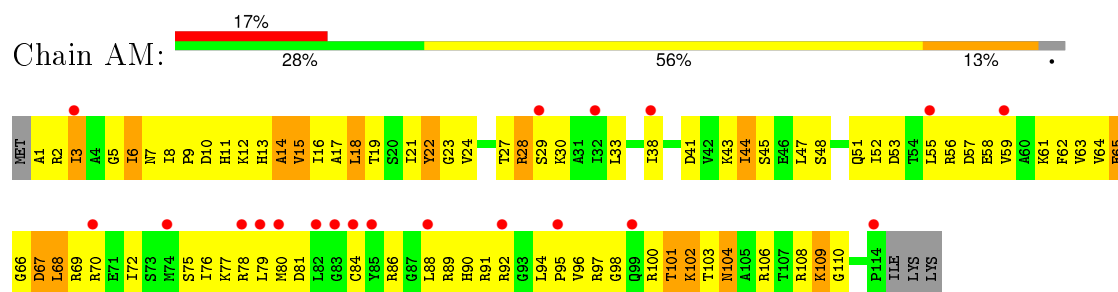
• Molecule 11: 30S RIBOSOMAL PROTEIN S12



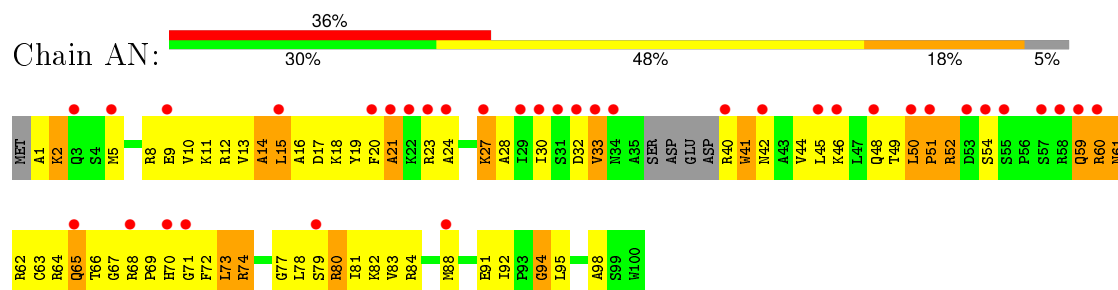
• Molecule 11: 30S RIBOSOMAL PROTEIN S12



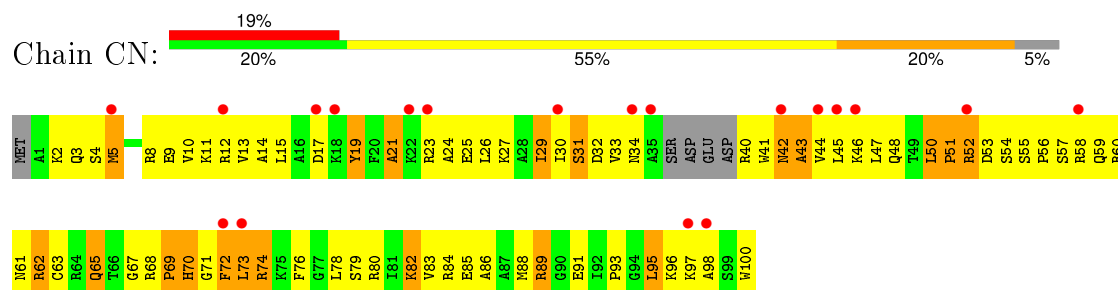
• Molecule 12: 30S RIBOSOMAL PROTEIN S13



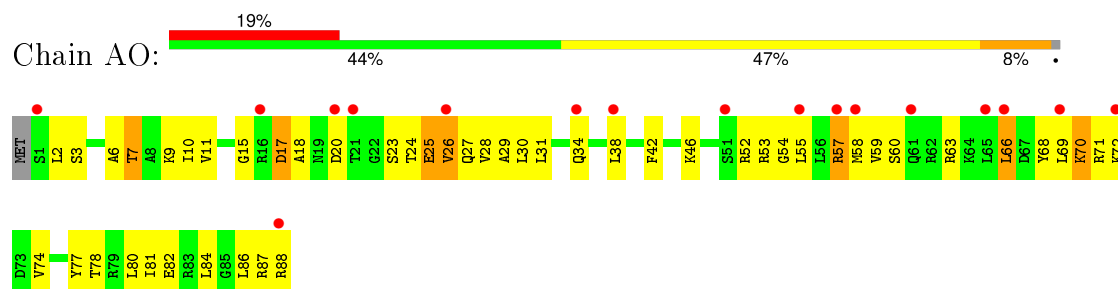
- Molecule 13: 30S RIBOSOMAL PROTEIN S14



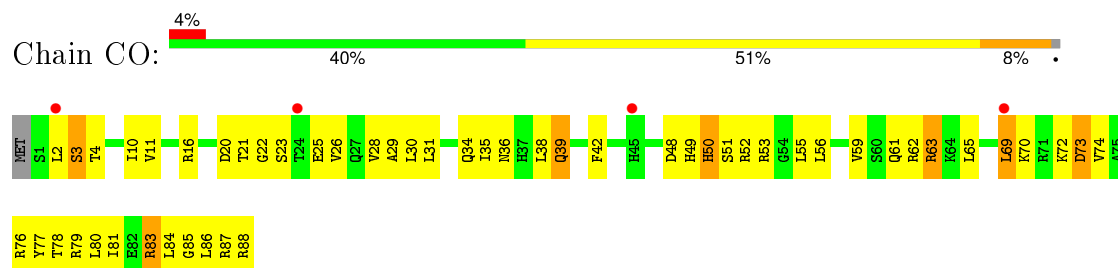
- Molecule 13: 30S RIBOSOMAL PROTEIN S14



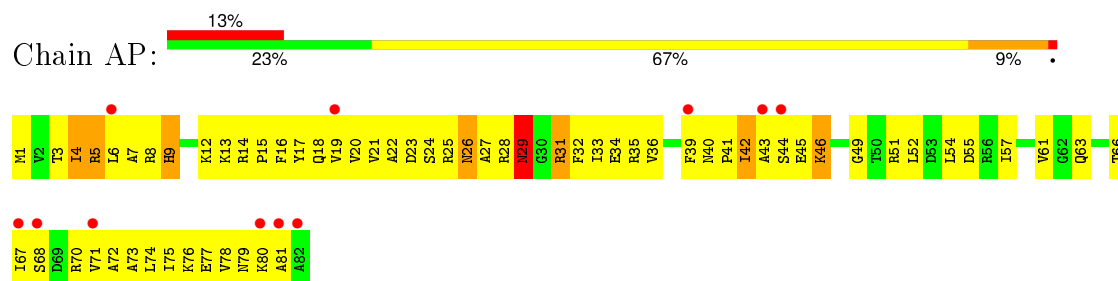
- Molecule 14: 30S RIBOSOMAL PROTEIN S15



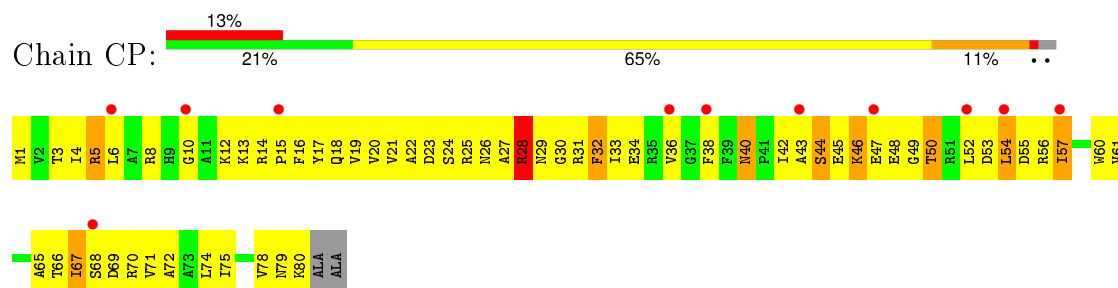
- Molecule 14: 30S RIBOSOMAL PROTEIN S15



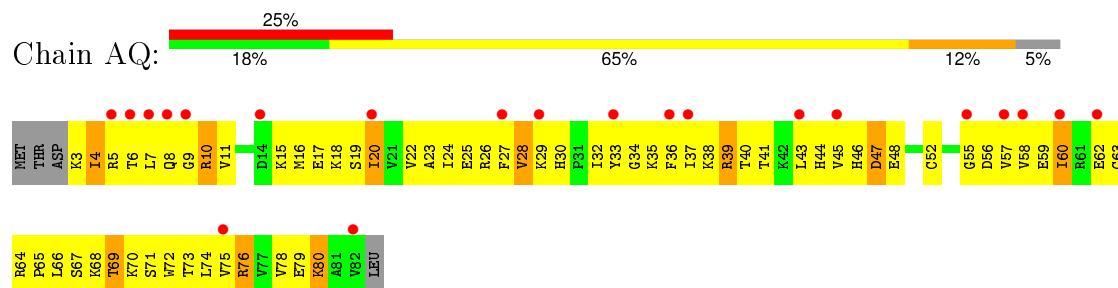
- Molecule 15: 30S RIBOSOMAL PROTEIN S16



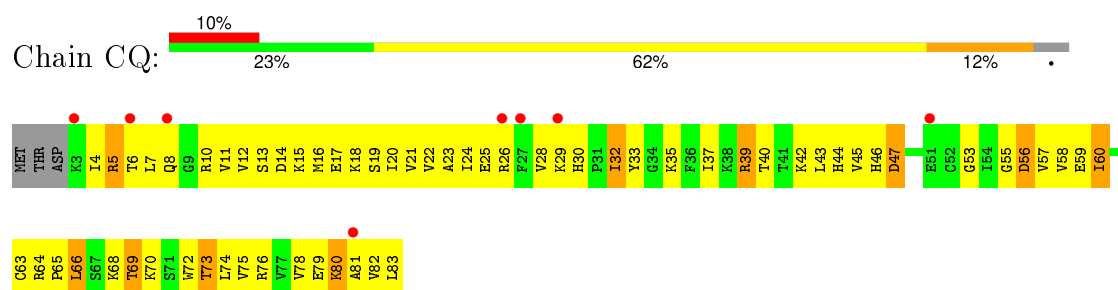
- Molecule 15: 30S RIBOSOMAL PROTEIN S16



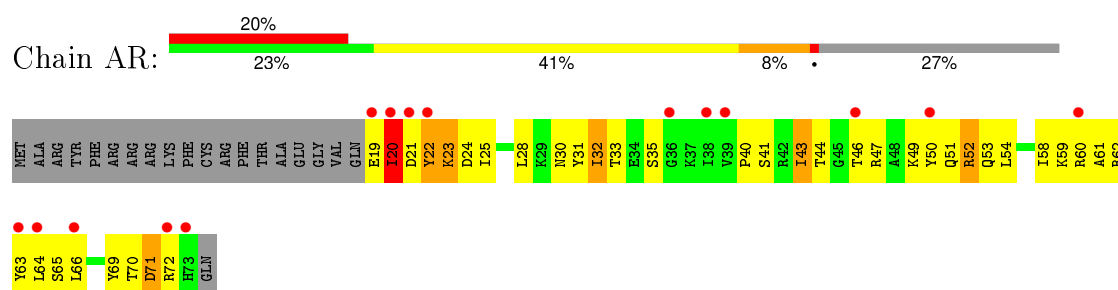
- Molecule 16: 30S RIBOSOMAL PROTEIN S17



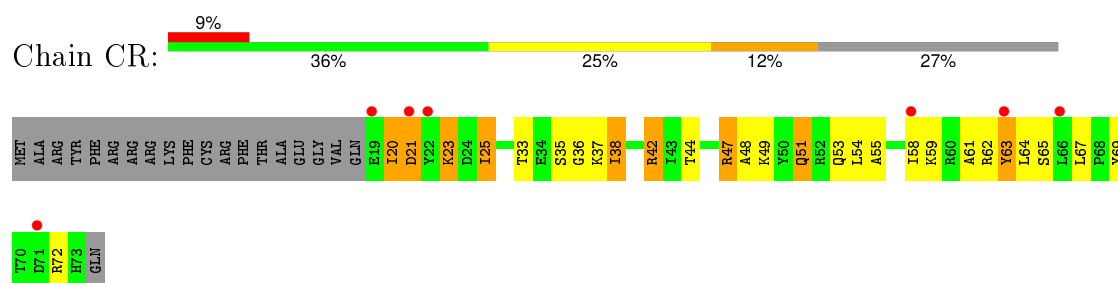
- Molecule 16: 30S RIBOSOMAL PROTEIN S17



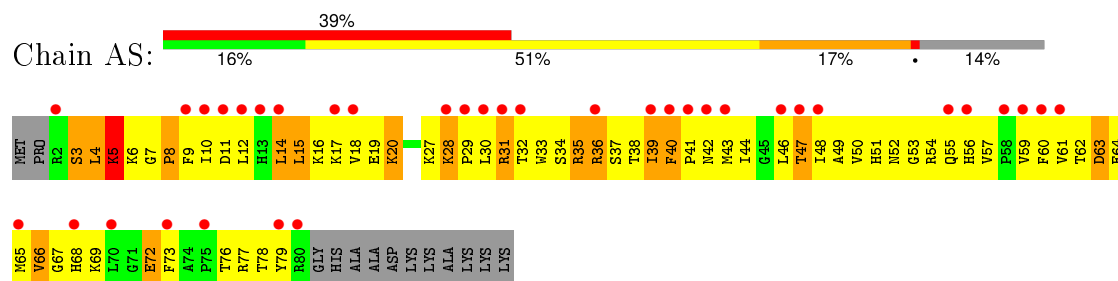
- Molecule 17: 30S RIBOSOMAL PROTEIN S18



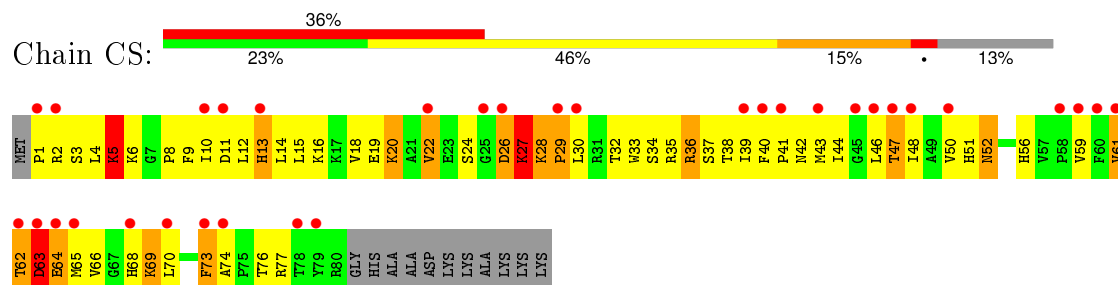
- Molecule 17: 30S RIBOSOMAL PROTEIN S18



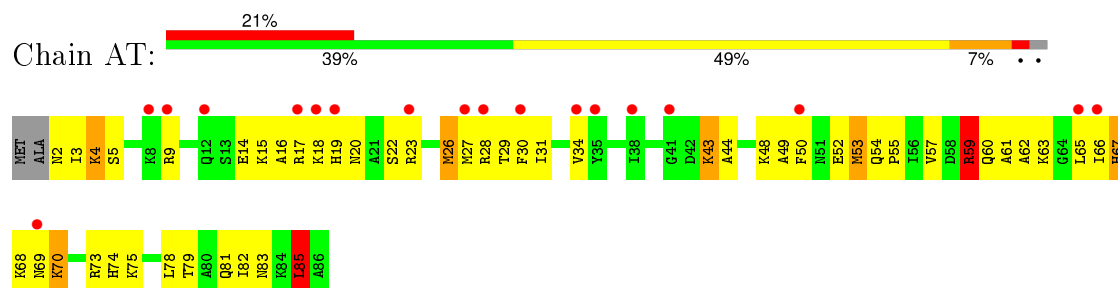
- Molecule 18: 30S RIBOSOMAL PROTEIN S19



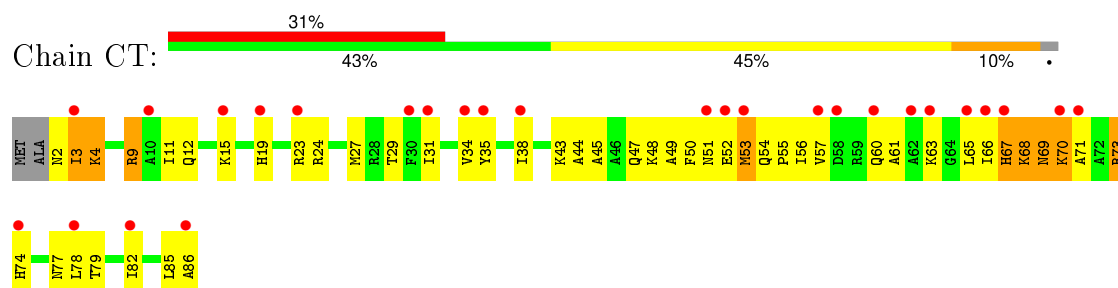
- Molecule 18: 30S RIBOSOMAL PROTEIN S19



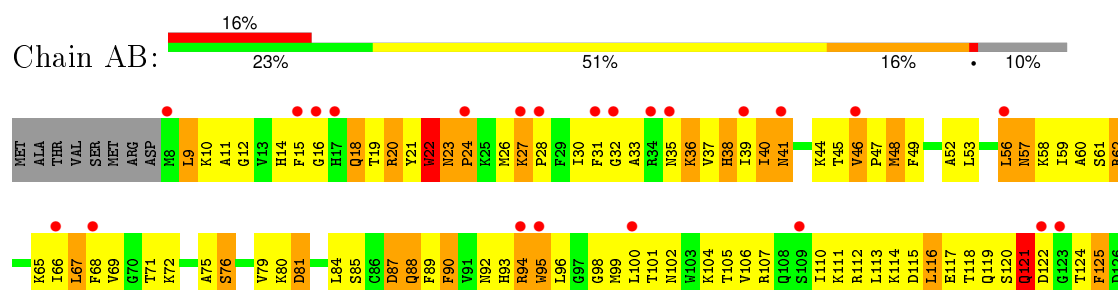
- Molecule 19: 30S RIBOSOMAL PROTEIN S20



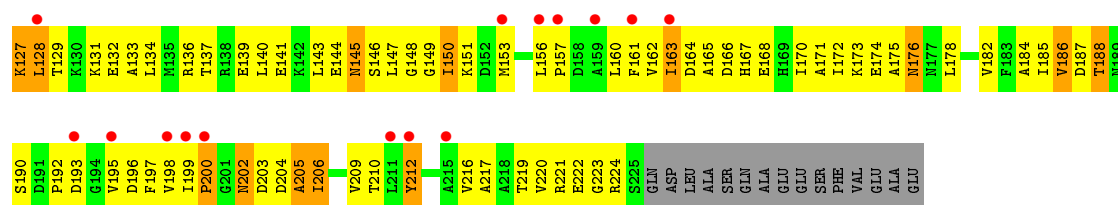
- Molecule 19: 30S RIBOSOMAL PROTEIN S20



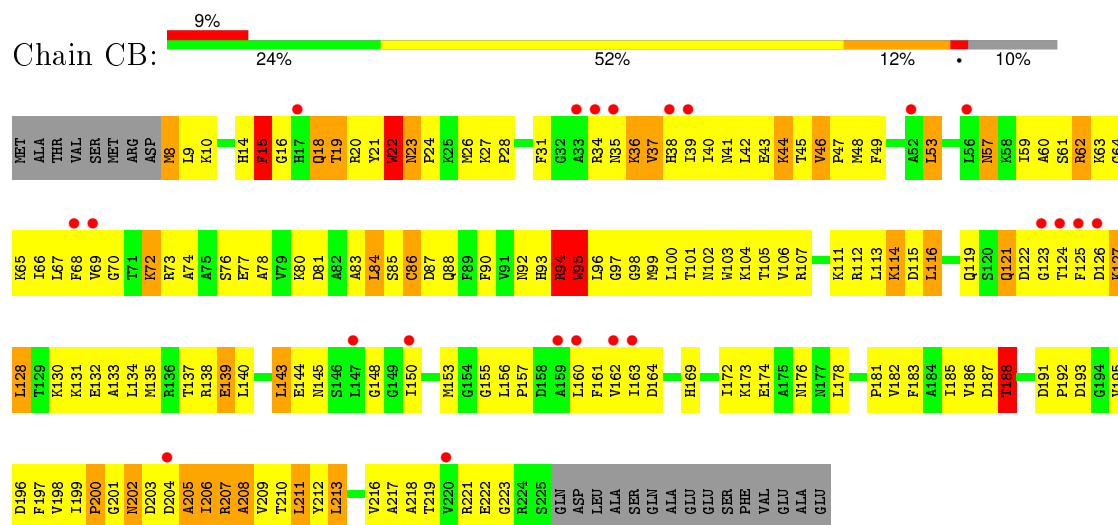
- Molecule 20: 30S RIBOSOMAL PROTEIN S2



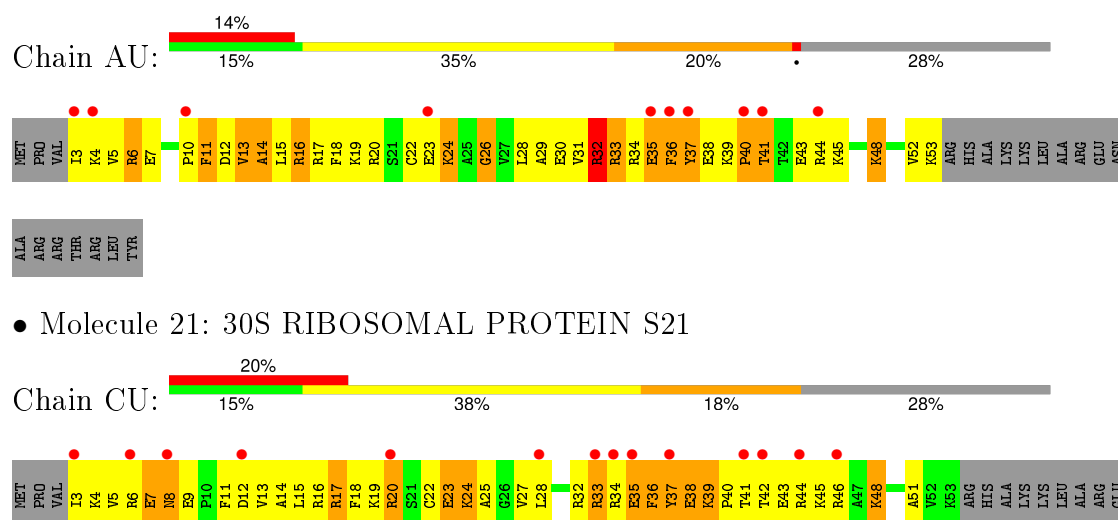




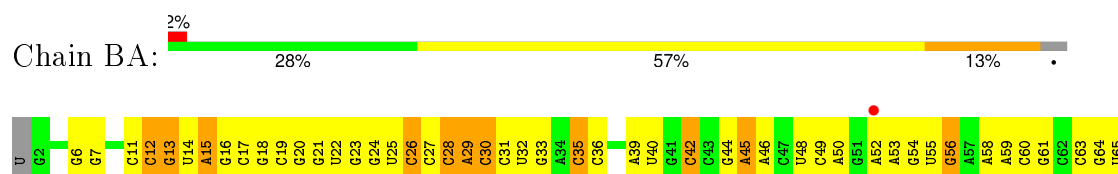
• Molecule 20: 30S RIBOSOMAL PROTEIN S2

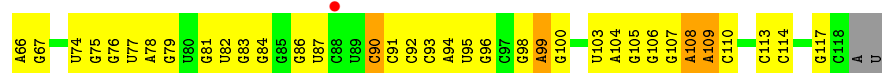


• Molecule 21: 30S RIBOSOMAL PROTEIN S21

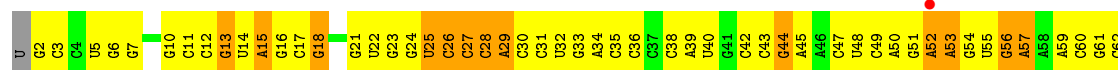


• Molecule 22: 5S RIBOSOMAL RNA

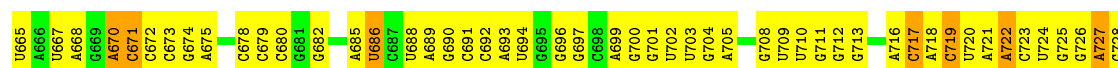
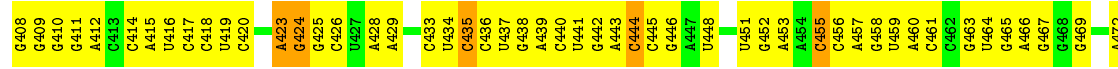
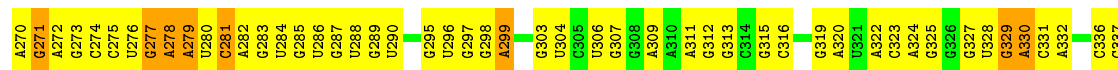
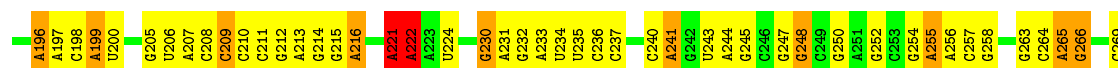
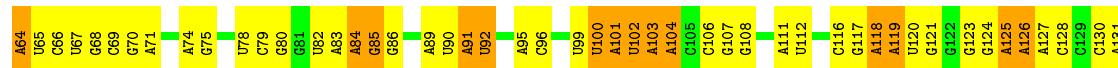
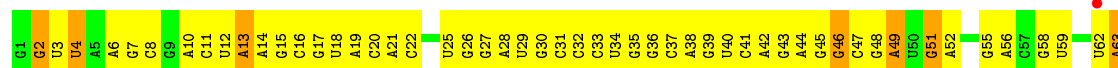




## ● Molecule 22: 5S RIBOSOMAL RNA

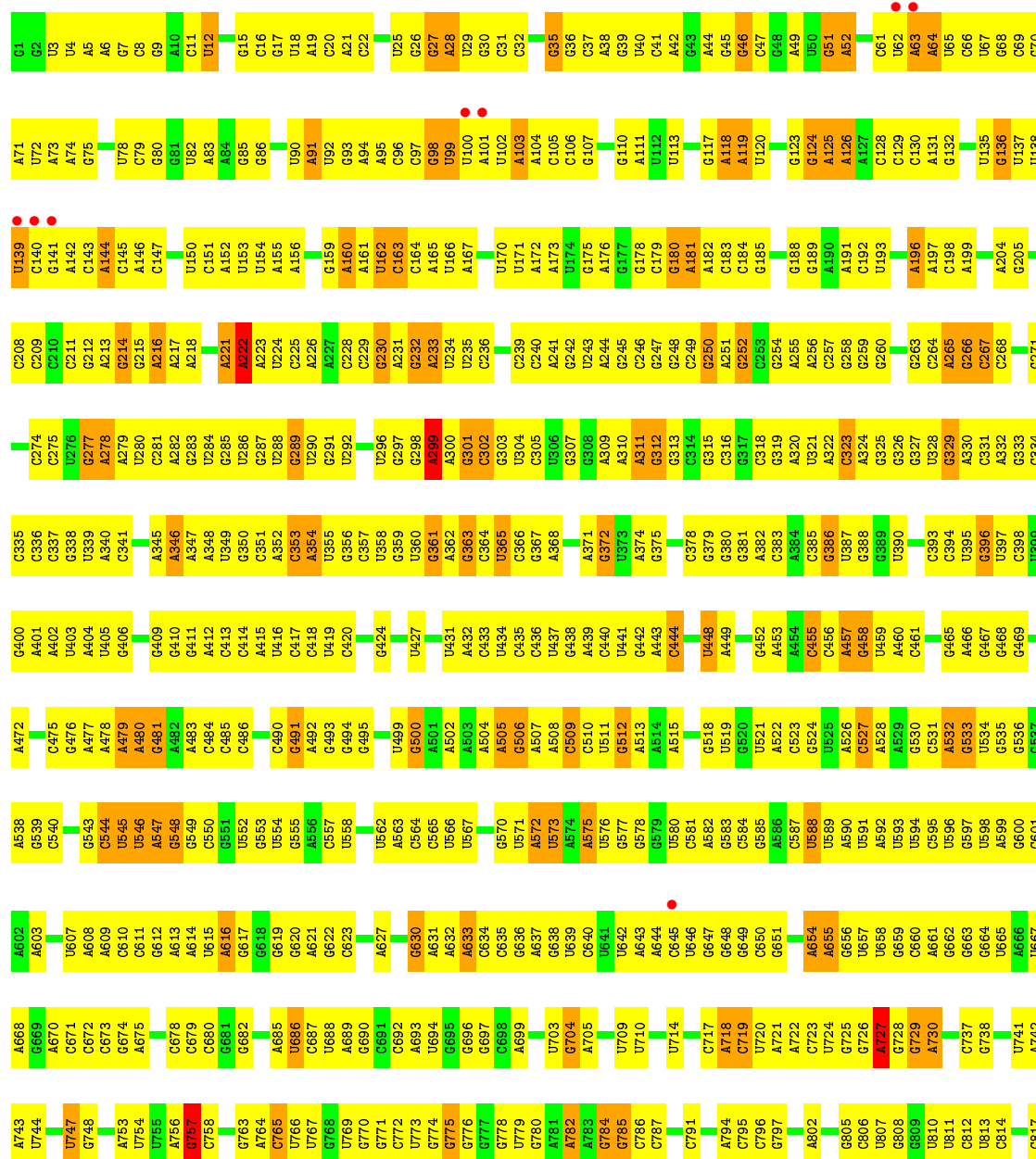


## ● Molecule 23: 23S RIBOSOMAL RNA



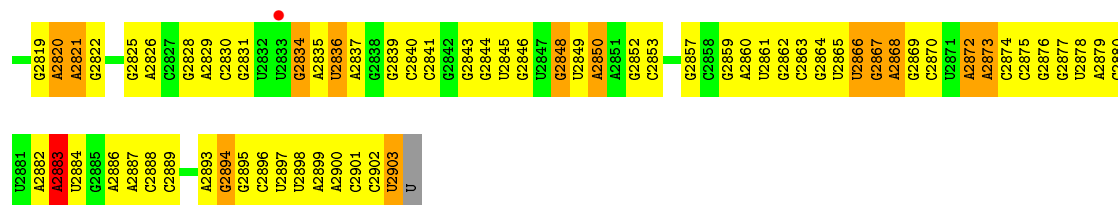
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C1670	U1594	G1529	C1462	U1402	A1327	A1260	C1197						G738	
C1595	G1530	C1463	C1463	U1403	A1328		U1198	G1068	C1005	A941	C876	U813	A739	
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C1600	A1535	U1468	U1468	G1407	G1337	A1268	U1203	A1073	A1010	A947	G	A819	U744	
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				U1412										
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G1475	C1541	G1346	G1475	A1413	A1346	A1274	C1211	U1079	G1016	G953	C	A825	A752	
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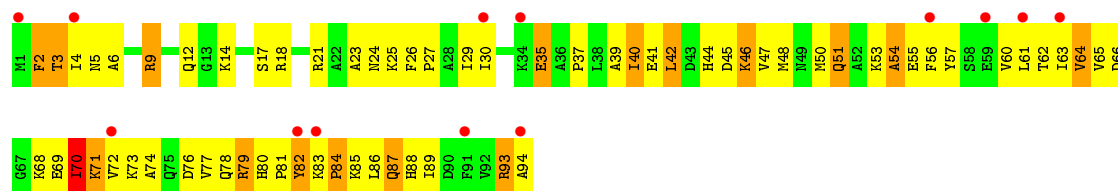


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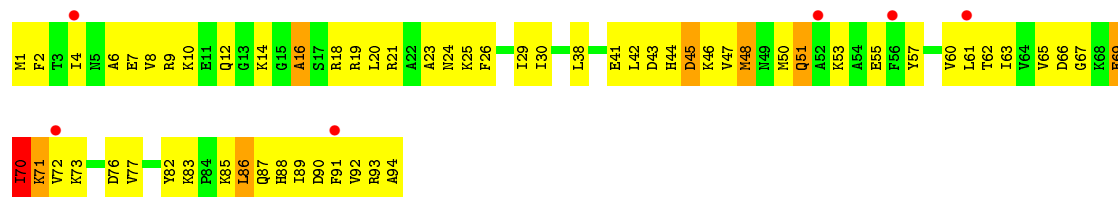




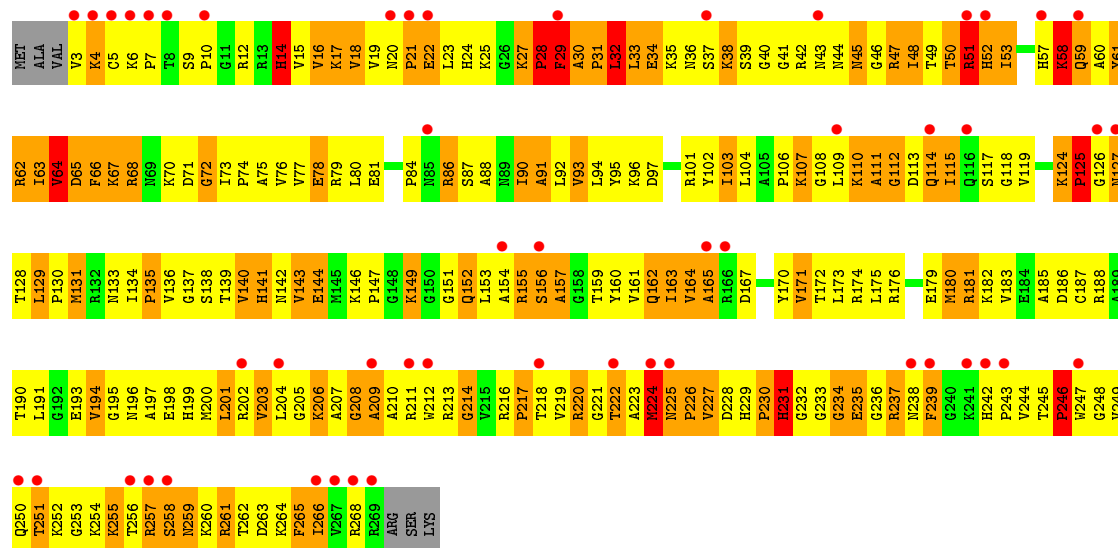
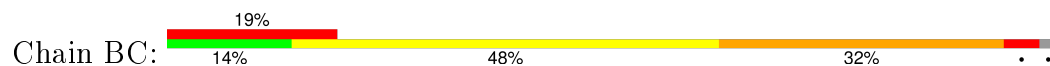
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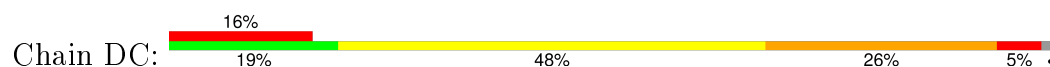
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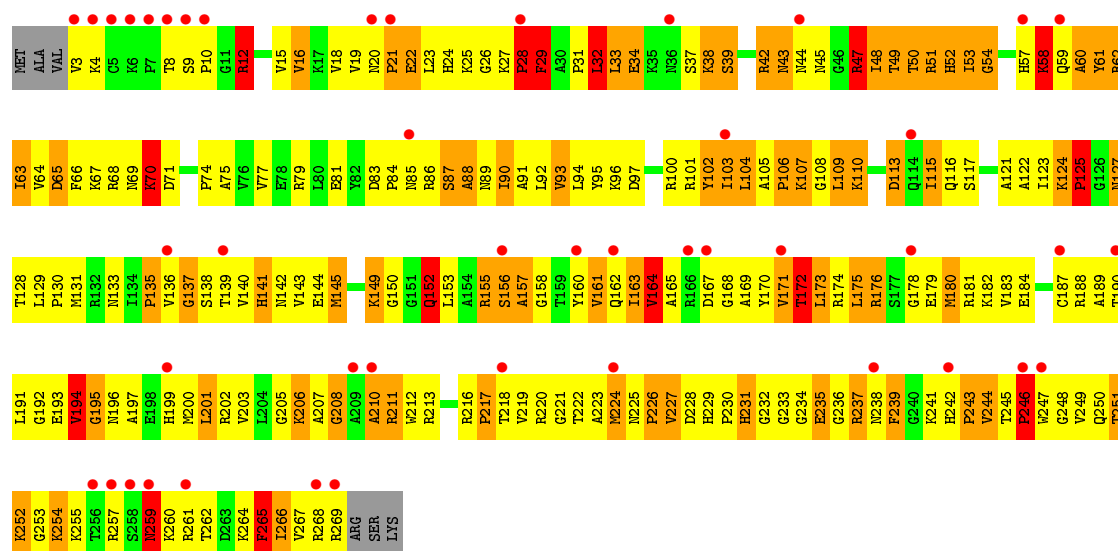
• Molecule 25: 50S RIBOSOMAL PROTEIN L2



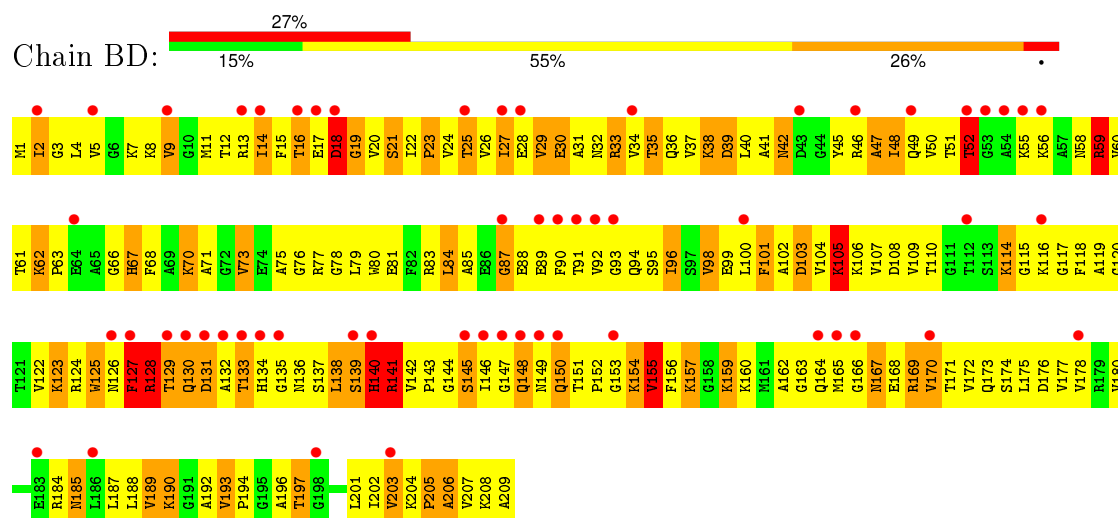
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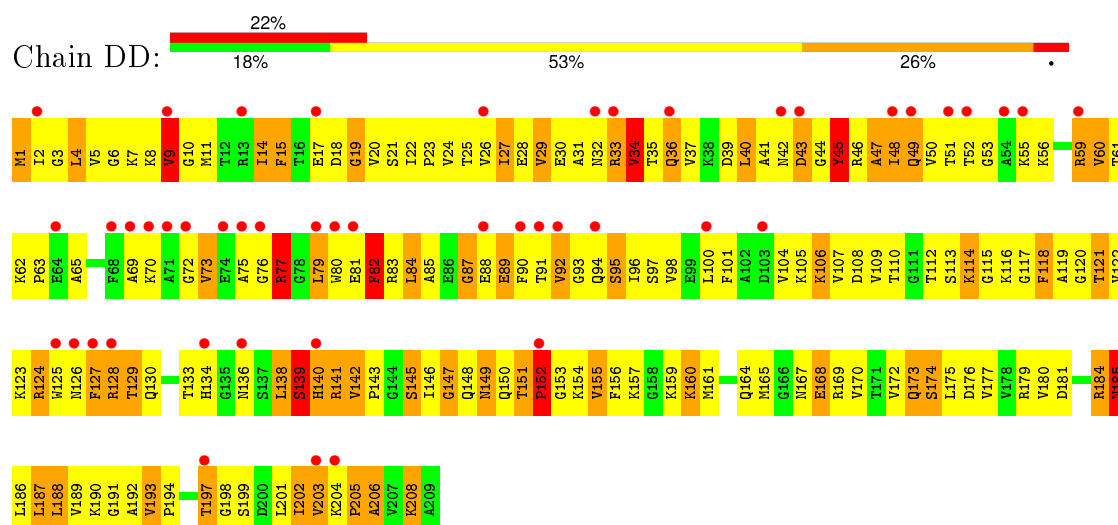




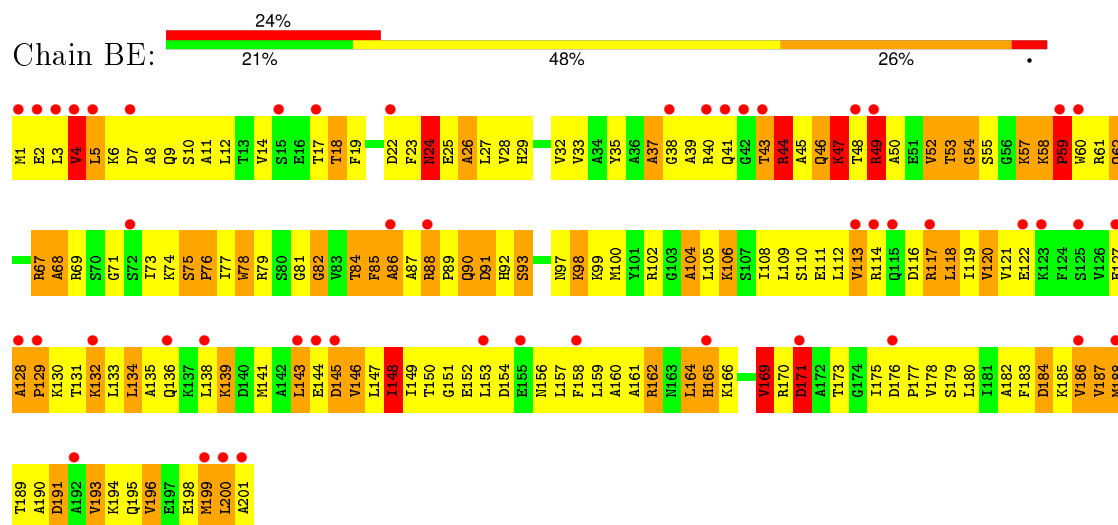
• Molecule 26: 50S RIBOSOMAL PROTEIN L3



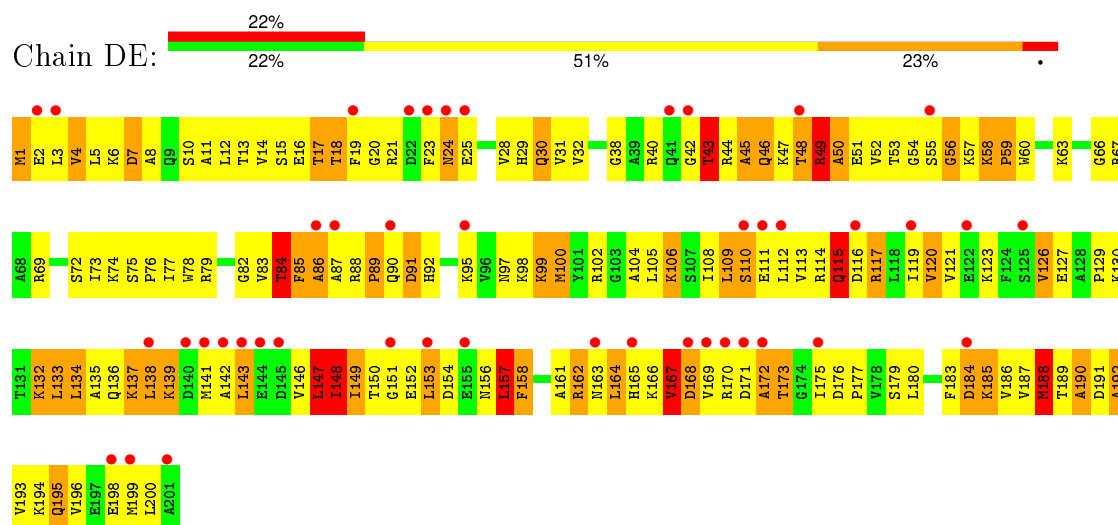
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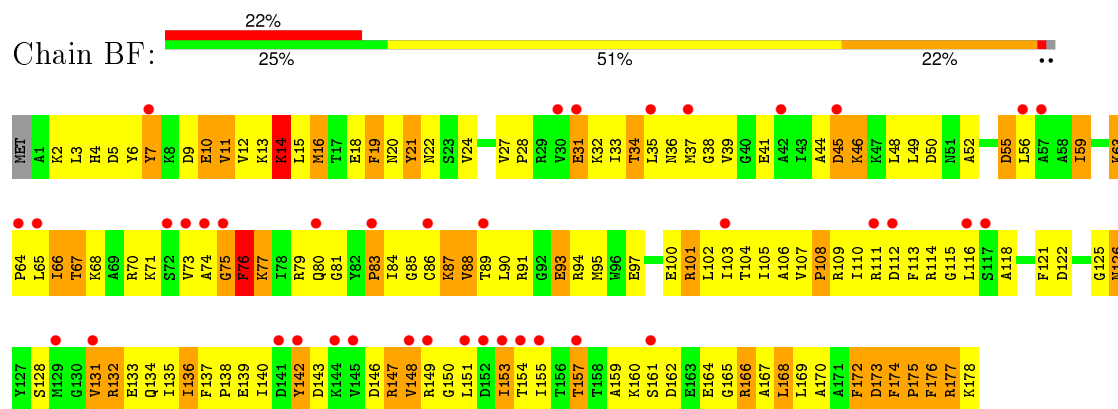
• Molecule 27: 50S RIBOSOMAL PROTEIN L4



• Molecule 27: 50S RIBOSOMAL PROTEIN L4

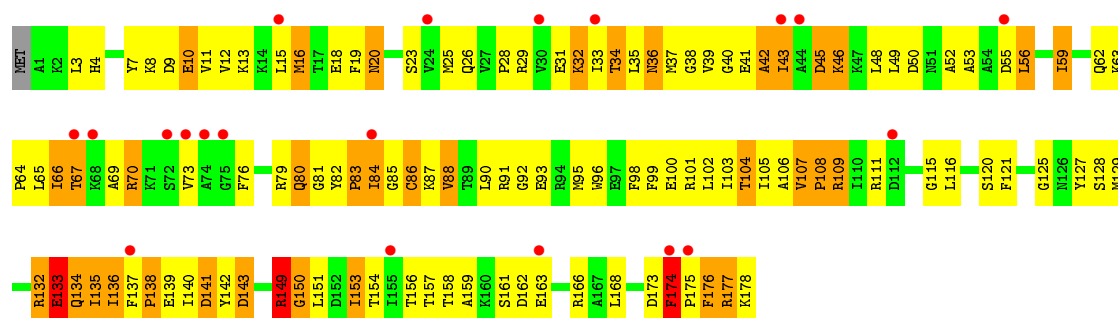


• Molecule 28: 50S RIBOSOMAL PROTEIN L5

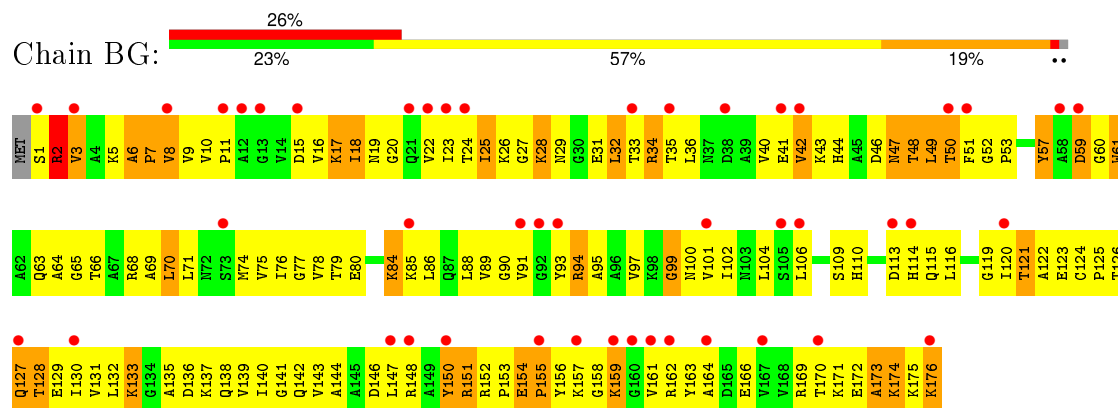


• Molecule 28: 50S RIBOSOMAL PROTEIN L5

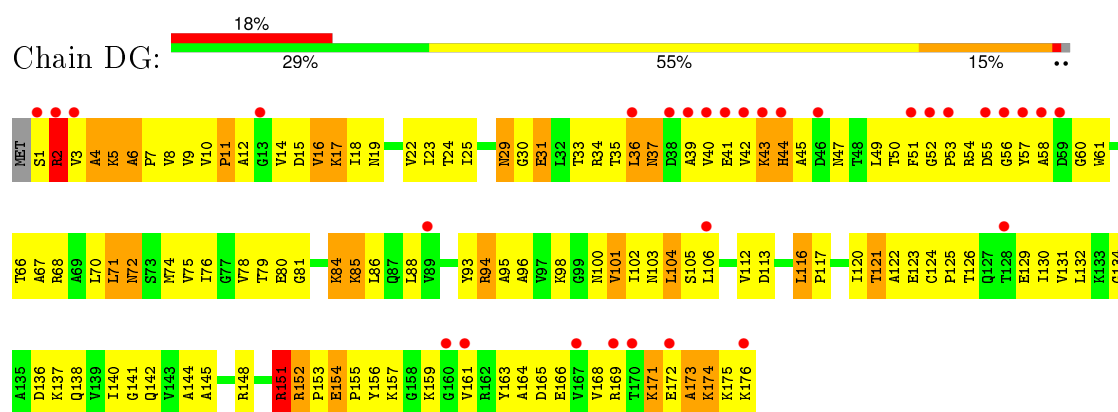




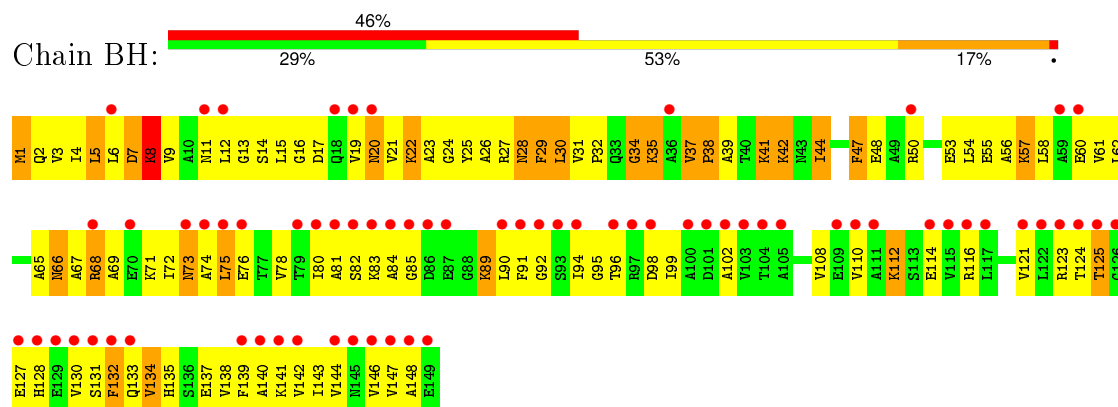
• Molecule 29: 50S RIBOSOMAL PROTEIN L6



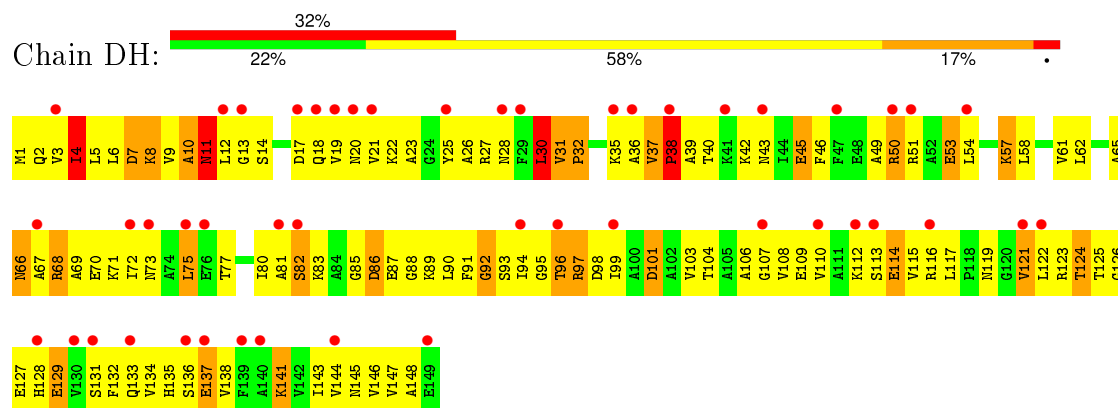
• Molecule 29: 50S RIBOSOMAL PROTEIN L6



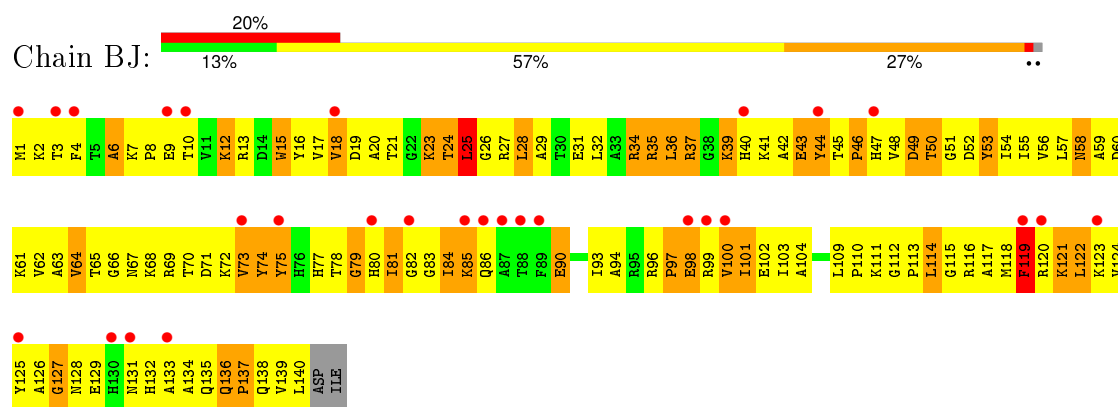
• Molecule 30: 50S RIBOSOMAL PROTEIN L9



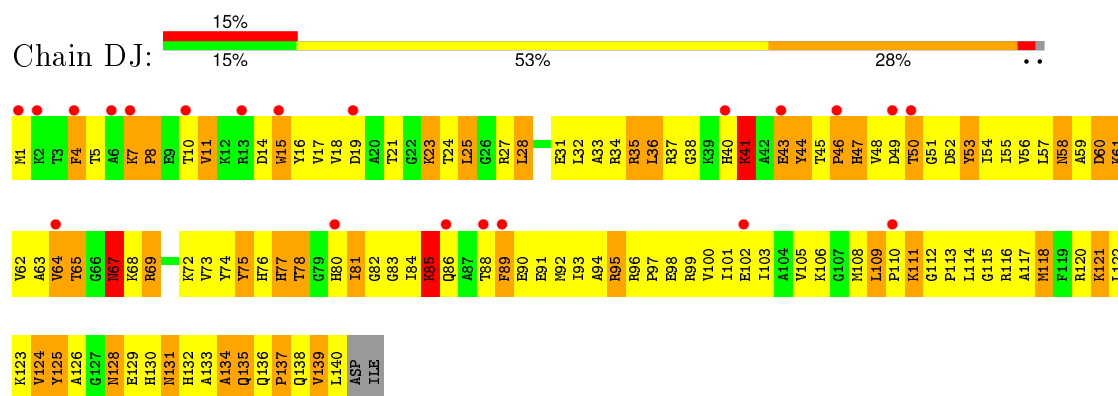
• Molecule 30: 50S RIBOSOMAL PROTEIN L9



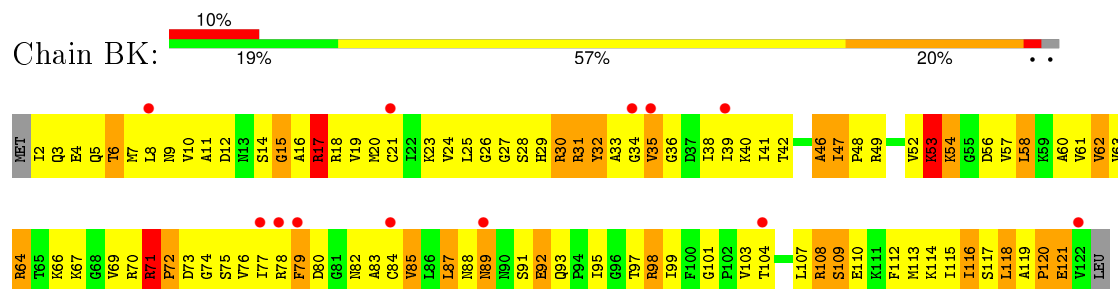
• Molecule 31: 50S RIBOSOMAL PROTEIN L13



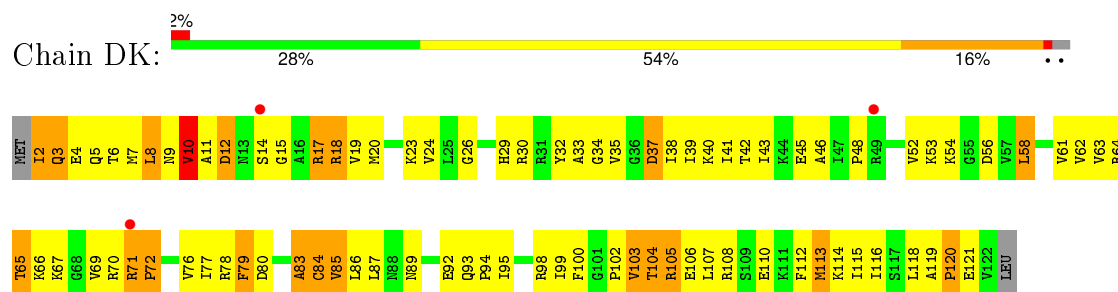
• Molecule 31: 50S RIBOSOMAL PROTEIN L13



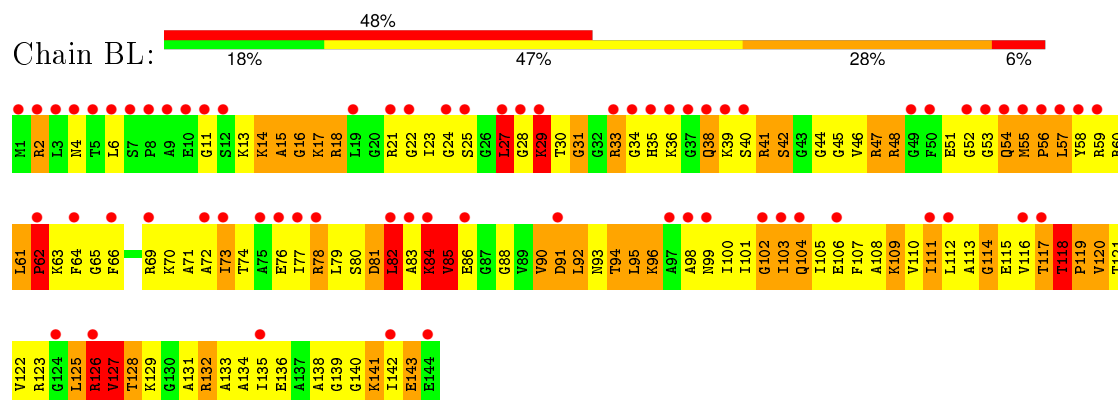
• Molecule 32: 50S RIBOSOMAL PROTEIN L14



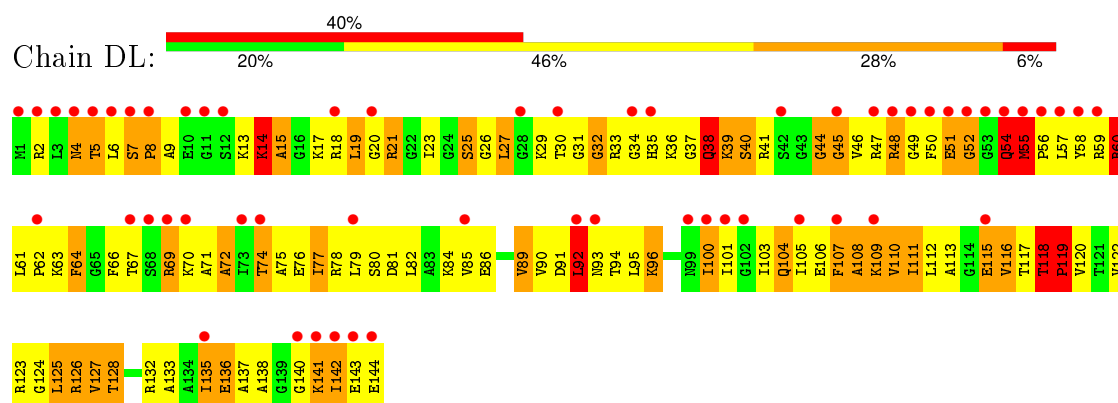
- Molecule 32: 50S RIBOSOMAL PROTEIN L14



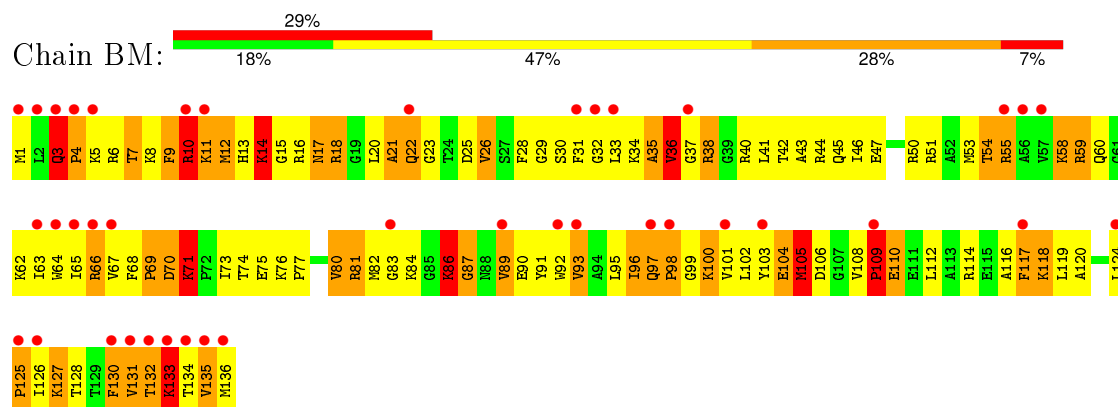
- Molecule 33: 50S RIBOSOMAL PROTEIN L15



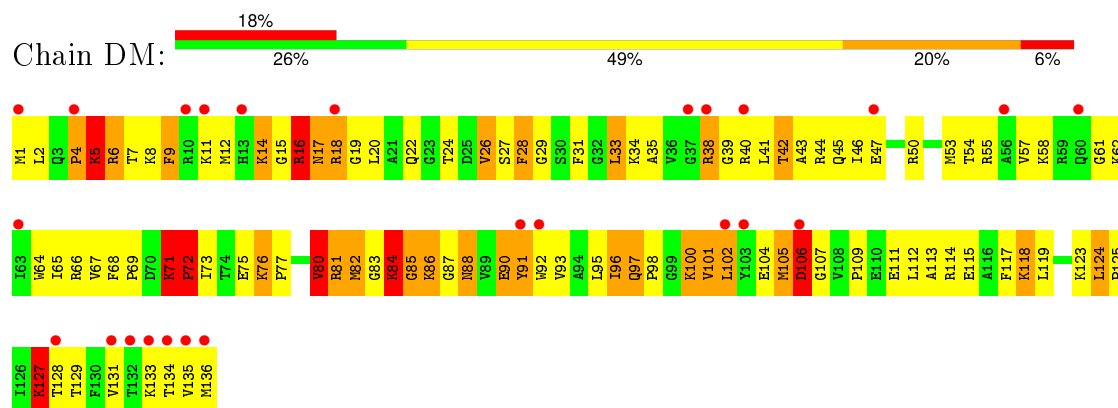
- Molecule 33: 50S RIBOSOMAL PROTEIN L15



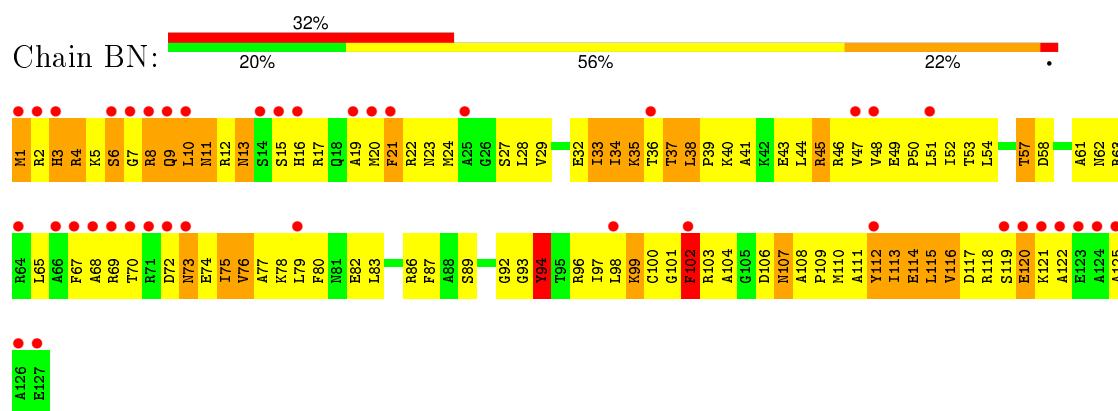
- Molecule 34: 50S RIBOSOMAL PROTEIN L16



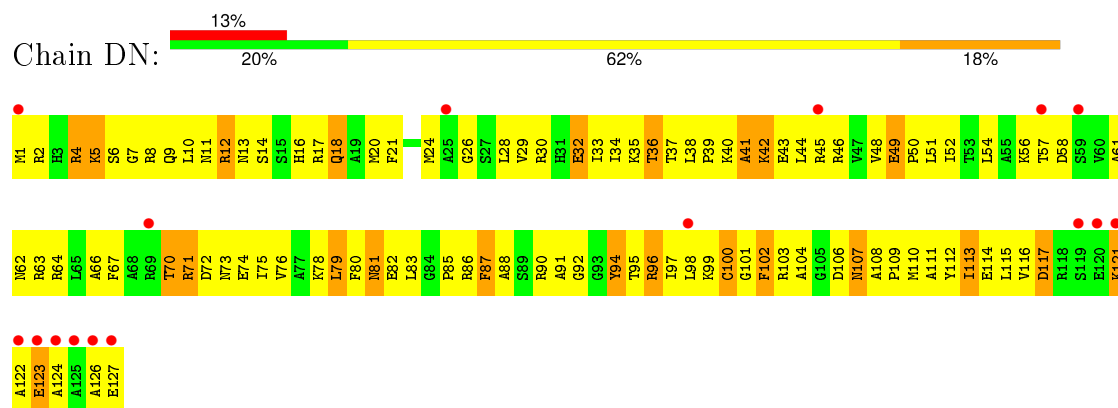
• Molecule 34: 50S RIBOSOMAL PROTEIN L16



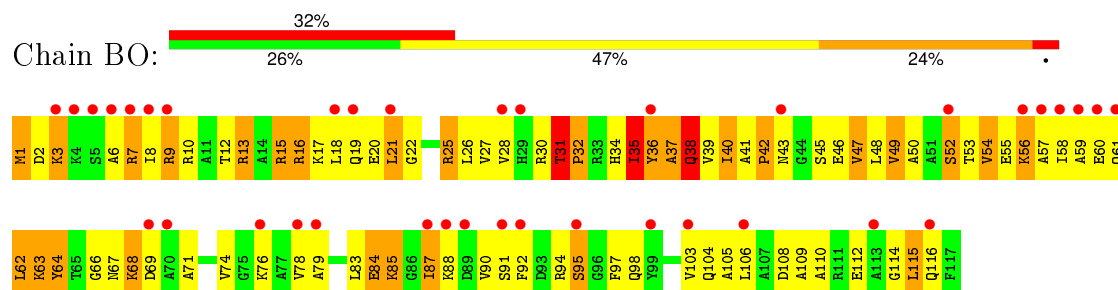
• Molecule 35: 50S RIBOSOMAL PROTEIN L17



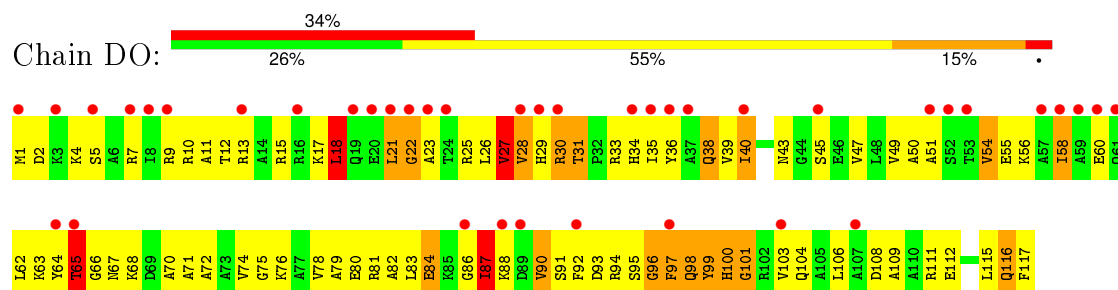
• Molecule 35: 50S RIBOSOMAL PROTEIN L17



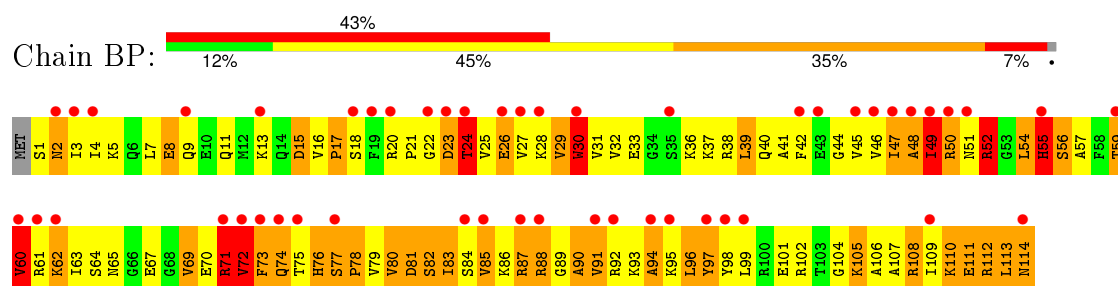
• Molecule 36: 50S RIBOSOMAL PROTEIN L18



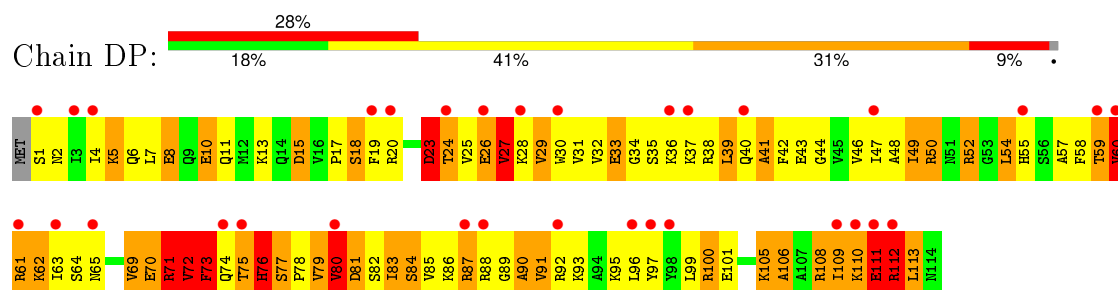
• Molecule 36: 50S RIBOSOMAL PROTEIN L18



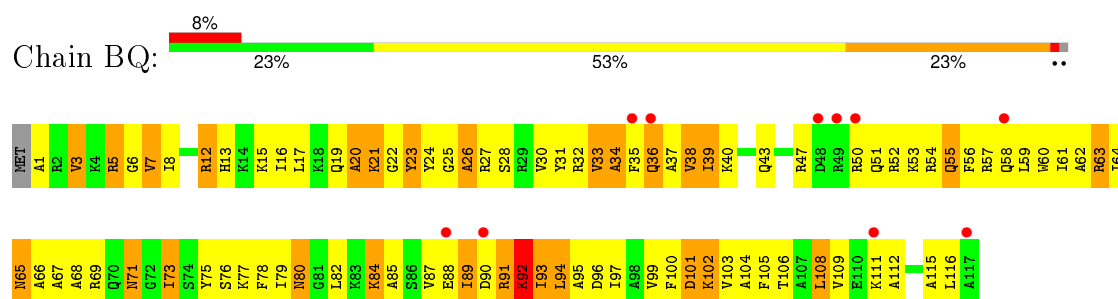
• Molecule 37: 50S RIBOSOMAL PROTEIN L19



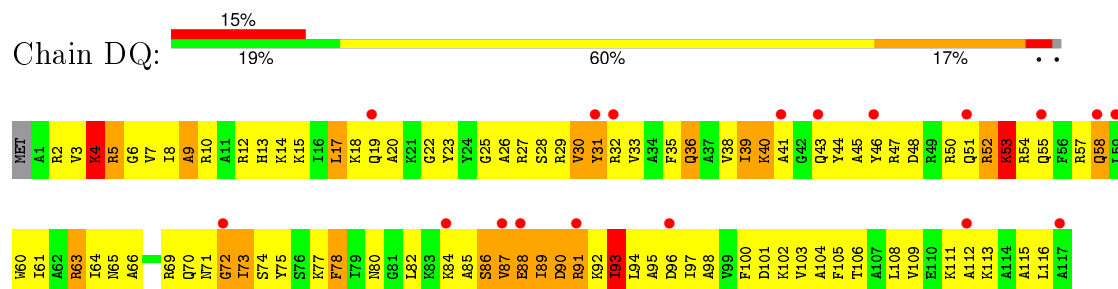
• Molecule 37: 50S RIBOSOMAL PROTEIN L19



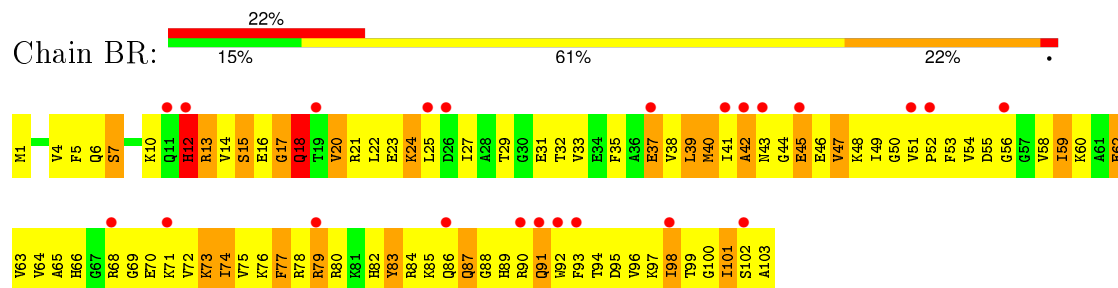
• Molecule 38: 50S RIBOSOMAL PROTEIN L20



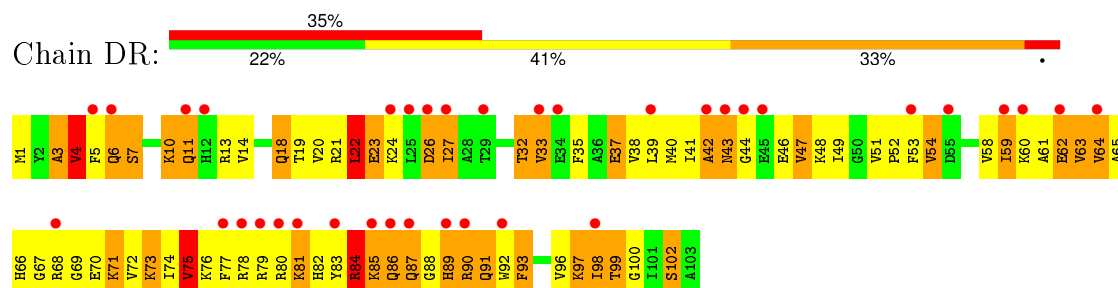
• Molecule 38: 50S RIBOSOMAL PROTEIN L20



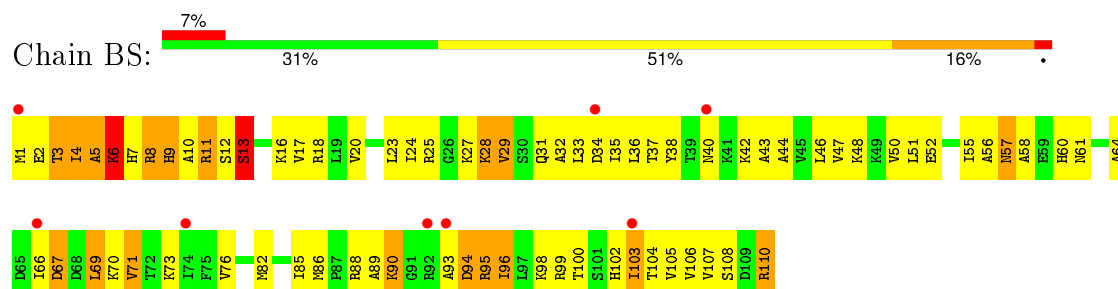
- Molecule 39: 50S RIBOSOMAL PROTEIN L21



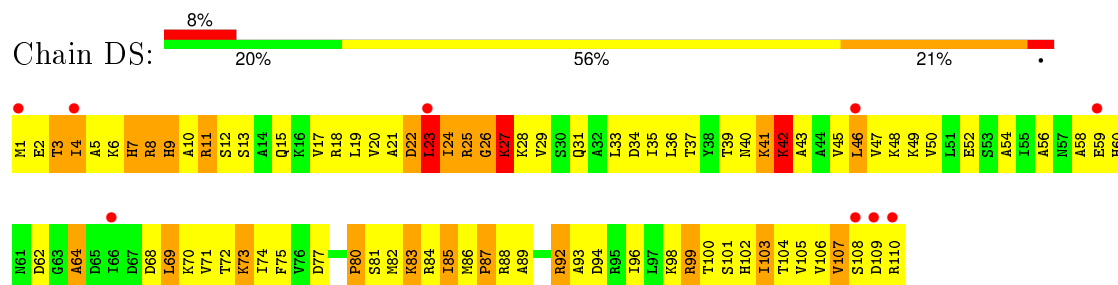
- Molecule 39: 50S RIBOSOMAL PROTEIN L21



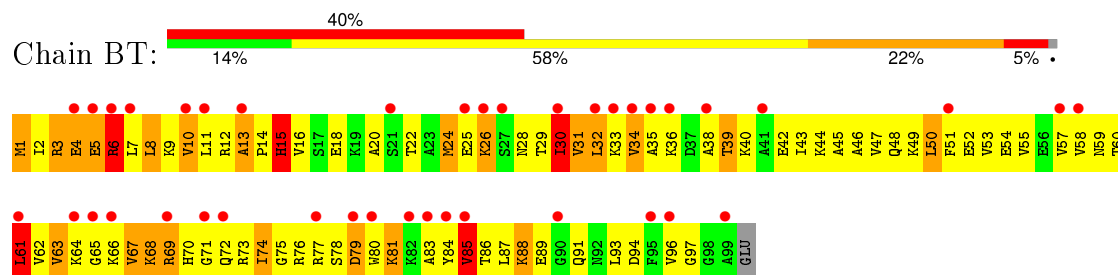
- Molecule 40: 50S RIBOSOMAL PROTEIN L22



- Molecule 40: 50S RIBOSOMAL PROTEIN L22

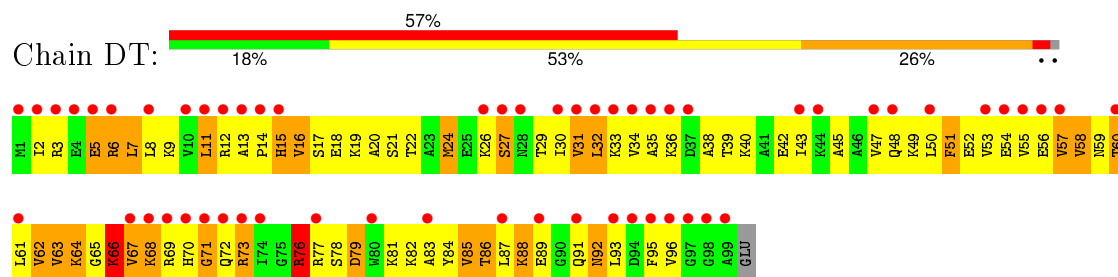


- Molecule 41: 50S RIBOSOMAL PROTEIN L23

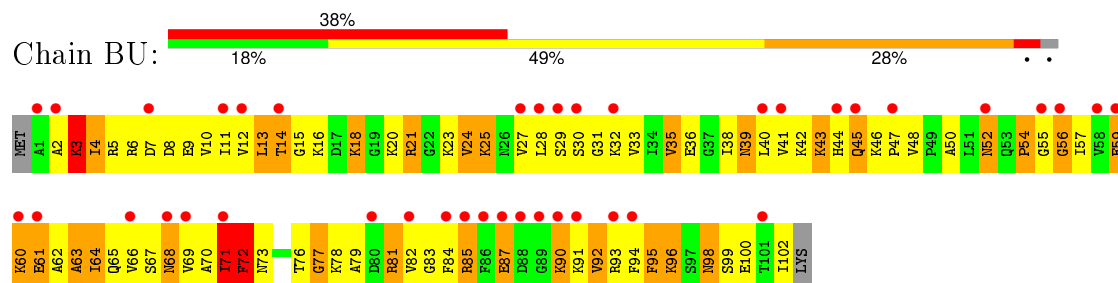




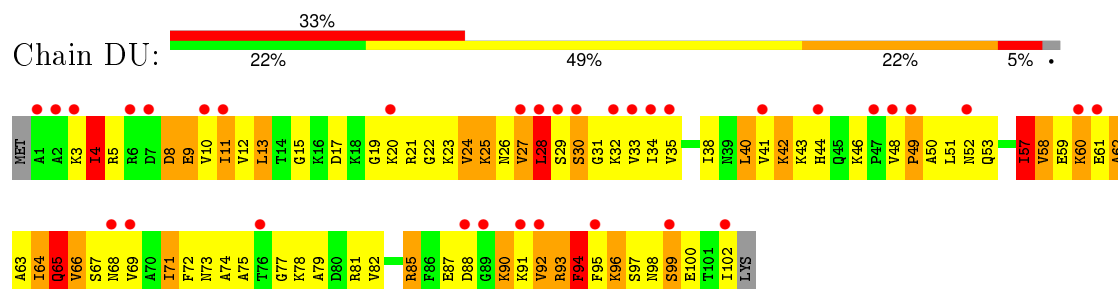
- Molecule 41: 50S RIBOSOMAL PROTEIN L23



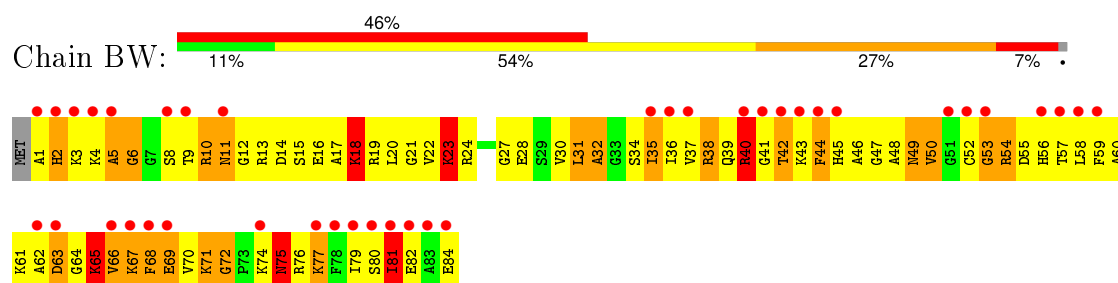
- Molecule 42: 50S RIBOSOMAL PROTEIN L24



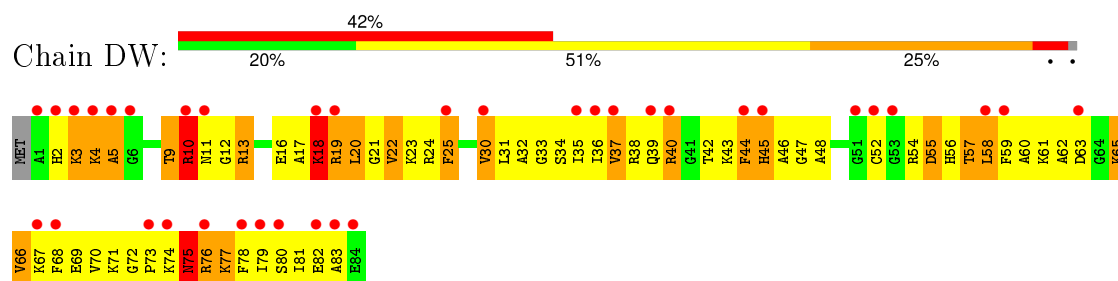
- Molecule 42: 50S RIBOSOMAL PROTEIN L24



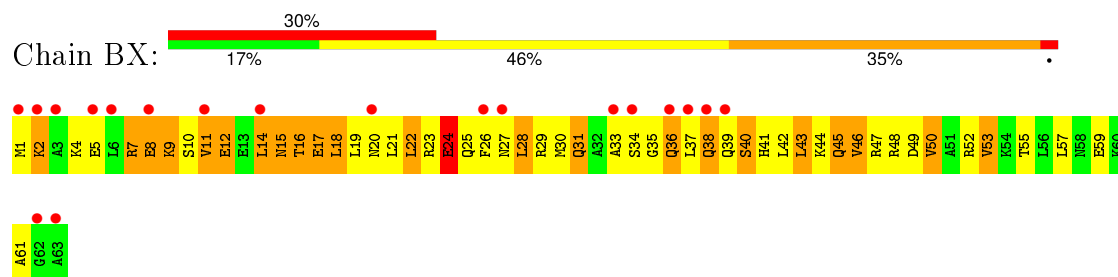
- Molecule 43: 50S RIBOSOMAL PROTEIN L27



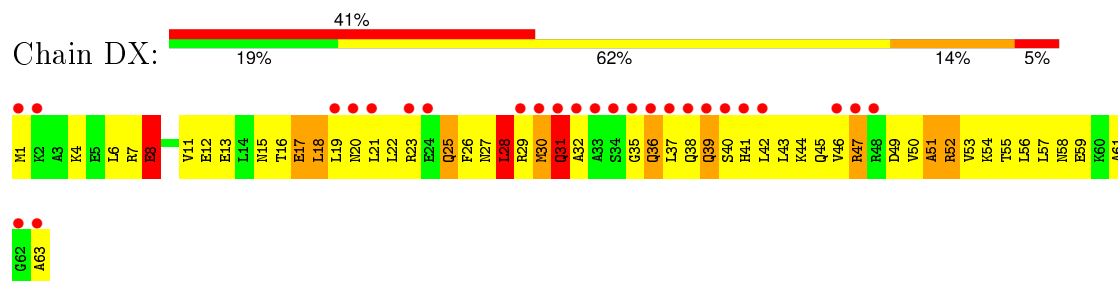
- Molecule 43: 50S RIBOSOMAL PROTEIN L27



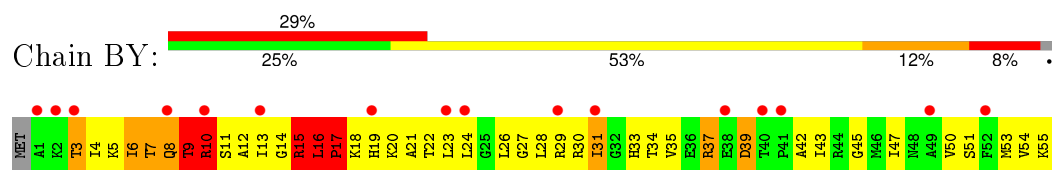
- Molecule 44: 50S RIBOSOMAL PROTEIN L29



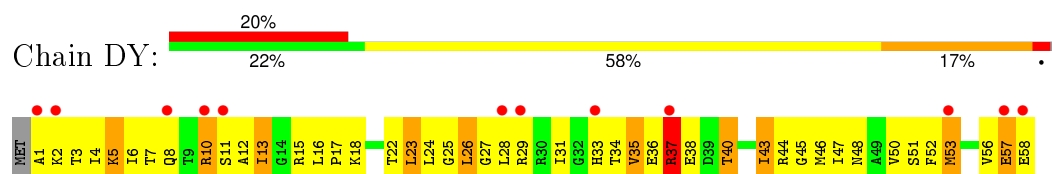
- Molecule 44: 50S RIBOSOMAL PROTEIN L29



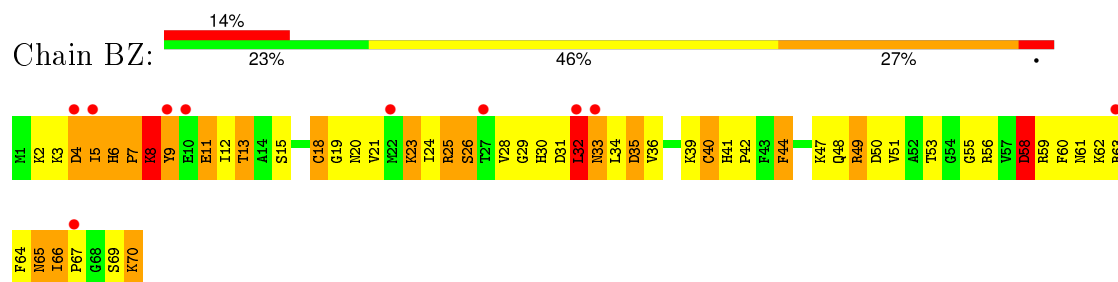
- Molecule 45: 50S RIBOSOMAL PROTEIN L30



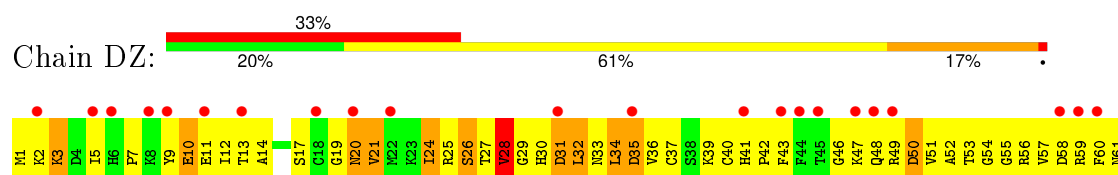
- Molecule 45: 50S RIBOSOMAL PROTEIN L30

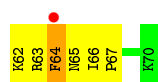


- Molecule 46: 50S RIBOSOMAL PROTEIN L31

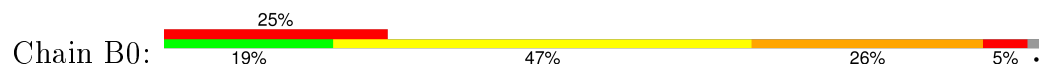


- Molecule 46: 50S RIBOSOMAL PROTEIN L31

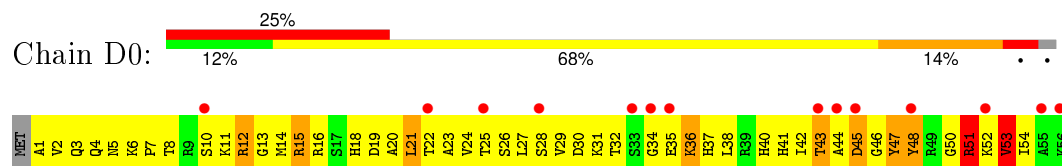




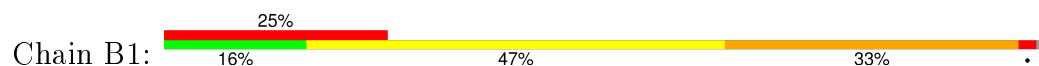
## ● Molecule 47: 50S RIBOSOMAL PROTEIN L32



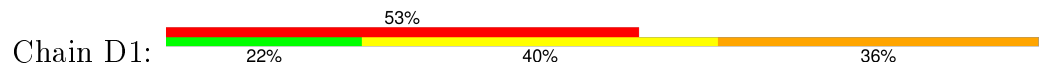
## ● Molecule 47: 50S RIBOSOMAL PROTEIN L32



## ● Molecule 48: 50S RIBOSOMAL PROTEIN L33



## ● Molecule 48: 50S RIBOSOMAL PROTEIN L33



## ● Molecule 49: 50S RIBOSOMAL PROTEIN L34

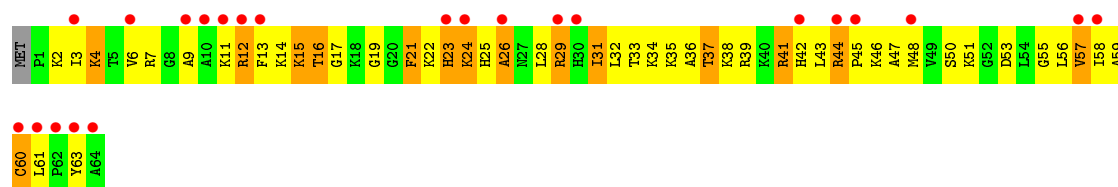


## ● Molecule 49: 50S RIBOSOMAL PROTEIN L34

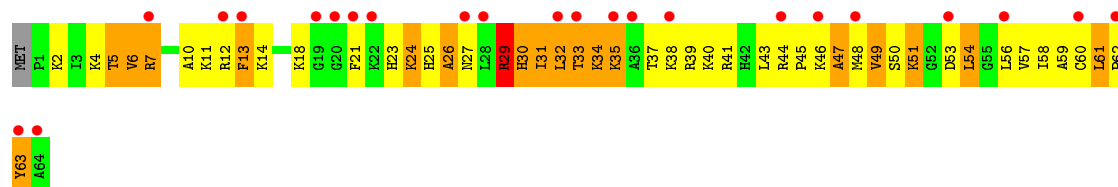


## ● Molecule 50: 50S RIBOSOMAL PROTEIN L35

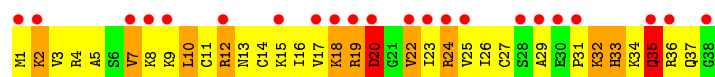
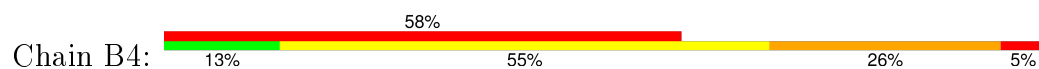




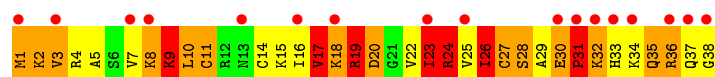
● Molecule 50: 50S RIBOSOMAL PROTEIN L35



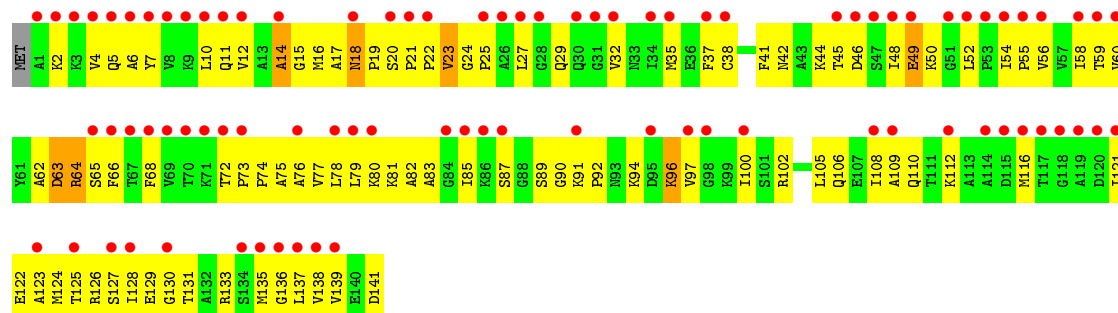
● Molecule 51: 50S RIBOSOMAL PROTEIN L36



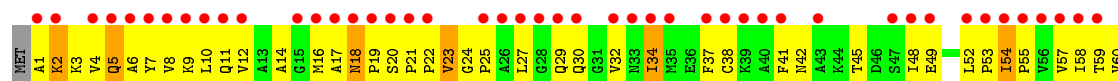
● Molecule 51: 50S RIBOSOMAL PROTEIN L36

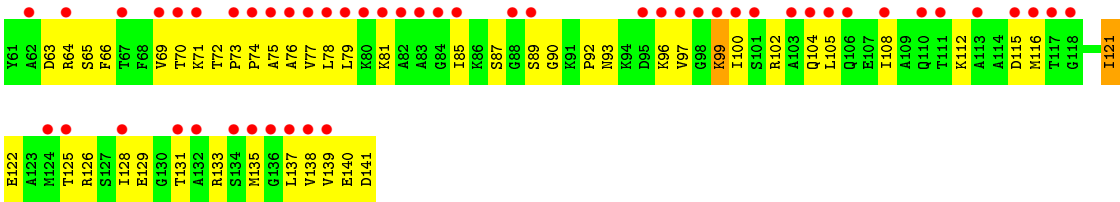


● Molecule 52: 50S RIBOSOMAL PROTEIN L11



● Molecule 52: 50S RIBOSOMAL PROTEIN L11





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	208.85Å 379.20Å 739.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.00 – 3.46 112.47 – 3.53	Depositor EDS
% Data completeness (in resolution range)	91.6 (70.00-3.46) 93.1 (112.47-3.53)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.56 (at 3.58Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.279 , 0.331 0.289 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	83.5	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 66.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 661147 reflections	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	284160	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.37% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 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: KSG, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	AA	0.23	0/36762	0.71	5/57350 (0.0%)
1	CA	0.23	0/36762	0.72	7/57350 (0.0%)
2	AC	0.23	0/1651	0.44	0/2225
2	CC	0.23	0/1651	0.47	0/2225
3	AD	0.23	0/1665	0.46	0/2227
3	CD	0.23	0/1665	0.45	0/2227
4	AE	0.23	0/1118	0.44	0/1504
4	CE	0.24	0/1118	0.45	0/1504
5	AF	0.24	0/835	0.46	0/1128
5	CF	0.24	0/835	0.47	0/1128
6	AG	0.23	0/1187	0.44	0/1591
6	CG	0.23	0/1211	0.45	0/1624
7	AH	0.23	0/989	0.44	0/1326
7	CH	0.24	0/989	0.45	0/1326
8	AI	0.24	0/1034	0.45	0/1375
8	CI	0.24	0/1034	0.45	0/1375
9	AJ	0.23	0/796	0.49	0/1077
9	CJ	0.22	0/796	0.49	0/1077
10	AK	0.24	0/893	0.46	0/1205
10	CK	0.24	0/893	0.46	0/1205
11	AL	0.22	0/969	0.46	0/1300
11	CL	0.22	0/969	0.47	0/1300
12	AM	0.21	0/892	0.47	0/1193
12	CM	0.21	0/884	0.46	0/1181
13	AN	0.24	0/785	0.45	0/1043
13	CN	0.24	0/785	0.44	0/1043
14	AO	0.23	0/724	0.45	0/966
14	CO	0.23	0/724	0.44	0/966
15	AP	0.26	0/659	0.44	0/884
15	CP	0.25	0/648	0.45	0/870
16	AQ	0.23	0/657	0.46	0/881
16	CQ	0.24	0/666	0.47	0/892

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AR	0.23	0/462	0.45	0/621
17	CR	0.23	0/462	0.45	0/621
18	AS	0.25	0/652	0.47	0/877
18	CS	0.25	0/660	0.46	0/888
19	AT	0.23	0/671	0.41	0/888
19	CT	0.23	0/671	0.42	0/888
20	AB	0.25	0/1735	0.46	0/2338
20	CB	0.25	0/1735	0.46	0/2338
21	AU	0.26	0/430	0.49	0/570
21	CU	0.26	0/430	0.48	0/570
22	BA	0.23	0/2803	0.69	0/4371
22	DA	0.25	0/2803	0.71	0/4371
23	BB	0.26	5/68314 (0.0%)	0.73	22/106569 (0.0%)
23	DB	0.26	5/68314 (0.0%)	0.73	18/106569 (0.0%)
24	BV	0.25	0/766	0.44	0/1025
24	DV	0.25	0/766	0.44	0/1025
25	BC	0.24	0/2092	0.56	0/2813
25	DC	0.23	0/2092	0.56	0/2813
26	BD	0.26	0/1586	0.54	0/2134
26	DD	0.26	0/1586	0.54	0/2134
27	BE	0.25	0/1571	0.54	0/2113
27	DE	0.25	0/1571	0.53	0/2113
28	BF	0.27	0/1444	0.62	0/1937
28	DF	0.26	0/1444	0.59	0/1937
29	BG	0.23	0/1343	0.52	0/1816
29	DG	0.23	0/1343	0.52	0/1816
30	BH	0.25	0/1122	0.51	0/1515
30	DH	0.25	0/1122	0.53	0/1515
31	BJ	0.24	0/1135	0.49	0/1529
31	DJ	0.23	0/1135	0.56	0/1529
32	BK	0.24	0/939	0.63	0/1258
32	DK	0.23	0/939	0.61	0/1258
33	BL	0.27	0/1062	0.72	0/1413
33	DL	0.28	0/1062	0.76	2/1413 (0.1%)
34	BM	0.27	0/1093	0.60	0/1460
34	DM	0.26	0/1093	0.58	0/1460
35	BN	0.24	0/1021	0.52	0/1364
35	DN	0.24	0/1021	0.47	0/1364
36	BO	0.24	0/910	0.50	0/1219
36	DO	0.23	0/910	0.46	0/1219
37	BP	0.26	0/929	0.84	3/1242 (0.2%)
37	DP	0.27	0/929	0.86	3/1242 (0.2%)
38	BQ	0.25	0/960	0.47	0/1278



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	DQ	0.26	0/960	0.50	0/1278
39	BR	0.30	0/829	0.60	0/1107
39	DR	0.26	0/829	0.55	0/1107
40	BS	0.22	0/864	0.50	0/1156
40	DS	0.22	0/864	0.51	0/1156
41	BT	0.24	0/784	0.50	0/1048
41	DT	0.25	0/784	0.54	0/1048
42	BU	0.26	0/787	0.54	0/1051
42	DU	0.25	0/787	0.61	1/1051 (0.1%)
43	BW	0.27	0/642	0.59	0/848
43	DW	0.27	0/642	0.53	0/848
44	BX	0.24	0/510	0.55	0/677
44	DX	0.23	0/510	0.50	0/677
45	BY	0.25	0/453	0.51	0/605
45	DY	0.24	0/453	0.54	0/605
46	BZ	0.28	0/559	0.67	0/745
46	DZ	0.28	0/559	0.61	0/745
47	B0	0.24	0/450	0.52	0/599
47	D0	0.25	0/450	0.58	0/599
48	B1	0.27	0/448	0.51	0/594
48	D1	0.27	0/448	0.50	0/594
49	B2	0.26	0/380	0.48	0/498
49	D2	0.26	0/380	0.47	0/498
50	B3	0.25	0/513	0.54	0/676
50	D3	0.25	0/513	0.51	0/676
51	B4	0.24	0/303	0.54	0/397
51	D4	0.24	0/303	0.53	0/397
52	BI	0.24	0/1046	0.50	0/1410
52	DI	0.26	0/1046	0.53	0/1410
All	All	0.25	10/306470 (0.0%)	0.68	61/458101 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	14
1	CA	0	16
23	BB	0	41
23	DB	1	41
47	D0	0	1
All	All	1	113

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	BB	1086	A	C5-C6	-17.07	1.25	1.41
23	DB	1086	A	C5-C6	-17.02	1.25	1.41
23	DB	1088	A	C6-N1	-10.55	1.28	1.35
23	BB	1088	A	C6-N1	-10.45	1.28	1.35
23	BB	1060	U	C2-N3	7.88	1.43	1.37

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	DB	2791	G	O5'-P-OP2	-26.15	79.33	110.70
23	BB	2791	G	O5'-P-OP1	-26.11	79.37	110.70
23	DB	2791	G	O5'-P-OP1	19.42	134.01	110.70
23	BB	2791	G	O5'-P-OP2	19.11	133.63	110.70
23	DB	2790	U	OP2-P-O3'	15.02	138.25	105.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	DB	2076	U	C3'

5 of 113 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	187	G	Sidechain
1	AA	281	G	Sidechain
1	AA	324	G	Sidechain
1	AA	437	U	Sidechain
1	AA	438	U	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32831	0	16521	1330	0
1	CA	32831	0	16521	1382	0
2	AC	1624	0	1699	184	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	CC	1624	0	1699	162	0
3	AD	1643	0	1710	173	0
3	CD	1643	0	1710	175	0
4	AE	1105	0	1148	108	0
4	CE	1105	0	1148	143	0
5	AF	817	0	808	73	0
5	CF	817	0	808	102	0
6	AG	1174	0	1230	104	0
6	CG	1196	0	1246	101	0
7	AH	979	0	1034	85	0
7	CH	979	0	1034	80	0
8	AI	1022	0	1070	156	0
8	CI	1022	0	1070	125	0
9	AJ	786	0	828	95	0
9	CJ	786	0	828	111	0
10	AK	877	0	887	104	0
10	CK	877	0	887	106	0
11	AL	955	0	1019	105	0
11	CL	955	0	1019	91	0
12	AM	883	0	944	88	0
12	CM	876	0	937	113	0
13	AN	774	0	827	104	0
13	CN	774	0	827	121	0
14	AO	716	0	742	53	0
14	CO	716	0	742	55	0
15	AP	649	0	666	78	0
15	CP	638	0	656	79	0
16	AQ	648	0	691	101	0
16	CQ	657	0	702	90	0
17	AR	455	0	478	42	0
17	CR	455	0	478	45	0
18	AS	637	0	665	87	0
18	CS	644	0	675	96	0
19	AT	665	0	714	59	0
19	CT	665	0	714	58	0
20	AB	1704	0	1732	195	0
20	CB	1704	0	1732	167	0
21	AU	425	0	449	68	0
21	CU	425	0	449	65	0
22	BA	2507	0	1270	84	0
22	DA	2507	0	1270	117	0
23	BB	60995	0	30678	2753	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	DB	60995	0	30677	2695	0
24	BV	753	0	780	100	0
24	DV	753	0	780	69	0
25	BC	2053	0	2122	451	0
25	DC	2053	0	2122	389	0
26	BD	1565	0	1616	379	0
26	DD	1565	0	1616	309	0
27	BE	1552	0	1619	279	0
27	DE	1552	0	1619	256	0
28	BF	1420	0	1460	170	0
28	DF	1420	0	1460	157	0
29	BG	1323	0	1374	166	0
29	DG	1323	0	1374	158	0
30	BH	1111	0	1148	173	0
30	DH	1111	0	1148	166	0
31	BJ	1112	0	1147	220	0
31	DJ	1112	0	1147	207	0
32	BK	930	0	1000	123	0
32	DK	930	0	1000	124	0
33	BL	1053	0	1129	277	0
33	DL	1053	0	1129	250	0
34	BM	1074	0	1157	238	0
34	DM	1074	0	1157	169	0
35	BN	1008	0	1045	186	0
35	DN	1008	0	1045	158	0
36	BO	900	0	935	128	0
36	DO	900	0	935	137	0
37	BP	917	0	965	198	0
37	DP	917	0	965	196	0
38	BQ	947	0	1022	199	0
38	DQ	947	0	1022	175	0
39	BR	816	0	839	170	0
39	DR	816	0	839	166	0
40	BS	857	0	922	124	0
40	DS	857	0	922	116	0
41	BT	777	0	840	148	0
41	DT	777	0	840	133	0
42	BU	779	0	834	163	0
42	DU	779	0	834	121	0
43	BW	634	0	656	161	0
43	DW	634	0	656	169	0
44	BX	509	0	543	77	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	DX	509	0	543	83	0
45	BY	449	0	491	60	0
45	DY	449	0	491	81	0
46	BZ	549	0	552	111	0
46	DZ	549	0	552	102	0
47	B0	444	0	461	74	0
47	D0	444	0	461	91	0
48	B1	441	0	485	80	0
48	D1	441	0	485	77	0
49	B2	377	0	418	59	0
49	D2	377	0	418	67	0
50	B3	504	0	574	115	0
50	D3	504	0	574	107	0
51	B4	302	0	343	63	0
51	D4	302	0	343	75	0
52	BI	1032	0	1088	121	0
52	DI	1032	0	1088	183	0
53	AA	26	0	23	3	0
53	CA	26	0	23	1	0
54	AA	60	0	0	0	0
54	BB	110	0	0	0	0
54	CA	62	0	0	0	0
54	DB	109	0	0	0	0
54	DE	1	0	0	0	0
54	DN	1	0	0	0	0
55	AA	289	0	0	1	0
55	AE	3	0	0	0	0
55	AK	2	0	0	0	0
55	AN	3	0	0	0	0
55	AP	2	0	0	0	0
55	AT	1	0	0	0	0
55	BB	497	0	0	11	0
55	BC	1	0	0	0	0
55	BE	5	0	0	0	0
55	BH	1	0	0	0	0
55	BL	2	0	0	0	0
55	BN	1	0	0	0	0
55	CA	293	0	0	1	0
55	CE	3	0	0	0	0
55	CK	1	0	0	0	0
55	CL	4	0	0	0	0
55	CN	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	CP	1	0	0	0	0
55	CT	3	0	0	0	0
55	D2	2	0	0	0	0
55	DB	501	0	0	10	0
55	DC	1	0	0	0	0
55	DD	1	0	0	0	0
55	DE	3	0	0	0	0
55	DL	1	0	0	0	0
55	DN	2	0	0	0	0
55	DT	1	0	0	0	0
All	All	284160	0	190815	19652	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 42.

The worst 5 of 19652 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)
23:DB:1099:G:O5'	52:DI:4:VAL:N	1.71	1.23
32:DK:78:ARG:HG2	37:DP:72:VAL:HG21	1.24	1.15
23:DB:1098:A:H3'	52:DI:3:LYS:CA	1.76	1.15
23:DB:587:C:H3'	33:DL:29:LYS:HD2	1.20	1.14
48:D1:29:LYS:HB2	48:D1:30:PRO:HD3	1.30	1.14

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AC	204/233 (88%)	144 (71%)	44 (22%)	16 (8%)	<b>1</b>	<b>13</b>
2	CC	204/233 (88%)	138 (68%)	46 (22%)	20 (10%)	<b>1</b>	<b>9</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AD	203/206 (98%)	133 (66%)	49 (24%)	21 (10%)	1	8
3	CD	203/206 (98%)	137 (68%)	49 (24%)	17 (8%)	1	12
4	AE	148/167 (89%)	110 (74%)	30 (20%)	8 (5%)	2	23
4	CE	148/167 (89%)	109 (74%)	30 (20%)	9 (6%)	2	19
5	AF	98/135 (73%)	68 (69%)	25 (26%)	5 (5%)	2	25
5	CF	98/135 (73%)	72 (74%)	18 (18%)	8 (8%)	1	12
6	AG	148/179 (83%)	105 (71%)	35 (24%)	8 (5%)	2	23
6	CG	150/179 (84%)	101 (67%)	37 (25%)	12 (8%)	1	13
7	AH	127/130 (98%)	108 (85%)	14 (11%)	5 (4%)	4	33
7	CH	127/130 (98%)	91 (72%)	29 (23%)	7 (6%)	2	23
8	AI	125/130 (96%)	84 (67%)	30 (24%)	11 (9%)	1	11
8	CI	125/130 (96%)	82 (66%)	30 (24%)	13 (10%)	1	8
9	AJ	96/103 (93%)	65 (68%)	20 (21%)	11 (12%)	0	7
9	CJ	96/103 (93%)	59 (62%)	18 (19%)	19 (20%)	0	1
10	AK	115/129 (89%)	75 (65%)	32 (28%)	8 (7%)	1	16
10	CK	115/129 (89%)	76 (66%)	30 (26%)	9 (8%)	1	13
11	AL	121/124 (98%)	73 (60%)	35 (29%)	13 (11%)	0	8
11	CL	121/124 (98%)	76 (63%)	28 (23%)	17 (14%)	0	4
12	AM	112/118 (95%)	89 (80%)	13 (12%)	10 (9%)	1	11
12	CM	111/118 (94%)	82 (74%)	17 (15%)	12 (11%)	0	8
13	AN	92/101 (91%)	64 (70%)	19 (21%)	9 (10%)	1	9
13	CN	92/101 (91%)	50 (54%)	26 (28%)	16 (17%)	0	2
14	AO	86/89 (97%)	66 (77%)	19 (22%)	1 (1%)	16	60
14	CO	86/89 (97%)	69 (80%)	15 (17%)	2 (2%)	8	46
15	AP	80/82 (98%)	60 (75%)	14 (18%)	6 (8%)	1	14
15	CP	78/82 (95%)	55 (70%)	14 (18%)	9 (12%)	0	7
16	AQ	78/84 (93%)	49 (63%)	25 (32%)	4 (5%)	2	25
16	CQ	79/84 (94%)	58 (73%)	15 (19%)	6 (8%)	1	14
17	AR	53/75 (71%)	31 (58%)	16 (30%)	6 (11%)	0	7
17	CR	53/75 (71%)	36 (68%)	13 (24%)	4 (8%)	1	14
18	AS	77/92 (84%)	54 (70%)	12 (16%)	11 (14%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	CS	78/92 (85%)	50 (64%)	17 (22%)	11 (14%)	0	4
19	AT	83/87 (95%)	68 (82%)	12 (14%)	3 (4%)	4	35
19	CT	83/87 (95%)	62 (75%)	16 (19%)	5 (6%)	2	20
20	AB	216/241 (90%)	148 (68%)	52 (24%)	16 (7%)	1	15
20	CB	216/241 (90%)	149 (69%)	41 (19%)	26 (12%)	0	6
21	AU	49/71 (69%)	23 (47%)	12 (24%)	14 (29%)	0	0
21	CU	49/71 (69%)	26 (53%)	18 (37%)	5 (10%)	1	9
24	BV	92/94 (98%)	61 (66%)	24 (26%)	7 (8%)	1	14
24	DV	92/94 (98%)	64 (70%)	23 (25%)	5 (5%)	2	23
25	BC	265/273 (97%)	94 (36%)	95 (36%)	76 (29%)	0	0
25	DC	265/273 (97%)	97 (37%)	101 (38%)	67 (25%)	0	1
26	BD	207/209 (99%)	87 (42%)	68 (33%)	52 (25%)	0	1
26	DD	207/209 (99%)	91 (44%)	72 (35%)	44 (21%)	0	1
27	BE	199/201 (99%)	101 (51%)	57 (29%)	41 (21%)	0	1
27	DE	199/201 (99%)	90 (45%)	63 (32%)	46 (23%)	0	1
28	BF	176/179 (98%)	99 (56%)	42 (24%)	35 (20%)	0	1
28	DF	176/179 (98%)	98 (56%)	49 (28%)	29 (16%)	0	2
29	BG	174/177 (98%)	112 (64%)	41 (24%)	21 (12%)	0	6
29	DG	174/177 (98%)	108 (62%)	51 (29%)	15 (9%)	1	11
30	BH	147/149 (99%)	83 (56%)	49 (33%)	15 (10%)	1	9
30	DH	147/149 (99%)	83 (56%)	46 (31%)	18 (12%)	0	6
31	BJ	138/142 (97%)	68 (49%)	43 (31%)	27 (20%)	0	2
31	DJ	138/142 (97%)	72 (52%)	36 (26%)	30 (22%)	0	1
32	BK	119/123 (97%)	73 (61%)	27 (23%)	19 (16%)	0	2
32	DK	119/123 (97%)	70 (59%)	30 (25%)	19 (16%)	0	2
33	BL	142/144 (99%)	56 (39%)	47 (33%)	39 (28%)	0	0
33	DL	142/144 (99%)	68 (48%)	35 (25%)	39 (28%)	0	0
34	BM	134/136 (98%)	64 (48%)	37 (28%)	33 (25%)	0	1
34	DM	134/136 (98%)	71 (53%)	43 (32%)	20 (15%)	0	3
35	BN	125/127 (98%)	68 (54%)	41 (33%)	16 (13%)	0	5
35	DN	125/127 (98%)	86 (69%)	29 (23%)	10 (8%)	1	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	BO	115/117 (98%)	61 (53%)	34 (30%)	20 (17%)	0	2
36	DO	115/117 (98%)	62 (54%)	33 (29%)	20 (17%)	0	2
37	BP	112/115 (97%)	37 (33%)	38 (34%)	37 (33%)	0	0
37	DP	112/115 (97%)	42 (38%)	37 (33%)	33 (30%)	0	0
38	BQ	115/118 (98%)	79 (69%)	23 (20%)	13 (11%)	0	7
38	DQ	115/118 (98%)	78 (68%)	21 (18%)	16 (14%)	0	4
39	BR	101/103 (98%)	39 (39%)	38 (38%)	24 (24%)	0	1
39	DR	101/103 (98%)	42 (42%)	30 (30%)	29 (29%)	0	0
40	BS	108/110 (98%)	58 (54%)	34 (32%)	16 (15%)	0	3
40	DS	108/110 (98%)	62 (57%)	26 (24%)	20 (18%)	0	2
41	BT	97/100 (97%)	38 (39%)	42 (43%)	17 (18%)	0	2
41	DT	97/100 (97%)	44 (45%)	28 (29%)	25 (26%)	0	1
42	BU	100/104 (96%)	36 (36%)	43 (43%)	21 (21%)	0	1
42	DU	100/104 (96%)	47 (47%)	34 (34%)	19 (19%)	0	2
43	BW	82/85 (96%)	35 (43%)	22 (27%)	25 (30%)	0	0
43	DW	82/85 (96%)	28 (34%)	31 (38%)	23 (28%)	0	0
44	BX	61/63 (97%)	20 (33%)	30 (49%)	11 (18%)	0	2
44	DX	61/63 (97%)	37 (61%)	15 (25%)	9 (15%)	0	3
45	BY	56/59 (95%)	29 (52%)	17 (30%)	10 (18%)	0	2
45	DY	56/59 (95%)	38 (68%)	15 (27%)	3 (5%)	2	23
46	BZ	68/70 (97%)	32 (47%)	23 (34%)	13 (19%)	0	2
46	DZ	68/70 (97%)	36 (53%)	22 (32%)	10 (15%)	0	3
47	B0	54/57 (95%)	27 (50%)	17 (32%)	10 (18%)	0	2
47	D0	54/57 (95%)	25 (46%)	20 (37%)	9 (17%)	0	2
48	B1	52/55 (94%)	22 (42%)	20 (38%)	10 (19%)	0	2
48	D1	52/55 (94%)	21 (40%)	18 (35%)	13 (25%)	0	1
49	B2	44/46 (96%)	22 (50%)	15 (34%)	7 (16%)	0	2
49	D2	44/46 (96%)	22 (50%)	10 (23%)	12 (27%)	0	0
50	B3	62/65 (95%)	26 (42%)	28 (45%)	8 (13%)	0	5
50	D3	62/65 (95%)	30 (48%)	21 (34%)	11 (18%)	0	2
51	B4	36/38 (95%)	17 (47%)	9 (25%)	10 (28%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	D4	36/38 (95%)	13 (36%)	10 (28%)	13 (36%)	0	0
52	BI	139/142 (98%)	122 (88%)	12 (9%)	5 (4%)	4	35
52	DI	139/142 (98%)	119 (86%)	15 (11%)	5 (4%)	4	35
All	All	11263/11954 (94%)	6605 (59%)	2995 (27%)	1663 (15%)	0	3

5 of 1663 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AC	2	GLN
2	AC	81	GLU
2	AC	91	ALA
3	AD	18	LEU
3	AD	25	ARG

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AC	170/190 (90%)	149 (88%)	21 (12%)	6	28
2	CC	170/190 (90%)	150 (88%)	20 (12%)	6	30
3	AD	172/173 (99%)	145 (84%)	27 (16%)	3	18
3	CD	172/173 (99%)	143 (83%)	29 (17%)	2	14
4	AE	113/126 (90%)	96 (85%)	17 (15%)	3	20
4	CE	113/126 (90%)	94 (83%)	19 (17%)	2	14
5	AF	87/116 (75%)	68 (78%)	19 (22%)	1	5
5	CF	87/116 (75%)	76 (87%)	11 (13%)	5	27
6	AG	123/147 (84%)	106 (86%)	17 (14%)	4	23
6	CG	125/147 (85%)	111 (89%)	14 (11%)	7	33
7	AH	104/105 (99%)	92 (88%)	12 (12%)	7	31
7	CH	104/105 (99%)	93 (89%)	11 (11%)	8	37
8	AI	105/107 (98%)	90 (86%)	15 (14%)	4	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	CI	105/107 (98%)	91 (87%)	14 (13%)	5	25
9	AJ	86/90 (96%)	70 (81%)	16 (19%)	2	9
9	CJ	86/90 (96%)	78 (91%)	8 (9%)	11	44
10	AK	90/99 (91%)	72 (80%)	18 (20%)	1	7
10	CK	90/99 (91%)	79 (88%)	11 (12%)	6	28
11	AL	103/104 (99%)	90 (87%)	13 (13%)	5	27
11	CL	103/104 (99%)	86 (84%)	17 (16%)	3	15
12	AM	92/96 (96%)	76 (83%)	16 (17%)	2	13
12	CM	91/96 (95%)	80 (88%)	11 (12%)	6	29
13	AN	79/84 (94%)	70 (89%)	9 (11%)	7	32
13	CN	79/84 (94%)	73 (92%)	6 (8%)	16	54
14	AO	76/77 (99%)	69 (91%)	7 (9%)	11	44
14	CO	76/77 (99%)	67 (88%)	9 (12%)	6	30
15	AP	65/65 (100%)	54 (83%)	11 (17%)	2	14
15	CP	65/65 (100%)	57 (88%)	8 (12%)	6	28
16	AQ	74/78 (95%)	64 (86%)	10 (14%)	5	25
16	CQ	75/78 (96%)	68 (91%)	7 (9%)	11	44
17	AR	48/65 (74%)	44 (92%)	4 (8%)	14	49
17	CR	48/65 (74%)	42 (88%)	6 (12%)	6	28
18	AS	70/79 (89%)	59 (84%)	11 (16%)	3	18
18	CS	71/79 (90%)	58 (82%)	13 (18%)	2	10
19	AT	65/66 (98%)	55 (85%)	10 (15%)	3	19
19	CT	65/66 (98%)	55 (85%)	10 (15%)	3	19
20	AB	180/199 (90%)	148 (82%)	32 (18%)	2	12
20	CB	180/199 (90%)	153 (85%)	27 (15%)	3	20
21	AU	44/61 (72%)	37 (84%)	7 (16%)	3	17
21	CU	44/61 (72%)	31 (70%)	13 (30%)	0	3
24	BV	78/78 (100%)	64 (82%)	14 (18%)	2	11
24	DV	78/78 (100%)	72 (92%)	6 (8%)	16	53
25	BC	213/218 (98%)	162 (76%)	51 (24%)	1	4
25	DC	213/218 (98%)	164 (77%)	49 (23%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	BD	164/164 (100%)	130 (79%)	34 (21%)	1	7
26	DD	164/164 (100%)	126 (77%)	38 (23%)	1	4
27	BE	165/165 (100%)	127 (77%)	38 (23%)	1	4
27	DE	165/165 (100%)	137 (83%)	28 (17%)	2	14
28	BF	149/150 (99%)	127 (85%)	22 (15%)	4	20
28	DF	149/150 (99%)	127 (85%)	22 (15%)	4	20
29	BG	137/138 (99%)	115 (84%)	22 (16%)	3	17
29	DG	137/138 (99%)	114 (83%)	23 (17%)	2	14
30	BH	114/114 (100%)	95 (83%)	19 (17%)	3	15
30	DH	114/114 (100%)	92 (81%)	22 (19%)	2	8
31	BJ	114/116 (98%)	93 (82%)	21 (18%)	2	10
31	DJ	114/116 (98%)	92 (81%)	22 (19%)	2	8
32	BK	102/104 (98%)	81 (79%)	21 (21%)	1	7
32	DK	102/104 (98%)	89 (87%)	13 (13%)	5	27
33	BL	103/103 (100%)	76 (74%)	27 (26%)	0	3
33	DL	103/103 (100%)	78 (76%)	25 (24%)	1	4
34	BM	109/109 (100%)	81 (74%)	28 (26%)	0	4
34	DM	109/109 (100%)	75 (69%)	34 (31%)	0	2
35	BN	103/103 (100%)	84 (82%)	19 (18%)	2	10
35	DN	103/103 (100%)	87 (84%)	16 (16%)	3	18
36	BO	87/87 (100%)	68 (78%)	19 (22%)	1	5
36	DO	87/87 (100%)	73 (84%)	14 (16%)	3	17
37	BP	99/100 (99%)	78 (79%)	21 (21%)	1	6
37	DP	99/100 (99%)	72 (73%)	27 (27%)	0	3
38	BQ	89/90 (99%)	72 (81%)	17 (19%)	2	9
38	DQ	89/90 (99%)	70 (79%)	19 (21%)	1	6
39	BR	84/84 (100%)	72 (86%)	12 (14%)	4	22
39	DR	84/84 (100%)	67 (80%)	17 (20%)	1	7
40	BS	93/93 (100%)	83 (89%)	10 (11%)	8	36
40	DS	93/93 (100%)	80 (86%)	13 (14%)	4	23
41	BT	83/84 (99%)	65 (78%)	18 (22%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	DT	83/84 (99%)	70 (84%)	13 (16%)	3	18
42	BU	83/85 (98%)	66 (80%)	17 (20%)	1	7
42	DU	83/85 (98%)	65 (78%)	18 (22%)	1	6
43	BW	62/63 (98%)	50 (81%)	12 (19%)	2	8
43	DW	62/63 (98%)	51 (82%)	11 (18%)	2	12
44	BX	55/55 (100%)	38 (69%)	17 (31%)	0	2
44	DX	55/55 (100%)	45 (82%)	10 (18%)	2	11
45	BY	48/49 (98%)	37 (77%)	11 (23%)	1	4
45	DY	48/49 (98%)	36 (75%)	12 (25%)	1	4
46	BZ	62/62 (100%)	46 (74%)	16 (26%)	0	3
46	DZ	62/62 (100%)	54 (87%)	8 (13%)	5	26
47	B0	47/48 (98%)	36 (77%)	11 (23%)	1	4
47	D0	47/48 (98%)	38 (81%)	9 (19%)	2	9
48	B1	48/49 (98%)	35 (73%)	13 (27%)	0	3
48	D1	48/49 (98%)	38 (79%)	10 (21%)	1	6
49	B2	38/38 (100%)	29 (76%)	9 (24%)	1	4
49	D2	38/38 (100%)	29 (76%)	9 (24%)	1	4
50	B3	51/52 (98%)	41 (80%)	10 (20%)	1	8
50	D3	51/52 (98%)	39 (76%)	12 (24%)	1	4
51	B4	34/34 (100%)	25 (74%)	9 (26%)	0	3
51	D4	34/34 (100%)	19 (56%)	15 (44%)	0	0
52	BI	109/110 (99%)	107 (98%)	2 (2%)	66	88
52	DI	109/110 (99%)	105 (96%)	4 (4%)	41	76
All	All	9341/9744 (96%)	7726 (83%)	1615 (17%)	2	13

5 of 1615 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
43	BW	69	GLU
5	CF	39	LEU
41	DT	64	LYS
45	BY	7	THR
50	B3	44	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 329 such sidechains are listed below:

Mol	Chain	Res	Type
43	BW	56	HIS
4	CE	131	ASN
40	DS	15	GLN
45	BY	19	HIS
2	CC	2	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1529/1542 (99%)	255 (16%)	24 (1%)
1	CA	1529/1542 (99%)	232 (15%)	24 (1%)
22	BA	116/120 (96%)	23 (19%)	0
22	DA	116/120 (96%)	22 (18%)	0
23	BB	2837/2904 (97%)	424 (14%)	13 (0%)
23	DB	2837/2904 (97%)	438 (15%)	18 (0%)
All	All	8964/9132 (98%)	1394 (15%)	79 (0%)

5 of 1394 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	7	A
1	AA	9	G
1	AA	14	U
1	AA	32	A
1	AA	39	G

5 of 79 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	BB	2425	A
1	CA	428	G
23	DB	2198	A
23	BB	2756	U
1	CA	279	A

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

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 345 ligands modelled in this entry, 343 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
53	KSG	AA	1601	-	24,27,27	2.46	3 (12%)	29,40,40	1.05	2 (6%)
53	KSG	CA	1601	-	24,27,27	2.32	4 (16%)	29,40,40	0.93	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	KSG	AA	1601	-	-	1/8/52/52	0/2/2/2
53	KSG	CA	1601	-	-	1/8/52/52	0/2/2/2

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	AA	1601	KSG	C14-C13	-9.89	1.49	1.53
53	CA	1601	KSG	C14-C13	-8.47	1.49	1.53
53	AA	1601	KSG	O7-C1	2.21	1.47	1.41
53	CA	1601	KSG	O1-C1	2.43	1.48	1.41
53	CA	1601	KSG	C1-C12	2.52	1.57	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	AA	1601	KSG	C1-O1-C2	-2.12	112.46	118.01
53	CA	1601	KSG	C6-C7-C2	2.12	114.26	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	AA	1601	KSG	C4-C3-C2	2.31	114.68	109.60

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
53	AA	1601	KSG	C2-O1-C1-C12
53	CA	1601	KSG	C2-O1-C1-C12

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
53	AA	1601	KSG	3	0
53	CA	1601	KSG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AA	1530/1542 (99%)	0.27	26 (1%) 73 66	15, 73, 149, 180	0
1	CA	1530/1542 (99%)	0.04	16 (1%) 84 78	7, 52, 134, 180	0
2	AC	206/233 (88%)	0.87	27 (13%) 5 5	7, 68, 138, 180	0
2	CC	206/233 (88%)	0.54	12 (5%) 26 23	6, 74, 126, 169	0
3	AD	205/206 (99%)	1.10	46 (22%) 1 1	27, 79, 147, 180	0
3	CD	205/206 (99%)	0.31	2 (0%) 84 78	5, 55, 113, 165	0
4	AE	150/167 (89%)	0.65	9 (6%) 25 22	15, 62, 120, 162	0
4	CE	150/167 (89%)	0.60	8 (5%) 30 26	6, 55, 112, 180	0
5	AF	100/135 (74%)	0.62	7 (7%) 19 18	18, 72, 133, 166	0
5	CF	100/135 (74%)	0.90	14 (14%) 4 4	12, 71, 132, 165	0
6	AG	150/179 (83%)	0.84	27 (18%) 2 2	22, 89, 143, 180	0
6	CG	152/179 (84%)	0.86	21 (13%) 4 5	19, 86, 147, 180	0
7	AH	129/130 (99%)	1.24	27 (20%) 1 1	14, 70, 141, 176	0
7	CH	129/130 (99%)	0.71	19 (14%) 3 4	5, 54, 114, 160	0
8	AI	127/130 (97%)	1.16	29 (22%) 1 1	18, 90, 146, 180	0
8	CI	127/130 (97%)	1.21	31 (24%) 1 1	23, 92, 156, 180	0
9	AJ	98/103 (95%)	1.28	28 (28%) 1 1	20, 82, 157, 180	0
9	CJ	98/103 (95%)	0.70	6 (6%) 25 22	34, 79, 135, 151	0
10	AK	117/129 (90%)	0.59	8 (6%) 20 19	7, 55, 138, 160	0
10	CK	117/129 (90%)	0.46	7 (5%) 25 22	11, 50, 105, 142	0
11	AL	123/124 (99%)	0.74	11 (8%) 12 12	21, 61, 128, 178	0
11	CL	123/124 (99%)	0.87	11 (8%) 12 12	5, 39, 119, 160	0
12	AM	114/118 (96%)	1.13	20 (17%) 2 2	44, 106, 159, 173	0
12	CM	113/118 (95%)	1.32	24 (21%) 1 1	26, 100, 157, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AN	96/101 (95%)	1.83	36 (37%) 0 0	15, 84, 151, 180	0
13	CN	96/101 (95%)	1.15	19 (19%) 1 2	21, 82, 139, 161	0
14	AO	88/89 (98%)	1.02	17 (19%) 2 2	18, 70, 114, 180	0
14	CO	88/89 (98%)	0.57	4 (4%) 37 31	14, 51, 112, 150	0
15	AP	82/82 (100%)	0.93	11 (13%) 4 5	27, 89, 142, 180	0
15	CP	80/82 (97%)	0.98	11 (13%) 4 5	5, 46, 145, 180	0
16	AQ	80/84 (95%)	1.53	21 (26%) 1 1	37, 91, 140, 180	0
16	CQ	81/84 (96%)	0.94	8 (9%) 9 11	12, 57, 119, 154	0
17	AR	55/75 (73%)	1.35	15 (27%) 1 1	18, 69, 147, 164	0
17	CR	55/75 (73%)	1.04	7 (12%) 5 6	13, 53, 126, 175	0
18	AS	79/92 (85%)	2.14	36 (45%) 0 0	59, 112, 174, 180	0
18	CS	80/92 (86%)	2.10	33 (41%) 0 0	48, 109, 172, 180	0
19	AT	85/87 (97%)	1.17	18 (21%) 1 1	36, 94, 142, 170	0
19	CT	85/87 (97%)	1.57	27 (31%) 1 1	17, 55, 118, 179	0
20	AB	218/241 (90%)	0.91	38 (17%) 2 2	28, 92, 142, 180	0
20	CB	218/241 (90%)	0.67	22 (10%) 9 10	27, 96, 157, 180	0
21	AU	51/71 (71%)	1.14	10 (19%) 1 2	26, 94, 153, 174	0
21	CU	51/71 (71%)	1.31	14 (27%) 1 1	29, 82, 163, 180	0
22	BA	117/120 (97%)	0.07	2 (1%) 73 66	39, 67, 125, 171	0
22	DA	117/120 (97%)	0.01	2 (1%) 73 66	34, 73, 116, 180	0
23	BB	2841/2904 (97%)	0.21	43 (1%) 76 70	9, 53, 144, 180	0
23	DB	2841/2904 (97%)	0.15	25 (0%) 85 79	5, 45, 143, 180	0
24	BV	94/94 (100%)	0.74	13 (13%) 4 5	26, 78, 134, 155	0
24	DV	94/94 (100%)	0.55	6 (6%) 23 21	34, 83, 139, 162	0
25	BC	267/273 (97%)	1.25	51 (19%) 2 2	5, 53, 143, 180	0
25	DC	267/273 (97%)	1.15	45 (16%) 2 2	5, 52, 158, 180	0
26	BD	209/209 (100%)	1.49	57 (27%) 1 1	9, 82, 157, 180	0
26	DD	209/209 (100%)	1.29	47 (22%) 1 1	5, 57, 142, 180	0
27	BE	201/201 (100%)	1.39	49 (24%) 1 1	5, 85, 162, 180	0
27	DE	201/201 (100%)	1.41	44 (21%) 1 1	6, 82, 170, 180	0
28	BF	178/179 (99%)	0.96	39 (21%) 1 1	39, 105, 168, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
28	DF	178/179 (99%)	0.81	20 (11%)	7	8	29, 96, 154, 180	0
29	BG	176/177 (99%)	1.35	46 (26%)	1	1	34, 100, 164, 180	0
29	DG	176/177 (99%)	0.94	31 (17%)	2	2	23, 88, 156, 180	0
30	BH	149/149 (100%)	2.44	69 (46%)	0	0	22, 126, 180, 180	0
30	DH	149/149 (100%)	1.58	47 (31%)	1	1	30, 106, 167, 180	0
31	BJ	140/142 (98%)	1.06	28 (20%)	1	2	11, 88, 153, 180	0
31	DJ	140/142 (98%)	0.89	21 (15%)	3	3	7, 66, 148, 176	0
32	BK	121/123 (98%)	0.77	12 (9%)	9	11	13, 60, 118, 152	0
32	DK	121/123 (98%)	0.61	3 (2%)	61	54	5, 36, 92, 134	0
33	BL	144/144 (100%)	2.69	69 (47%)	0	0	15, 86, 167, 180	0
33	DL	144/144 (100%)	2.22	57 (39%)	0	0	5, 81, 156, 180	0
34	BM	136/136 (100%)	1.64	40 (29%)	1	1	13, 71, 175, 180	0
34	DM	136/136 (100%)	1.21	25 (18%)	2	2	11, 70, 164, 180	0
35	BN	127/127 (100%)	1.61	41 (32%)	1	0	17, 78, 169, 180	0
35	DN	127/127 (100%)	1.12	16 (12%)	5	6	5, 48, 159, 180	0
36	BO	117/117 (100%)	1.87	37 (31%)	1	1	26, 91, 167, 180	0
36	DO	117/117 (100%)	1.86	40 (34%)	0	0	5, 91, 172, 180	0
37	BP	114/115 (99%)	1.91	49 (42%)	0	0	18, 98, 172, 180	0
37	DP	114/115 (99%)	1.55	32 (28%)	1	1	7, 65, 166, 180	0
38	BQ	117/118 (99%)	0.56	10 (8%)	13	13	13, 66, 146, 174	0
38	DQ	117/118 (99%)	0.94	18 (15%)	3	3	6, 57, 158, 180	0
39	BR	103/103 (100%)	1.16	23 (22%)	1	1	24, 105, 167, 180	0
39	DR	103/103 (100%)	1.75	36 (34%)	0	0	25, 92, 157, 180	0
40	BS	110/110 (100%)	0.71	8 (7%)	18	17	9, 63, 133, 180	0
40	DS	110/110 (100%)	0.81	9 (8%)	14	14	5, 46, 137, 180	0
41	BT	99/100 (99%)	1.73	40 (40%)	0	0	25, 81, 162, 180	0
41	DT	99/100 (99%)	2.70	57 (57%)	0	0	15, 86, 168, 180	0
42	BU	102/104 (98%)	2.35	40 (39%)	0	0	17, 91, 169, 180	0
42	DU	102/104 (98%)	1.91	34 (33%)	0	0	30, 110, 171, 180	0
43	BW	84/85 (98%)	2.75	39 (46%)	0	0	10, 86, 159, 180	0
43	DW	84/85 (98%)	2.52	36 (42%)	0	0	16, 86, 168, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
44	BX	63/63 (100%)	1.86	19 (30%)	1	1	20, 97, 160, 180	0
44	DX	63/63 (100%)	2.81	26 (41%)	0	0	38, 110, 169, 180	0
45	BY	58/59 (98%)	1.66	17 (29%)	1	1	13, 86, 157, 180	0
45	DY	58/59 (98%)	1.28	12 (20%)	1	1	5, 79, 136, 150	0
46	BZ	70/70 (100%)	0.96	10 (14%)	4	4	19, 66, 145, 180	0
46	DZ	70/70 (100%)	1.49	23 (32%)	0	0	5, 68, 141, 180	0
47	B0	56/57 (98%)	1.48	14 (25%)	1	1	26, 95, 180, 180	0
47	D0	56/57 (98%)	1.68	14 (25%)	1	1	10, 70, 159, 177	0
48	B1	54/55 (98%)	1.50	14 (25%)	1	1	24, 97, 160, 180	0
48	D1	54/55 (98%)	2.85	29 (53%)	0	0	8, 82, 158, 180	0
49	B2	46/46 (100%)	1.42	11 (23%)	1	1	6, 51, 154, 174	0
49	D2	46/46 (100%)	1.19	7 (15%)	3	3	9, 55, 131, 150	0
50	B3	64/65 (98%)	2.07	23 (35%)	0	0	19, 61, 155, 180	0
50	D3	64/65 (98%)	2.05	23 (35%)	0	0	5, 61, 139, 178	0
51	B4	38/38 (100%)	2.87	22 (57%)	0	0	30, 102, 170, 180	0
51	D4	38/38 (100%)	2.80	17 (44%)	0	0	14, 111, 175, 180	0
52	BI	141/142 (99%)	2.63	86 (60%)	0	0	52, 152, 180, 180	0
52	DI	141/142 (99%)	2.83	97 (68%)	0	0	83, 160, 180, 180	0
All	All	20439/21086 (96%)	0.80	2703 (13%)	4	5	5, 67, 155, 180	0

The worst 5 of 2703 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
33	BL	98	ALA	17.5
36	BO	58	ILE	17.1
33	BL	8	PRO	16.2
41	DT	4	GLU	15.3
42	BU	29	SER	15.2

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	DB	3082	1/1	0.82	0.29	6.31	61,61,61,61	0
54	MG	BB	3086	1/1	0.95	0.29	5.28	94,94,94,94	0
53	KSG	CA	1601	26/26	0.83	0.33	3.77	53,53,53,53	0
53	KSG	AA	1601	26/26	0.83	0.30	2.61	53,53,53,53	0
54	MG	BB	3100	1/1	0.73	0.22	2.09	37,37,37,37	1
54	MG	DB	3025	1/1	0.91	0.26	1.72	20,20,20,20	0
54	MG	BB	3078	1/1	0.95	0.28	1.33	49,49,49,49	0
54	MG	AA	1631	1/1	0.68	0.26	1.07	143,143,143,143	0
54	MG	DB	3086	1/1	0.94	0.24	0.94	25,25,25,25	0
54	MG	DB	3094	1/1	0.89	0.21	0.64	33,33,33,33	0
54	MG	BB	3110	1/1	0.92	0.22	0.58	79,79,79,79	0
54	MG	DN	201	1/1	0.94	0.26	0.13	38,38,38,38	0
54	MG	DB	3067	1/1	0.91	0.28	-0.22	11,11,11,11	0
54	MG	BB	3081	1/1	0.81	0.21	-0.24	34,34,34,34	0
54	MG	BB	3012	1/1	0.97	0.19	-0.37	75,75,75,75	0
54	MG	DB	3085	1/1	0.86	0.21	-0.48	64,64,64,64	0
54	MG	AA	1608	1/1	0.66	0.19	-0.49	57,57,57,57	0
54	MG	AA	1616	1/1	0.71	0.20	-0.58	86,86,86,86	0
54	MG	BB	3034	1/1	0.67	0.23	-0.62	42,42,42,42	0
54	MG	BB	3018	1/1	0.75	0.22	-0.75	42,42,42,42	0
54	MG	BB	3073	1/1	0.92	0.21	-0.79	55,55,55,55	0
54	MG	BB	3048	1/1	0.84	0.14	-0.83	39,39,39,39	0
54	MG	DB	3109	1/1	0.92	0.19	-0.86	57,57,57,57	0
54	MG	DB	3050	1/1	0.92	0.20	-0.87	42,42,42,42	0
54	MG	DB	3056	1/1	0.90	0.12	-0.88	67,67,67,67	0
54	MG	BB	3005	1/1	0.85	0.15	-1.07	13,13,13,13	0
54	MG	DB	3062	1/1	0.80	0.12	-1.08	24,24,24,24	0
54	MG	BB	3062	1/1	0.92	0.21	-1.11	34,34,34,34	0
54	MG	AA	1602	1/1	0.83	0.19	-1.18	34,34,34,34	0
54	MG	DB	3055	1/1	0.93	0.20	-1.19	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	AA	1653	1/1	0.92	0.15	-1.21	30,30,30,30	0
54	MG	DB	3012	1/1	0.91	0.17	-1.24	6,6,6,6	0
54	MG	DB	3003	1/1	0.87	0.13	-1.27	8,8,8,8	0
54	MG	CA	1615	1/1	0.95	0.14	-1.36	54,54,54,54	0
54	MG	BB	3092	1/1	0.94	0.16	-1.43	56,56,56,56	0
54	MG	BB	3088	1/1	0.90	0.16	-1.45	25,25,25,25	0
54	MG	AA	1610	1/1	0.98	0.15	-1.48	10,10,10,10	0
54	MG	DB	3029	1/1	0.85	0.19	-1.52	22,22,22,22	0
54	MG	DB	3024	1/1	0.85	0.12	-1.52	27,27,27,27	0
54	MG	BB	3098	1/1	0.94	0.15	-1.62	49,49,49,49	0
54	MG	DB	3076	1/1	0.89	0.15	-1.67	69,69,69,69	0
54	MG	DB	3027	1/1	0.88	0.15	-1.75	37,37,37,37	0
54	MG	DB	3046	1/1	0.95	0.18	-1.76	18,18,18,18	0
54	MG	CA	1640	1/1	0.80	0.12	-1.85	139,139,139,139	0
54	MG	DB	3001	1/1	0.93	0.17	-1.89	5,5,5,5	0
54	MG	CA	1642	1/1	0.91	0.13	-1.93	70,70,70,70	0
54	MG	BB	3029	1/1	0.97	0.10	-1.97	7,7,7,7	0
54	MG	CA	1613	1/1	0.94	0.10	-2.14	63,63,63,63	0
54	MG	DB	3108	1/1	0.75	0.12	-2.15	24,24,24,24	0
54	MG	DB	3092	1/1	0.95	0.06	-2.25	16,16,16,16	0
54	MG	CA	1617	1/1	0.92	0.07	-2.29	45,45,45,45	0
54	MG	BB	3065	1/1	0.84	0.14	-2.31	47,47,47,47	0
54	MG	BB	3096	1/1	0.90	0.12	-2.36	39,39,39,39	0
54	MG	BB	3040	1/1	0.95	0.14	-2.44	18,18,18,18	0
54	MG	BB	3103	1/1	0.96	0.14	-2.50	11,11,11,11	0
54	MG	BB	3087	1/1	0.92	0.10	-2.53	53,53,53,53	0
54	MG	BB	3021	1/1	0.82	0.17	-2.64	24,24,24,24	0
54	MG	BB	3094	1/1	0.83	0.14	-2.84	16,16,16,16	0
54	MG	DB	3014	1/1	0.94	0.14	-2.85	28,28,28,28	0
54	MG	BB	3051	1/1	0.86	0.10	-2.87	74,74,74,74	0
54	MG	DB	3010	1/1	0.93	0.08	-2.87	8,8,8,8	0
54	MG	AA	1661	1/1	0.79	0.05	-2.90	83,83,83,83	0
54	MG	DB	3022	1/1	0.93	0.07	-2.92	5,5,5,5	0
54	MG	CA	1602	1/1	0.90	0.12	-2.93	8,8,8,8	0
54	MG	AA	1604	1/1	0.89	0.11	-2.98	25,25,25,25	0
54	MG	DB	3034	1/1	0.92	0.11	-3.01	84,84,84,84	0
54	MG	BB	3023	1/1	0.93	0.10	-3.04	27,27,27,27	0
54	MG	BB	3056	1/1	0.93	0.14	-3.04	37,37,37,37	0
54	MG	DB	3072	1/1	0.97	0.10	-3.12	5,5,5,5	0
54	MG	BB	3090	1/1	0.89	0.11	-3.14	65,65,65,65	0
54	MG	DB	3097	1/1	0.96	0.13	-3.16	19,19,19,19	0
54	MG	CA	1647	1/1	0.91	0.12	-3.26	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	AA	1654	1/1	0.80	0.11	-3.34	81,81,81,81	0
54	MG	DB	3090	1/1	0.95	0.15	-3.38	106,106,106,106	0
54	MG	DB	3077	1/1	0.97	0.13	-3.54	41,41,41,41	0
54	MG	CA	1634	1/1	0.94	0.09	-3.55	46,46,46,46	0
54	MG	AA	1638	1/1	0.95	0.11	-3.56	88,88,88,88	0
54	MG	CA	1606	1/1	0.94	0.08	-3.56	30,30,30,30	0
54	MG	BB	3037	1/1	0.95	0.10	-3.58	21,21,21,21	0
54	MG	DB	3068	1/1	0.95	0.12	-3.80	49,49,49,49	0
54	MG	BB	3085	1/1	0.93	0.11	-3.80	67,67,67,67	0
54	MG	AA	1643	1/1	0.97	0.07	-3.80	116,116,116,116	0
54	MG	CA	1618	1/1	0.98	0.08	-3.87	26,26,26,26	0
54	MG	CA	1658	1/1	0.90	0.07	-3.90	18,18,18,18	0
54	MG	DB	3106	1/1	0.89	0.12	-4.07	7,7,7,7	0
54	MG	DB	3083	1/1	0.92	0.13	-4.28	18,18,18,18	0
54	MG	BB	3026	1/1	0.91	0.12	-4.30	25,25,25,25	0
54	MG	BB	3011	1/1	0.97	0.12	-4.40	9,9,9,9	0
54	MG	AA	1651	1/1	0.92	0.05	-4.46	64,64,64,64	0
54	MG	BB	3052	1/1	0.90	0.09	-4.47	27,27,27,27	0
54	MG	DB	3009	1/1	0.91	0.11	-4.50	10,10,10,10	0
54	MG	BB	3083	1/1	0.88	0.14	-4.55	25,25,25,25	0
54	MG	DB	3096	1/1	0.99	0.17	-4.66	31,31,31,31	0
54	MG	DB	3101	1/1	0.95	0.13	-4.78	30,30,30,30	0
54	MG	BB	3035	1/1	0.96	0.12	-4.84	25,25,25,25	0
54	MG	BB	3013	1/1	0.91	0.09	-4.84	36,36,36,36	0
54	MG	CA	1635	1/1	0.93	0.11	-4.88	91,91,91,91	0
54	MG	CA	1657	1/1	0.92	0.13	-4.93	51,51,51,51	0
54	MG	BB	3019	1/1	0.93	0.14	-4.94	22,22,22,22	0
54	MG	AA	1611	1/1	0.95	0.06	-5.02	57,57,57,57	0
54	MG	DB	3087	1/1	0.96	0.12	-5.05	40,40,40,40	0
54	MG	DB	3007	1/1	0.82	0.14	-5.11	15,15,15,15	0
54	MG	DB	3026	1/1	0.88	0.14	-5.12	30,30,30,30	0
54	MG	BB	3079	1/1	0.94	0.06	-5.43	32,32,32,32	0
54	MG	DB	3075	1/1	0.81	0.14	-5.59	42,42,42,42	0
54	MG	BB	3108	1/1	0.90	0.13	-5.83	22,22,22,22	0
54	MG	BB	3069	1/1	0.96	0.08	-6.08	8,8,8,8	0
54	MG	CA	1648	1/1	0.96	0.06	-6.19	39,39,39,39	0
54	MG	CA	1619	1/1	0.96	0.07	-6.23	9,9,9,9	0
54	MG	BB	3061	1/1	0.94	0.06	-6.51	33,33,33,33	0
54	MG	DB	3002	1/1	0.91	0.13	-6.55	20,20,20,20	0
54	MG	BB	3002	1/1	0.98	0.09	-6.63	9,9,9,9	0
54	MG	DB	3054	1/1	0.97	0.10	-6.69	32,32,32,32	0
54	MG	CA	1645	1/1	0.96	0.07	-7.12	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DB	3078	1/1	0.97	0.08	-10.26	5,5,5,5	0
54	MG	BB	3001	1/1	0.85	0.11	-11.21	28,28,28,28	0
54	MG	BB	3004	1/1	0.92	0.08	-	39,39,39,39	0
54	MG	BB	3017	1/1	0.89	0.10	-	54,54,54,54	0
54	MG	DB	3060	1/1	0.83	0.10	-	105,105,105,105	0
54	MG	DB	3035	1/1	0.83	0.16	-	24,24,24,24	0
54	MG	AA	1620	1/1	0.74	0.29	-	116,116,116,116	0
54	MG	DB	3103	1/1	0.82	0.17	-	61,61,61,61	0
54	MG	BB	3076	1/1	0.85	0.12	-	43,43,43,43	0
54	MG	AA	1659	1/1	0.97	0.20	-	157,157,157,157	0
54	MG	CA	1659	1/1	0.91	0.25	-	88,88,88,88	0
54	MG	AA	1625	1/1	0.86	0.40	-	81,81,81,81	0
54	MG	AA	1614	1/1	0.73	0.15	-	67,67,67,67	0
54	MG	CA	1620	1/1	0.96	0.14	-	32,32,32,32	0
54	MG	AA	1627	1/1	0.75	0.33	-	17,17,17,17	1
54	MG	BB	3032	1/1	0.92	0.14	-	31,31,31,31	0
54	MG	DB	3043	1/1	0.94	0.07	-	7,7,7,7	0
54	MG	CA	1637	1/1	0.84	0.15	-	107,107,107,107	0
54	MG	BB	3022	1/1	0.96	0.14	-	55,55,55,55	0
54	MG	AA	1605	1/1	0.92	0.12	-	30,30,30,30	0
54	MG	DB	3005	1/1	0.98	0.09	-	6,6,6,6	0
54	MG	AA	1628	1/1	0.71	0.16	-	63,63,63,63	0
54	MG	DB	3053	1/1	0.88	0.10	-	37,37,37,37	0
54	MG	AA	1609	1/1	0.49	0.20	-	119,119,119,119	0
54	MG	AA	1607	1/1	0.81	0.08	-	82,82,82,82	0
54	MG	BB	3093	1/1	0.92	0.17	-	5,5,5,5	1
54	MG	CA	1646	1/1	0.95	0.05	-	94,94,94,94	0
54	MG	DB	3061	1/1	0.89	0.11	-	48,48,48,48	0
54	MG	DB	3015	1/1	0.87	0.15	-	69,69,69,69	0
54	MG	DB	3006	1/1	0.98	0.08	-	16,16,16,16	0
54	MG	CA	1610	1/1	0.97	0.16	-	61,61,61,61	0
54	MG	AA	1615	1/1	0.30	0.19	-	72,72,72,72	0
54	MG	BB	3084	1/1	0.80	0.11	-	19,19,19,19	0
54	MG	DB	3051	1/1	0.94	0.15	-	57,57,57,57	0
54	MG	AA	1650	1/1	0.44	0.23	-	133,133,133,133	0
54	MG	BB	3014	1/1	0.84	0.17	-	33,33,33,33	0
54	MG	DB	3069	1/1	0.93	0.09	-	50,50,50,50	0
54	MG	AA	1649	1/1	0.85	0.10	-	102,102,102,102	0
54	MG	AA	1660	1/1	0.80	0.10	-	95,95,95,95	0
54	MG	CA	1607	1/1	0.88	0.13	-	126,126,126,126	0
54	MG	CA	1643	1/1	0.95	0.10	-	62,62,62,62	0
54	MG	BB	3024	1/1	0.90	0.17	-	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	CA	1625	1/1	0.96	0.14	-	24,24,24,24	0
54	MG	CA	1644	1/1	0.82	0.12	-	59,59,59,59	0
54	MG	DB	3020	1/1	0.94	0.24	-	41,41,41,41	0
54	MG	AA	1613	1/1	0.80	0.20	-	108,108,108,108	0
54	MG	CA	1652	1/1	0.94	0.13	-	20,20,20,20	0
54	MG	BB	3007	1/1	0.88	0.14	-	57,57,57,57	0
54	MG	AA	1655	1/1	0.80	0.10	-	67,67,67,67	0
54	MG	DB	3098	1/1	0.88	0.11	-	9,9,9,9	0
54	MG	DB	3032	1/1	0.87	0.11	-	29,29,29,29	0
54	MG	DB	3059	1/1	0.73	0.15	-	75,75,75,75	0
54	MG	BB	3063	1/1	0.87	0.17	-	27,27,27,27	0
54	MG	DB	3042	1/1	0.90	0.16	-	5,5,5,5	0
54	MG	DB	3028	1/1	0.83	0.18	-	29,29,29,29	0
54	MG	BB	3071	1/1	0.91	0.19	-	38,38,38,38	0
54	MG	AA	1640	1/1	0.82	0.10	-	42,42,42,42	0
54	MG	BB	3030	1/1	0.93	0.08	-	45,45,45,45	0
54	MG	CA	1660	1/1	0.96	0.21	-	27,27,27,27	0
54	MG	DB	3021	1/1	0.93	0.12	-	25,25,25,25	0
54	MG	CA	1611	1/1	0.96	0.04	-	43,43,43,43	0
54	MG	BB	3045	1/1	0.97	0.05	-	40,40,40,40	0
54	MG	DB	3066	1/1	0.93	0.15	-	12,12,12,12	0
54	MG	AA	1618	1/1	0.92	0.12	-	102,102,102,102	0
54	MG	BB	3031	1/1	0.86	0.18	-	46,46,46,46	0
54	MG	BB	3080	1/1	0.91	0.09	-	42,42,42,42	0
54	MG	CA	1636	1/1	0.92	0.14	-	13,13,13,13	0
54	MG	AA	1630	1/1	0.95	0.10	-	20,20,20,20	0
54	MG	BB	3060	1/1	0.82	0.16	-	81,81,81,81	0
54	MG	CA	1631	1/1	0.58	0.25	-	21,21,21,21	1
54	MG	BB	3049	1/1	0.89	0.15	-	12,12,12,12	0
54	MG	CA	1654	1/1	0.97	0.19	-	32,32,32,32	0
54	MG	DB	3037	1/1	0.94	0.10	-	8,8,8,8	0
54	MG	BB	3059	1/1	0.90	0.10	-	16,16,16,16	0
54	MG	AA	1621	1/1	0.73	0.14	-	96,96,96,96	0
54	MG	DB	3099	1/1	0.96	0.17	-	11,11,11,11	0
54	MG	BB	3082	1/1	0.64	0.39	-	63,63,63,63	0
54	MG	CA	1629	1/1	0.62	0.61	-	62,62,62,62	1
54	MG	AA	1633	1/1	0.82	0.15	-	92,92,92,92	0
54	MG	BB	3020	1/1	0.96	0.07	-	38,38,38,38	0
54	MG	CA	1626	1/1	0.95	0.11	-	17,17,17,17	0
54	MG	BB	3016	1/1	0.92	0.18	-	19,19,19,19	0
54	MG	CA	1653	1/1	0.95	0.07	-	48,48,48,48	0
54	MG	BB	3010	1/1	0.89	0.16	-	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DB	3052	1/1	0.78	0.25	-	42,42,42,42	0
54	MG	DB	3079	1/1	0.93	0.14	-	7,7,7,7	0
54	MG	AA	1657	1/1	0.81	0.27	-	83,83,83,83	0
54	MG	AA	1622	1/1	0.96	0.06	-	16,16,16,16	0
54	MG	AA	1612	1/1	0.80	0.12	-	52,52,52,52	0
54	MG	DB	3019	1/1	0.99	0.03	-	8,8,8,8	0
54	MG	CA	1656	1/1	0.97	0.10	-	60,60,60,60	0
54	MG	CA	1603	1/1	0.94	0.12	-	32,32,32,32	0
54	MG	DB	3045	1/1	0.95	0.07	-	45,45,45,45	0
54	MG	DB	3033	1/1	0.77	0.26	-	88,88,88,88	0
54	MG	CA	1633	1/1	0.96	0.10	-	50,50,50,50	0
54	MG	DB	3071	1/1	0.72	0.13	-	27,27,27,27	0
54	MG	DB	3089	1/1	0.97	0.28	-	28,28,28,28	0
54	MG	BB	3106	1/1	0.92	0.25	-	62,62,62,62	0
54	MG	CA	1605	1/1	0.96	0.09	-	37,37,37,37	0
54	MG	DB	3039	1/1	0.93	0.11	-	5,5,5,5	0
54	MG	BB	3075	1/1	0.91	0.25	-	35,35,35,35	0
54	MG	DB	3084	1/1	0.97	0.17	-	18,18,18,18	0
54	MG	CA	1616	1/1	0.59	0.26	-	153,153,153,153	0
54	MG	BB	3003	1/1	0.94	0.11	-	23,23,23,23	0
54	MG	AA	1635	1/1	0.97	0.07	-	75,75,75,75	0
54	MG	CA	1638	1/1	0.88	0.21	-	60,60,60,60	0
54	MG	BB	3097	1/1	0.72	0.13	-	96,96,96,96	0
54	MG	BB	3041	1/1	0.81	0.18	-	47,47,47,47	0
54	MG	DB	3100	1/1	0.94	0.14	-	6,6,6,6	0
54	MG	AA	1606	1/1	0.91	0.06	-	28,28,28,28	0
54	MG	BB	3008	1/1	0.74	0.16	-	82,82,82,82	0
54	MG	BB	3095	1/1	0.98	0.06	-	48,48,48,48	0
54	MG	DB	3104	1/1	0.94	0.19	-	44,44,44,44	0
54	MG	CA	1628	1/1	0.85	0.34	-	38,38,38,38	1
54	MG	CA	1604	1/1	0.95	0.15	-	49,49,49,49	0
54	MG	CA	1621	1/1	0.92	0.09	-	46,46,46,46	0
54	MG	BB	3058	1/1	0.97	0.12	-	33,33,33,33	0
54	MG	DB	3017	1/1	0.74	0.23	-	22,22,22,22	0
54	MG	BB	3089	1/1	0.93	0.23	-	82,82,82,82	0
54	MG	AA	1636	1/1	0.94	0.14	-	83,83,83,83	0
54	MG	BB	3074	1/1	0.87	0.12	-	7,7,7,7	0
54	MG	DB	3095	1/1	0.91	0.09	-	44,44,44,44	0
54	MG	AA	1644	1/1	0.95	0.17	-	81,81,81,81	0
54	MG	BB	3099	1/1	0.89	0.13	-	58,58,58,58	0
54	MG	BB	3064	1/1	0.88	0.16	-	71,71,71,71	0
54	MG	AA	1647	1/1	0.87	0.60	-	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	CA	1632	1/1	0.94	0.12	-	34,34,34,34	0
54	MG	AA	1656	1/1	0.86	0.14	-	100,100,100,100	0
54	MG	AA	1642	1/1	0.83	0.15	-	107,107,107,107	0
54	MG	AA	1617	1/1	0.87	0.13	-	65,65,65,65	0
54	MG	CA	1627	1/1	0.85	0.19	-	114,114,114,114	0
54	MG	BB	3036	1/1	0.89	0.10	-	29,29,29,29	0
54	MG	CA	1624	1/1	0.32	0.29	-	162,162,162,162	0
54	MG	CA	1630	1/1	0.86	0.09	-	49,49,49,49	0
54	MG	BB	3091	1/1	0.89	0.16	-	42,42,42,42	0
54	MG	BB	3015	1/1	0.97	0.10	-	23,23,23,23	0
54	MG	DB	3018	1/1	0.92	0.12	-	39,39,39,39	0
54	MG	AA	1624	1/1	0.88	0.12	-	25,25,25,25	1
54	MG	AA	1658	1/1	0.80	0.12	-	113,113,113,113	0
54	MG	BB	3033	1/1	0.75	0.25	-	113,113,113,113	0
54	MG	DB	3038	1/1	0.94	0.08	-	33,33,33,33	0
54	MG	DB	3031	1/1	0.97	0.10	-	40,40,40,40	0
54	MG	AA	1652	1/1	0.88	0.14	-	105,105,105,105	0
54	MG	BB	3006	1/1	0.95	0.08	-	20,20,20,20	0
54	MG	DB	3011	1/1	0.94	0.17	-	23,23,23,23	0
54	MG	CA	1609	1/1	0.78	0.19	-	132,132,132,132	0
54	MG	BB	3039	1/1	0.91	0.13	-	26,26,26,26	0
54	MG	DB	3080	1/1	0.89	0.12	-	34,34,34,34	0
54	MG	BB	3101	1/1	0.89	0.10	-	14,14,14,14	0
54	MG	DB	3036	1/1	0.94	0.17	-	25,25,25,25	0
54	MG	DB	3081	1/1	0.91	0.15	-	110,110,110,110	0
54	MG	DB	3065	1/1	0.95	0.16	-	25,25,25,25	0
54	MG	DB	3093	1/1	0.86	0.76	-	48,48,48,48	1
54	MG	BB	3046	1/1	0.82	0.17	-	63,63,63,63	0
54	MG	AA	1639	1/1	0.46	0.19	-	141,141,141,141	0
54	MG	AA	1603	1/1	0.80	0.14	-	74,74,74,74	0
54	MG	DB	3057	1/1	0.81	0.20	-	56,56,56,56	1
54	MG	DB	3040	1/1	0.85	0.20	-	28,28,28,28	0
54	MG	BB	3047	1/1	0.69	0.29	-	128,128,128,128	0
54	MG	BB	3067	1/1	0.85	0.16	-	56,56,56,56	0
54	MG	DB	3088	1/1	0.96	0.21	-	51,51,51,51	0
54	MG	DB	3070	1/1	0.94	0.07	-	60,60,60,60	0
54	MG	BB	3077	1/1	0.74	0.16	-	37,37,37,37	0
54	MG	BB	3043	1/1	0.88	0.24	-	63,63,63,63	0
54	MG	DB	3049	1/1	0.78	0.10	-	79,79,79,79	0
54	MG	BB	3038	1/1	0.91	0.13	-	82,82,82,82	0
54	MG	CA	1649	1/1	0.94	0.31	-	86,86,86,86	0
54	MG	CA	1623	1/1	0.50	0.14	-	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BB	3050	1/1	0.95	0.13	-	20,20,20,20	0
54	MG	DB	3073	1/1	0.94	0.11	-	44,44,44,44	0
54	MG	CA	1662	1/1	0.97	0.11	-	38,38,38,38	0
54	MG	BB	3044	1/1	0.95	0.07	-	39,39,39,39	0
54	MG	BB	3107	1/1	0.82	0.13	-	37,37,37,37	0
54	MG	BB	3057	1/1	0.86	0.18	-	19,19,19,19	0
54	MG	CA	1608	1/1	0.87	0.06	-	31,31,31,31	0
54	MG	AA	1629	1/1	0.96	0.10	-	62,62,62,62	0
54	MG	BB	3028	1/1	0.80	0.22	-	66,66,66,66	0
54	MG	DB	3048	1/1	0.95	0.07	-	7,7,7,7	0
54	MG	CA	1655	1/1	0.95	0.05	-	26,26,26,26	0
54	MG	DB	3102	1/1	0.95	0.10	-	13,13,13,13	0
54	MG	BB	3053	1/1	0.87	0.12	-	36,36,36,36	0
54	MG	BB	3070	1/1	0.98	0.09	-	55,55,55,55	0
54	MG	AA	1648	1/1	0.97	0.12	-	31,31,31,31	0
54	MG	AA	1634	1/1	0.90	0.19	-	73,73,73,73	0
54	MG	DB	3023	1/1	0.78	0.08	-	44,44,44,44	0
54	MG	DB	3016	1/1	0.80	0.14	-	25,25,25,25	0
54	MG	BB	3072	1/1	0.88	0.12	-	26,26,26,26	0
54	MG	AA	1632	1/1	0.93	0.07	-	44,44,44,44	0
54	MG	CA	1641	1/1	0.94	0.08	-	40,40,40,40	0
54	MG	AA	1619	1/1	0.74	0.13	-	33,33,33,33	0
54	MG	DB	3041	1/1	0.97	0.13	-	29,29,29,29	0
54	MG	CA	1650	1/1	0.94	0.08	-	67,67,67,67	0
54	MG	BB	3054	1/1	0.92	0.11	-	77,77,77,77	0
54	MG	CA	1622	1/1	0.63	0.34	-	132,132,132,132	0
54	MG	BB	3042	1/1	0.88	0.07	-	74,74,74,74	0
54	MG	DB	3091	1/1	0.97	0.16	-	39,39,39,39	0
54	MG	BB	3009	1/1	0.95	0.08	-	35,35,35,35	0
54	MG	DB	3063	1/1	0.98	0.11	-	42,42,42,42	0
54	MG	DB	3044	1/1	0.80	0.09	-	58,58,58,58	0
54	MG	DB	3058	1/1	0.85	0.20	-	132,132,132,132	0
54	MG	CA	1651	1/1	0.84	0.16	-	122,122,122,122	0
54	MG	AA	1641	1/1	0.95	0.09	-	72,72,72,72	0
54	MG	DB	3105	1/1	0.94	0.08	-	24,24,24,24	0
54	MG	CA	1639	1/1	0.93	0.04	-	41,41,41,41	0
54	MG	DB	3008	1/1	0.96	0.18	-	39,39,39,39	0
54	MG	AA	1646	1/1	0.92	0.15	-	103,103,103,103	0
54	MG	DB	3047	1/1	0.89	0.09	-	29,29,29,29	0
54	MG	BB	3025	1/1	0.97	0.16	-	67,67,67,67	0
54	MG	DB	3064	1/1	0.77	0.27	-	66,66,66,66	1
54	MG	AA	1623	1/1	0.88	0.32	-	143,143,143,143	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	AA	1626	1/1	0.61	0.43	-	82,82,82,82	1
54	MG	BB	3104	1/1	0.88	0.13	-	33,33,33,33	0
54	MG	CA	1663	1/1	0.92	0.15	-	20,20,20,20	0
54	MG	BB	3055	1/1	0.95	0.12	-	19,19,19,19	0
54	MG	AA	1645	1/1	0.89	0.16	-	97,97,97,97	0
54	MG	CA	1661	1/1	0.89	0.29	-	67,67,67,67	0
54	MG	DB	3013	1/1	0.67	0.20	-	32,32,32,32	0
54	MG	BB	3068	1/1	0.92	0.12	-	39,39,39,39	0
54	MG	DB	3074	1/1	0.97	0.13	-	12,12,12,12	0
54	MG	AA	1637	1/1	0.67	0.62	-	115,115,115,115	0
54	MG	CA	1614	1/1	0.93	0.13	-	97,97,97,97	0
54	MG	BB	3027	1/1	0.93	0.07	-	29,29,29,29	0
54	MG	BB	3105	1/1	0.87	0.15	-	33,33,33,33	0
54	MG	BB	3102	1/1	0.91	0.11	-	34,34,34,34	0
54	MG	DB	3004	1/1	0.94	0.15	-	38,38,38,38	0
54	MG	DB	3107	1/1	0.85	0.13	-	19,19,19,19	0
54	MG	DE	301	1/1	0.80	0.16	-	69,69,69,69	0
54	MG	CA	1612	1/1	0.87	0.10	-	71,71,71,71	0
54	MG	BB	3066	1/1	0.88	0.13	-	42,42,42,42	0
54	MG	DB	3030	1/1	0.92	0.17	-	11,11,11,11	0
54	MG	BB	3109	1/1	0.90	0.15	-	33,33,33,33	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.