



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 03:37 am BST

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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

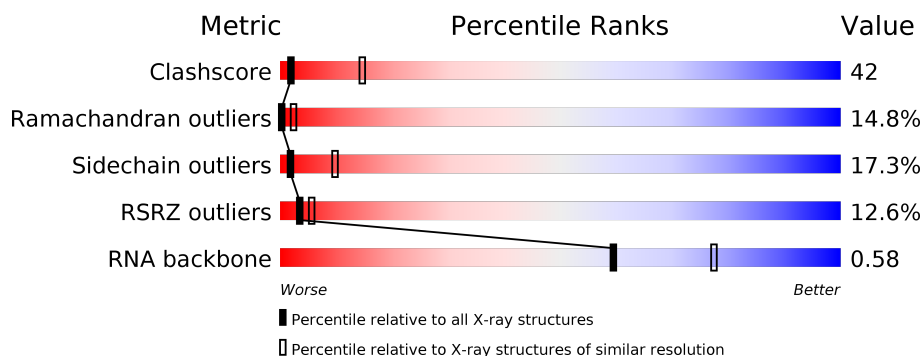
# 1 Overall quality at a glance

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	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)
RNA backbone	3102	1036 (3.96-2.96)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1542	<div> <div>23%</div> <div>63%</div> <div>13%</div> <div>•</div> </div>
1	CA	1542	<div> <div>22%</div> <div>64%</div> <div>12%</div> <div>•</div> </div>
2	AC	233	<div> <div>11%</div> <div>25%</div> <div>52%</div> <div>11%</div> <div>•</div> <div>12%</div> </div>
2	CC	233	<div> <div>5%</div> <div>30%</div> <div>45%</div> <div>12%</div> <div>•</div> <div>12%</div> </div>
3	AD	206	<div> <div>22%</div> <div>31%</div> <div>51%</div> <div>16%</div> <div>•</div> </div>
3	CD	206	<div> <div>27%</div> <div>56%</div> <div>16%</div> </div>

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Mol	Chain	Length	Quality of chain
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	
16	AQ	84	

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Mol	Chain	Length	Quality of chain
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	
28	DF	179	



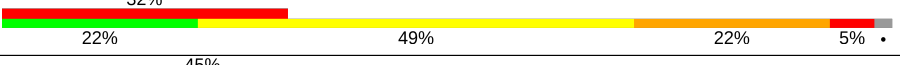
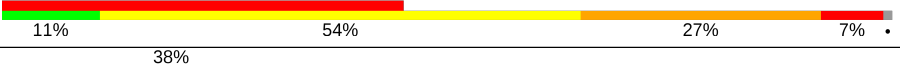
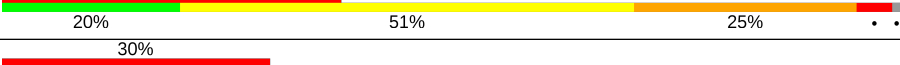

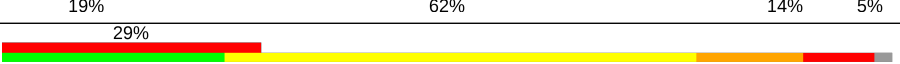
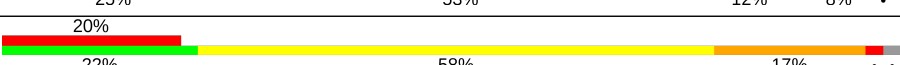
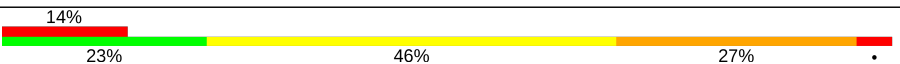
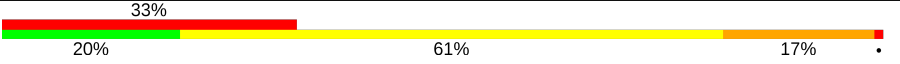
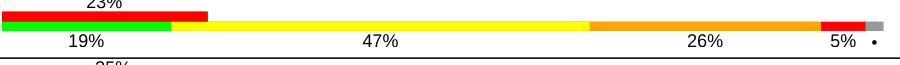
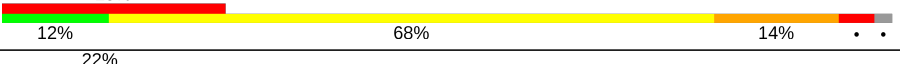


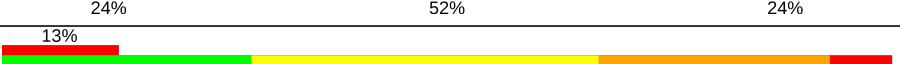
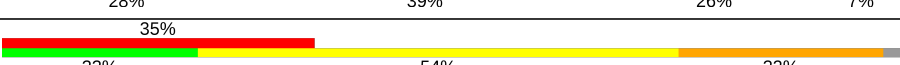
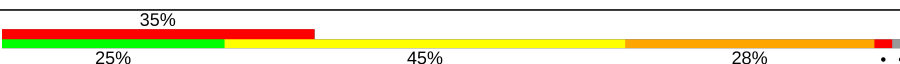





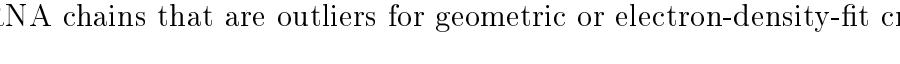
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Mol	Chain	Length	Quality of chain
29	BG	177	
29	DG	177	
30	BH	149	
30	DH	149	
31	BJ	142	
31	DJ	142	
32	BK	123	
32	DK	123	
33	BL	144	
33	DL	144	
34	BM	136	
34	DM	136	
35	BN	127	
35	DN	127	
36	BO	117	
36	DO	117	
37	BP	115	
37	DP	115	
38	BQ	118	
38	DQ	118	
39	BR	103	
39	DR	103	
40	BS	110	
40	DS	110	
41	BT	100	

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Mol	Chain	Length	Quality of chain
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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	AA	1626	-	-	-	X
54	MG	AA	1637	-	-	-	X
54	MG	CA	1629	-	-	-	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			

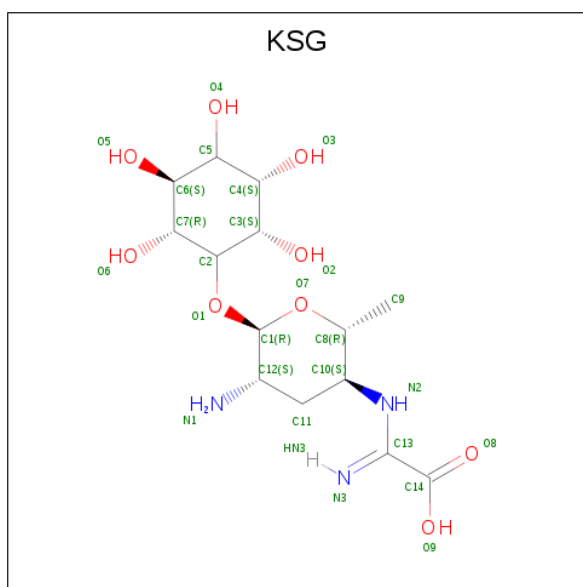
- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L36.

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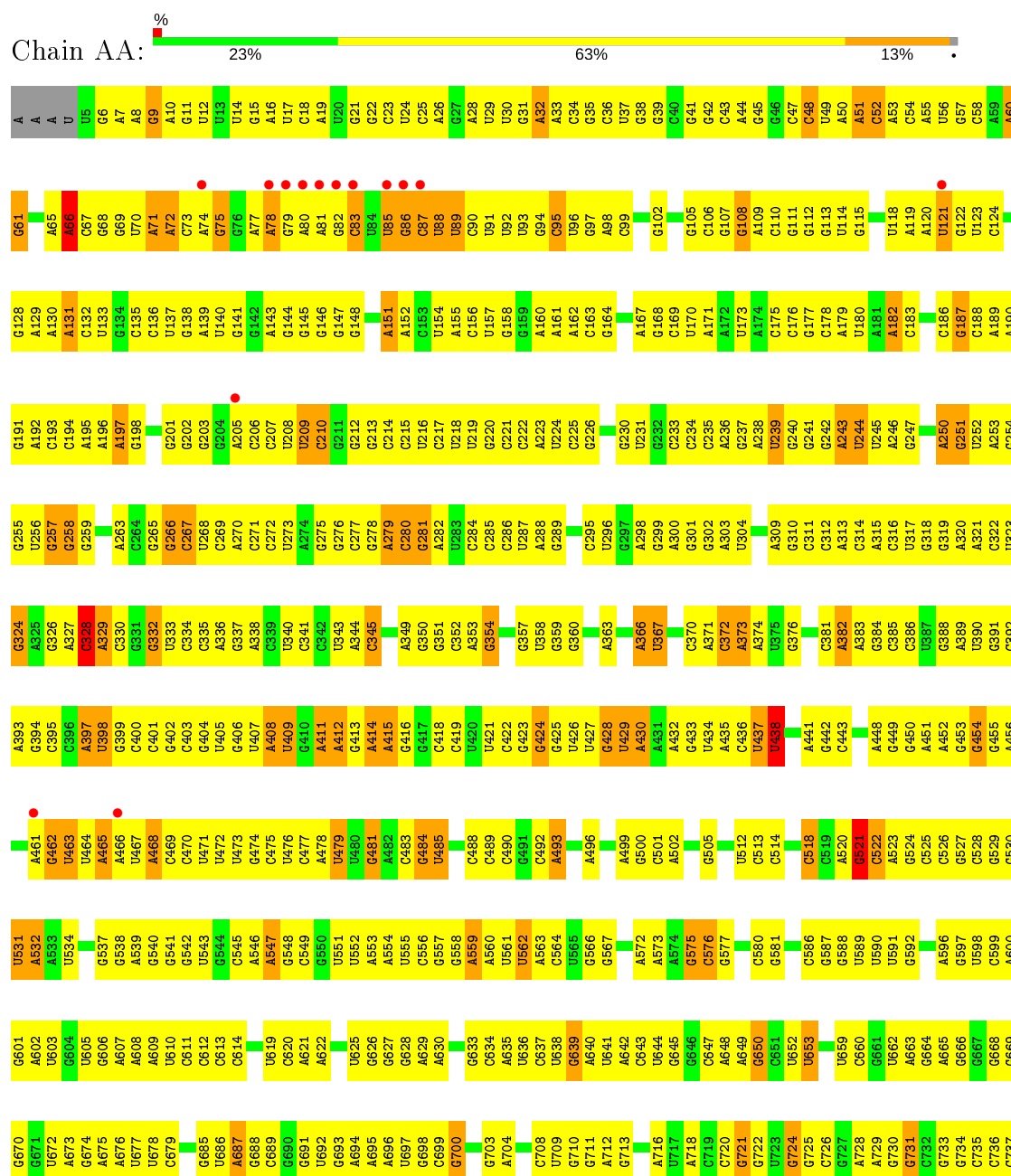
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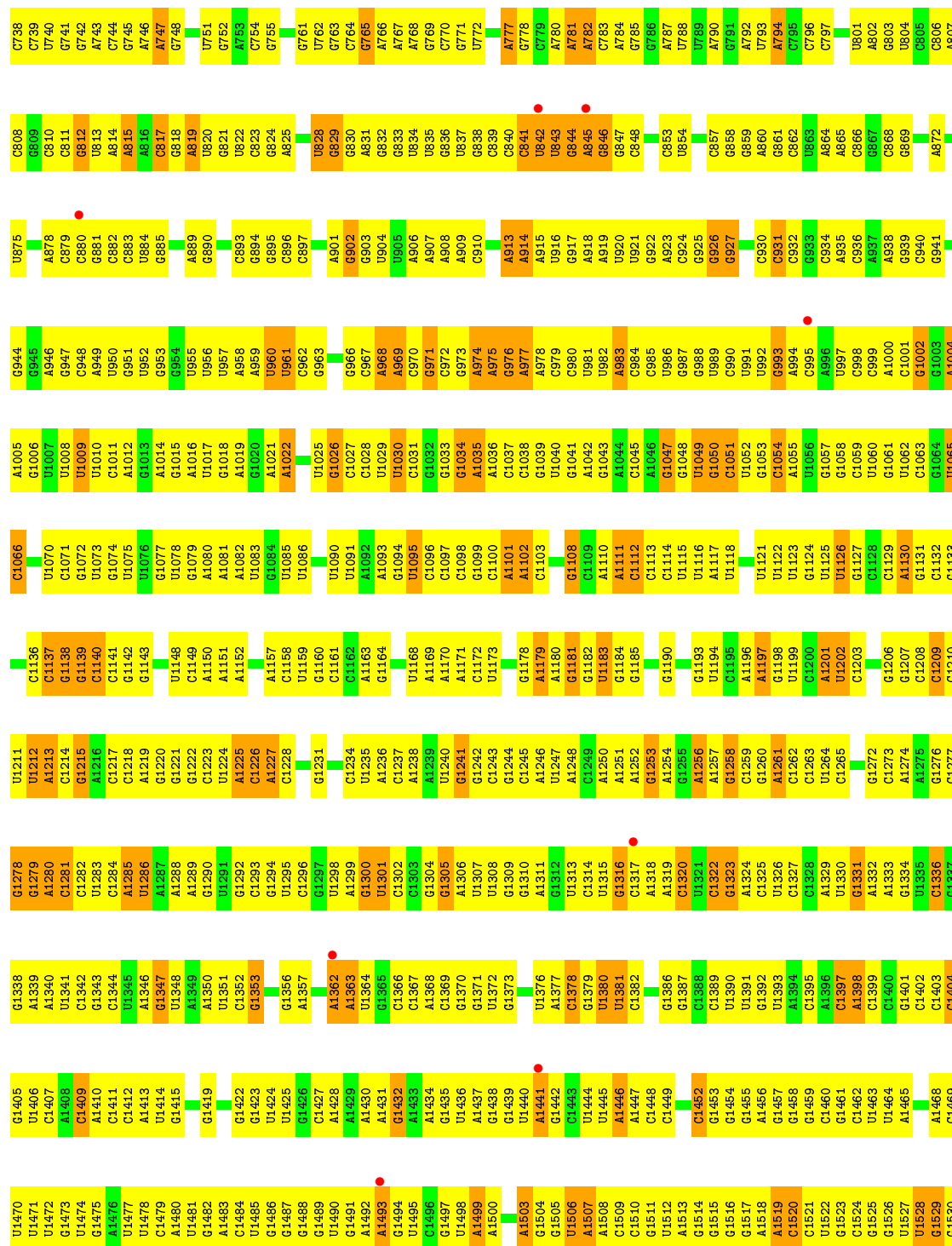
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	DE	3	Total 3	O 3	0	0
55	DL	1	Total 1	O 1	0	0
55	DN	2	Total 2	O 2	0	0
55	DT	1	Total 1	O 1	0	0
55	D2	2	Total 2	O 2	0	0

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

#### • Molecule 1: 16S RIBOSOMAL RNA

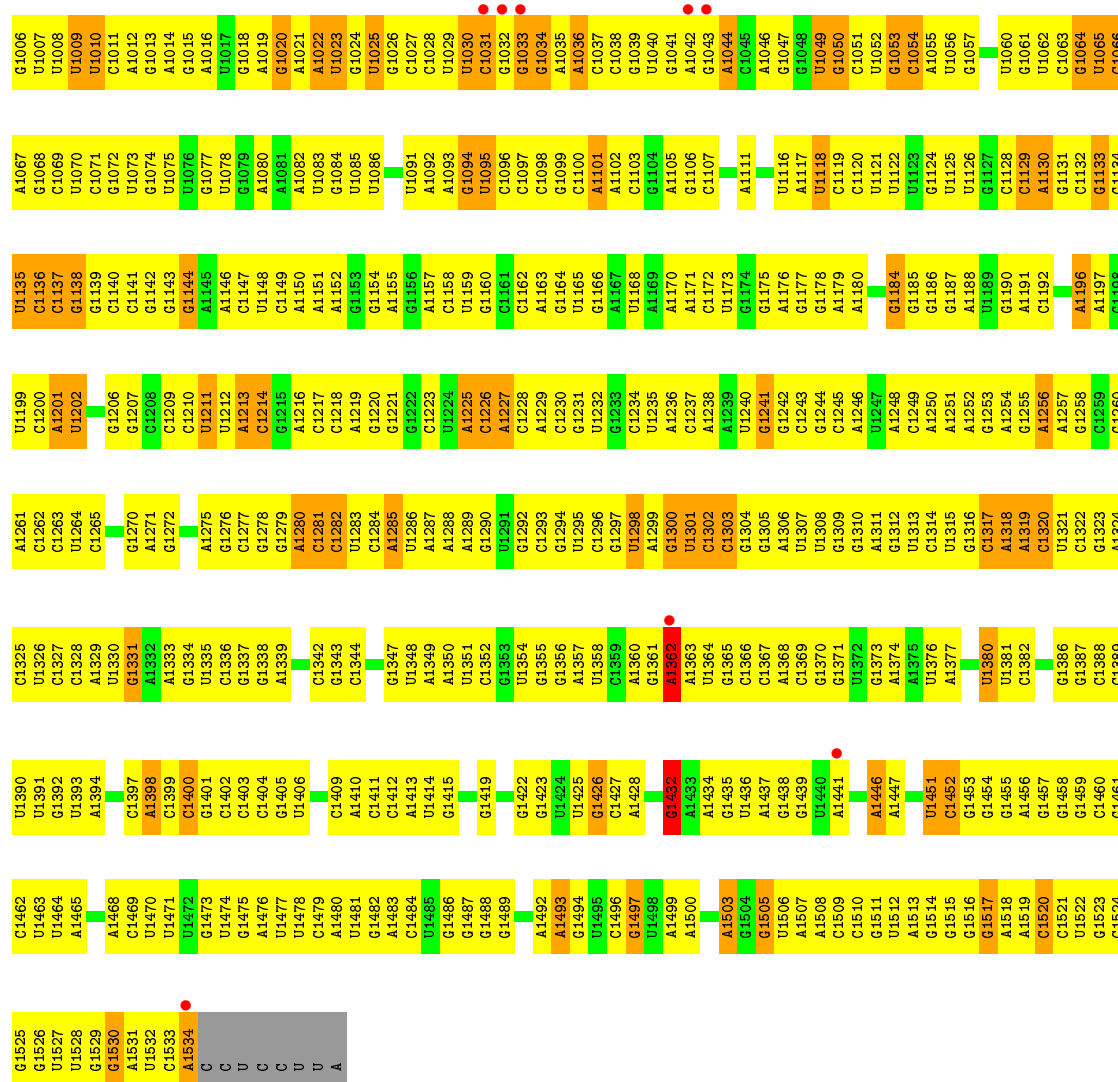




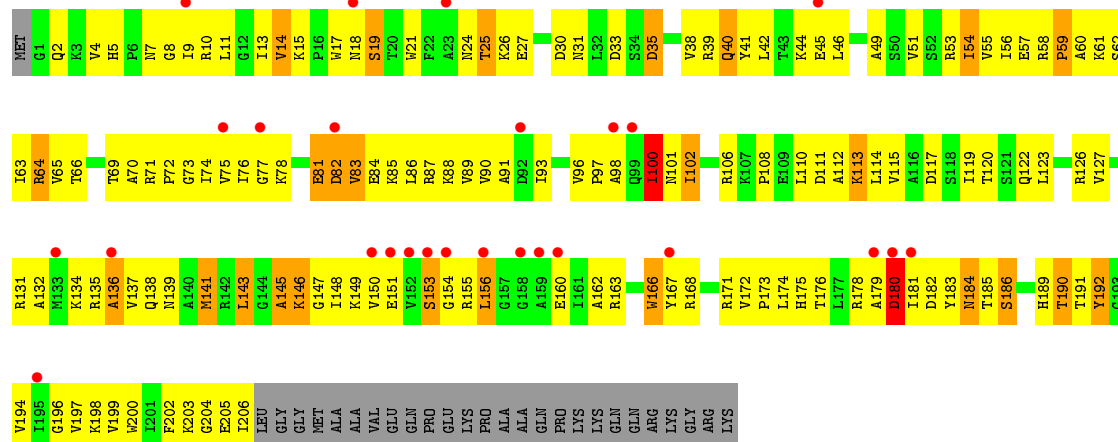
# Molecule 1: 16S RIBOSOMAL RNA





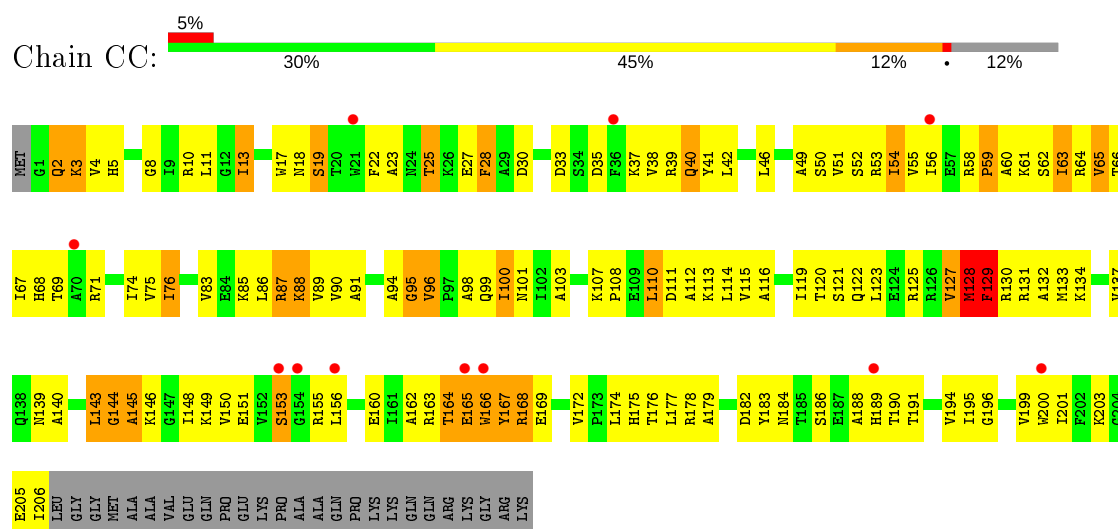


## • Molecule 2: 30S RIBOSOMAL PROTEIN S3

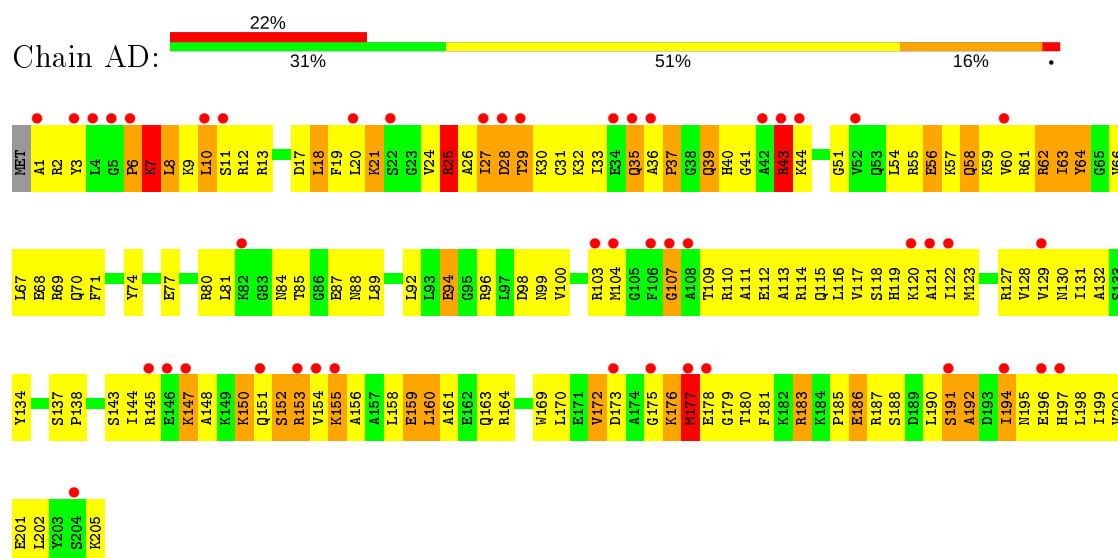


## • Molecule 2: 30S RIBOSOMAL PROTEIN S3

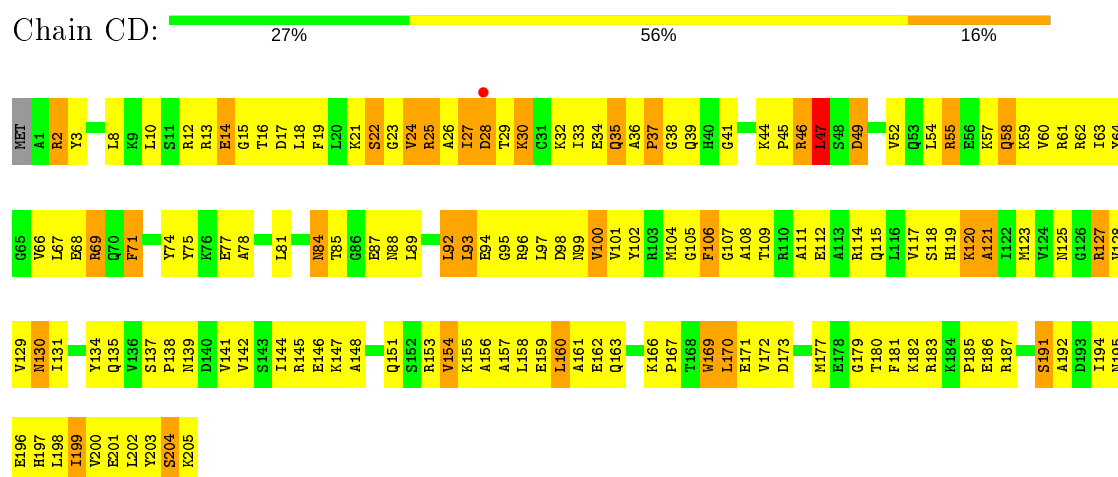




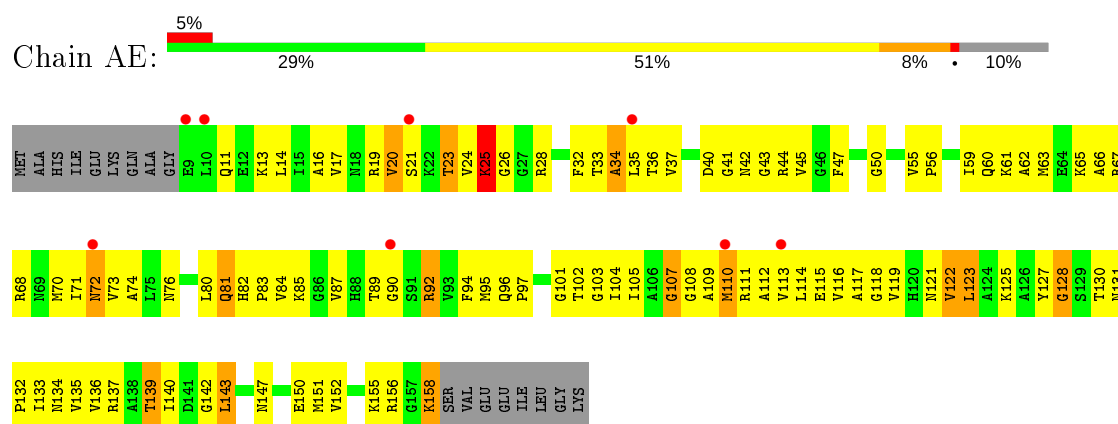
• Molecule 3: 30S RIBOSOMAL PROTEIN S4



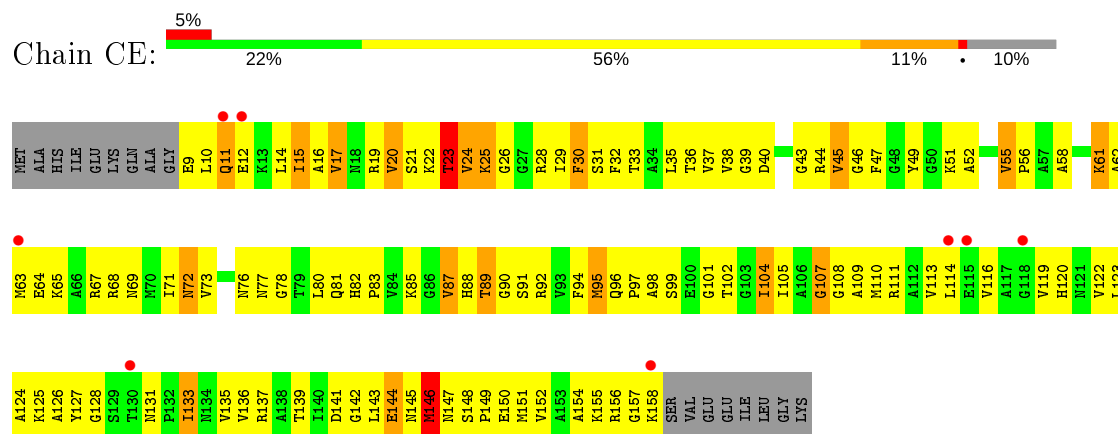
• Molecule 3: 30S RIBOSOMAL PROTEIN S4



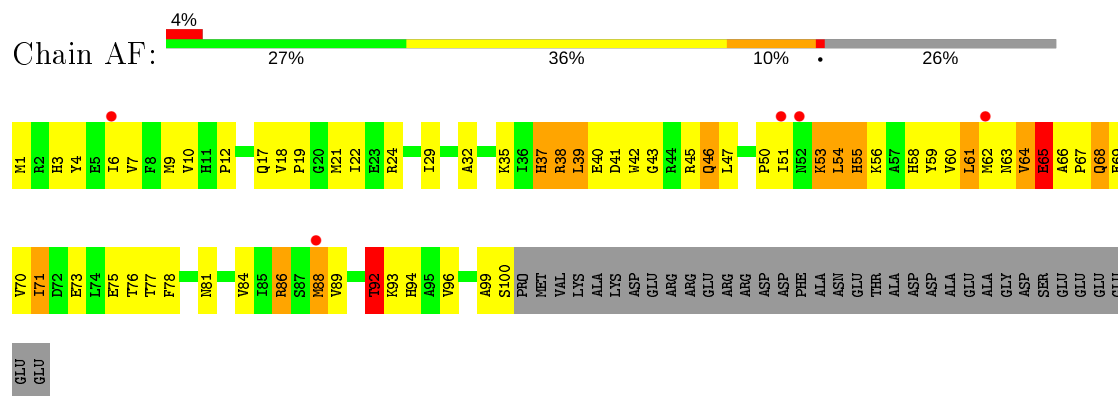
• Molecule 4: 30S RIBOSOMAL PROTEIN S5



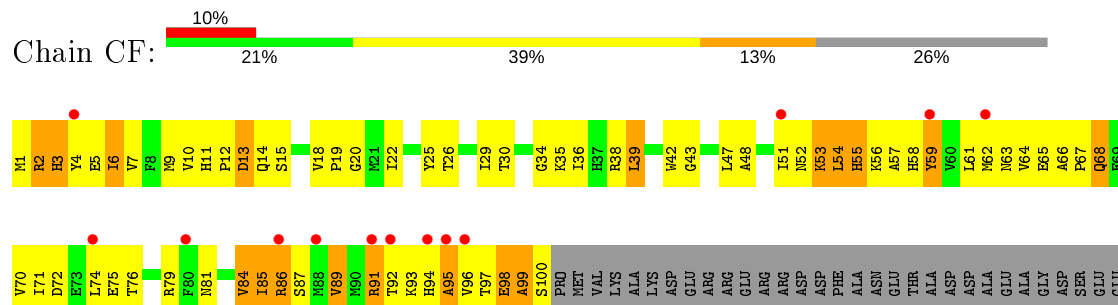
• Molecule 4: 30S RIBOSOMAL PROTEIN S5



• Molecule 5: 30S RIBOSOMAL PROTEIN S6

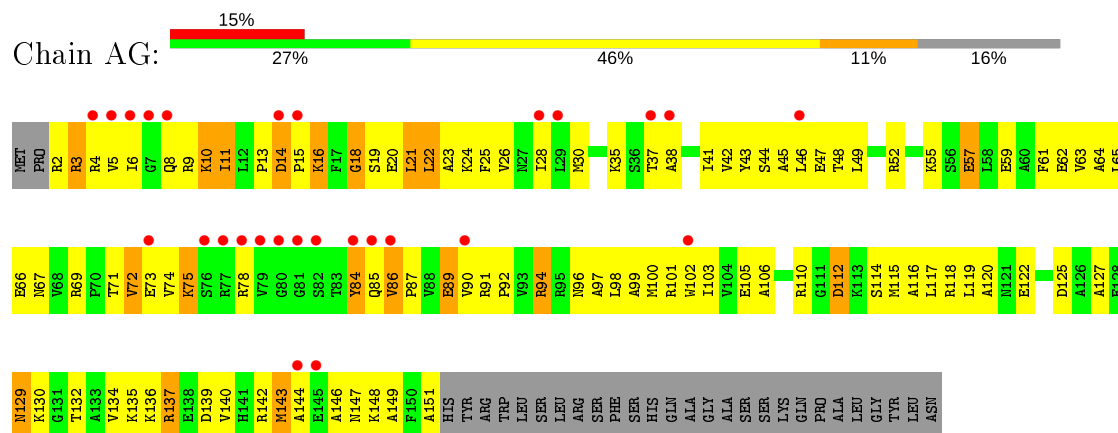


• Molecule 5: 30S RIBOSOMAL PROTEIN S6



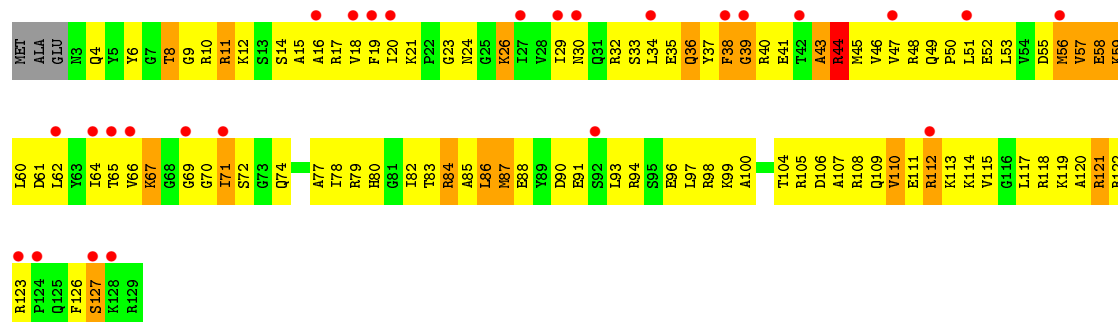
GLU  
GLU  
GLU  
GLU

• Molecule 6: 30S RIBOSOMAL PROTEIN S7

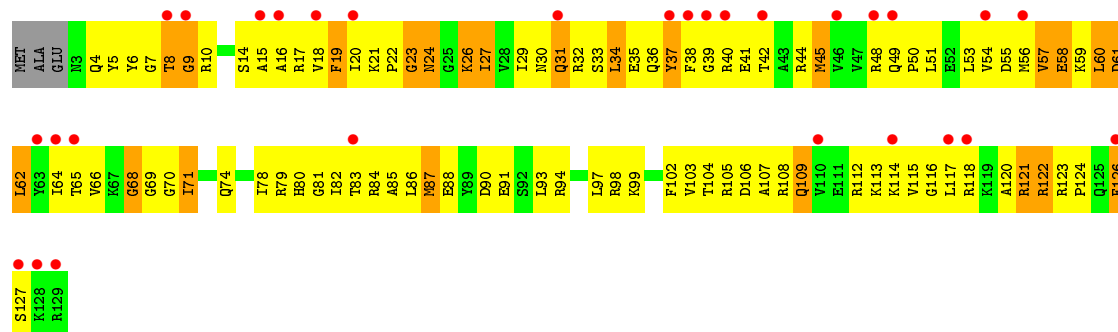




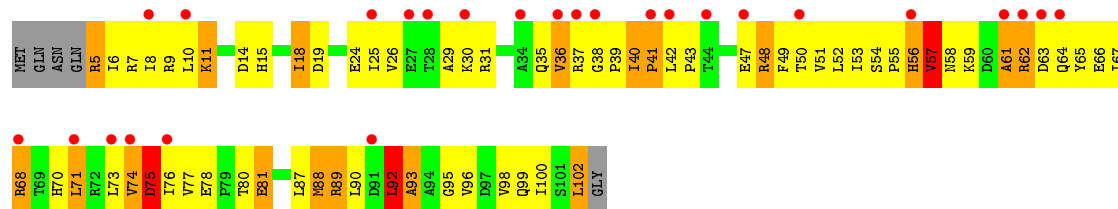
• Molecule 8: 30S RIBOSOMAL PROTEIN S9



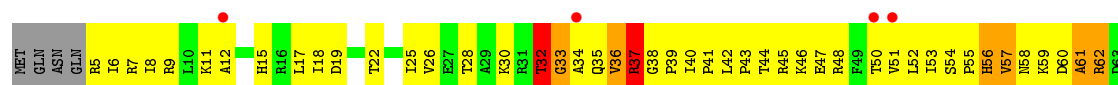
• Molecule 8: 30S RIBOSOMAL PROTEIN S9



• Molecule 9: 30S RIBOSOMAL PROTEIN S10



• Molecule 9: 30S RIBOSOMAL PROTEIN S10

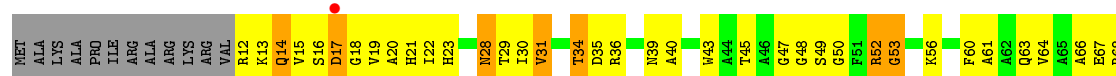




• Molecule 10: 30S RIBOSOMAL PROTEIN S11



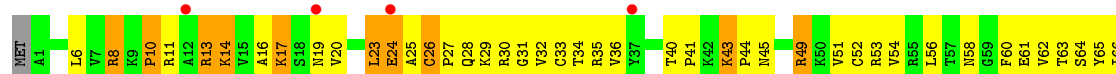
• Molecule 10: 30S RIBOSOMAL PROTEIN S11



• Molecule 11: 30S RIBOSOMAL PROTEIN S12



• Molecule 11: 30S RIBOSOMAL PROTEIN S12

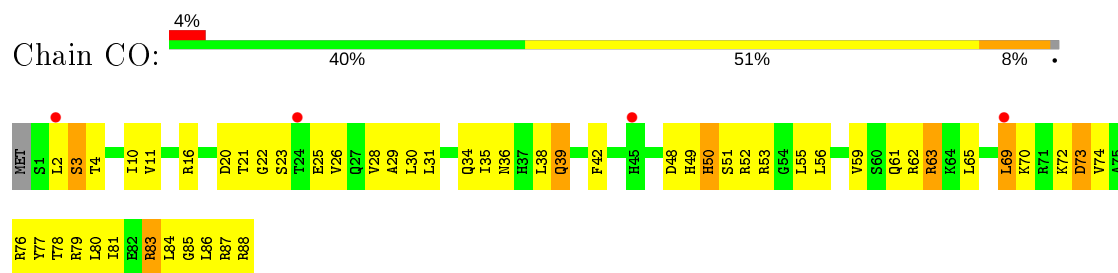


• Molecule 12: 30S RIBOSOMAL PROTEIN S13

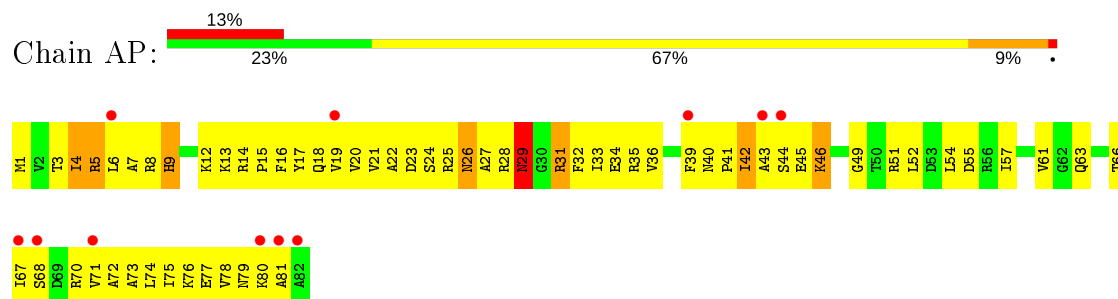




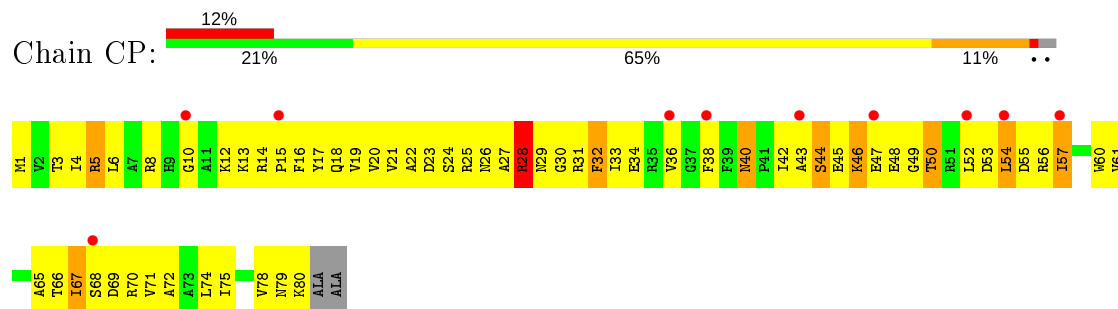
## • Molecule 14: 30S RIBOSOMAL PROTEIN S15



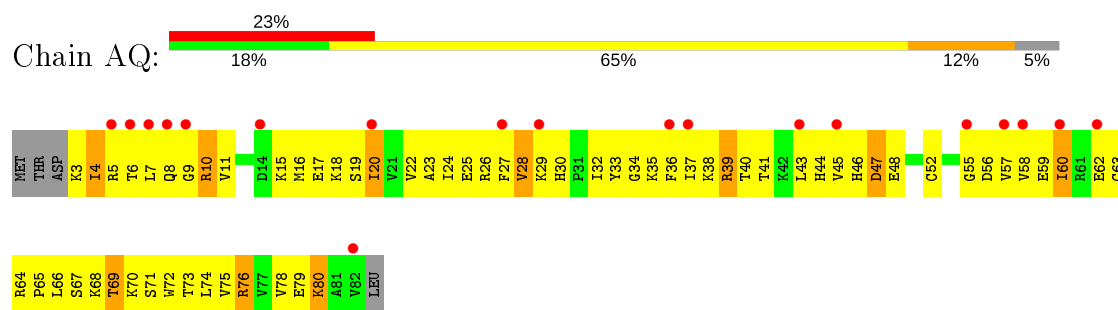
## • Molecule 15: 30S RIBOSOMAL PROTEIN S16



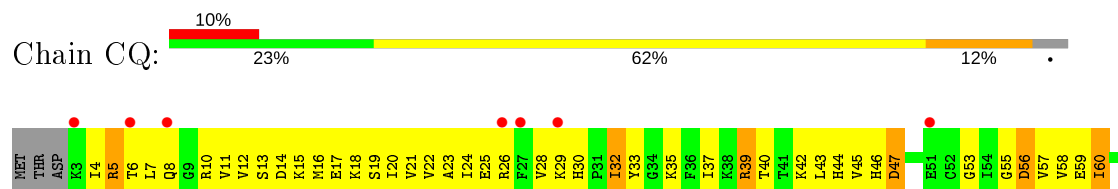
## • Molecule 15: 30S RIBOSOMAL PROTEIN S16



## • Molecule 16: 30S RIBOSOMAL PROTEIN S17

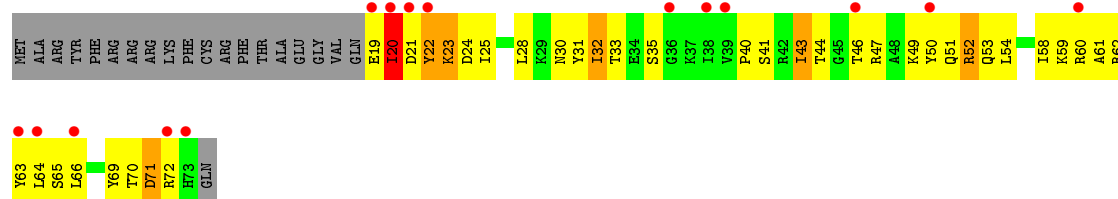
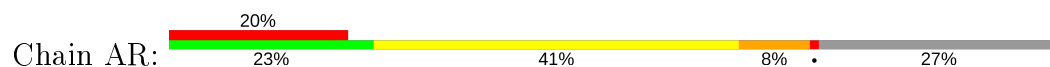


## • Molecule 16: 30S RIBOSOMAL PROTEIN S17

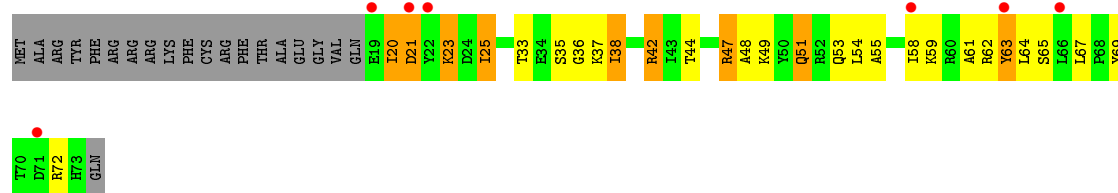




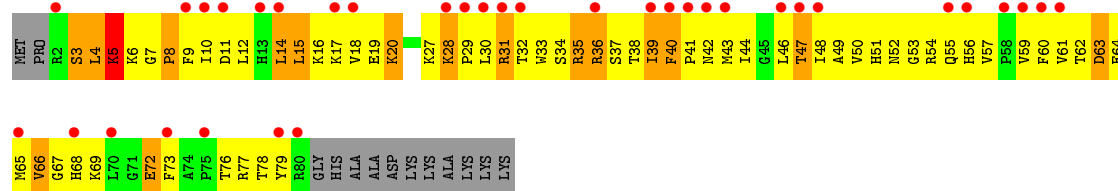
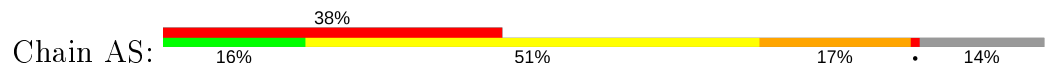
• Molecule 17: 30S RIBOSOMAL PROTEIN S18



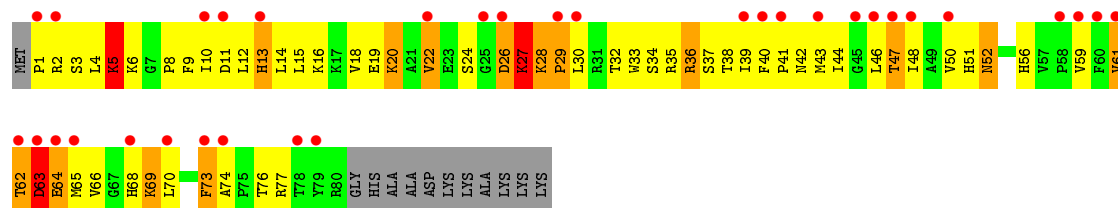
• Molecule 17: 30S RIBOSOMAL PROTEIN S18



• Molecule 18: 30S RIBOSOMAL PROTEIN S19



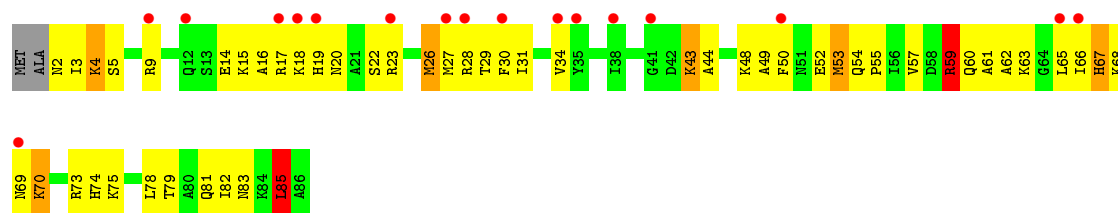
• Molecule 18: 30S RIBOSOMAL PROTEIN S19



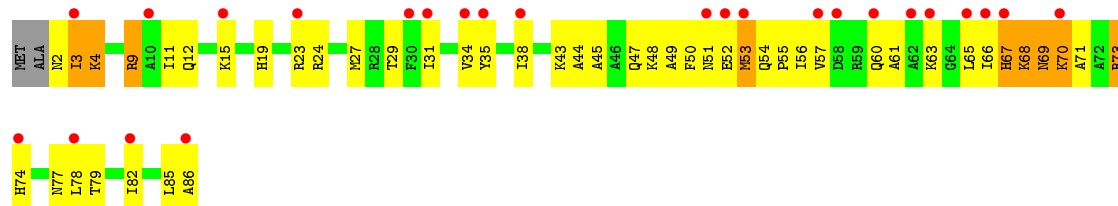
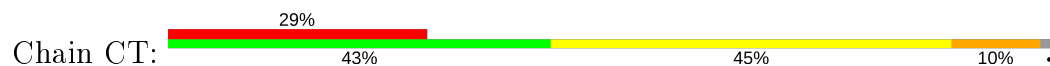
• Molecule 19: 30S RIBOSOMAL PROTEIN S20



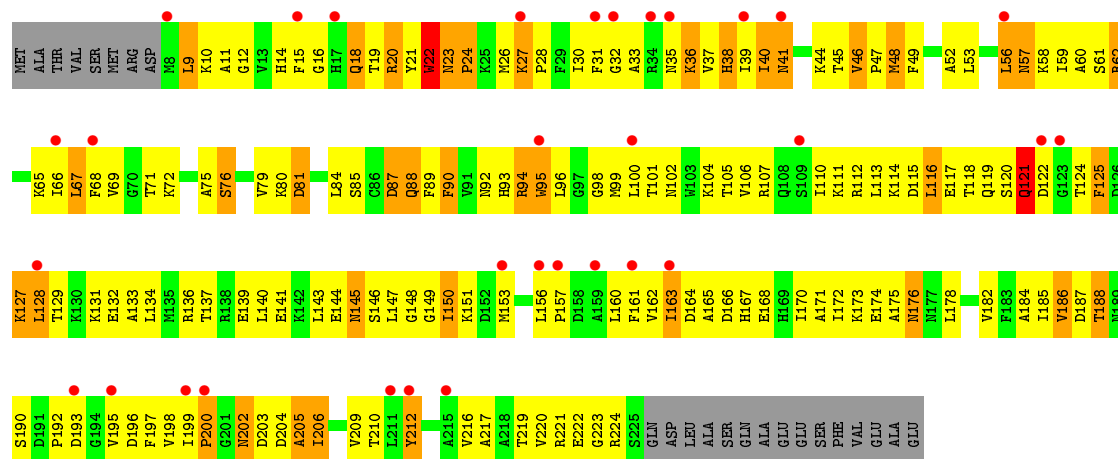




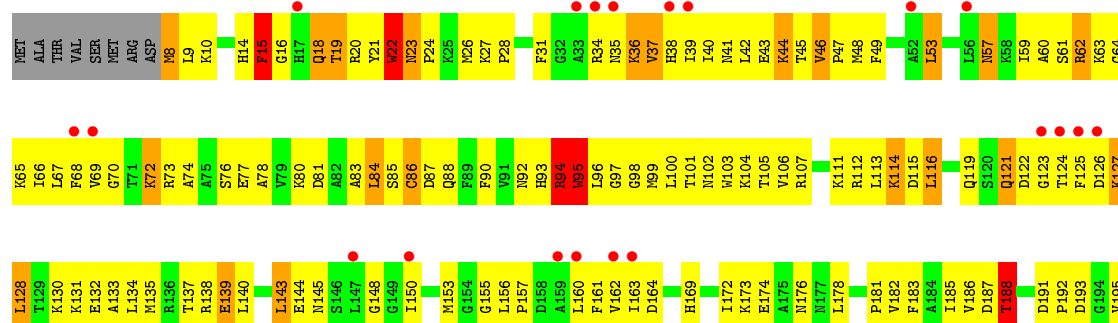
• Molecule 19: 30S RIBOSOMAL PROTEIN S20



• Molecule 20: 30S RIBOSOMAL PROTEIN S2



• Molecule 20: 30S RIBOSOMAL PROTEIN S2

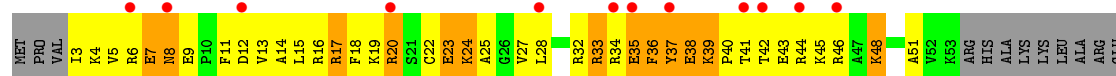
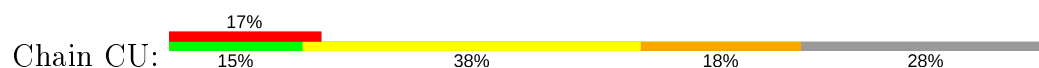




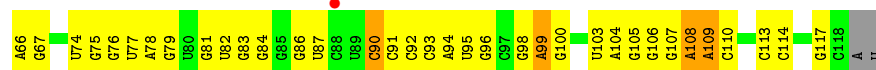
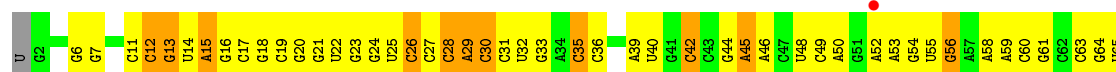
• Molecule 21: 30S RIBOSOMAL PROTEIN S21



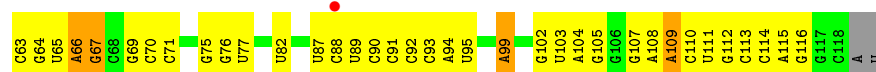
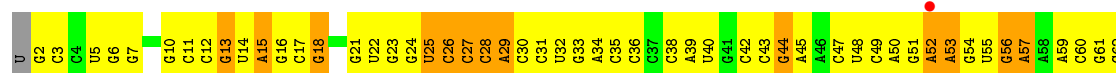
• Molecule 21: 30S RIBOSOMAL PROTEIN S21



• Molecule 22: 5S RIBOSOMAL RNA



• Molecule 22: 5S RIBOSOMAL RNA



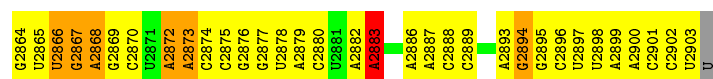
• Molecule 23: 23S RIBOSOMAL RNA



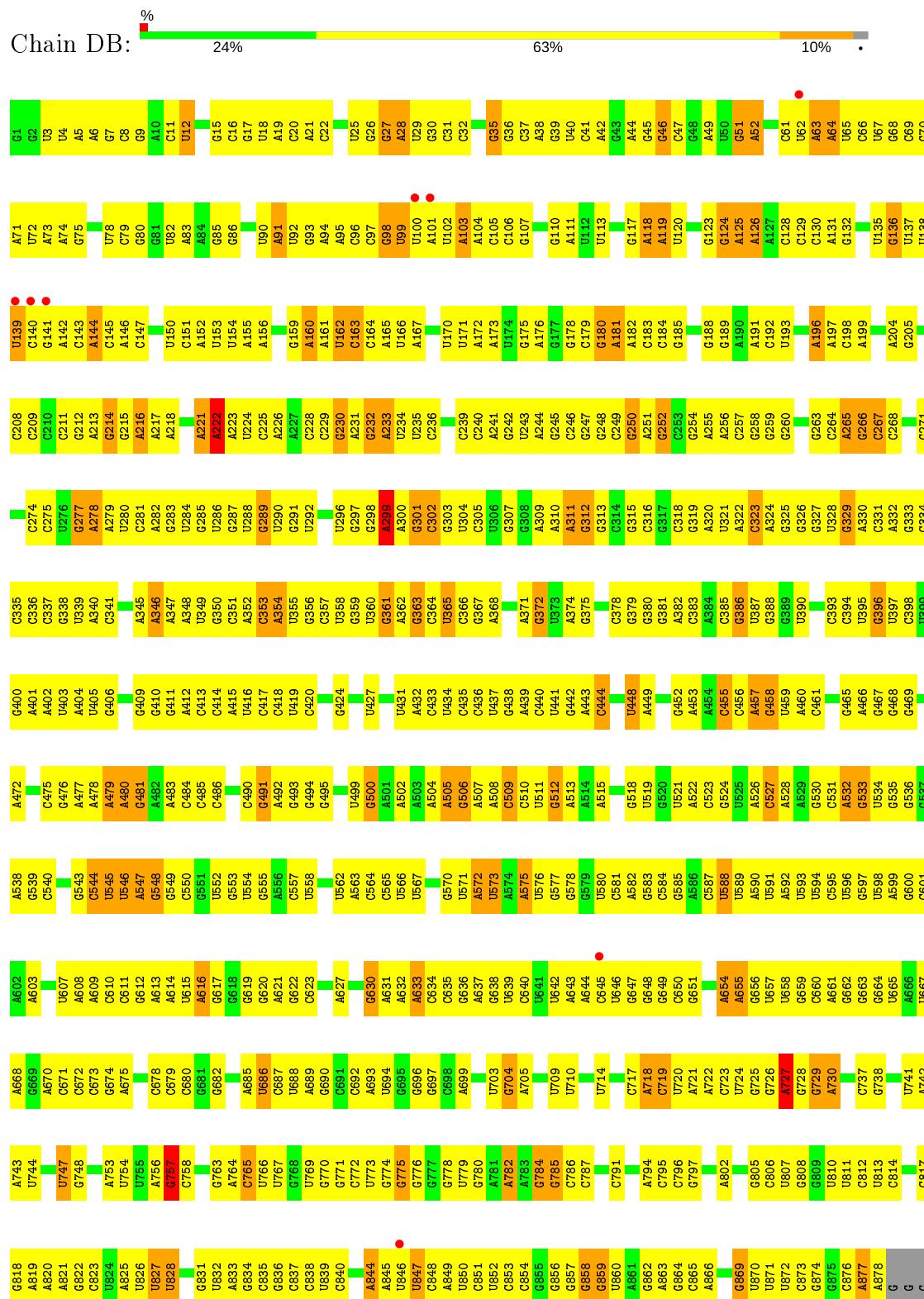
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C935	U872	G808	C731	U667	A602	A538	G474	G409	U339	A271	A197	U133	U65	G2
A936				A668	A603	G539		G410	C341	A272	C198	G134	C66	U3
C937		U811	C737	G669		C540	A477	G411		G273	C197	U135	U67	U4
A941	C876	U812	A738	C670	U607	C541	A478	A412	A346	C274	A199	G136	G68	A5
G942	A877	U813	G759	A671	A608	G542	A479	C413	A347	C275	U200	U137	C69	A6
A943	A878	C814	C740	C672	A609	G543	A480	C414		G276		U138	C70	G7
	G		U741	C544	C610	C544	G481	A415		U277		U139	A71	C8
	G	C817	A742	U545	C611	U545	A482	U416	G350	A278	U206	C140		G9
C946	G	G818	G743	U546	G612	U546	A483	C417	A352	A279	U207	G141	A74	A10
A947	G	A819	U744	A547	G613	A547	C484	C418	G351	U280	C208	A142	G75	C11
C948	U	G820		G548	A614	G548	C485	U419	C353	C281	C209	C143	U12	U12
G949	U	A821	U747	C550	U615	C550		C420	U355	A282	C210	A144	A13	A13
C950	C	G822	G748		A616					G283	C211	C145	A14	A14
C951	A	C823		G553	G617		C490	A423	U356	G284	G212	A146	G15	G15
G952	U	U824	A751	U554	G618		G491	G424	C357	U285	G213	C147	C16	C16
C953	C	A825	A752	U554	G619	G554	A492	A425	U358	G286	G214	U148	G17	G17
G954	C	U826	A753	G555	G620	G555	G494	G426	G359	U287	G215	A149	U82	U18
U955	C	U827	U754	A556	A621	A556	G495	U427	U360	U288	A216	U150	A83	U18
G956	G	U828	U755	C557	G622	C557	G496	A428	G361	U289		C151	A84	A19
C957	A	A829	A756	U558	C623	U558	G497	A429	A362	U290	A221	A152	C85	C20
U958	C	G830	C757	G559	C624	G559	G498		G363		A222	U153	C86	A21
A959	U	G831	G758	C560		C560	U499	C433	C364	G295	A223	U154	A89	U25
A960	U	U832	G759	U561	A627	U561	G500	U434	U365	U296	U224	A155	U90	G26
C961	A	A833	G760	A562		A562	A501	C435	C366	G297		A156	A91	G27
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C971	C908	G843	C772	U574	U639	U574	U511	C445	C378	A309	C240	U166	A103	G36
A972	A909	A844	U773	A574	C640	A574	G512	G446	G379	A310	A241	A167	A104	C37
U973	A910	U845	G774	U575	U641	U575	A513	A447	G380	A311	G242	G168	G105	A38
G974	A911	U846	G775	U576	U642	U576	A514	U448	G381	G312	U243	G169	C106	G39
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G997	U932	G805	G664	A599	U665	A599	G535		G406	C336		C130	U62	U62
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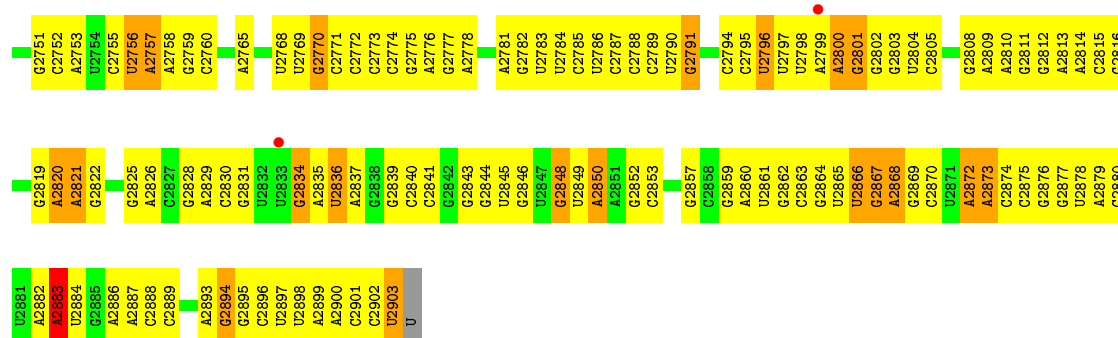
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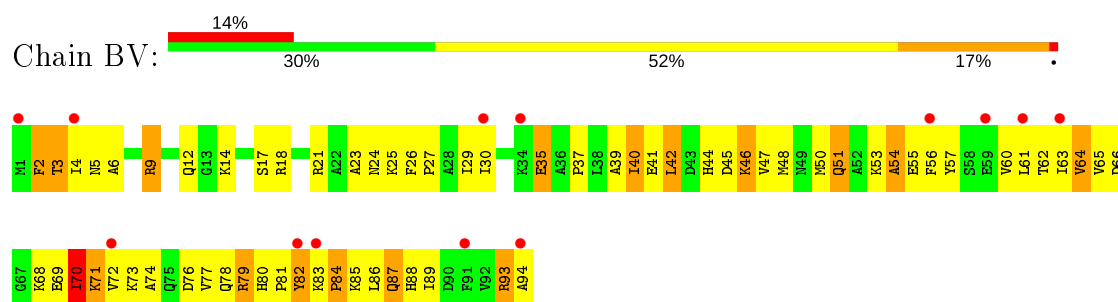
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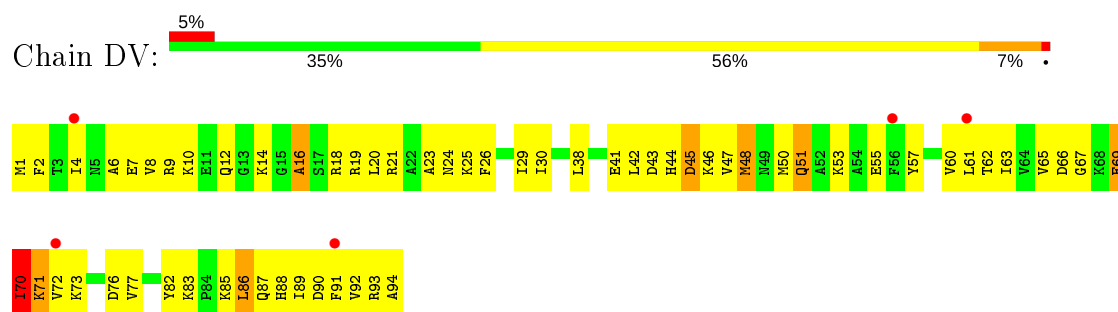




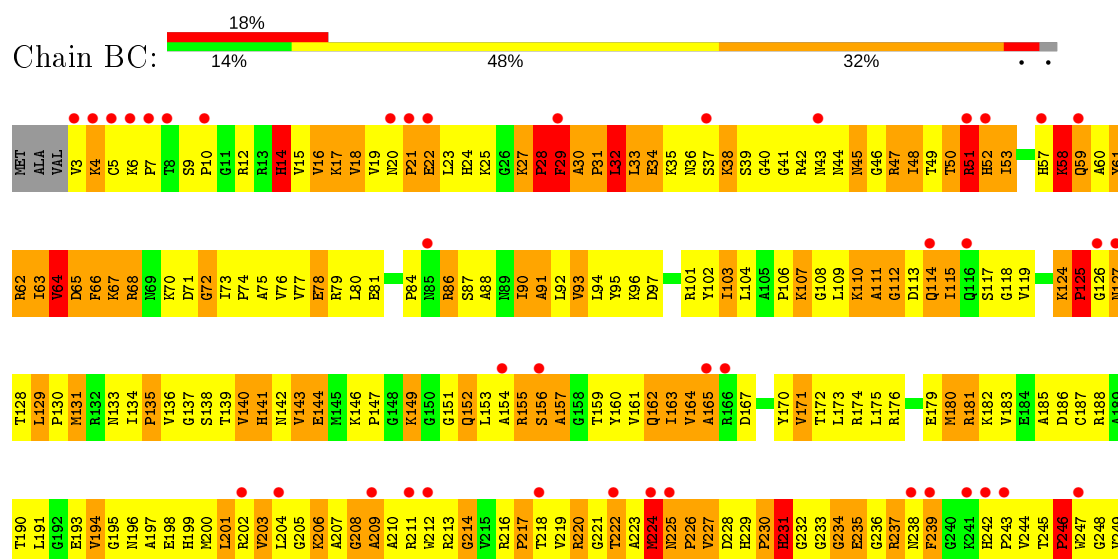
• Molecule 24: 50S RIBOSOMAL PROTEIN L25



• Molecule 24: 50S RIBOSOMAL PROTEIN L25

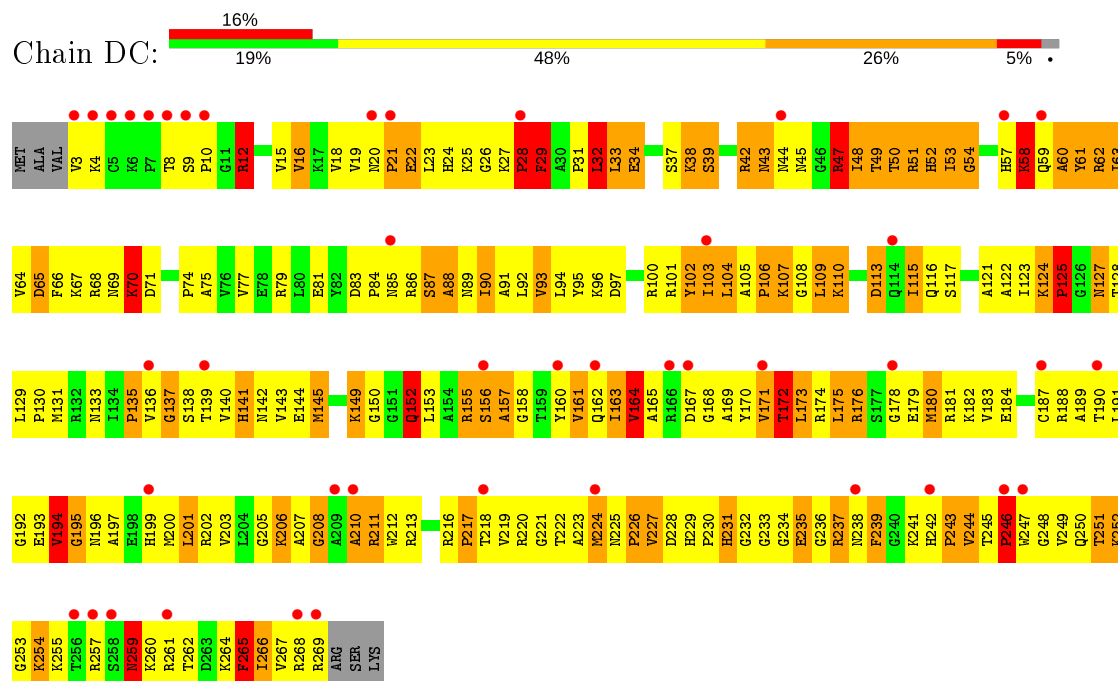


• Molecule 25: 50S RIBOSOMAL PROTEIN L2

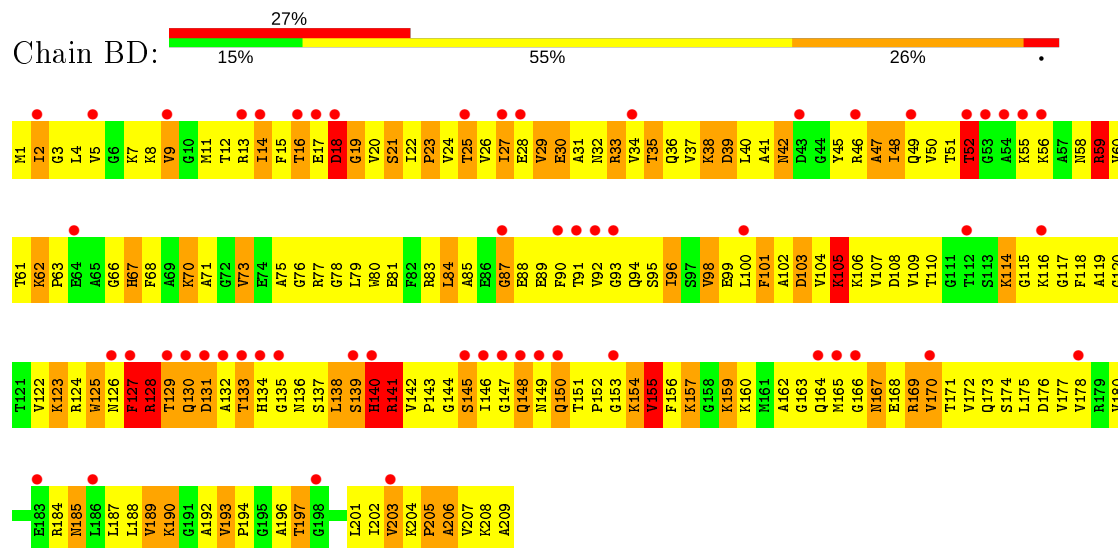




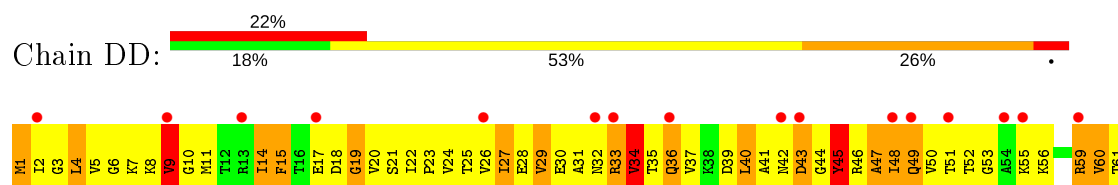
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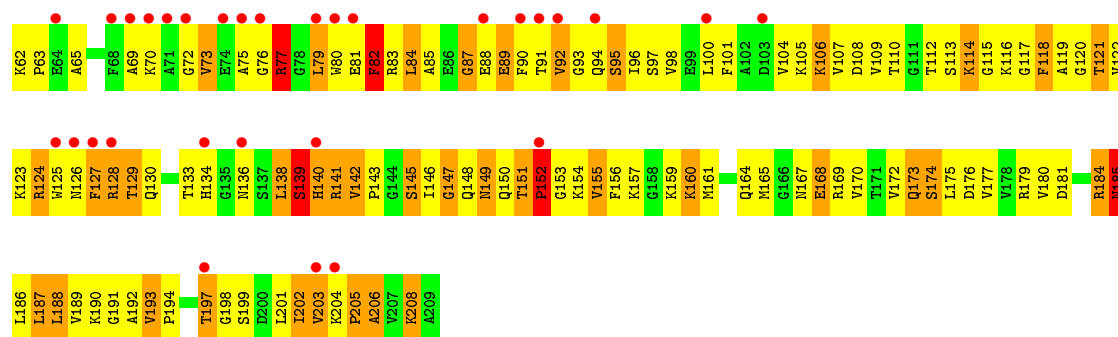


• Molecule 26: 50S RIBOSOMAL PROTEIN L3

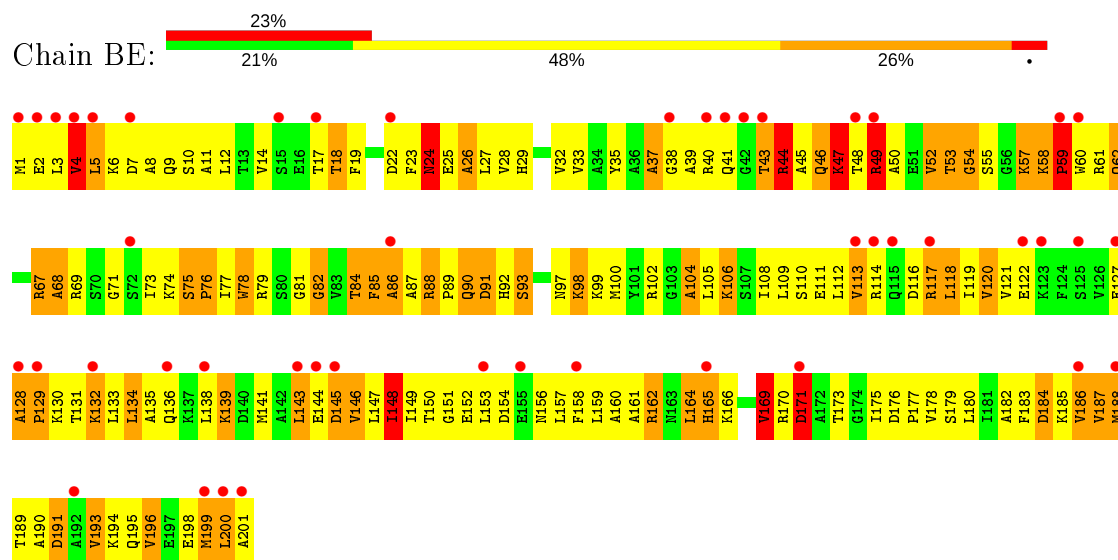


• Molecule 26: 50S RIBOSOMAL PROTEIN L3

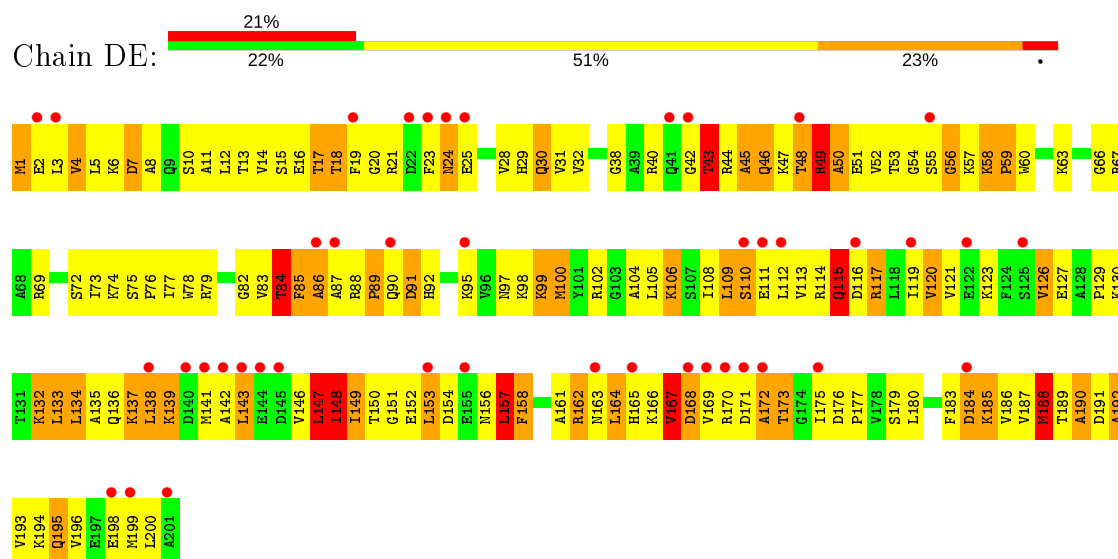




• Molecule 27: 50S RIBOSOMAL PROTEIN L4

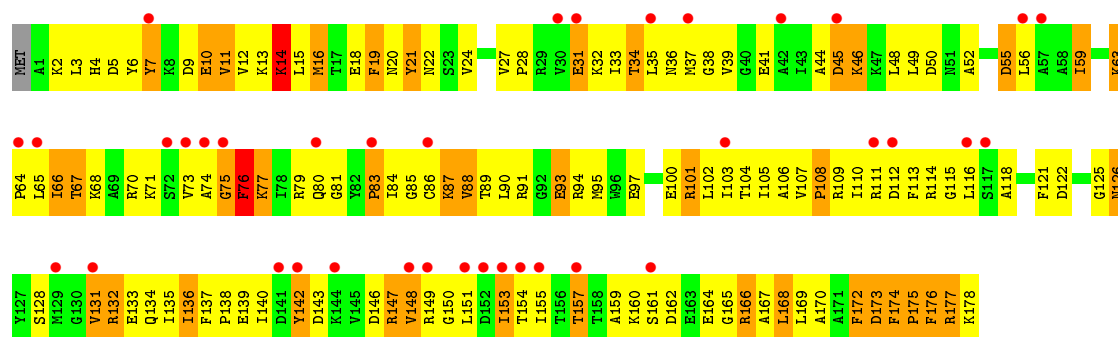


• Molecule 27: 50S RIBOSOMAL PROTEIN L4

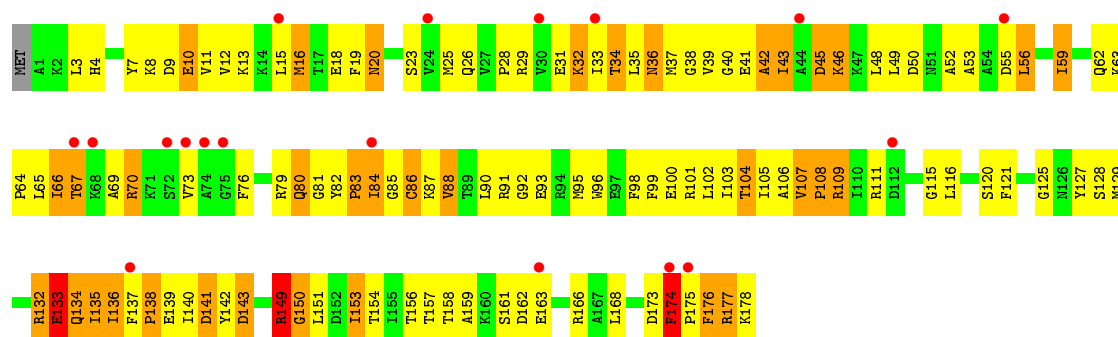


• Molecule 28: 50S RIBOSOMAL PROTEIN L5

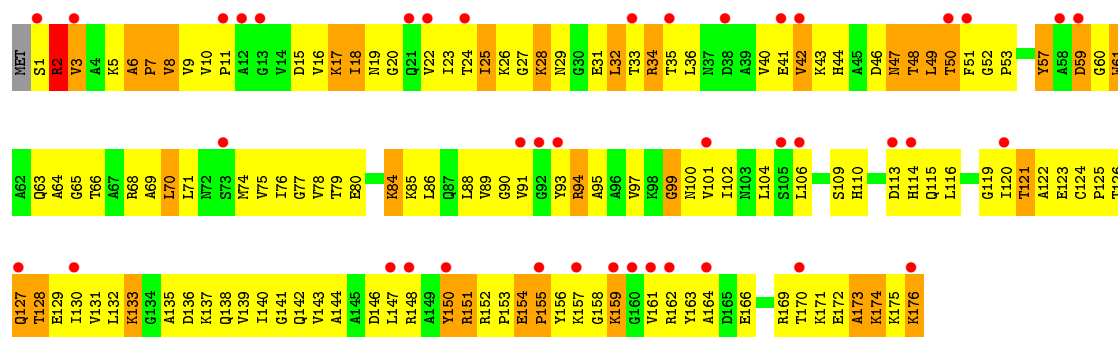




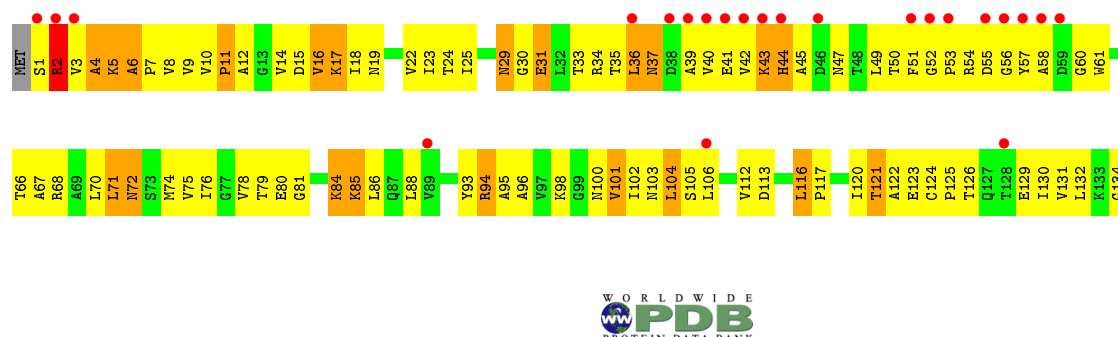
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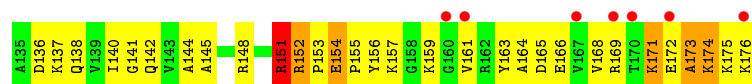


• Molecule 29: 50S RIBOSOMAL PROTEIN L6

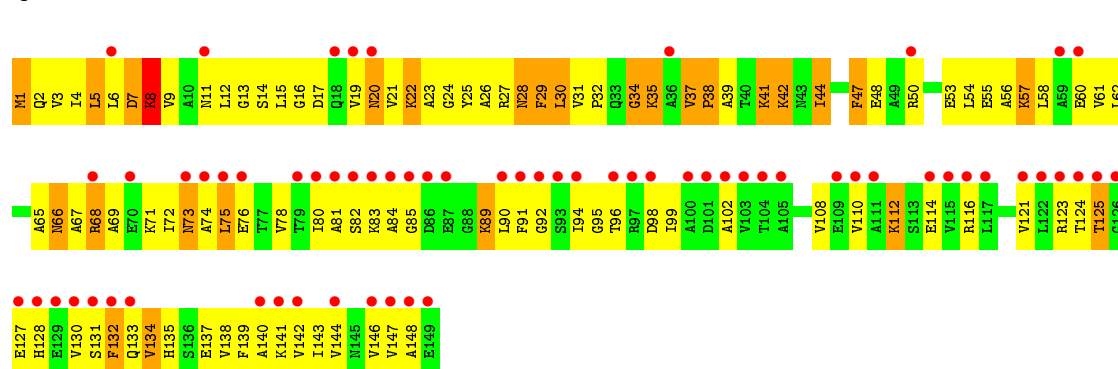


• Molecule 29: 50S RIBOSOMAL PROTEIN L6

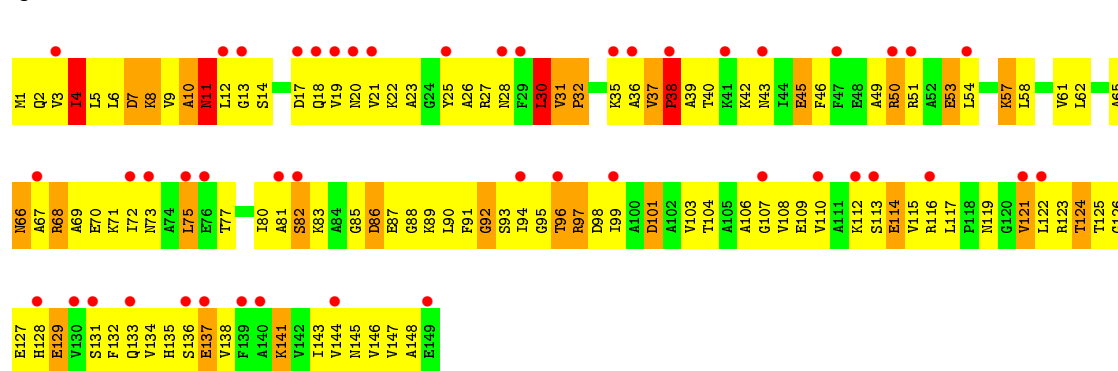




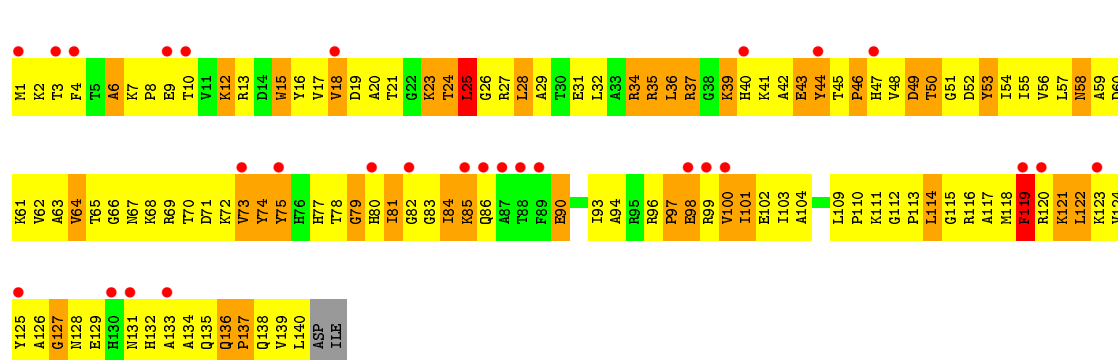
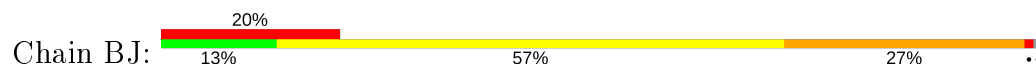
• Molecule 30: 50S RIBOSOMAL PROTEIN L9



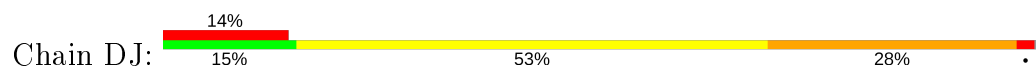
• Molecule 30: 50S RIBOSOMAL PROTEIN L9

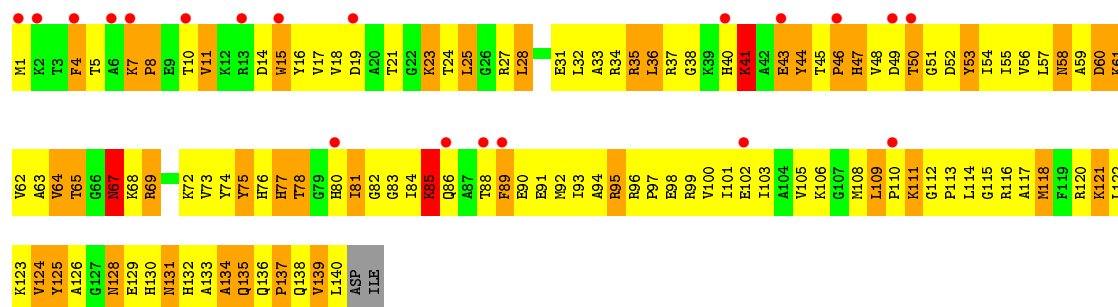


• Molecule 31: 50S RIBOSOMAL PROTEIN L13

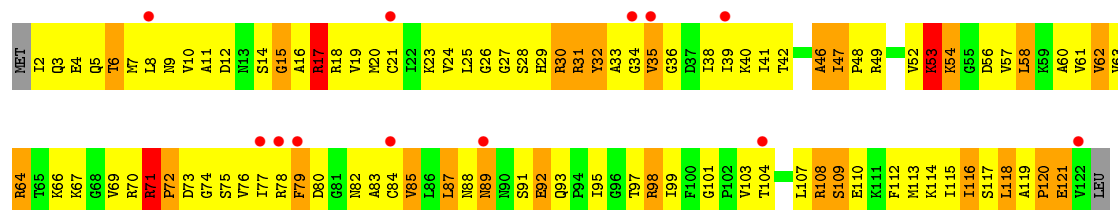


• Molecule 31: 50S RIBOSOMAL PROTEIN L13

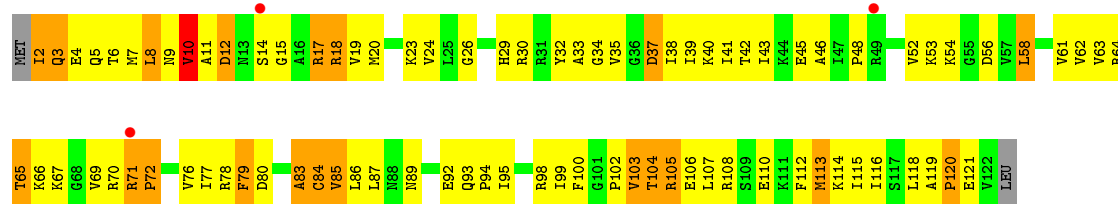




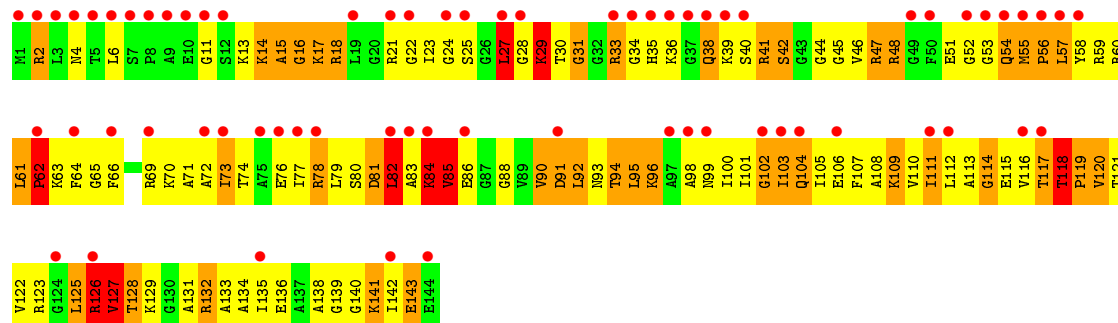
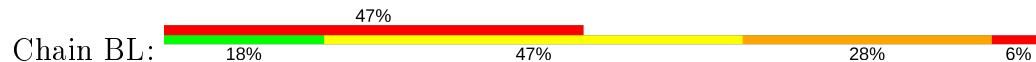
• Molecule 32: 50S RIBOSOMAL PROTEIN L14



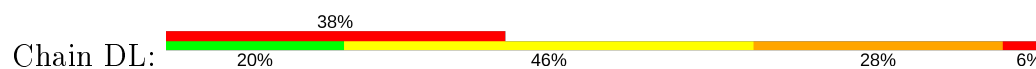
• Molecule 32: 50S RIBOSOMAL PROTEIN L14

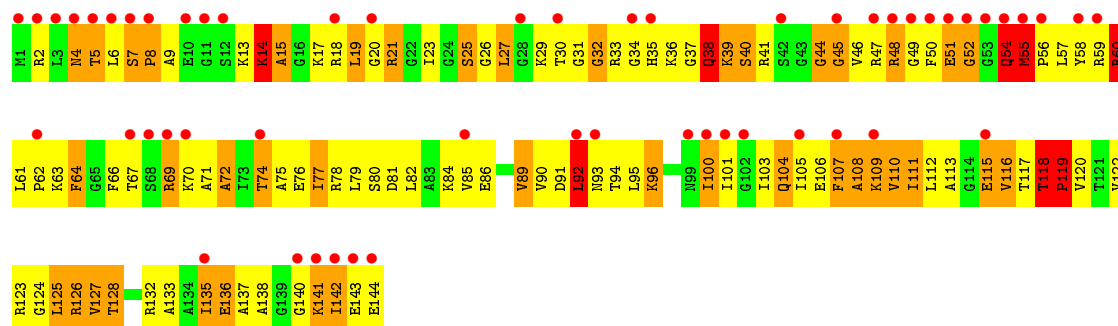


• Molecule 33: 50S RIBOSOMAL PROTEIN L15

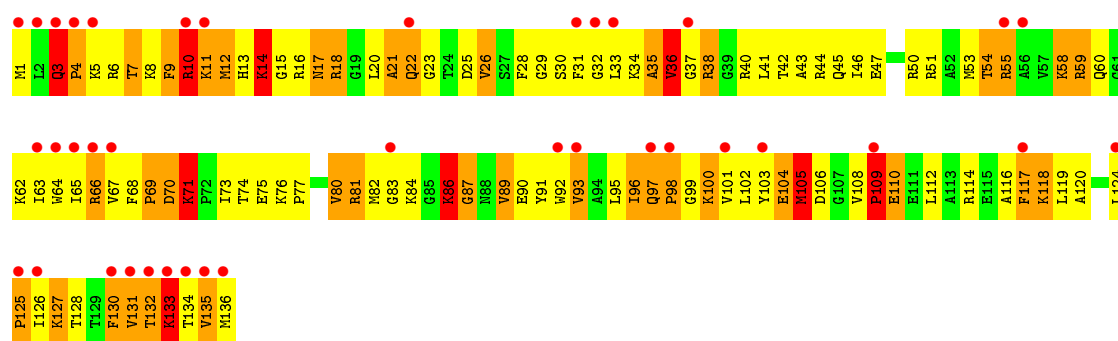
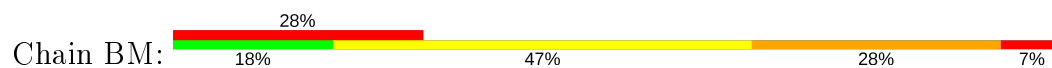


• Molecule 33: 50S RIBOSOMAL PROTEIN L15

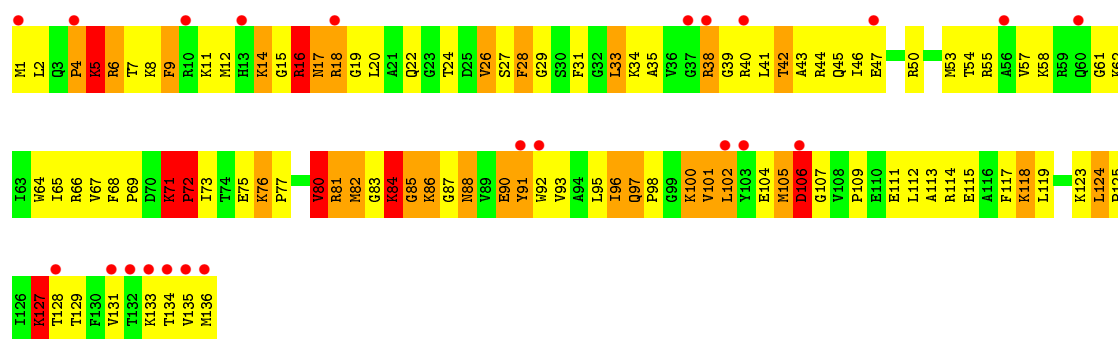
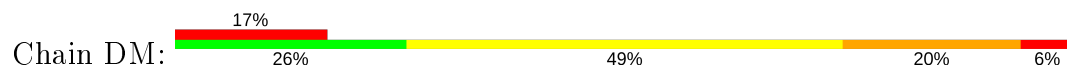




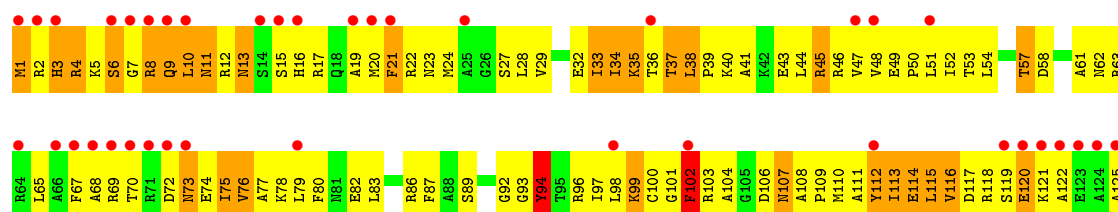
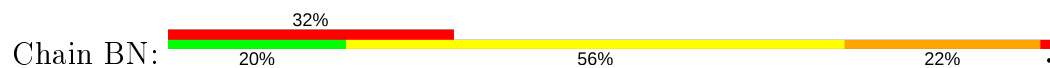
• Molecule 34: 50S RIBOSOMAL PROTEIN L16



• Molecule 34: 50S RIBOSOMAL PROTEIN L16

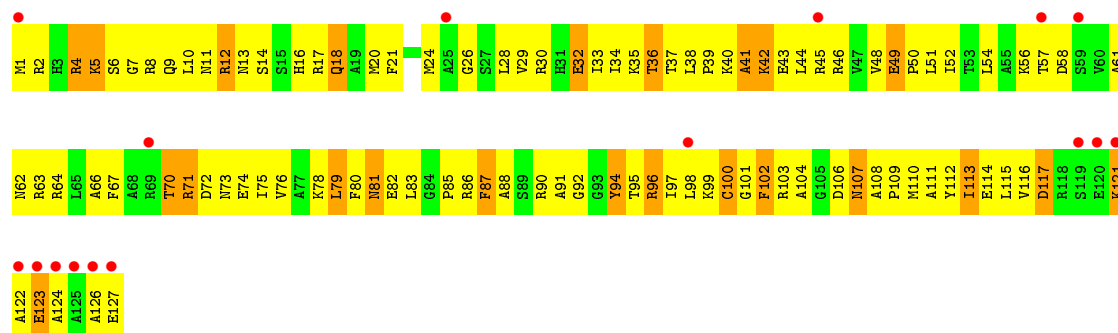


• Molecule 35: 50S RIBOSOMAL PROTEIN L17

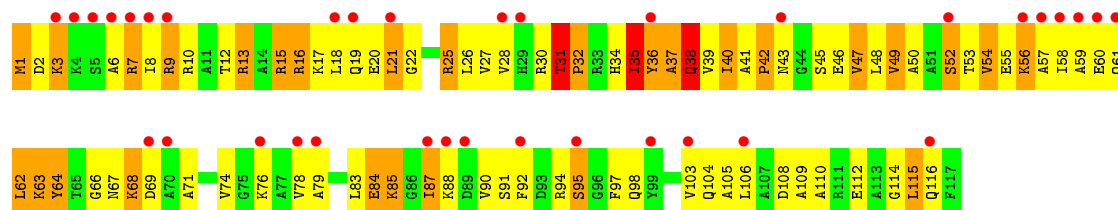




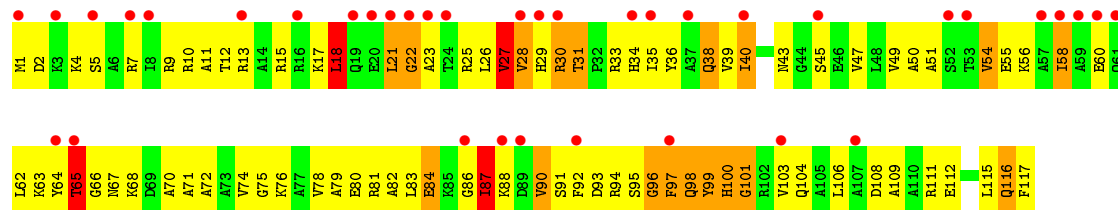
• Molecule 35: 50S RIBOSOMAL PROTEIN L17



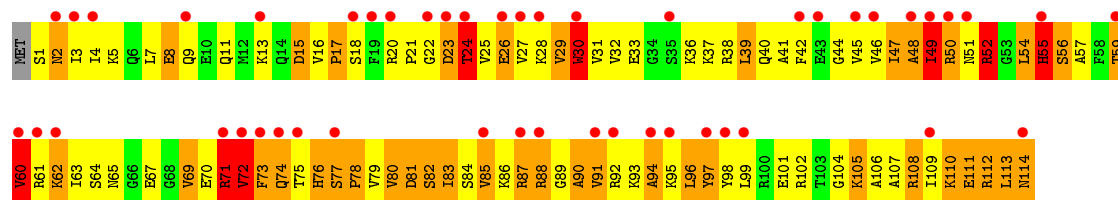
• Molecule 36: 50S RIBOSOMAL PROTEIN L18



• Molecule 36: 50S RIBOSOMAL PROTEIN L18

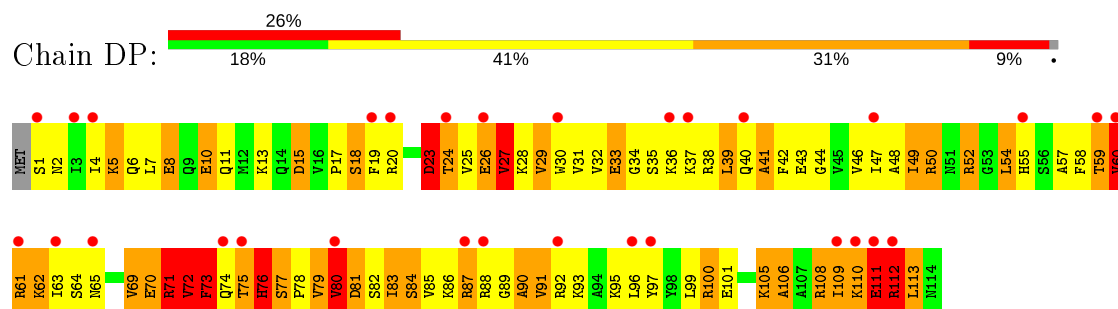


• Molecule 37: 50S RIBOSOMAL PROTEIN L19

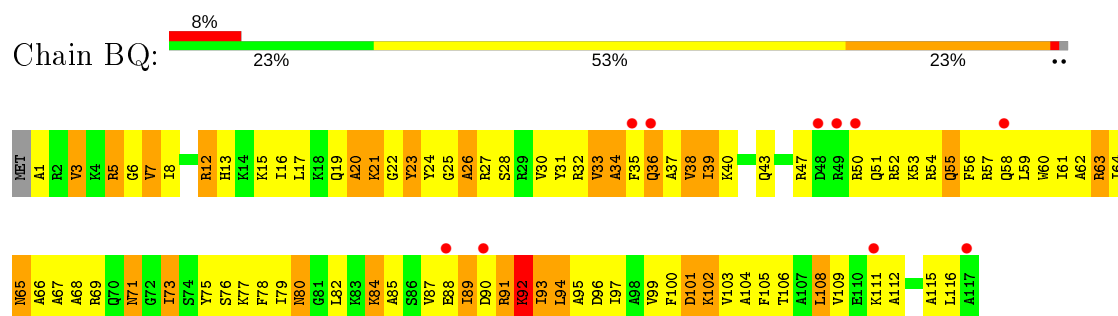




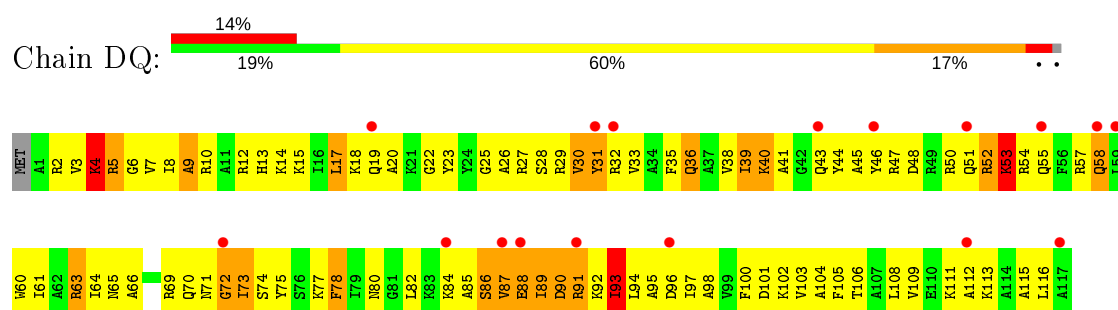
• Molecule 37: 50S RIBOSOMAL PROTEIN L19



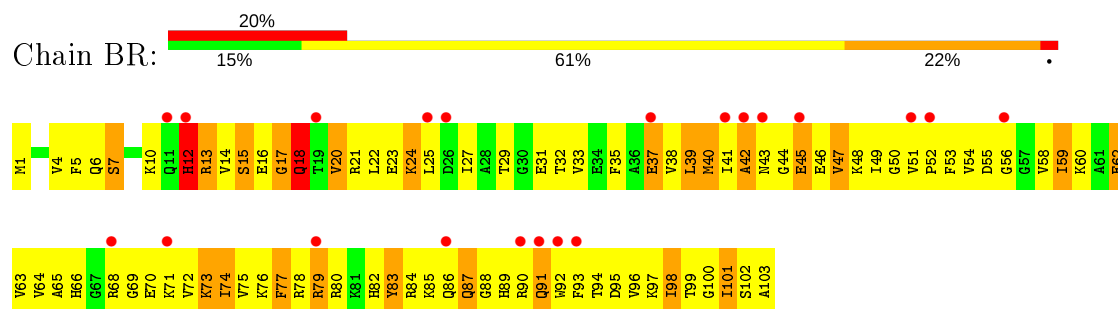
• Molecule 38: 50S RIBOSOMAL PROTEIN L20



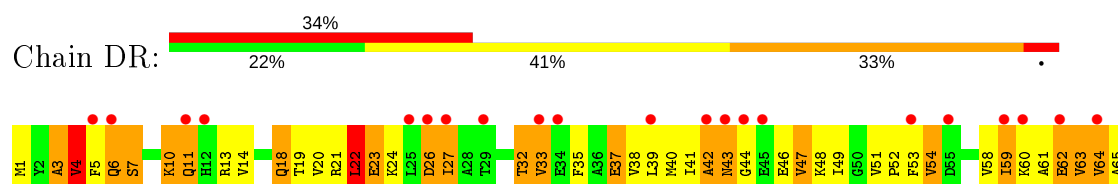
• Molecule 38: 50S RIBOSOMAL PROTEIN L20

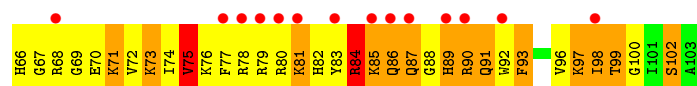


• Molecule 39: 50S RIBOSOMAL PROTEIN L21

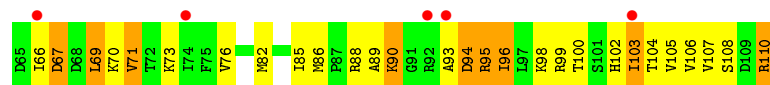
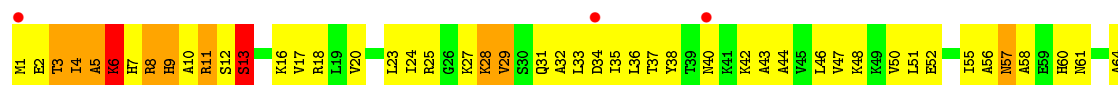


• Molecule 39: 50S RIBOSOMAL PROTEIN L21

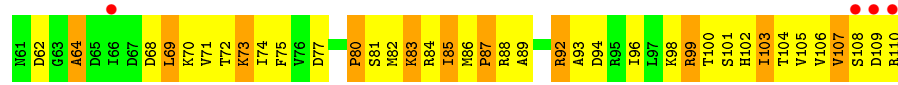
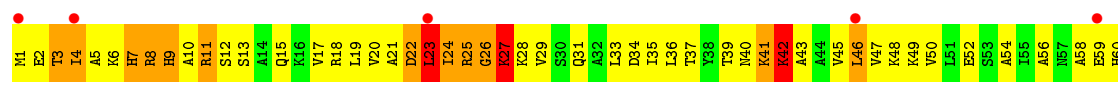




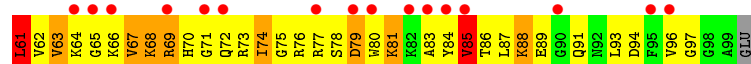
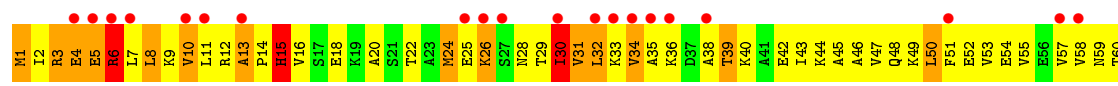
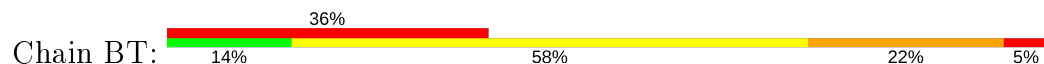
• Molecule 40: 50S RIBOSOMAL PROTEIN L22



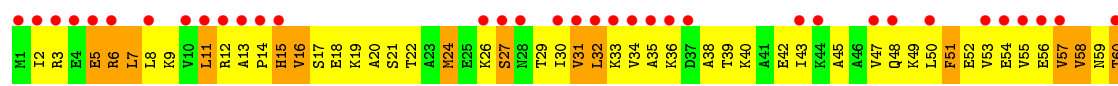
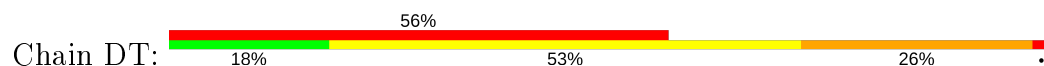
• Molecule 40: 50S RIBOSOMAL PROTEIN L22



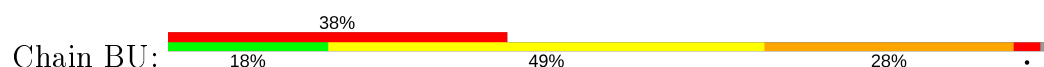
• Molecule 41: 50S RIBOSOMAL PROTEIN L23

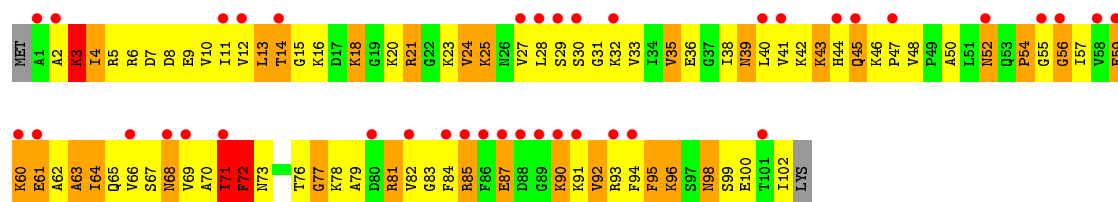


• Molecule 41: 50S RIBOSOMAL PROTEIN L23

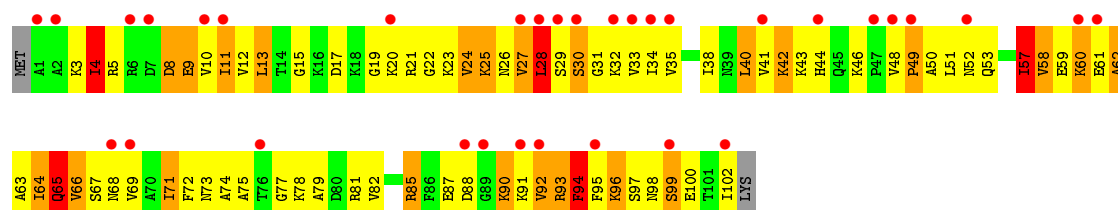


• Molecule 42: 50S RIBOSOMAL PROTEIN L24

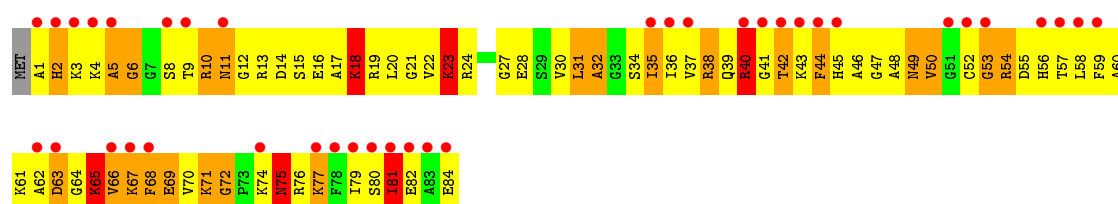
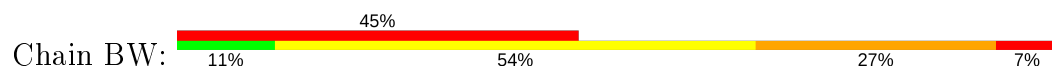




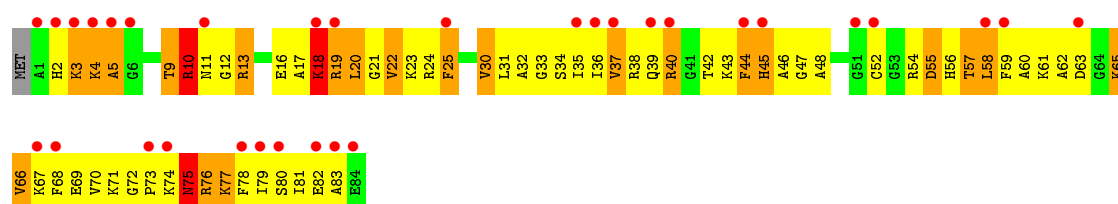
• Molecule 42: 50S RIBOSOMAL PROTEIN L24



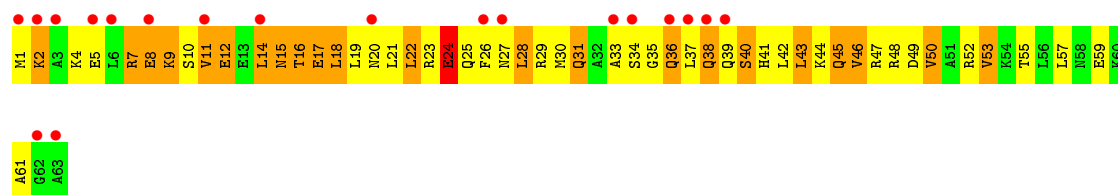
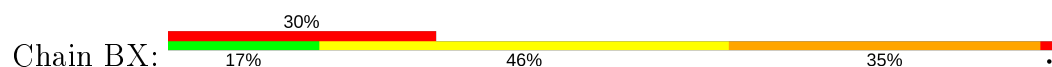
• Molecule 43: 50S RIBOSOMAL PROTEIN L27



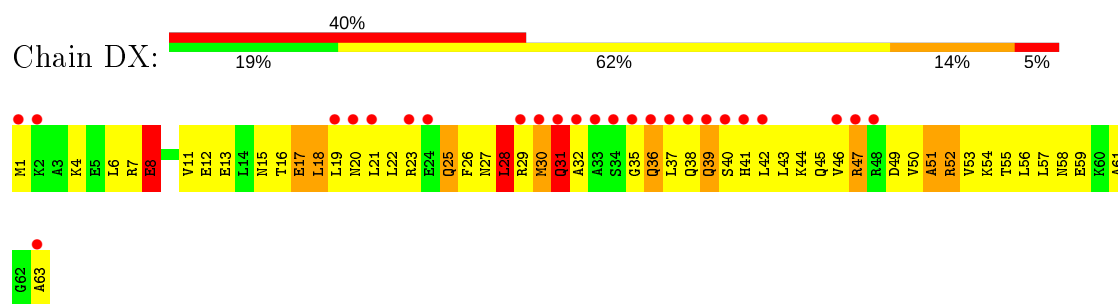
• Molecule 43: 50S RIBOSOMAL PROTEIN L27



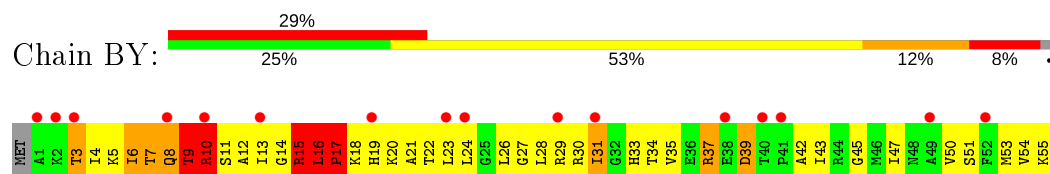
• Molecule 44: 50S RIBOSOMAL PROTEIN L29



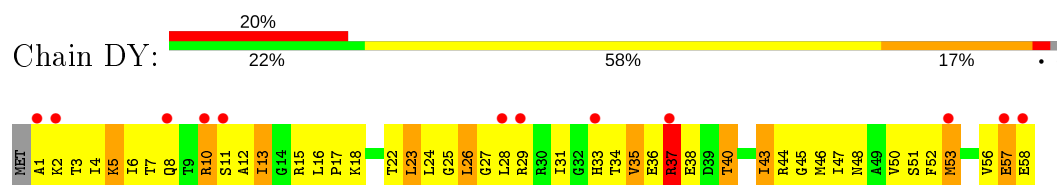
• Molecule 44: 50S RIBOSOMAL PROTEIN L29



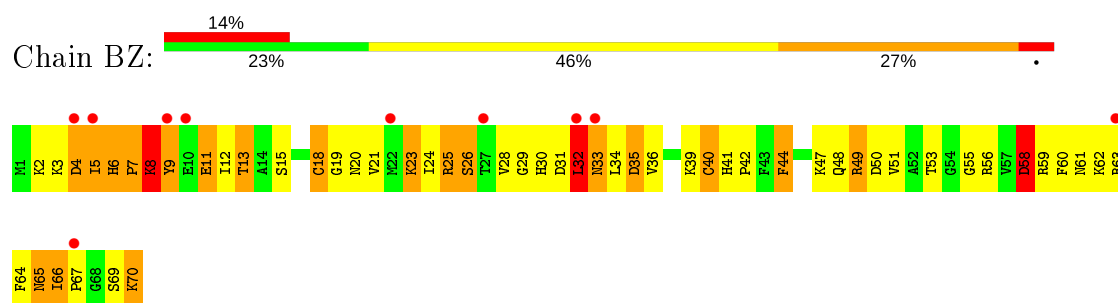
• Molecule 45: 50S RIBOSOMAL PROTEIN L30



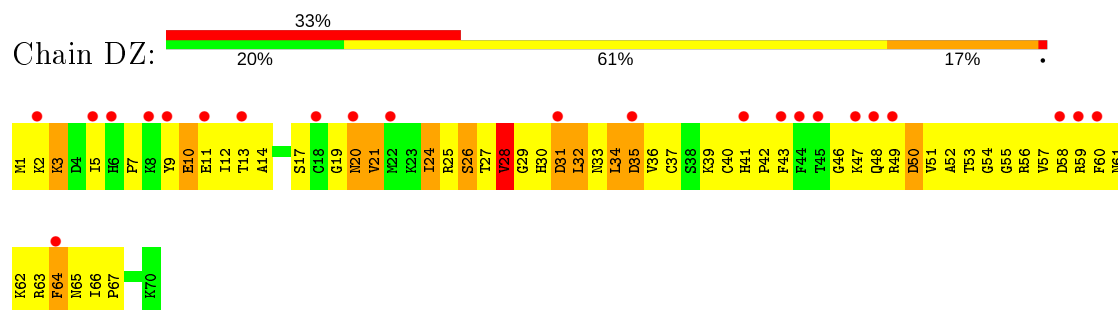
• Molecule 45: 50S RIBOSOMAL PROTEIN L30



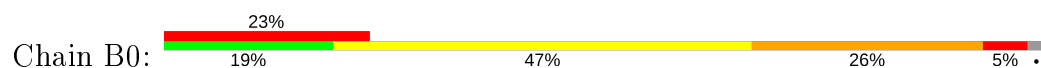
• Molecule 46: 50S RIBOSOMAL PROTEIN L31

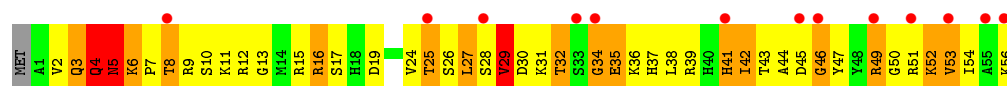


• Molecule 46: 50S RIBOSOMAL PROTEIN L31

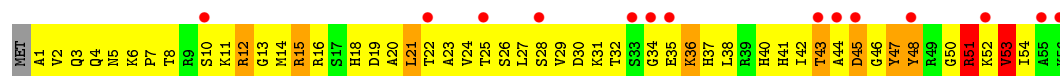


• Molecule 47: 50S RIBOSOMAL PROTEIN L32

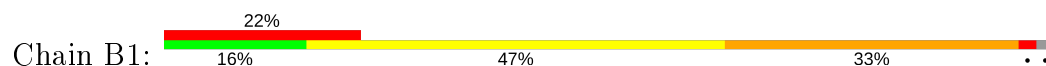




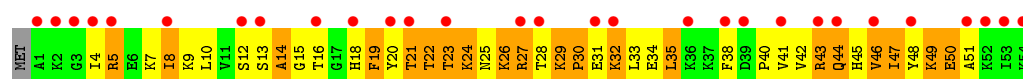
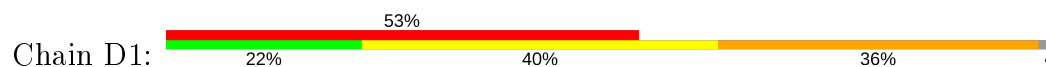
• Molecule 47: 50S RIBOSOMAL PROTEIN L32



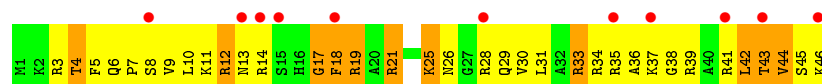
• Molecule 48: 50S RIBOSOMAL PROTEIN L33



• Molecule 48: 50S RIBOSOMAL PROTEIN L33



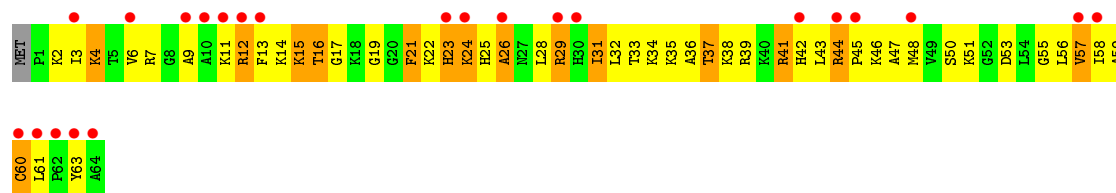
• Molecule 49: 50S RIBOSOMAL PROTEIN L34



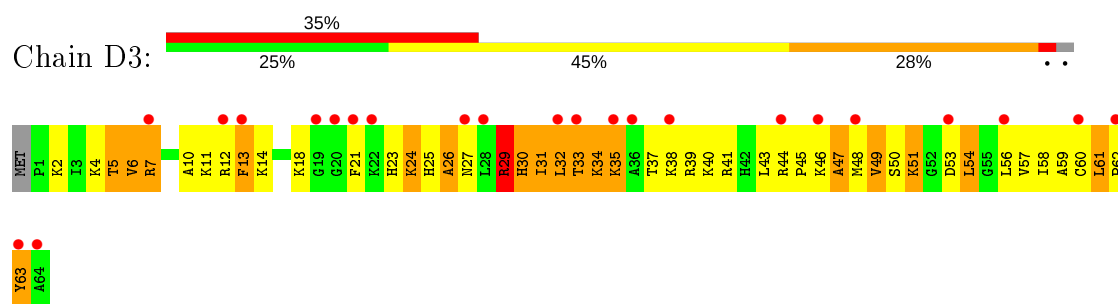
• Molecule 49: 50S RIBOSOMAL PROTEIN L34



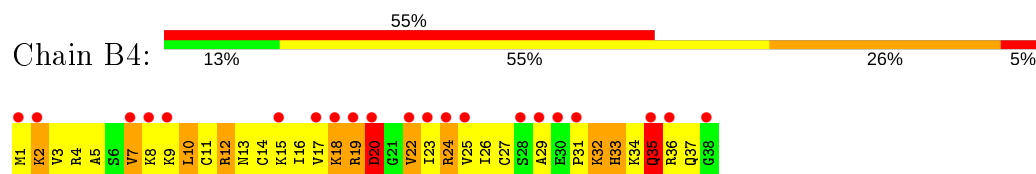
• Molecule 50: 50S RIBOSOMAL PROTEIN L35



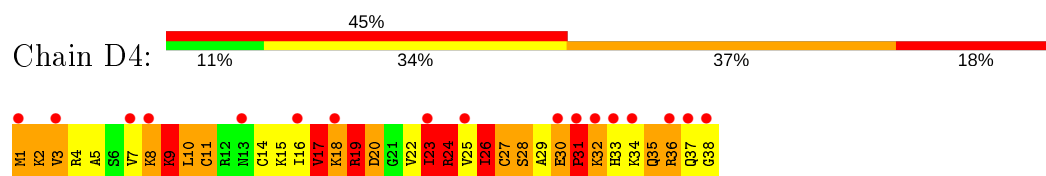
• Molecule 50: 50S RIBOSOMAL PROTEIN L35



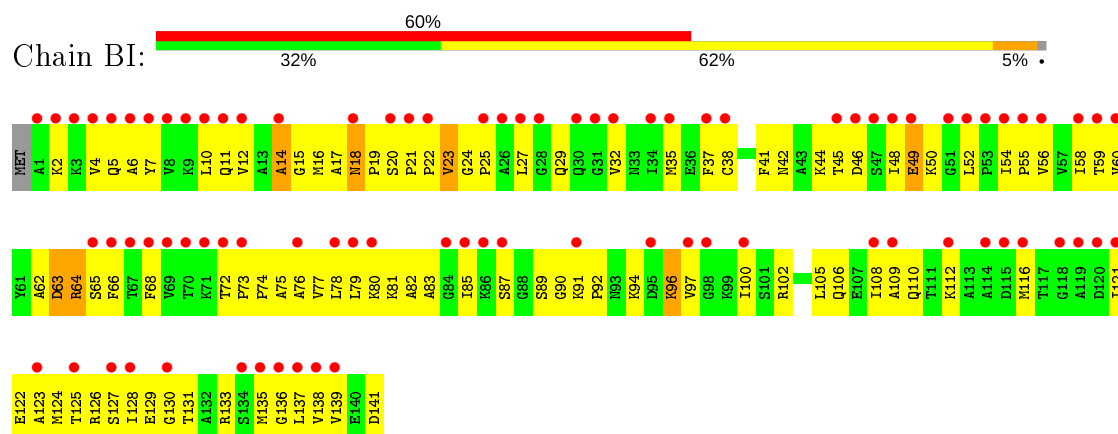
- Molecule 51: 50S RIBOSOMAL PROTEIN L36



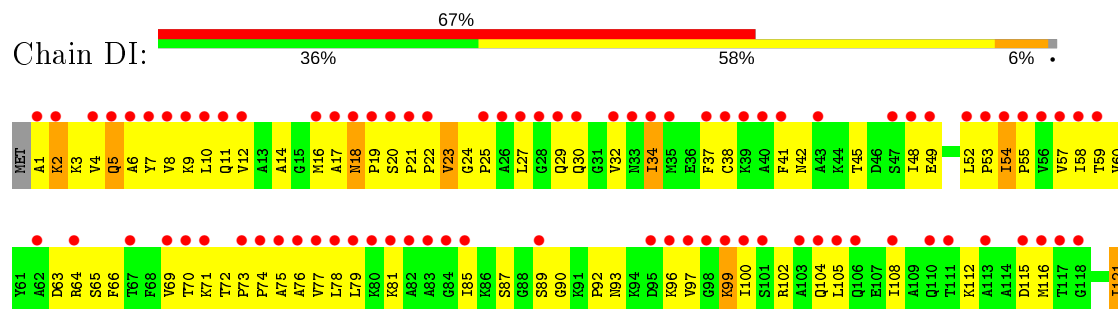
- Molecule 51: 50S RIBOSOMAL PROTEIN L36

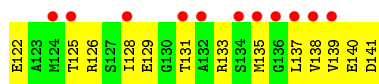


- Molecule 52: 50S RIBOSOMAL PROTEIN L11



- 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 0.287 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
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 , 66.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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>9</b>
2	CC	204/233 (88%)	138 (68%)	46 (22%)	20 (10%)	<b>0</b>	<b>6</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AD	203/206 (98%)	133 (66%)	49 (24%)	21 (10%)	0	6
3	CD	203/206 (98%)	137 (68%)	49 (24%)	17 (8%)	1	8
4	AE	148/167 (89%)	110 (74%)	30 (20%)	8 (5%)	2	16
4	CE	148/167 (89%)	109 (74%)	30 (20%)	9 (6%)	1	13
5	AF	98/135 (73%)	68 (69%)	25 (26%)	5 (5%)	2	17
5	CF	98/135 (73%)	72 (74%)	18 (18%)	8 (8%)	1	8
6	AG	148/179 (83%)	105 (71%)	35 (24%)	8 (5%)	2	16
6	CG	150/179 (84%)	101 (67%)	37 (25%)	12 (8%)	1	9
7	AH	127/130 (98%)	108 (85%)	14 (11%)	5 (4%)	3	24
7	CH	127/130 (98%)	91 (72%)	29 (23%)	7 (6%)	2	16
8	AI	125/130 (96%)	84 (67%)	30 (24%)	11 (9%)	1	7
8	CI	125/130 (96%)	82 (66%)	30 (24%)	13 (10%)	0	6
9	AJ	96/103 (93%)	65 (68%)	20 (21%)	11 (12%)	0	5
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	11
10	CK	115/129 (89%)	76 (66%)	30 (26%)	9 (8%)	1	9
11	AL	121/124 (98%)	73 (60%)	35 (29%)	13 (11%)	0	5
11	CL	121/124 (98%)	76 (63%)	28 (23%)	17 (14%)	0	3
12	AM	112/118 (95%)	89 (80%)	13 (12%)	10 (9%)	1	7
12	CM	111/118 (94%)	82 (74%)	17 (15%)	12 (11%)	0	5
13	AN	92/101 (91%)	64 (70%)	19 (21%)	9 (10%)	0	6
13	CN	92/101 (91%)	50 (54%)	26 (28%)	16 (17%)	0	2
14	AO	86/89 (97%)	66 (77%)	19 (22%)	1 (1%)	13	48
14	CO	86/89 (97%)	69 (80%)	15 (17%)	2 (2%)	6	34
15	AP	80/82 (98%)	60 (75%)	14 (18%)	6 (8%)	1	10
15	CP	78/82 (95%)	55 (70%)	14 (18%)	9 (12%)	0	5
16	AQ	78/84 (93%)	49 (63%)	25 (32%)	4 (5%)	2	17
16	CQ	79/84 (94%)	58 (73%)	15 (19%)	6 (8%)	1	9
17	AR	53/75 (71%)	31 (58%)	16 (30%)	6 (11%)	0	5
17	CR	53/75 (71%)	36 (68%)	13 (24%)	4 (8%)	1	10
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	3
19	AT	83/87 (95%)	68 (82%)	12 (14%)	3 (4%)	3	25
19	CT	83/87 (95%)	62 (75%)	16 (19%)	5 (6%)	1	14
20	AB	216/241 (90%)	148 (68%)	52 (24%)	16 (7%)	1	10
20	CB	216/241 (90%)	149 (69%)	41 (19%)	26 (12%)	0	4
21	AU	49/71 (69%)	23 (47%)	12 (24%)	14 (29%)	0	0
21	CU	49/71 (69%)	26 (53%)	18 (37%)	5 (10%)	0	6
24	BV	92/94 (98%)	61 (66%)	24 (26%)	7 (8%)	1	9
24	DV	92/94 (98%)	64 (70%)	23 (25%)	5 (5%)	2	16
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	0
26	BD	207/209 (99%)	87 (42%)	68 (33%)	52 (25%)	0	0
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	4
29	DG	174/177 (98%)	108 (62%)	51 (29%)	15 (9%)	1	8
30	BH	147/149 (99%)	83 (56%)	49 (33%)	15 (10%)	0	6
30	DH	147/149 (99%)	83 (56%)	46 (31%)	18 (12%)	0	4
31	BJ	138/142 (97%)	68 (49%)	43 (31%)	27 (20%)	0	1
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	0
34	DM	134/136 (98%)	71 (53%)	43 (32%)	20 (15%)	0	2
35	BN	125/127 (98%)	68 (54%)	41 (33%)	16 (13%)	0	3
35	DN	125/127 (98%)	86 (69%)	29 (23%)	10 (8%)	1	9

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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	5
38	DQ	115/118 (98%)	78 (68%)	21 (18%)	16 (14%)	0	3
39	BR	101/103 (98%)	39 (39%)	38 (38%)	24 (24%)	0	0
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	2
40	DS	108/110 (98%)	62 (57%)	26 (24%)	20 (18%)	0	1
41	BT	97/100 (97%)	38 (39%)	42 (43%)	17 (18%)	0	1
41	DT	97/100 (97%)	44 (45%)	28 (29%)	25 (26%)	0	0
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	1
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	1
44	DX	61/63 (97%)	37 (61%)	15 (25%)	9 (15%)	0	2
45	BY	56/59 (95%)	29 (52%)	17 (30%)	10 (18%)	0	1
45	DY	56/59 (95%)	38 (68%)	15 (27%)	3 (5%)	2	16
46	BZ	68/70 (97%)	32 (47%)	23 (34%)	13 (19%)	0	1
46	DZ	68/70 (97%)	36 (53%)	22 (32%)	10 (15%)	0	2
47	B0	54/57 (95%)	27 (50%)	17 (32%)	10 (18%)	0	1
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	1
48	D1	52/55 (94%)	21 (40%)	18 (35%)	13 (25%)	0	0
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	3
50	D3	62/65 (95%)	30 (48%)	21 (34%)	11 (18%)	0	1
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%)	3	25
52	DI	139/142 (98%)	119 (86%)	15 (11%)	5 (4%)	3	25
All	All	11263/11954 (94%)	6605 (59%)	2995 (27%)	1663 (15%)	0	2

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%)	4	22
2	CC	170/190 (90%)	150 (88%)	20 (12%)	5	23
3	AD	172/173 (99%)	145 (84%)	27 (16%)	2	14
3	CD	172/173 (99%)	143 (83%)	29 (17%)	2	11
4	AE	113/126 (90%)	96 (85%)	17 (15%)	3	15
4	CE	113/126 (90%)	94 (83%)	19 (17%)	2	11
5	AF	87/116 (75%)	68 (78%)	19 (22%)	1	4
5	CF	87/116 (75%)	76 (87%)	11 (13%)	4	21
6	AG	123/147 (84%)	106 (86%)	17 (14%)	3	18
6	CG	125/147 (85%)	111 (89%)	14 (11%)	6	25
7	AH	104/105 (99%)	92 (88%)	12 (12%)	5	24
7	CH	104/105 (99%)	93 (89%)	11 (11%)	6	28
8	AI	105/107 (98%)	90 (86%)	15 (14%)	3	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	CI	105/107 (98%)	91 (87%)	14 (13%)	4	19
9	AJ	86/90 (96%)	70 (81%)	16 (19%)	1	7
9	CJ	86/90 (96%)	78 (91%)	8 (9%)	9	34
10	AK	90/99 (91%)	72 (80%)	18 (20%)	1	5
10	CK	90/99 (91%)	79 (88%)	11 (12%)	5	22
11	AL	103/104 (99%)	90 (87%)	13 (13%)	4	21
11	CL	103/104 (99%)	86 (84%)	17 (16%)	2	12
12	AM	92/96 (96%)	76 (83%)	16 (17%)	2	9
12	CM	91/96 (95%)	80 (88%)	11 (12%)	5	22
13	AN	79/84 (94%)	70 (89%)	9 (11%)	5	24
13	CN	79/84 (94%)	73 (92%)	6 (8%)	13	42
14	AO	76/77 (99%)	69 (91%)	7 (9%)	9	34
14	CO	76/77 (99%)	67 (88%)	9 (12%)	5	23
15	AP	65/65 (100%)	54 (83%)	11 (17%)	2	11
15	CP	65/65 (100%)	57 (88%)	8 (12%)	4	22
16	AQ	74/78 (95%)	64 (86%)	10 (14%)	4	19
16	CQ	75/78 (96%)	68 (91%)	7 (9%)	9	34
17	AR	48/65 (74%)	44 (92%)	4 (8%)	11	38
17	CR	48/65 (74%)	42 (88%)	6 (12%)	4	21
18	AS	70/79 (89%)	59 (84%)	11 (16%)	2	14
18	CS	71/79 (90%)	58 (82%)	13 (18%)	1	7
19	AT	65/66 (98%)	55 (85%)	10 (15%)	2	14
19	CT	65/66 (98%)	55 (85%)	10 (15%)	2	14
20	AB	180/199 (90%)	148 (82%)	32 (18%)	2	8
20	CB	180/199 (90%)	153 (85%)	27 (15%)	3	15
21	AU	44/61 (72%)	37 (84%)	7 (16%)	2	13
21	CU	44/61 (72%)	31 (70%)	13 (30%)	0	2
24	BV	78/78 (100%)	64 (82%)	14 (18%)	2	8
24	DV	78/78 (100%)	72 (92%)	6 (8%)	13	42
25	BC	213/218 (98%)	162 (76%)	51 (24%)	0	3
25	DC	213/218 (98%)	164 (77%)	49 (23%)	1	3

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	DT	83/84 (99%)	70 (84%)	13 (16%)	2	14
42	BU	83/85 (98%)	66 (80%)	17 (20%)	1	5
42	DU	83/85 (98%)	65 (78%)	18 (22%)	1	4
43	BW	62/63 (98%)	50 (81%)	12 (19%)	1	6
43	DW	62/63 (98%)	51 (82%)	11 (18%)	2	9
44	BX	55/55 (100%)	38 (69%)	17 (31%)	0	2
44	DX	55/55 (100%)	45 (82%)	10 (18%)	1	8
45	BY	48/49 (98%)	37 (77%)	11 (23%)	1	3
45	DY	48/49 (98%)	36 (75%)	12 (25%)	0	3
46	BZ	62/62 (100%)	46 (74%)	16 (26%)	0	2
46	DZ	62/62 (100%)	54 (87%)	8 (13%)	4	20
47	B0	47/48 (98%)	36 (77%)	11 (23%)	1	3
47	D0	47/48 (98%)	38 (81%)	9 (19%)	1	6
48	B1	48/49 (98%)	35 (73%)	13 (27%)	0	2
48	D1	48/49 (98%)	38 (79%)	10 (21%)	1	5
49	B2	38/38 (100%)	29 (76%)	9 (24%)	1	3
49	D2	38/38 (100%)	29 (76%)	9 (24%)	1	3
50	B3	51/52 (98%)	41 (80%)	10 (20%)	1	6
50	D3	51/52 (98%)	39 (76%)	12 (24%)	1	3
51	B4	34/34 (100%)	25 (74%)	9 (26%)	0	2
51	D4	34/34 (100%)	19 (56%)	15 (44%)	0	0
52	BI	109/110 (99%)	107 (98%)	2 (2%)	59	81
52	DI	109/110 (99%)	105 (96%)	4 (4%)	34	64
All	All	9341/9744 (96%)	7726 (83%)	1615 (17%)	2	10

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	2.02	5 (20%)	29,40,40	1.07	3 (10%)
53	KSG	CA	1601	-	24,27,27	1.97	4 (16%)	29,40,40	0.97	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	-	-	2/8/52/52	0/2/2/2
53	KSG	CA	1601	-	-	2/8/52/52	0/2/2/2

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	AA	1601	KSG	C14-C13	-6.75	1.49	1.53
53	CA	1601	KSG	C14-C13	-5.75	1.49	1.53
53	AA	1601	KSG	C1-C12	2.65	1.57	1.52
53	CA	1601	KSG	C1-C12	2.60	1.57	1.52
53	CA	1601	KSG	O7-C1	2.58	1.48	1.41

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	AA	1601	KSG	C1-O1-C2	-2.22	112.46	117.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	AA	1601	KSG	C4-C3-C2	2.19	114.68	109.68
53	AA	1601	KSG	C5-C4-C3	2.09	114.47	110.82
53	CA	1601	KSG	C6-C7-C2	2.01	114.26	109.68

There are no chirality outliers.

All (4) torsion outliers are listed below:

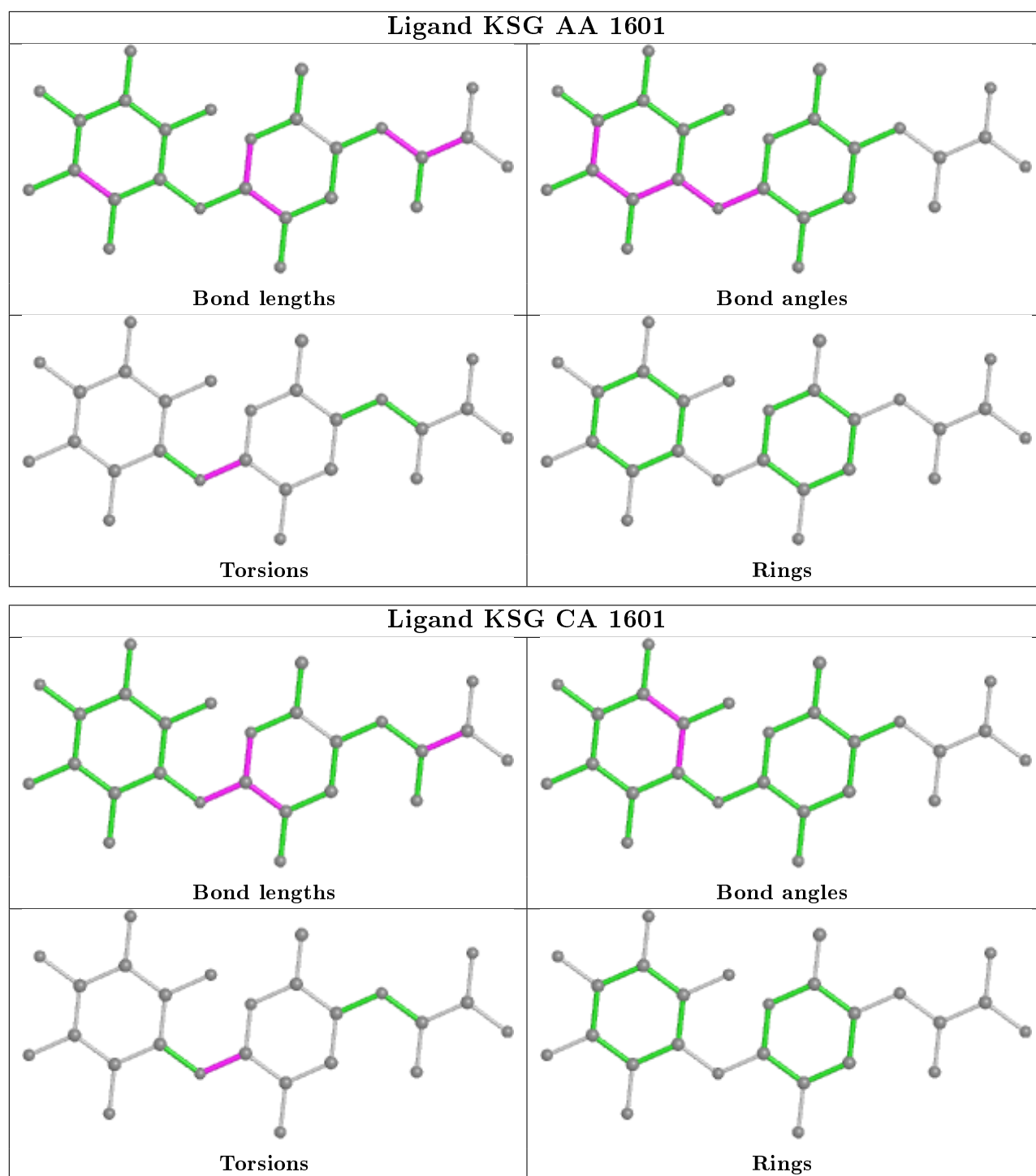
Mol	Chain	Res	Type	Atoms
53	CA	1601	KSG	C12-C1-O1-C2
53	AA	1601	KSG	C12-C1-O1-C2
53	CA	1601	KSG	O7-C1-O1-C2
53	AA	1601	KSG	O7-C1-O1-C2

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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%)	0.23	23 (1%) 73 71	15, 73, 149, 180	0
1	CA	1530/1542 (99%)	0.01	14 (0%) 84 81	7, 52, 134, 180	0
2	AC	206/233 (88%)	0.84	26 (12%) 3 5	7, 68, 138, 180	0
2	CC	206/233 (88%)	0.51	11 (5%) 26 26	6, 74, 126, 169	0
3	AD	205/206 (99%)	1.05	46 (22%) 0 0	27, 79, 147, 180	0
3	CD	205/206 (99%)	0.28	1 (0%) 91 89	5, 55, 113, 165	0
4	AE	150/167 (89%)	0.61	8 (5%) 26 26	15, 62, 120, 162	0
4	CE	150/167 (89%)	0.57	8 (5%) 26 26	6, 55, 112, 180	0
5	AF	100/135 (74%)	0.58	5 (5%) 28 28	18, 72, 133, 166	0
5	CF	100/135 (74%)	0.86	13 (13%) 3 5	12, 71, 132, 165	0
6	AG	150/179 (83%)	0.81	27 (18%) 1 2	22, 89, 143, 180	0
6	CG	152/179 (84%)	0.82	21 (13%) 2 4	19, 86, 147, 180	0
7	AH	129/130 (99%)	1.20	27 (20%) 1 1	14, 70, 141, 176	0
7	CH	129/130 (99%)	0.68	18 (13%) 2 4	5, 54, 114, 160	0
8	AI	127/130 (97%)	1.11	26 (20%) 1 1	18, 90, 146, 180	0
8	CI	127/130 (97%)	1.16	29 (22%) 0 1	23, 92, 156, 180	0
9	AJ	98/103 (95%)	1.23	26 (26%) 0 0	20, 82, 157, 180	0
9	CJ	98/103 (95%)	0.67	5 (5%) 28 27	34, 79, 135, 151	0
10	AK	117/129 (90%)	0.56	7 (5%) 21 22	7, 55, 138, 160	0
10	CK	117/129 (90%)	0.43	7 (5%) 21 22	11, 50, 105, 142	0
11	AL	123/124 (99%)	0.70	10 (8%) 12 14	21, 61, 128, 178	0
11	CL	123/124 (99%)	0.84	11 (8%) 9 12	5, 39, 119, 160	0
12	AM	114/118 (96%)	1.09	20 (17%) 1 2	44, 106, 159, 173	0
12	CM	113/118 (95%)	1.27	22 (19%) 1 1	26, 100, 157, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
13	AN	96/101 (95%)	1.76	33 (34%)	0	0	15, 84, 151, 180	0
13	CN	96/101 (95%)	1.09	16 (16%)	1	2	21, 82, 139, 161	0
14	AO	88/89 (98%)	0.98	17 (19%)	1	1	18, 70, 114, 180	0
14	CO	88/89 (98%)	0.53	4 (4%)	33	32	14, 51, 112, 150	0
15	AP	82/82 (100%)	0.89	11 (13%)	3	4	27, 89, 142, 180	0
15	CP	80/82 (97%)	0.94	10 (12%)	3	6	5, 46, 145, 180	0
16	AQ	80/84 (95%)	1.47	19 (23%)	0	0	37, 91, 140, 180	0
16	CQ	81/84 (96%)	0.90	8 (9%)	7	9	12, 57, 119, 154	0
17	AR	55/75 (73%)	1.30	15 (27%)	0	0	18, 69, 147, 164	0
17	CR	55/75 (73%)	0.99	7 (12%)	3	5	13, 53, 126, 175	0
18	AS	79/92 (85%)	2.06	35 (44%)	0	0	59, 112, 174, 180	0
18	CS	80/92 (86%)	2.04	33 (41%)	0	0	48, 109, 172, 180	0
19	AT	85/87 (97%)	1.13	17 (20%)	1	1	36, 94, 142, 170	0
19	CT	85/87 (97%)	1.51	25 (29%)	0	0	17, 55, 118, 179	0
20	AB	218/241 (90%)	0.87	32 (14%)	2	3	28, 92, 142, 180	0
20	CB	218/241 (90%)	0.64	22 (10%)	7	9	27, 96, 157, 180	0
21	AU	51/71 (71%)	1.09	10 (19%)	1	1	26, 94, 153, 174	0
21	CU	51/71 (71%)	1.26	12 (23%)	0	0	29, 82, 163, 180	0
22	BA	117/120 (97%)	0.04	2 (1%)	70	67	39, 67, 125, 171	0
22	DA	117/120 (97%)	-0.01	2 (1%)	70	67	34, 73, 116, 180	0
23	BB	2841/2904 (97%)	0.17	40 (1%)	75	72	9, 53, 144, 180	0
23	DB	2841/2904 (97%)	0.12	21 (0%)	87	85	5, 45, 143, 180	0
24	BV	94/94 (100%)	0.72	13 (13%)	2	4	26, 78, 134, 155	0
24	DV	94/94 (100%)	0.52	5 (5%)	26	26	34, 83, 139, 162	0
25	BC	267/273 (97%)	1.20	50 (18%)	1	2	5, 53, 143, 180	0
25	DC	267/273 (97%)	1.10	43 (16%)	1	2	5, 52, 158, 180	0
26	BD	209/209 (100%)	1.44	56 (26%)	0	0	9, 82, 157, 180	0
26	DD	209/209 (100%)	1.24	46 (22%)	0	1	5, 57, 142, 180	0
27	BE	201/201 (100%)	1.34	47 (23%)	0	0	5, 85, 162, 180	0
27	DE	201/201 (100%)	1.36	43 (21%)	0	1	6, 82, 170, 180	0
28	BF	178/179 (99%)	0.93	37 (20%)	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%)	0.77	18 (10%)	7	9	29, 96, 154, 180	0
29	BG	176/177 (99%)	1.31	41 (23%)	0	0	34, 100, 164, 180	0
29	DG	176/177 (99%)	0.91	30 (17%)	1	2	23, 88, 156, 180	0
30	BH	149/149 (100%)	2.37	66 (44%)	0	0	22, 126, 180, 180	0
30	DH	149/149 (100%)	1.53	47 (31%)	0	0	30, 106, 167, 180	0
31	BJ	140/142 (98%)	1.02	28 (20%)	1	1	11, 88, 153, 180	0
31	DJ	140/142 (98%)	0.85	20 (14%)	2	4	7, 66, 148, 176	0
32	BK	121/123 (98%)	0.74	12 (9%)	7	9	13, 60, 118, 152	0
32	DK	121/123 (98%)	0.58	3 (2%)	57	54	5, 36, 92, 134	0
33	BL	144/144 (100%)	2.61	67 (46%)	0	0	15, 86, 167, 180	0
33	DL	144/144 (100%)	2.15	54 (37%)	0	0	5, 81, 156, 180	0
34	BM	136/136 (100%)	1.58	38 (27%)	0	0	13, 71, 175, 180	0
34	DM	136/136 (100%)	1.16	23 (16%)	1	2	11, 70, 164, 180	0
35	BN	127/127 (100%)	1.56	41 (32%)	0	0	17, 78, 169, 180	0
35	DN	127/127 (100%)	1.08	16 (12%)	3	5	5, 48, 159, 180	0
36	BO	117/117 (100%)	1.82	35 (29%)	0	0	26, 91, 167, 180	0
36	DO	117/117 (100%)	1.80	37 (31%)	0	0	5, 91, 172, 180	0
37	BP	114/115 (99%)	1.85	47 (41%)	0	0	18, 98, 172, 180	0
37	DP	114/115 (99%)	1.49	30 (26%)	0	0	7, 65, 166, 180	0
38	BQ	117/118 (99%)	0.53	10 (8%)	10	13	13, 66, 146, 174	0
38	DQ	117/118 (99%)	0.90	17 (14%)	2	3	6, 57, 158, 180	0
39	BR	103/103 (100%)	1.12	21 (20%)	1	1	24, 105, 167, 180	0
39	DR	103/103 (100%)	1.70	35 (33%)	0	0	25, 92, 157, 180	0
40	BS	110/110 (100%)	0.68	8 (7%)	15	17	9, 63, 133, 180	0
40	DS	110/110 (100%)	0.78	9 (8%)	11	14	5, 46, 137, 180	0
41	BT	99/100 (99%)	1.67	36 (36%)	0	0	25, 81, 162, 180	0
41	DT	99/100 (99%)	2.63	56 (56%)	0	0	15, 86, 168, 180	0
42	BU	102/104 (98%)	2.27	39 (38%)	0	0	17, 91, 169, 180	0
42	DU	102/104 (98%)	1.85	33 (32%)	0	0	30, 110, 171, 180	0
43	BW	84/85 (98%)	2.68	38 (45%)	0	0	10, 86, 159, 180	0
43	DW	84/85 (98%)	2.45	32 (38%)	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%)	1.79	19 (30%)	0	0	20, 97, 160, 180	0
44	DX	63/63 (100%)	2.73	25 (39%)	0	0	38, 110, 169, 180	0
45	BY	58/59 (98%)	1.60	17 (29%)	0	0	13, 86, 157, 180	0
45	DY	58/59 (98%)	1.24	12 (20%)	1	1	5, 79, 136, 150	0
46	BZ	70/70 (100%)	0.92	10 (14%)	2	4	19, 66, 145, 180	0
46	DZ	70/70 (100%)	1.44	23 (32%)	0	0	5, 68, 141, 180	0
47	B0	56/57 (98%)	1.42	13 (23%)	0	0	26, 95, 180, 180	0
47	D0	56/57 (98%)	1.62	14 (25%)	0	0	10, 70, 159, 177	0
48	B1	54/55 (98%)	1.45	12 (22%)	0	1	24, 97, 160, 180	0
48	D1	54/55 (98%)	2.77	29 (53%)	0	0	8, 82, 158, 180	0
49	B2	46/46 (100%)	1.36	11 (23%)	0	0	6, 51, 154, 174	0
49	D2	46/46 (100%)	1.14	6 (13%)	3	5	9, 55, 131, 150	0
50	B3	64/65 (98%)	1.99	23 (35%)	0	0	19, 61, 155, 180	0
50	D3	64/65 (98%)	1.98	23 (35%)	0	0	5, 61, 139, 178	0
51	B4	38/38 (100%)	2.78	21 (55%)	0	0	30, 102, 170, 180	0
51	D4	38/38 (100%)	2.72	17 (44%)	0	0	14, 111, 175, 180	0
52	BI	141/142 (99%)	2.56	85 (60%)	0	0	52, 152, 180, 180	0
52	DI	141/142 (99%)	2.75	95 (67%)	0	0	83, 160, 180, 180	0
All	All	20439/21086 (96%)	0.76	2584 (12%)	3	5	5, 67, 155, 180	0

The worst 5 of 2584 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
33	BL	98	ALA	17.2
36	BO	58	ILE	16.8
33	BL	8	PRO	15.7
41	DT	4	GLU	15.1
42	BU	29	SER	14.8

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	AA	1615	1/1	0.30	0.19	72,72,72,72	0
54	MG	CA	1624	1/1	0.30	0.29	162,162,162,162	0
54	MG	AA	1650	1/1	0.44	0.23	133,133,133,133	0
54	MG	AA	1639	1/1	0.46	0.19	141,141,141,141	0
54	MG	AA	1609	1/1	0.49	0.19	119,119,119,119	0
54	MG	CA	1623	1/1	0.50	0.14	77,77,77,77	0
54	MG	CA	1631	1/1	0.58	0.26	21,21,21,21	1
54	MG	CA	1616	1/1	0.59	0.26	153,153,153,153	0
54	MG	AA	1626	1/1	0.61	0.43	82,82,82,82	1
54	MG	CA	1629	1/1	0.62	0.61	62,62,62,62	1
54	MG	CA	1622	1/1	0.63	0.34	132,132,132,132	0
54	MG	BB	3082	1/1	0.64	0.39	63,63,63,63	0
54	MG	AA	1608	1/1	0.66	0.18	57,57,57,57	0
54	MG	DB	3013	1/1	0.66	0.20	32,32,32,32	0
54	MG	AA	1637	1/1	0.66	0.62	115,115,115,115	0
54	MG	BB	3034	1/1	0.67	0.22	42,42,42,42	0
54	MG	AA	1631	1/1	0.68	0.25	143,143,143,143	0
54	MG	BB	3047	1/1	0.70	0.29	128,128,128,128	0
54	MG	AA	1628	1/1	0.71	0.16	63,63,63,63	0
54	MG	AA	1616	1/1	0.71	0.20	86,86,86,86	0
54	MG	BB	3100	1/1	0.72	0.22	37,37,37,37	1
54	MG	DB	3059	1/1	0.72	0.15	75,75,75,75	0
54	MG	BB	3097	1/1	0.72	0.13	96,96,96,96	0
54	MG	DB	3071	1/1	0.72	0.13	27,27,27,27	0
54	MG	AA	1614	1/1	0.73	0.15	67,67,67,67	0
54	MG	AA	1621	1/1	0.73	0.14	96,96,96,96	0
54	MG	AA	1620	1/1	0.74	0.29	116,116,116,116	0
54	MG	AA	1619	1/1	0.74	0.13	33,33,33,33	0
54	MG	BB	3033	1/1	0.74	0.26	113,113,113,113	0
54	MG	BB	3077	1/1	0.74	0.16	37,37,37,37	0
54	MG	BB	3008	1/1	0.74	0.16	82,82,82,82	0
54	MG	DB	3017	1/1	0.74	0.23	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	AA	1627	1/1	0.75	0.33	17,17,17,17	1
54	MG	BB	3018	1/1	0.75	0.22	42,42,42,42	0
54	MG	DB	3033	1/1	0.76	0.26	88,88,88,88	0
54	MG	DB	3108	1/1	0.76	0.11	24,24,24,24	0
54	MG	DB	3064	1/1	0.77	0.27	66,66,66,66	1
54	MG	DB	3049	1/1	0.77	0.10	79,79,79,79	0
54	MG	DB	3052	1/1	0.78	0.25	42,42,42,42	0
54	MG	CA	1609	1/1	0.78	0.19	132,132,132,132	0
54	MG	DB	3044	1/1	0.79	0.09	58,58,58,58	0
54	MG	BB	3084	1/1	0.79	0.11	19,19,19,19	0
54	MG	DB	3023	1/1	0.79	0.08	44,44,44,44	0
54	MG	AA	1661	1/1	0.79	0.05	83,83,83,83	0
54	MG	AA	1603	1/1	0.80	0.14	74,74,74,74	0
54	MG	AA	1655	1/1	0.80	0.10	67,67,67,67	0
54	MG	AA	1613	1/1	0.80	0.20	108,108,108,108	0
54	MG	BB	3028	1/1	0.80	0.23	66,66,66,66	0
54	MG	AA	1612	1/1	0.80	0.11	52,52,52,52	0
54	MG	AA	1658	1/1	0.80	0.12	113,113,113,113	0
54	MG	DB	3016	1/1	0.80	0.14	25,25,25,25	0
54	MG	DB	3062	1/1	0.80	0.12	24,24,24,24	0
54	MG	AA	1654	1/1	0.80	0.11	81,81,81,81	0
54	MG	CA	1640	1/1	0.80	0.12	139,139,139,139	0
54	MG	AA	1660	1/1	0.80	0.10	95,95,95,95	0
54	MG	DE	301	1/1	0.80	0.16	69,69,69,69	0
54	MG	DB	3057	1/1	0.81	0.20	56,56,56,56	1
54	MG	AA	1657	1/1	0.81	0.27	83,83,83,83	0
54	MG	BB	3046	1/1	0.81	0.17	63,63,63,63	0
54	MG	AA	1607	1/1	0.81	0.08	82,82,82,82	0
54	MG	BB	3081	1/1	0.81	0.21	34,34,34,34	0
54	MG	DB	3075	1/1	0.81	0.14	42,42,42,42	0
54	MG	BB	3041	1/1	0.81	0.18	47,47,47,47	0
54	MG	DB	3007	1/1	0.82	0.14	15,15,15,15	0
54	MG	DB	3103	1/1	0.82	0.17	61,61,61,61	0
54	MG	BB	3107	1/1	0.82	0.13	37,37,37,37	0
54	MG	BB	3060	1/1	0.82	0.16	81,81,81,81	0
54	MG	CA	1644	1/1	0.82	0.12	59,59,59,59	0
54	MG	AA	1640	1/1	0.82	0.10	42,42,42,42	0
54	MG	BB	3021	1/1	0.82	0.17	24,24,24,24	0
54	MG	AA	1633	1/1	0.82	0.15	92,92,92,92	0
54	MG	DB	3082	1/1	0.83	0.29	61,61,61,61	0
54	MG	DB	3060	1/1	0.83	0.10	105,105,105,105	0
54	MG	DB	3028	1/1	0.83	0.18	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	AA	1602	1/1	0.83	0.19	34,34,34,34	0
54	MG	AA	1642	1/1	0.83	0.15	107,107,107,107	0
54	MG	BB	3094	1/1	0.83	0.15	16,16,16,16	0
54	MG	BB	3048	1/1	0.83	0.14	39,39,39,39	0
53	KSG	CA	1601	26/26	0.83	0.33	53,53,53,53	0
54	MG	DB	3035	1/1	0.83	0.16	24,24,24,24	0
53	KSG	AA	1601	26/26	0.83	0.30	53,53,53,53	0
54	MG	CA	1637	1/1	0.84	0.15	107,107,107,107	0
54	MG	BB	3014	1/1	0.84	0.17	33,33,33,33	0
54	MG	CA	1627	1/1	0.84	0.19	114,114,114,114	0
54	MG	BB	3065	1/1	0.84	0.14	47,47,47,47	0
54	MG	CA	1628	1/1	0.84	0.33	38,38,38,38	1
54	MG	CA	1651	1/1	0.84	0.16	122,122,122,122	0
54	MG	BB	3076	1/1	0.85	0.12	43,43,43,43	0
54	MG	DB	3029	1/1	0.85	0.19	22,22,22,22	0
54	MG	BB	3067	1/1	0.85	0.16	56,56,56,56	0
54	MG	DB	3058	1/1	0.85	0.20	132,132,132,132	0
54	MG	AA	1625	1/1	0.85	0.41	81,81,81,81	0
54	MG	BB	3001	1/1	0.85	0.11	28,28,28,28	0
54	MG	AA	1649	1/1	0.85	0.10	102,102,102,102	0
54	MG	DB	3107	1/1	0.85	0.13	19,19,19,19	0
54	MG	DB	3024	1/1	0.85	0.12	27,27,27,27	0
54	MG	BB	3005	1/1	0.85	0.15	13,13,13,13	0
54	MG	DB	3040	1/1	0.85	0.20	28,28,28,28	0
54	MG	DB	3085	1/1	0.86	0.21	64,64,64,64	0
54	MG	AA	1656	1/1	0.86	0.14	100,100,100,100	0
54	MG	BB	3031	1/1	0.86	0.18	46,46,46,46	0
54	MG	BB	3051	1/1	0.86	0.10	74,74,74,74	0
54	MG	CA	1630	1/1	0.86	0.09	49,49,49,49	0
54	MG	DB	3093	1/1	0.86	0.76	48,48,48,48	1
54	MG	BB	3053	1/1	0.86	0.12	36,36,36,36	0
54	MG	AA	1624	1/1	0.87	0.12	25,25,25,25	1
54	MG	DB	3032	1/1	0.87	0.11	29,29,29,29	0
54	MG	BB	3042	1/1	0.87	0.07	74,74,74,74	0
54	MG	BB	3057	1/1	0.87	0.18	19,19,19,19	0
54	MG	CA	1608	1/1	0.87	0.06	31,31,31,31	0
54	MG	BB	3074	1/1	0.87	0.12	7,7,7,7	0
54	MG	BB	3063	1/1	0.87	0.17	27,27,27,27	0
54	MG	AA	1647	1/1	0.87	0.60	84,84,84,84	0
54	MG	DB	3015	1/1	0.87	0.15	69,69,69,69	0
54	MG	AA	1617	1/1	0.87	0.13	65,65,65,65	0
54	MG	BB	3105	1/1	0.87	0.15	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DB	3003	1/1	0.87	0.13	8,8,8,8	0
54	MG	CA	1612	1/1	0.87	0.10	71,71,71,71	0
54	MG	BB	3083	1/1	0.88	0.14	25,25,25,25	0
54	MG	BB	3007	1/1	0.88	0.15	57,57,57,57	0
54	MG	BB	3064	1/1	0.88	0.16	71,71,71,71	0
54	MG	DB	3098	1/1	0.88	0.11	9,9,9,9	0
54	MG	BB	3043	1/1	0.88	0.24	63,63,63,63	0
54	MG	AA	1604	1/1	0.88	0.11	25,25,25,25	0
54	MG	CA	1638	1/1	0.88	0.21	60,60,60,60	0
54	MG	CA	1607	1/1	0.88	0.13	126,126,126,126	0
54	MG	DB	3053	1/1	0.88	0.10	37,37,37,37	0
54	MG	DB	3027	1/1	0.88	0.15	37,37,37,37	0
54	MG	AA	1652	1/1	0.88	0.14	105,105,105,105	0
54	MG	AA	1623	1/1	0.88	0.32	143,143,143,143	0
54	MG	BB	3099	1/1	0.88	0.13	58,58,58,58	0
54	MG	BB	3072	1/1	0.88	0.12	26,26,26,26	0
54	MG	BB	3066	1/1	0.88	0.13	42,42,42,42	0
54	MG	BB	3017	1/1	0.89	0.10	54,54,54,54	0
54	MG	BB	3090	1/1	0.89	0.11	65,65,65,65	0
54	MG	DB	3094	1/1	0.89	0.21	33,33,33,33	0
54	MG	BB	3091	1/1	0.89	0.16	42,42,42,42	0
54	MG	DB	3061	1/1	0.89	0.11	48,48,48,48	0
54	MG	DB	3047	1/1	0.89	0.09	29,29,29,29	0
54	MG	CA	1658	1/1	0.89	0.07	18,18,18,18	0
54	MG	BB	3010	1/1	0.89	0.16	74,74,74,74	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	BB	3049	1/1	0.89	0.15	12,12,12,12	0
54	MG	BB	3104	1/1	0.89	0.13	33,33,33,33	0
54	MG	BB	3101	1/1	0.89	0.10	14,14,14,14	0
54	MG	DB	3080	1/1	0.89	0.12	34,34,34,34	0
54	MG	BB	3088	1/1	0.89	0.16	25,25,25,25	0
54	MG	DB	3076	1/1	0.89	0.15	69,69,69,69	0
54	MG	DB	3026	1/1	0.89	0.14	30,30,30,30	0
54	MG	BB	3036	1/1	0.89	0.10	29,29,29,29	0
54	MG	BB	3080	1/1	0.90	0.09	42,42,42,42	0
54	MG	AA	1634	1/1	0.90	0.19	73,73,73,73	0
54	MG	DB	3106	1/1	0.90	0.12	7,7,7,7	0
54	MG	BB	3024	1/1	0.90	0.17	22,22,22,22	0
54	MG	BB	3109	1/1	0.90	0.15	33,33,33,33	0
54	MG	BB	3108	1/1	0.90	0.13	22,22,22,22	0
54	MG	DB	3056	1/1	0.90	0.12	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BB	3052	1/1	0.90	0.09	27,27,27,27	0
54	MG	DB	3042	1/1	0.90	0.16	5,5,5,5	0
54	MG	CA	1602	1/1	0.90	0.12	8,8,8,8	0
54	MG	DB	3081	1/1	0.91	0.16	110,110,110,110	0
54	MG	BB	3093	1/1	0.91	0.16	5,5,5,5	1
54	MG	BB	3075	1/1	0.91	0.25	35,35,35,35	0
54	MG	DB	3009	1/1	0.91	0.11	10,10,10,10	0
54	MG	BB	3073	1/1	0.91	0.21	55,55,55,55	0
54	MG	CA	1642	1/1	0.91	0.13	70,70,70,70	0
54	MG	DB	3025	1/1	0.91	0.26	20,20,20,20	0
54	MG	CA	1659	1/1	0.91	0.25	88,88,88,88	0
54	MG	BB	3026	1/1	0.91	0.12	25,25,25,25	0
54	MG	DB	3034	1/1	0.91	0.11	84,84,84,84	0
54	MG	BB	3038	1/1	0.91	0.14	82,82,82,82	0
54	MG	AA	1606	1/1	0.91	0.06	28,28,28,28	0
54	MG	BB	3071	1/1	0.91	0.19	38,38,38,38	0
54	MG	BB	3096	1/1	0.91	0.12	39,39,39,39	0
54	MG	BB	3013	1/1	0.91	0.09	36,36,36,36	0
54	MG	DB	3067	1/1	0.91	0.28	11,11,11,11	0
54	MG	DB	3012	1/1	0.91	0.17	6,6,6,6	0
54	MG	BB	3059	1/1	0.91	0.10	16,16,16,16	0
54	MG	DB	3095	1/1	0.91	0.09	44,44,44,44	0
54	MG	BB	3039	1/1	0.91	0.13	26,26,26,26	0
54	MG	DB	3002	1/1	0.91	0.13	20,20,20,20	0
54	MG	CA	1647	1/1	0.91	0.12	40,40,40,40	0
54	MG	AA	1651	1/1	0.92	0.05	64,64,64,64	0
54	MG	BB	3016	1/1	0.92	0.18	19,19,19,19	0
54	MG	AA	1653	1/1	0.92	0.15	30,30,30,30	0
54	MG	BB	3087	1/1	0.92	0.11	53,53,53,53	0
54	MG	BB	3068	1/1	0.92	0.12	39,39,39,39	0
54	MG	DB	3018	1/1	0.92	0.12	39,39,39,39	0
54	MG	BB	3102	1/1	0.92	0.11	34,34,34,34	0
54	MG	AA	1646	1/1	0.92	0.15	103,103,103,103	0
54	MG	BB	3110	1/1	0.92	0.22	79,79,79,79	0
54	MG	CA	1636	1/1	0.92	0.14	13,13,13,13	0
54	MG	BB	3062	1/1	0.92	0.21	34,34,34,34	0
54	MG	AA	1605	1/1	0.92	0.12	30,30,30,30	0
54	MG	CA	1657	1/1	0.92	0.13	51,51,51,51	0
54	MG	DB	3030	1/1	0.92	0.17	11,11,11,11	0
54	MG	AA	1618	1/1	0.92	0.12	102,102,102,102	0
54	MG	BB	3004	1/1	0.92	0.08	39,39,39,39	0
54	MG	DB	3083	1/1	0.92	0.13	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BB	3032	1/1	0.92	0.14	31,31,31,31	0
54	MG	CA	1617	1/1	0.92	0.06	45,45,45,45	0
54	MG	BB	3106	1/1	0.92	0.25	62,62,62,62	0
54	MG	DB	3109	1/1	0.92	0.19	57,57,57,57	0
54	MG	DB	3050	1/1	0.92	0.20	42,42,42,42	0
54	MG	DB	3066	1/1	0.93	0.15	12,12,12,12	0
54	MG	BB	3023	1/1	0.93	0.10	27,27,27,27	0
54	MG	CA	1635	1/1	0.93	0.11	91,91,91,91	0
54	MG	DB	3039	1/1	0.93	0.11	5,5,5,5	0
54	MG	DB	3022	1/1	0.93	0.07	5,5,5,5	0
54	MG	DB	3001	1/1	0.93	0.17	5,5,5,5	0
54	MG	DB	3055	1/1	0.93	0.20	20,20,20,20	0
54	MG	DB	3069	1/1	0.93	0.09	50,50,50,50	0
54	MG	CA	1663	1/1	0.93	0.15	20,20,20,20	0
54	MG	CA	1639	1/1	0.93	0.04	41,41,41,41	0
54	MG	DB	3021	1/1	0.93	0.12	25,25,25,25	0
54	MG	DB	3079	1/1	0.93	0.14	7,7,7,7	0
54	MG	CA	1614	1/1	0.93	0.13	97,97,97,97	0
54	MG	AA	1632	1/1	0.93	0.07	44,44,44,44	0
54	MG	BB	3027	1/1	0.93	0.07	29,29,29,29	0
54	MG	BB	3019	1/1	0.93	0.13	22,22,22,22	0
54	MG	BB	3054	1/1	0.93	0.11	77,77,77,77	0
54	MG	BB	3030	1/1	0.93	0.08	45,45,45,45	0
54	MG	CA	1621	1/1	0.93	0.09	46,46,46,46	0
54	MG	BB	3056	1/1	0.93	0.14	37,37,37,37	0
54	MG	BB	3085	1/1	0.93	0.11	67,67,67,67	0
54	MG	BB	3089	1/1	0.93	0.23	82,82,82,82	0
54	MG	DB	3036	1/1	0.94	0.17	25,25,25,25	0
54	MG	DB	3037	1/1	0.94	0.10	8,8,8,8	0
54	MG	DB	3038	1/1	0.94	0.08	33,33,33,33	0
54	MG	CA	1650	1/1	0.94	0.08	67,67,67,67	0
54	MG	BB	3079	1/1	0.94	0.06	32,32,32,32	0
54	MG	CA	1632	1/1	0.94	0.12	34,34,34,34	0
54	MG	DB	3043	1/1	0.94	0.07	7,7,7,7	0
54	MG	BB	3061	1/1	0.94	0.06	33,33,33,33	0
54	MG	BB	3003	1/1	0.94	0.11	23,23,23,23	0
54	MG	DB	3051	1/1	0.94	0.15	57,57,57,57	0
54	MG	DB	3105	1/1	0.94	0.08	24,24,24,24	0
54	MG	DB	3100	1/1	0.94	0.14	6,6,6,6	0
54	MG	DB	3070	1/1	0.94	0.07	60,60,60,60	0
54	MG	DN	201	1/1	0.94	0.26	38,38,38,38	0
54	MG	DB	3020	1/1	0.94	0.24	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	CA	1649	1/1	0.94	0.30	86,86,86,86	0
54	MG	CA	1613	1/1	0.94	0.10	63,63,63,63	0
54	MG	BB	3098	1/1	0.94	0.15	49,49,49,49	0
54	MG	DB	3073	1/1	0.94	0.11	44,44,44,44	0
54	MG	DB	3086	1/1	0.94	0.24	25,25,25,25	0
54	MG	CA	1652	1/1	0.94	0.13	20,20,20,20	0
54	MG	DB	3104	1/1	0.94	0.19	44,44,44,44	0
54	MG	CA	1641	1/1	0.94	0.08	40,40,40,40	0
54	MG	BB	3092	1/1	0.94	0.16	56,56,56,56	0
54	MG	AA	1636	1/1	0.94	0.14	83,83,83,83	0
54	MG	CA	1603	1/1	0.94	0.12	32,32,32,32	0
54	MG	DB	3011	1/1	0.94	0.17	23,23,23,23	0
54	MG	CA	1606	1/1	0.94	0.08	30,30,30,30	0
54	MG	DB	3014	1/1	0.94	0.14	28,28,28,28	0
54	MG	CA	1634	1/1	0.94	0.09	46,46,46,46	0
54	MG	DB	3010	1/1	0.94	0.08	8,8,8,8	0
54	MG	AA	1644	1/1	0.95	0.17	81,81,81,81	0
54	MG	BB	3078	1/1	0.95	0.28	49,49,49,49	0
54	MG	CA	1626	1/1	0.95	0.10	17,17,17,17	0
54	MG	CA	1604	1/1	0.95	0.15	49,49,49,49	0
54	MG	BB	3086	1/1	0.95	0.29	94,94,94,94	0
54	MG	BB	3009	1/1	0.95	0.08	35,35,35,35	0
54	MG	CA	1653	1/1	0.95	0.07	48,48,48,48	0
54	MG	BB	3040	1/1	0.95	0.14	18,18,18,18	0
54	MG	CA	1643	1/1	0.95	0.10	62,62,62,62	0
54	MG	CA	1611	1/1	0.95	0.04	43,43,43,43	0
54	MG	AA	1641	1/1	0.95	0.09	72,72,72,72	0
54	MG	DB	3101	1/1	0.95	0.13	30,30,30,30	0
54	MG	DB	3068	1/1	0.95	0.11	49,49,49,49	0
54	MG	DB	3008	1/1	0.95	0.19	39,39,39,39	0
54	MG	BB	3050	1/1	0.95	0.13	20,20,20,20	0
54	MG	BB	3037	1/1	0.95	0.10	21,21,21,21	0
54	MG	BB	3044	1/1	0.95	0.07	39,39,39,39	0
54	MG	DB	3065	1/1	0.95	0.16	25,25,25,25	0
54	MG	DB	3046	1/1	0.95	0.18	18,18,18,18	0
54	MG	DB	3090	1/1	0.95	0.15	106,106,106,106	0
54	MG	BB	3006	1/1	0.95	0.08	20,20,20,20	0
54	MG	BB	3055	1/1	0.95	0.12	19,19,19,19	0
54	MG	AA	1638	1/1	0.95	0.11	88,88,88,88	0
54	MG	DB	3048	1/1	0.95	0.07	7,7,7,7	0
54	MG	AA	1630	1/1	0.95	0.10	20,20,20,20	0
54	MG	DB	3045	1/1	0.95	0.07	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	CA	1646	1/1	0.95	0.05	94,94,94,94	0
54	MG	BB	3035	1/1	0.95	0.12	25,25,25,25	0
54	MG	DB	3092	1/1	0.95	0.06	16,16,16,16	0
54	MG	AA	1611	1/1	0.95	0.06	57,57,57,57	0
54	MG	DB	3004	1/1	0.95	0.15	38,38,38,38	0
54	MG	CA	1605	1/1	0.95	0.09	37,37,37,37	0
54	MG	CA	1615	1/1	0.95	0.14	54,54,54,54	0
54	MG	DB	3102	1/1	0.95	0.11	13,13,13,13	0
54	MG	CA	1620	1/1	0.95	0.14	32,32,32,32	0
54	MG	CA	1655	1/1	0.95	0.05	26,26,26,26	0
54	MG	AA	1629	1/1	0.96	0.10	62,62,62,62	0
54	MG	DB	3097	1/1	0.96	0.13	19,19,19,19	0
54	MG	CA	1619	1/1	0.96	0.07	9,9,9,9	0
54	MG	CA	1654	1/1	0.96	0.19	32,32,32,32	0
54	MG	DB	3088	1/1	0.96	0.21	51,51,51,51	0
54	MG	BB	3103	1/1	0.96	0.14	11,11,11,11	0
54	MG	BB	3069	1/1	0.96	0.08	8,8,8,8	0
54	MG	AA	1622	1/1	0.96	0.06	16,16,16,16	0
54	MG	DB	3099	1/1	0.96	0.17	11,11,11,11	0
54	MG	DB	3087	1/1	0.96	0.12	40,40,40,40	0
54	MG	AA	1635	1/1	0.96	0.07	75,75,75,75	0
54	MG	CA	1645	1/1	0.96	0.08	28,28,28,28	0
54	MG	CA	1648	1/1	0.96	0.06	39,39,39,39	0
54	MG	CA	1660	1/1	0.96	0.21	27,27,27,27	0
54	MG	BB	3020	1/1	0.96	0.07	38,38,38,38	0
54	MG	CA	1625	1/1	0.96	0.14	24,24,24,24	0
54	MG	CA	1633	1/1	0.96	0.10	50,50,50,50	0
54	MG	BB	3022	1/1	0.96	0.14	55,55,55,55	0
54	MG	DB	3072	1/1	0.97	0.10	5,5,5,5	0
54	MG	CA	1662	1/1	0.97	0.11	38,38,38,38	0
54	MG	DB	3089	1/1	0.97	0.28	28,28,28,28	0
54	MG	BB	3045	1/1	0.97	0.05	40,40,40,40	0
54	MG	AA	1643	1/1	0.97	0.07	116,116,116,116	0
54	MG	DB	3041	1/1	0.97	0.13	29,29,29,29	0
54	MG	BB	3011	1/1	0.97	0.12	9,9,9,9	0
54	MG	CA	1656	1/1	0.97	0.10	60,60,60,60	0
54	MG	DB	3091	1/1	0.97	0.16	39,39,39,39	0
54	MG	DB	3031	1/1	0.97	0.10	40,40,40,40	0
54	MG	DB	3074	1/1	0.97	0.13	12,12,12,12	0
54	MG	AA	1648	1/1	0.97	0.12	31,31,31,31	0
54	MG	BB	3029	1/1	0.97	0.10	7,7,7,7	0
54	MG	DB	3054	1/1	0.97	0.10	32,32,32,32	0

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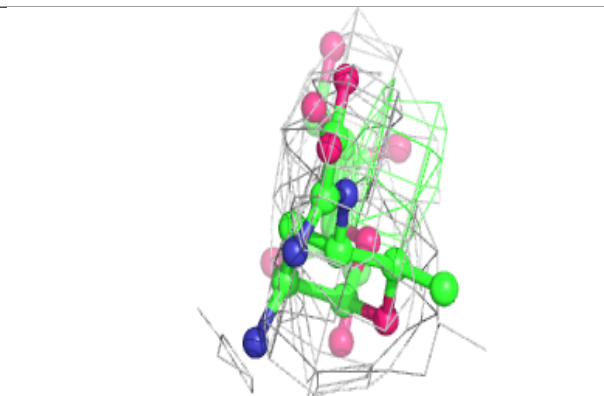
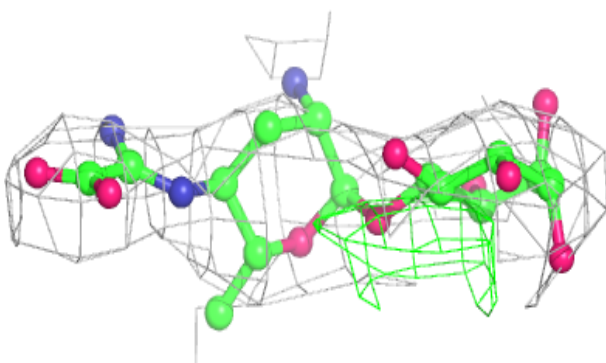
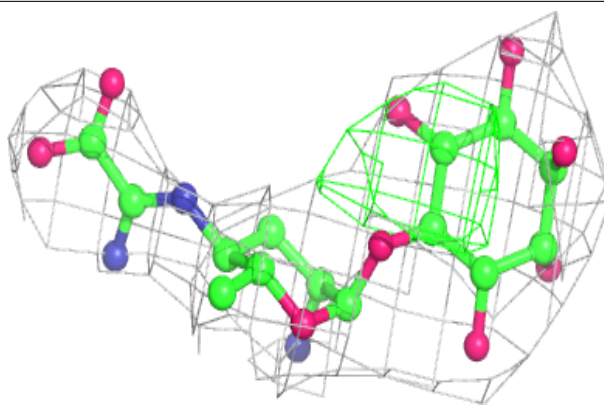
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	CA	1610	1/1	0.97	0.16	61,61,61,61	0
54	MG	BB	3015	1/1	0.97	0.10	23,23,23,23	0
54	MG	BB	3012	1/1	0.97	0.19	75,75,75,75	0
54	MG	DB	3077	1/1	0.97	0.12	41,41,41,41	0
54	MG	BB	3058	1/1	0.97	0.12	33,33,33,33	0
54	MG	DB	3078	1/1	0.97	0.08	5,5,5,5	0
54	MG	DB	3084	1/1	0.97	0.18	18,18,18,18	0
54	MG	BB	3025	1/1	0.97	0.15	67,67,67,67	0
54	MG	AA	1659	1/1	0.97	0.20	157,157,157,157	0
54	MG	AA	1610	1/1	0.98	0.16	10,10,10,10	0
54	MG	DB	3005	1/1	0.98	0.09	6,6,6,6	0
54	MG	DB	3063	1/1	0.98	0.11	42,42,42,42	0
54	MG	BB	3070	1/1	0.98	0.09	55,55,55,55	0
54	MG	DB	3006	1/1	0.98	0.08	16,16,16,16	0
54	MG	BB	3095	1/1	0.98	0.06	48,48,48,48	0
54	MG	CA	1618	1/1	0.98	0.08	26,26,26,26	0
54	MG	BB	3002	1/1	0.98	0.09	9,9,9,9	0
54	MG	DB	3096	1/1	0.99	0.17	31,31,31,31	0
54	MG	DB	3019	1/1	0.99	0.03	8,8,8,8	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

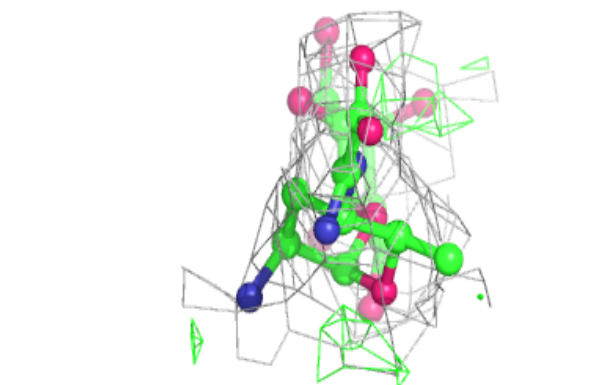
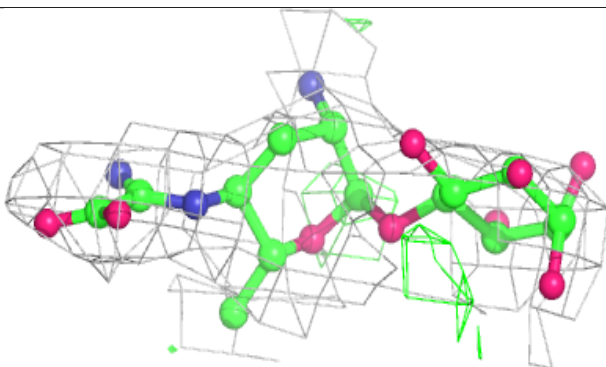
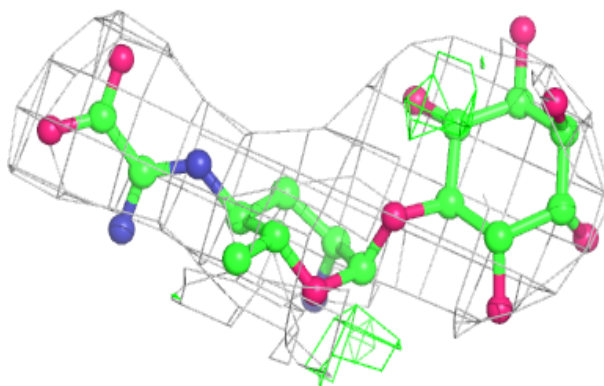


**Electron density around KSG CA 1601:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around KSG AA 1601:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.