



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 02:40 am BST

PDB ID : 4V5Y  
Title : Crystal structure of the bacterial ribosome from Escherichia coli in complex with paromomycin and ribosome recycling factor (RRF).  
Authors : Borovinskaya, M.A.; Pai, R.D.; Zhang, W.; Schuwirth, B.-S.; Holton, J.M.; Hirokawa, G.; Kaji, H.; Kaji, A.; Cate, J.H.D.  
Deposited on : 2007-06-19  
Resolution : 4.45 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

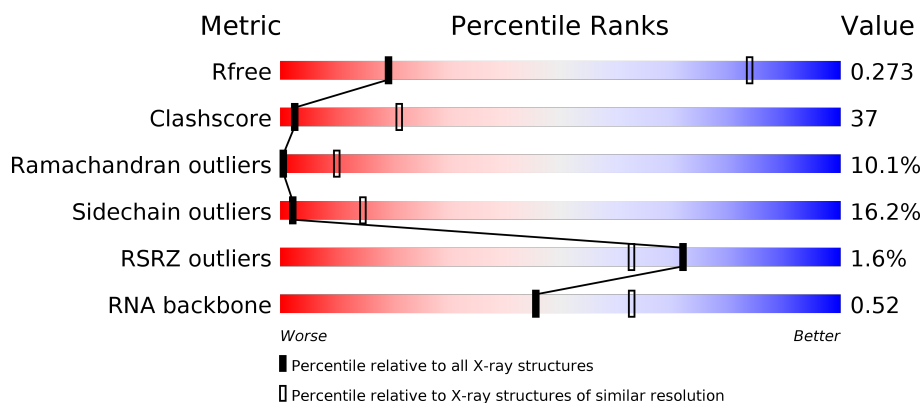
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.45 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1051 (5.12-3.80)
Clashscore	141614	1119 (5.12-3.80)
Ramachandran outliers	138981	1065 (5.12-3.80)
Sidechain outliers	138945	1047 (5.12-3.80)
RSRZ outliers	127900	1099 (5.20-3.70)
RNA backbone	3102	1060 (5.90-3.00)

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>64%</div> <div>12%</div> <div>.</div> </div>
1	CA	1542	<div> <div>24%</div> <div>63%</div> <div>11%</div> <div>.</div> </div>
2	AC	232	<div> <div>2%</div> <div>28%</div> <div>47%</div> <div>13%</div> <div>11%</div> </div>
2	CC	232	<div> <div>30%</div> <div>45%</div> <div>13%</div> <div>11%</div> </div>

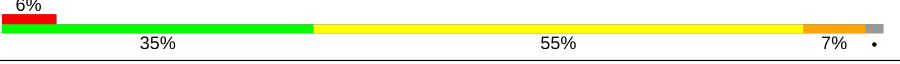

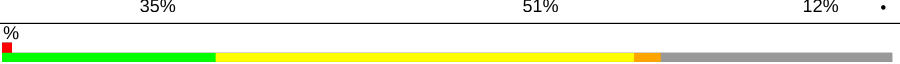
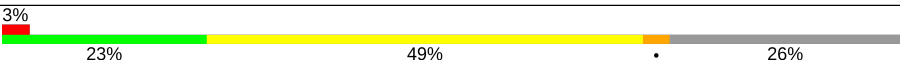
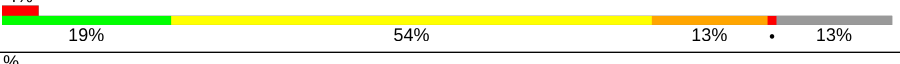
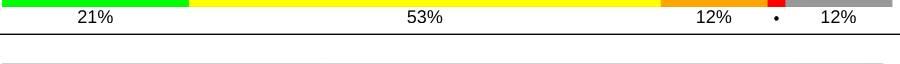
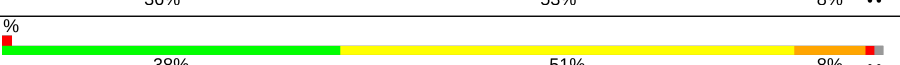
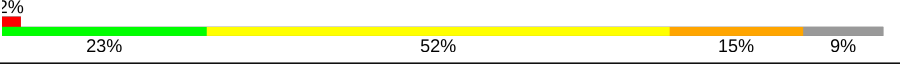
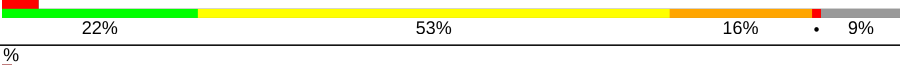

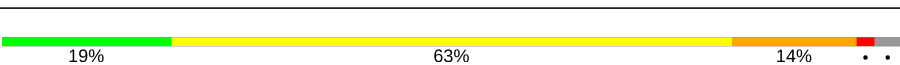
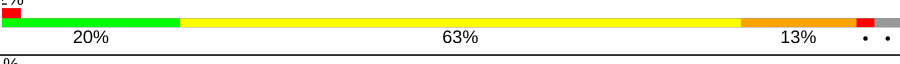
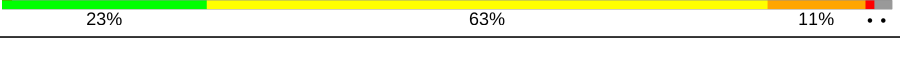
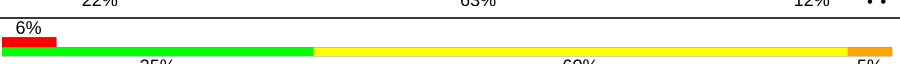

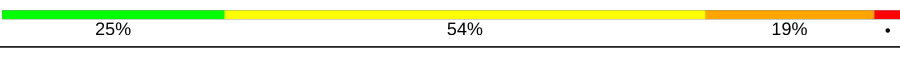
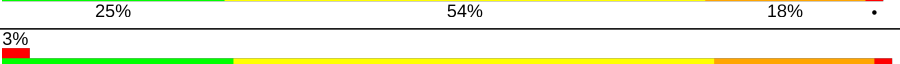
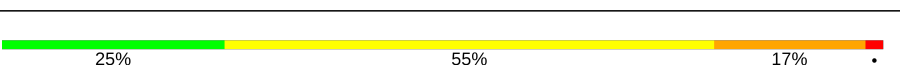
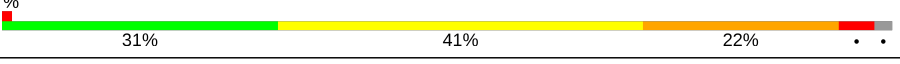
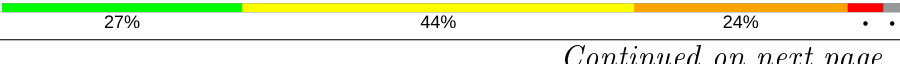



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Mol	Chain	Length	Quality of chain
3	AD	205	
3	CD	205	
4	AE	166	
4	CE	166	
5	AF	135	
5	CF	135	
6	AG	178	
6	CG	178	
7	AH	129	
7	CH	129	
8	AI	129	
8	CI	129	
9	AJ	103	
9	CJ	103	
10	AK	128	
10	CK	128	
11	AL	123	
11	CL	123	
12	AM	117	
12	CM	117	
13	AN	100	
13	CN	100	
14	AO	89	
14	CO	89	
15	AP	82	



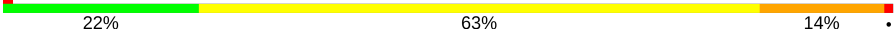
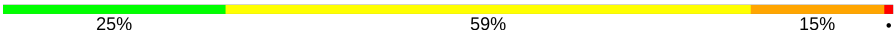
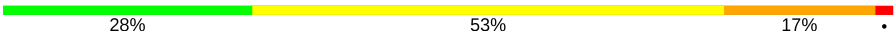
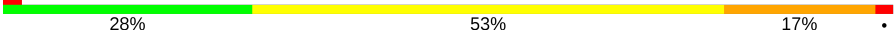
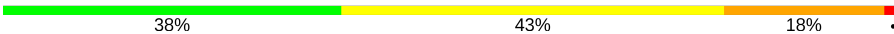
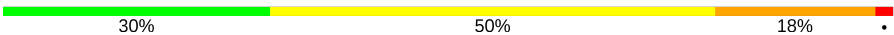
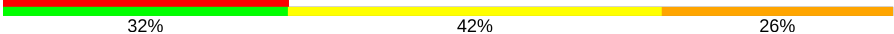
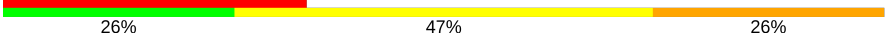
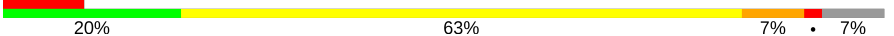
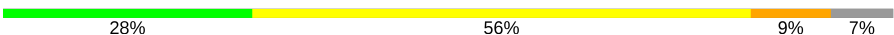
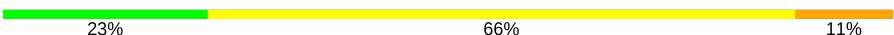





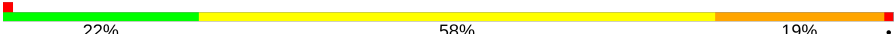
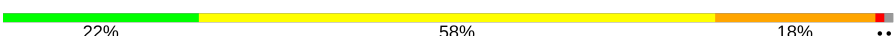
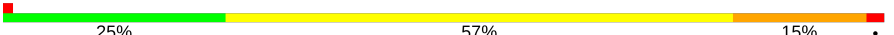
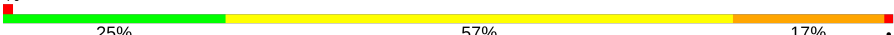



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Mol	Chain	Length	Quality of chain
15	CP	82	
16	AQ	83	
16	CQ	83	
17	AR	74	
17	CR	74	
18	AS	91	
18	CS	91	
19	AT	86	
19	CT	86	
20	AB	240	
20	CB	240	
21	AU	70	
21	CU	70	
22	BA	120	
22	DA	120	
23	BB	2904	
23	DB	2904	
24	BI	141	
24	DI	141	
25	BC	272	
25	DC	272	
26	BD	209	
26	DD	209	
27	BK	123	
27	DK	123	

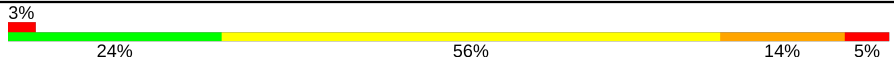
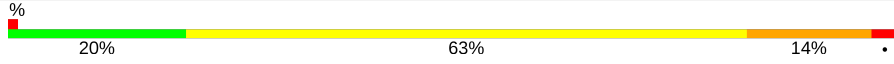
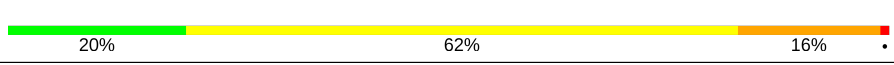
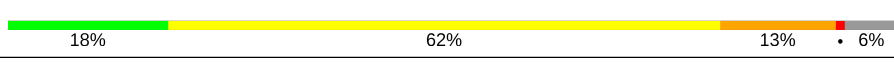
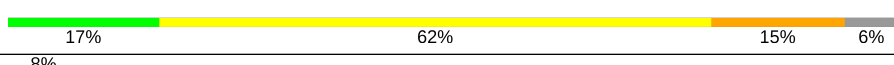
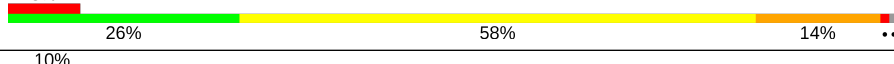
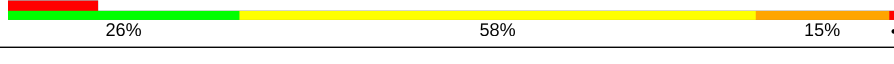
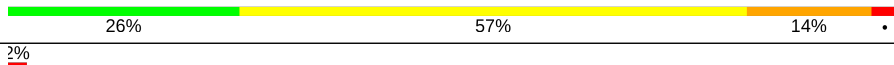
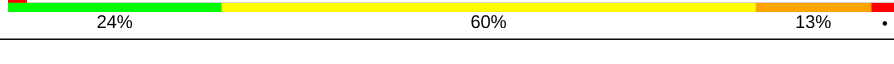
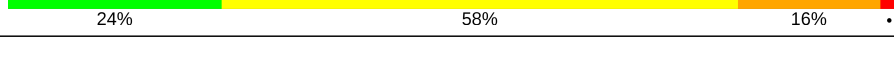
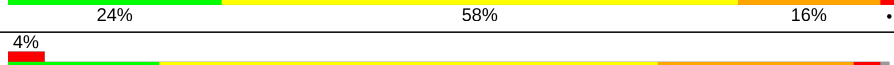
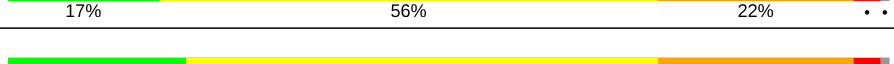
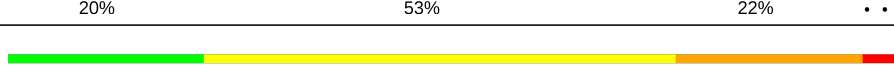
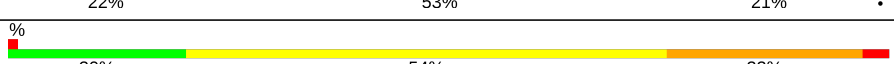
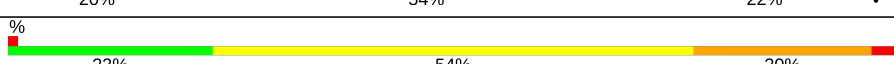
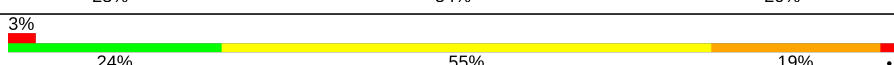
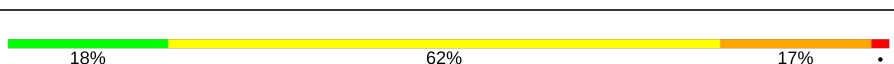
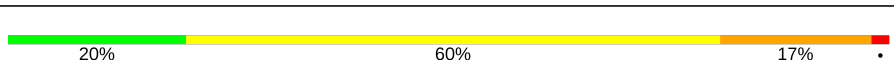
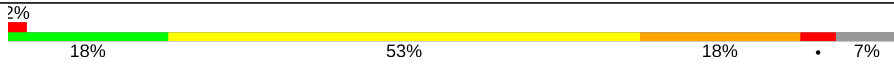
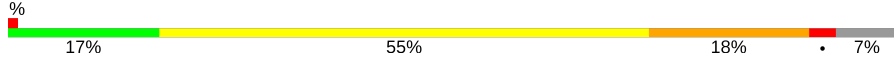
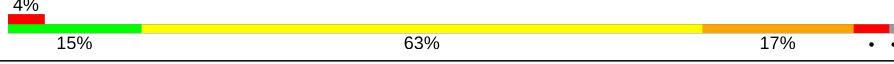
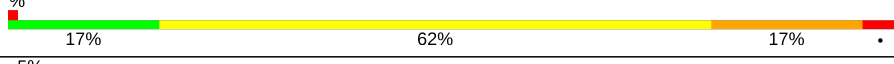

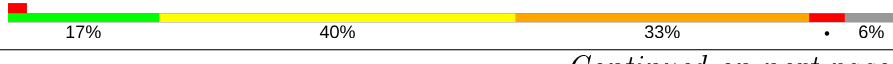

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Mol	Chain	Length	Quality of chain
28	BP	114	
28	DP	114	
29	BE	201	
29	DE	201	
30	BY	58	
30	DY	58	
31	B0	56	
31	D0	56	
32	B4	38	
32	D4	38	
33	B1	54	
33	D1	54	
34	B3	64	
34	D3	64	
35	BV	94	
35	DV	94	
36	B2	46	
36	D2	46	
37	BL	144	
37	DL	144	
38	BM	136	
38	DM	136	
39	BX	63	
39	DX	63	
40	BH	149	

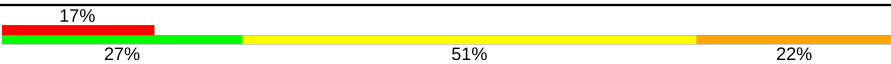

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Mol	Chain	Length	Quality of chain
40	DH	149	
41	BJ	142	
41	DJ	142	
42	BN	127	
42	DN	127	
43	BO	117	
43	DO	117	
44	BQ	117	
44	DQ	117	
45	BS	110	
45	DS	110	
46	BU	103	
46	DU	103	
47	BF	178	
47	DF	178	
48	BG	176	
48	DG	176	
49	BR	103	
49	DR	103	
50	BT	100	
50	DT	100	
51	BZ	78	
51	DZ	78	
52	BW	84	
52	DW	84	

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Mol	Chain	Length	Quality of chain
53	B6	185	
53	D6	185	

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	1608	-	-	-	X
54	MG	AA	1626	-	-	-	X
54	MG	AA	1632	-	-	-	X
54	MG	AA	1639	-	-	-	X
54	MG	AA	1657	-	-	-	X
54	MG	AA	1659	-	-	-	X
54	MG	CA	1608	-	-	-	X
54	MG	CA	1657	-	-	-	X
54	MG	CE	201	-	-	-	X
54	MG	DB	3052	-	-	-	X
55	PAR	BB	3111	-	-	-	X

## 2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 287128 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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 rRNA.

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 L11.

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

- Molecule 25 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			
25	DC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	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 L14.

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

- Molecule 28 is a protein called 50S ribosomal protein L19.

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

- Molecule 29 is a protein called 50S ribosomal protein L4.

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

- Molecule 30 is a protein called 50S ribosomal protein L30.

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

- Molecule 31 is a protein called 50S ribosomal protein L32.

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

- Molecule 32 is a protein called 50S ribosomal protein L36.

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

- Molecule 33 is a protein called 50S ribosomal protein L33.

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

- Molecule 34 is a protein called 50S ribosomal protein L35.

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

- Molecule 35 is a protein called 50S ribosomal protein L25.

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

- Molecule 36 is a protein called 50S ribosomal protein L34.

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

- Molecule 37 is a protein called 50S ribosomal protein L15.

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

- Molecule 38 is a protein called 50S ribosomal protein L16.

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

- Molecule 39 is a protein called 50S ribosomal protein L29.

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

- Molecule 40 is a protein called 50S ribosomal protein L9.

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

- Molecule 41 is a protein called 50S ribosomal protein L13.

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

- Molecule 42 is a protein called 50S ribosomal protein L17.

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

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

- Molecule 43 is a protein called 50S ribosomal protein L18.

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

- Molecule 44 is a protein called 50S ribosomal protein L20.

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

- Molecule 45 is a protein called 50S ribosomal protein L22.

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

- Molecule 46 is a protein called 50S ribosomal protein L24.

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

- Molecule 47 is a protein called 50S ribosomal protein L5.

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



- Molecule 48 is a protein called 50S ribosomal protein L6.

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

- Molecule 49 is a protein called 50S ribosomal protein L21.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BZ	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			
51	DZ	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			

- Molecule 52 is a protein called 50S ribosomal protein L27.

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

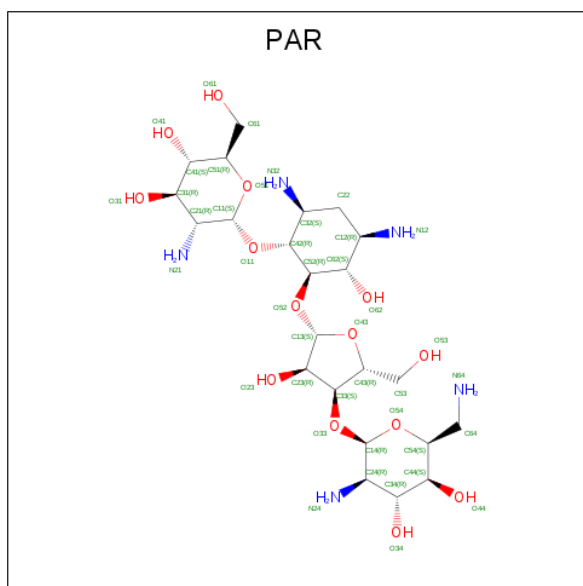
- Molecule 53 is a protein called 50S ribosomal protein RRF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B6	185	Total	C	N	O	S	0	0	0
			1478	924	270	282	2			
53	D6	185	Total	C	N	O	S	0	0	0
			1478	924	270	282	2			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	DB	111	Total	Mg	0	0
			111	111		
54	BB	110	Total	Mg	0	0
			110	110		
54	AA	60	Total	Mg	0	0
			60	60		
54	CA	61	Total	Mg	0	0
			61	61		
54	CE	1	Total	Mg	0	0
			1	1		

- Molecule 55 is PAROMOMYCIN (three-letter code: PAR) (formula: C<sub>23</sub>H<sub>45</sub>N<sub>5</sub>O<sub>14</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
55	AA	1	Total	C	N	O	0	0
			42	23	5	14		
55	BB	1	Total	C	N	O	0	0
			42	23	5	14		
55	CA	1	Total	C	N	O	0	0
			42	23	5	14		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
55	DB	1	Total	C	N	O	0	0
			42	23	5	14		

- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 57 is water.

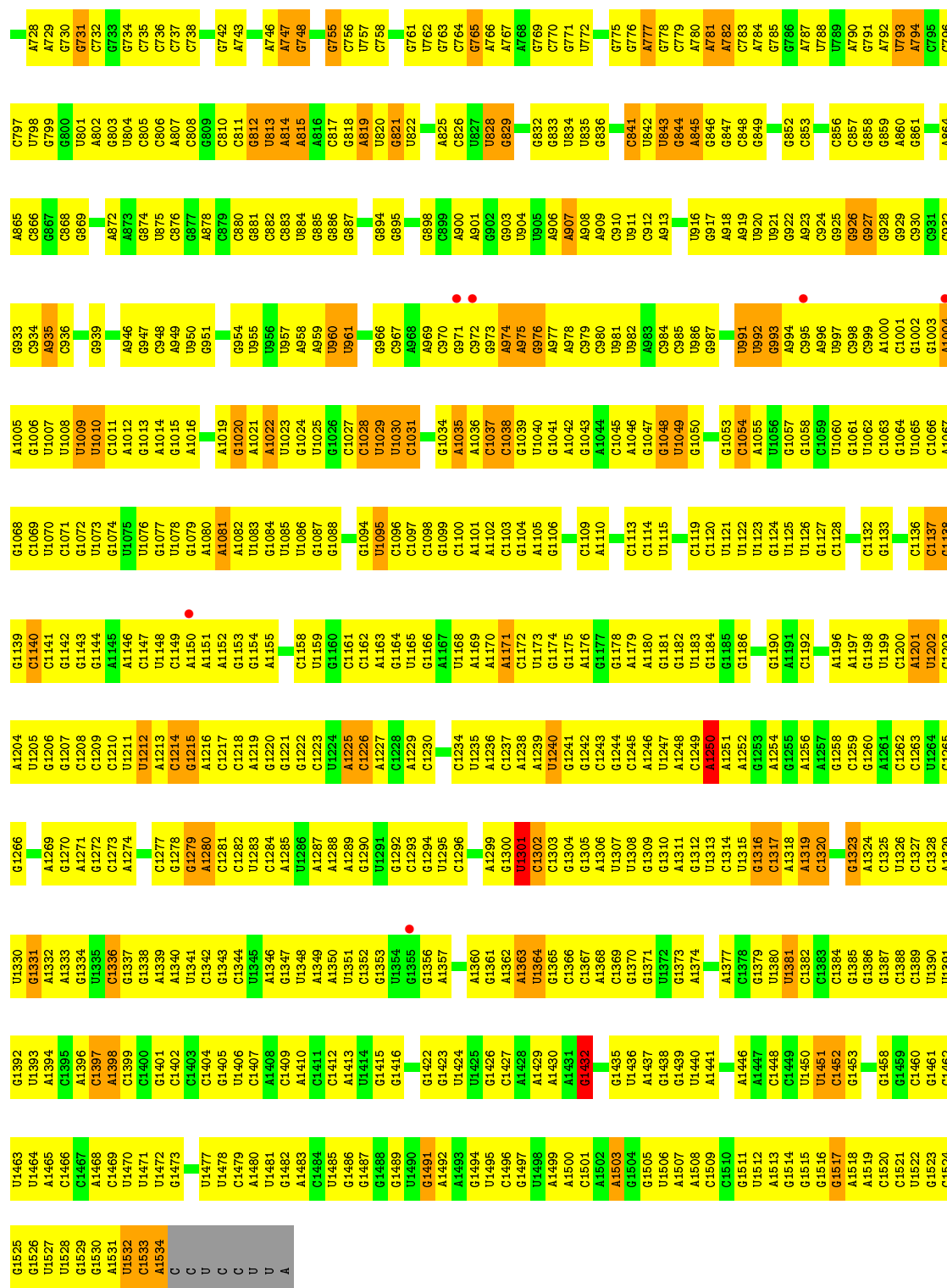
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	AA	291	Total	O	0	0
			291	291		
57	AL	3	Total	O	0	0
			3	3		
57	AN	4	Total	O	0	0
			4	4		
57	AT	2	Total	O	0	0
			2	2		
57	BB	495	Total	O	0	0
			495	495		
57	BC	6	Total	O	0	0
			6	6		
57	BD	1	Total	O	0	0
			1	1		
57	BE	2	Total	O	0	0
			2	2		
57	BL	1	Total	O	0	0
			1	1		
57	BT	1	Total	O	0	0
			1	1		
57	CA	296	Total	O	0	0
			296	296		
57	CE	3	Total	O	0	0
			3	3		
57	CL	4	Total	O	0	0
			4	4		
57	CN	4	Total	O	0	0
			4	4		

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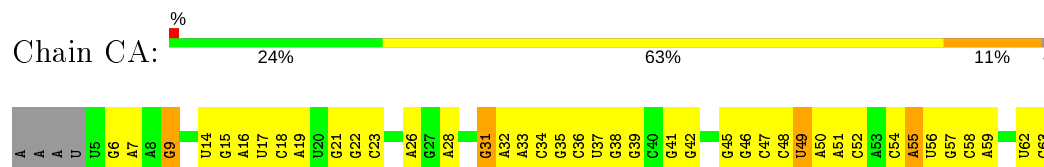
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	CP	1	Total 1	O 1	0	0
57	CT	1	Total 1	O 1	0	0
57	DB	502	Total 502	O 502	0	0
57	DC	4	Total 4	O 4	0	0
57	DD	1	Total 1	O 1	0	0
57	DE	1	Total 1	O 1	0	0
57	DL	2	Total 2	O 2	0	0
57	DQ	1	Total 1	O 1	0	0
57	DR	1	Total 1	O 1	0	0

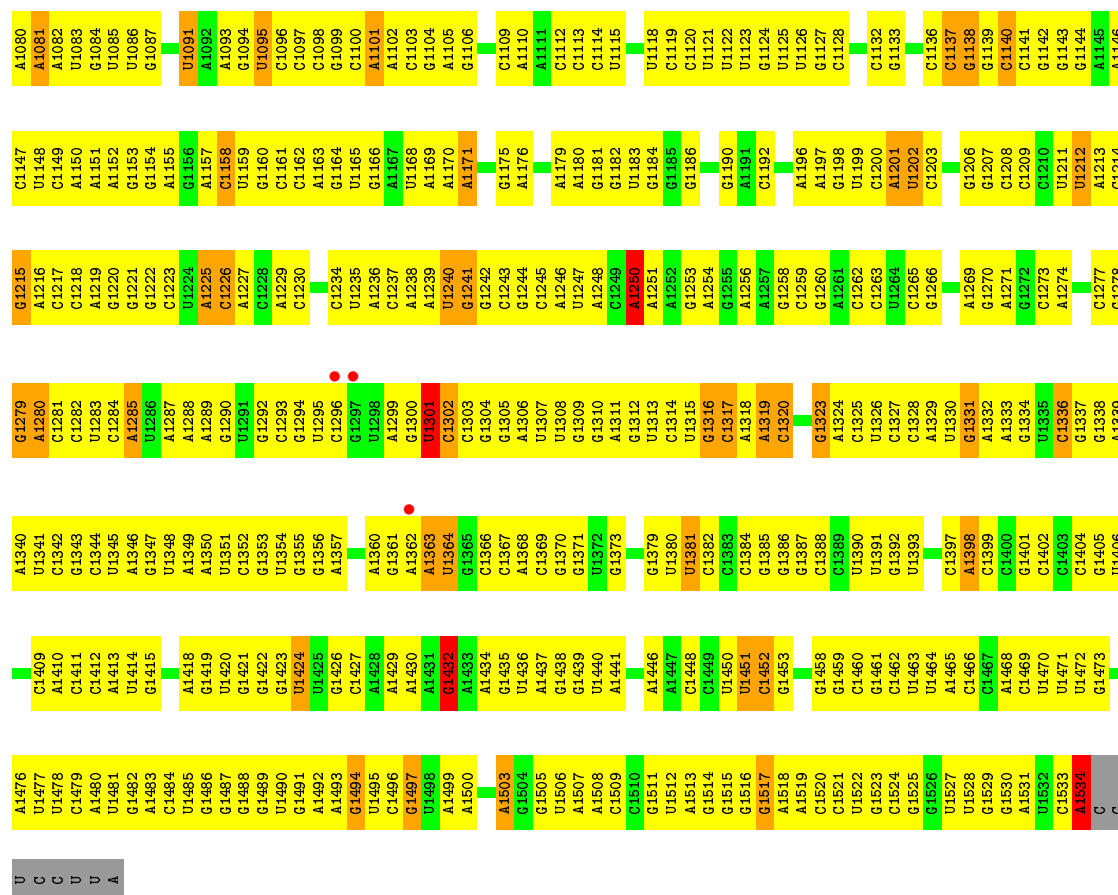




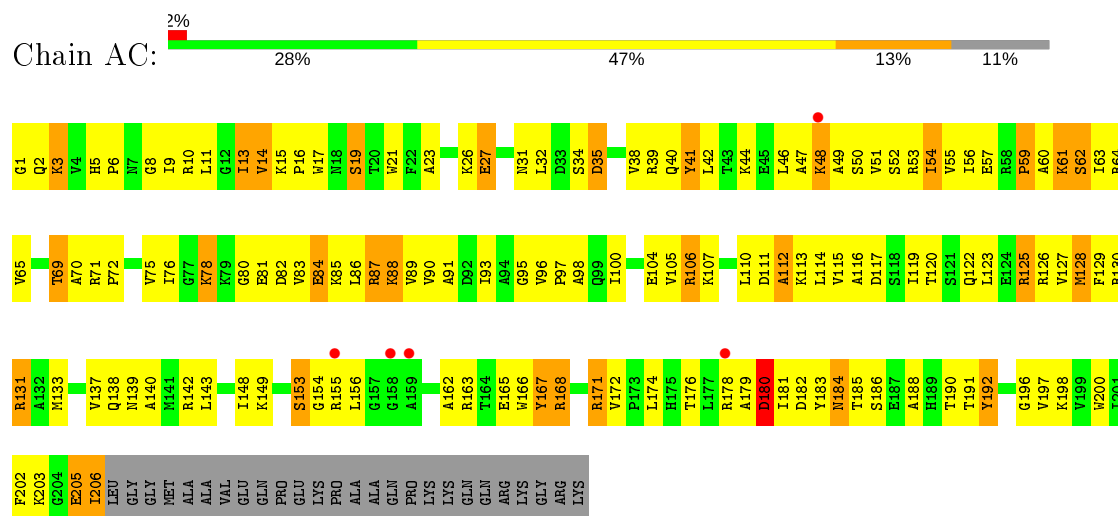
- Molecule 1: 16S rRNA



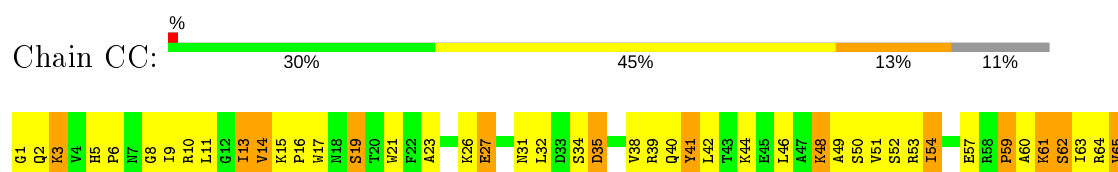
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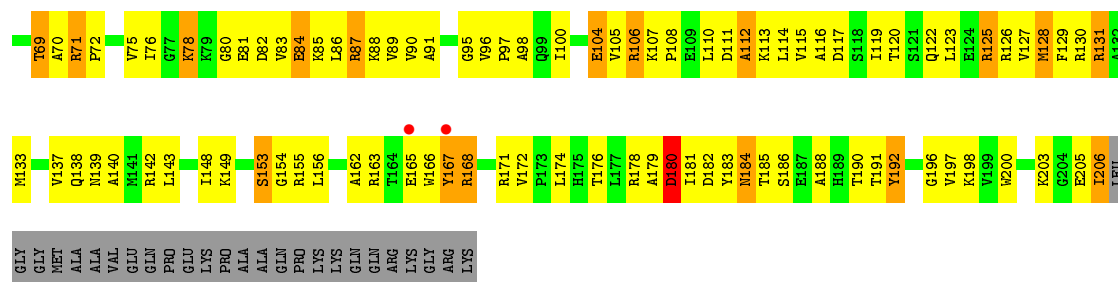
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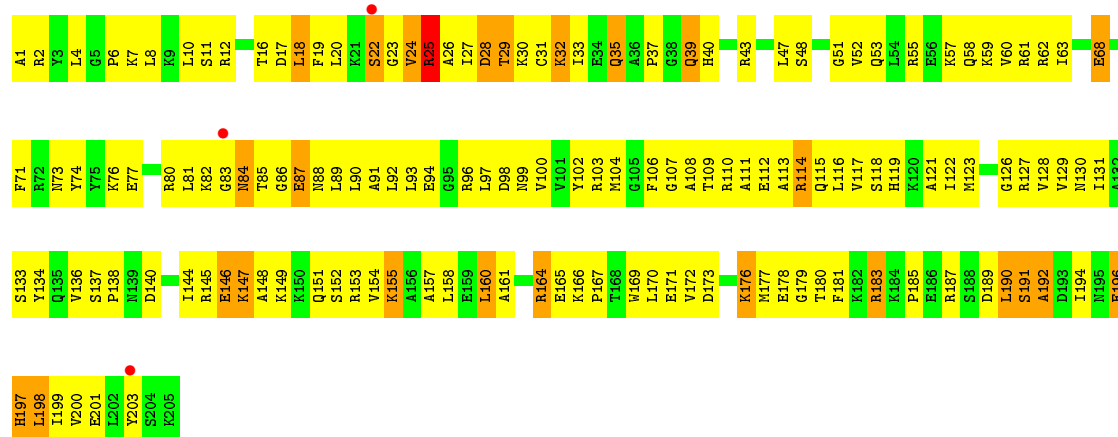
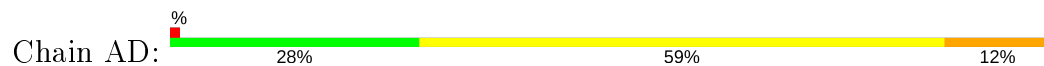
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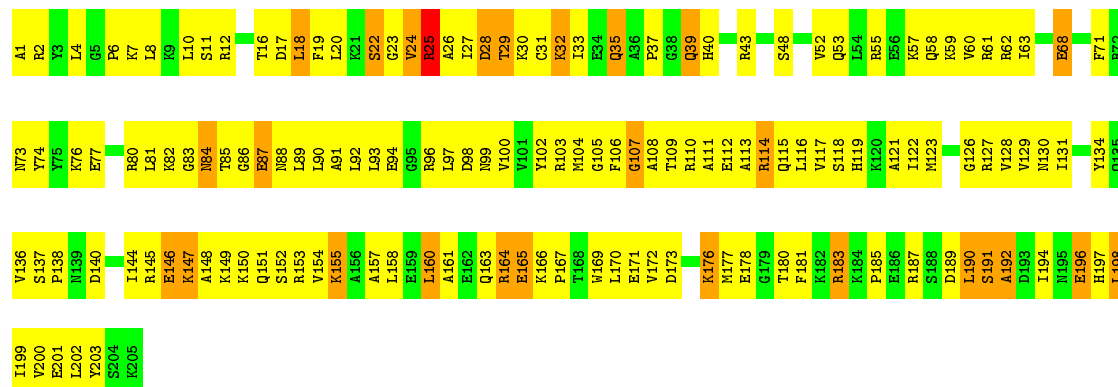




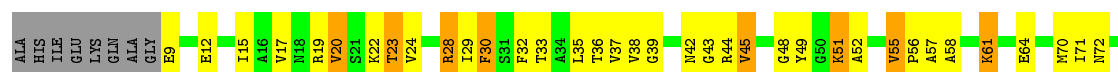
• Molecule 3: 30S ribosomal protein S4



• Molecule 3: 30S ribosomal protein S4

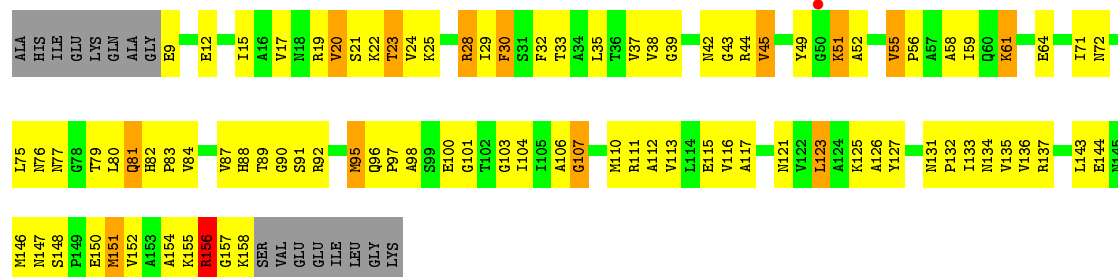


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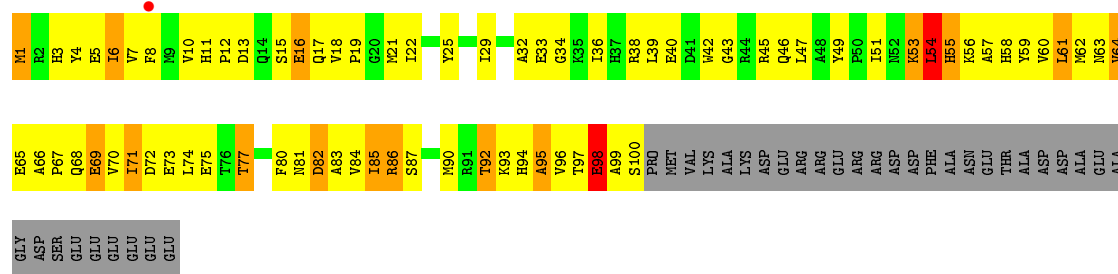
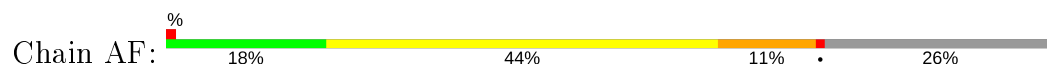




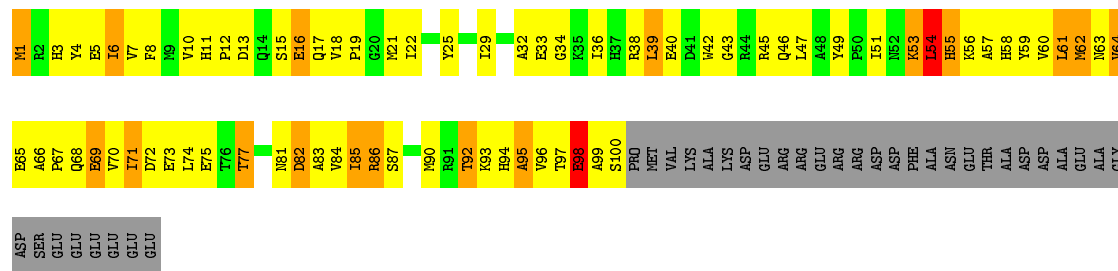
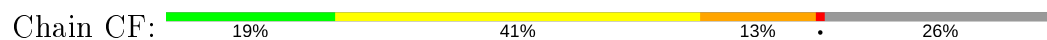
• Molecule 4: 30S ribosomal protein S5



• Molecule 5: 30S ribosomal protein S6

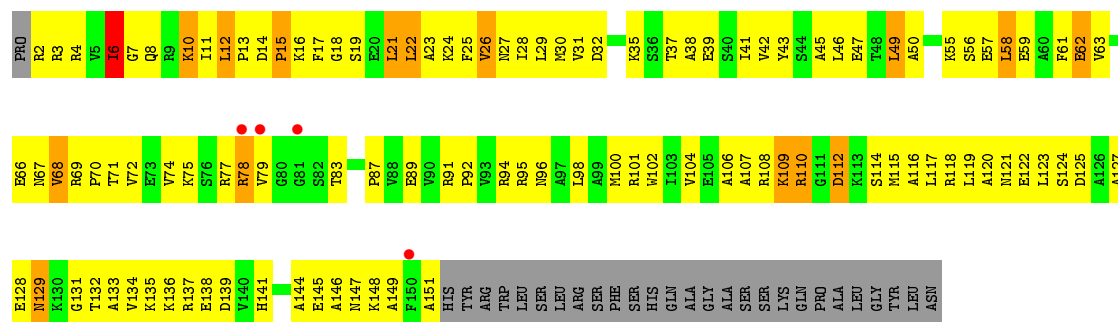


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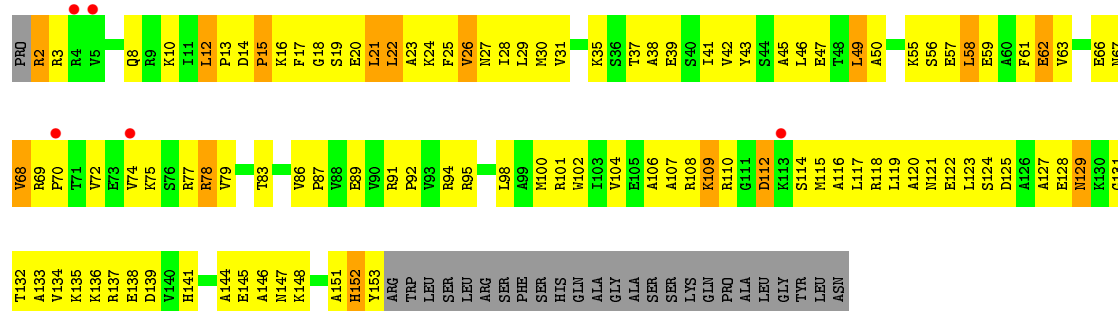


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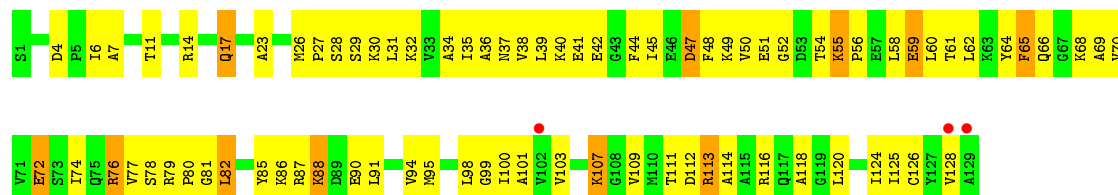
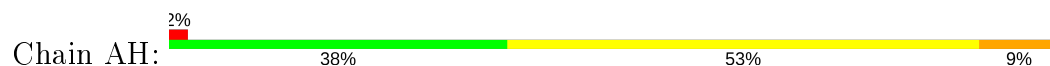




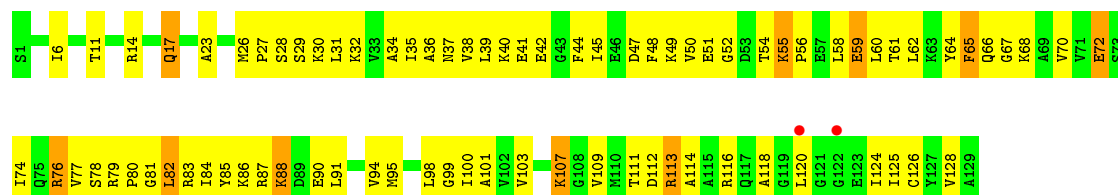
• Molecule 6: 30S ribosomal protein S7



• Molecule 7: 30S ribosomal protein S8

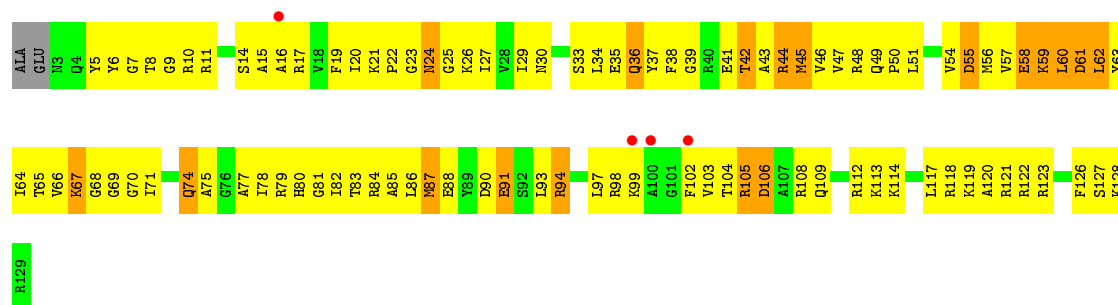


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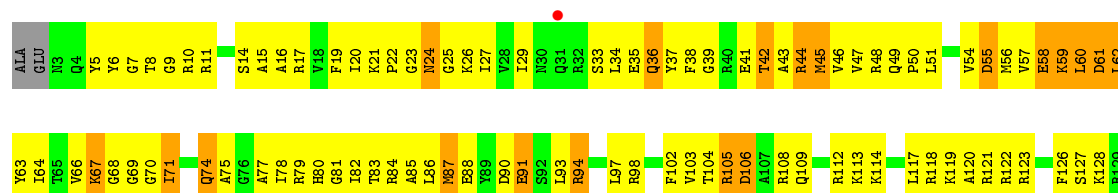


• Molecule 8: 30S ribosomal protein S9

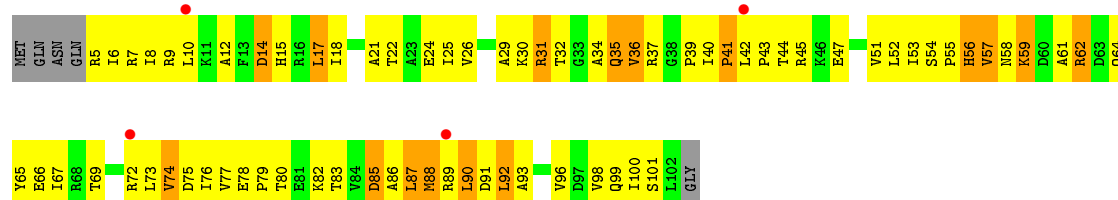




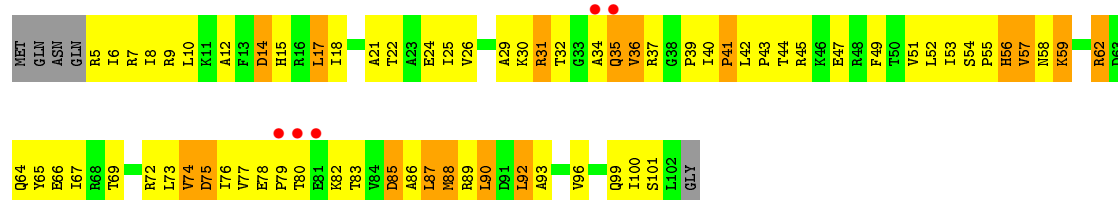
• Molecule 8: 30S ribosomal protein S9



• Molecule 9: 30S ribosomal protein S10

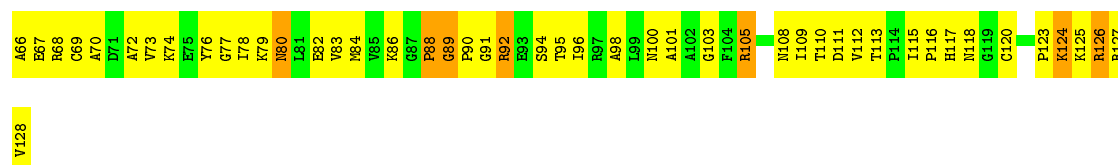


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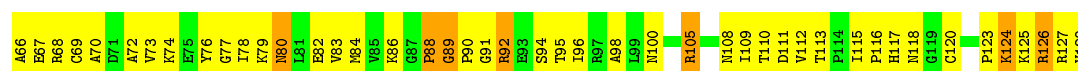


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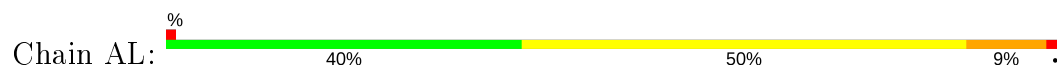




- Molecule 10: 30S ribosomal protein S11



- Molecule 11: 30S ribosomal protein S12



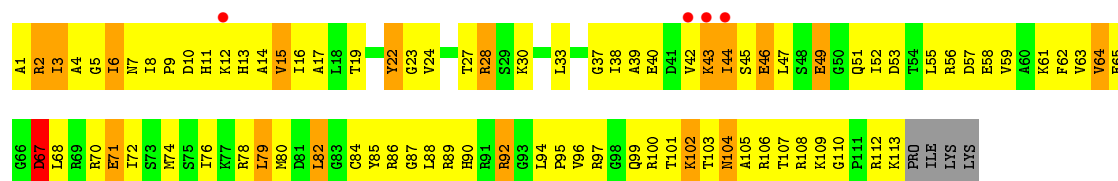
- Molecule 11: 30S ribosomal protein S12



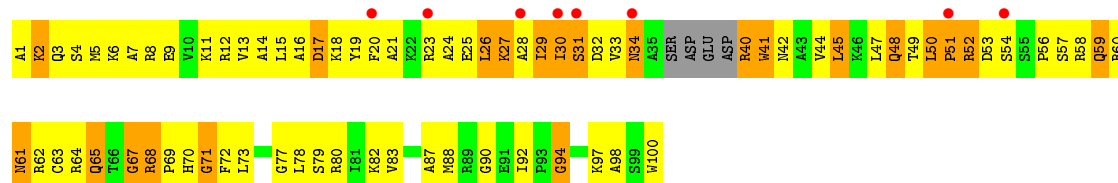
- Molecule 12: 30S ribosomal protein S13



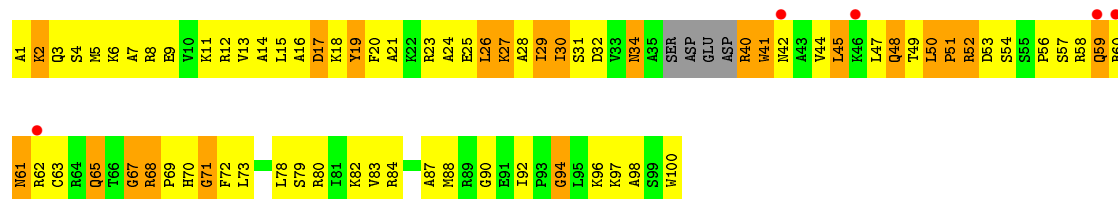
- Molecule 12: 30S ribosomal protein S13



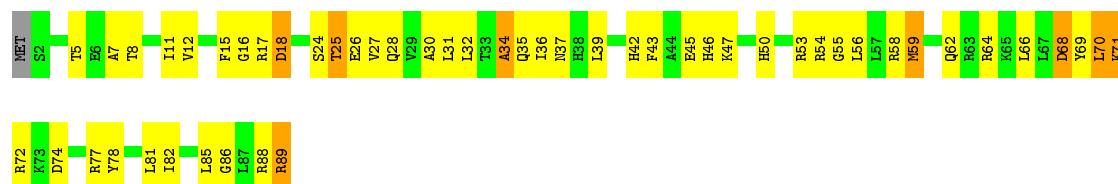
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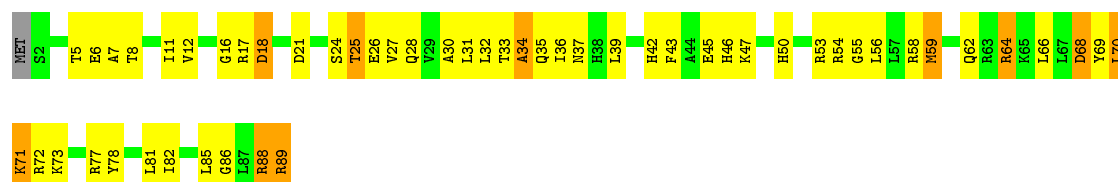
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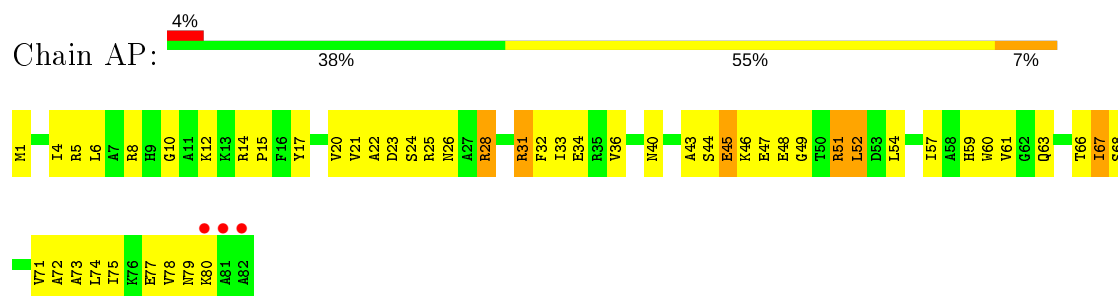
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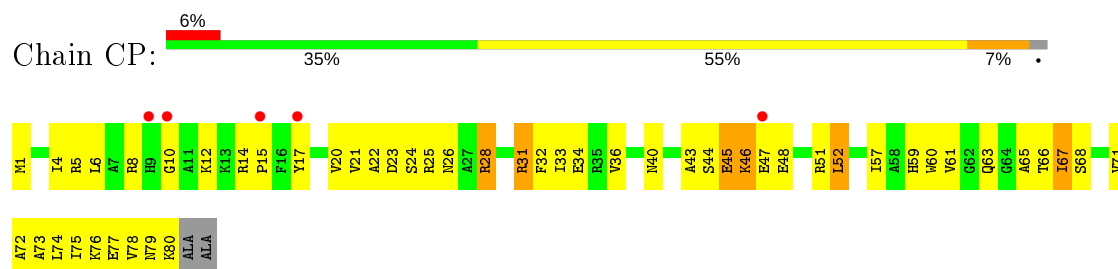
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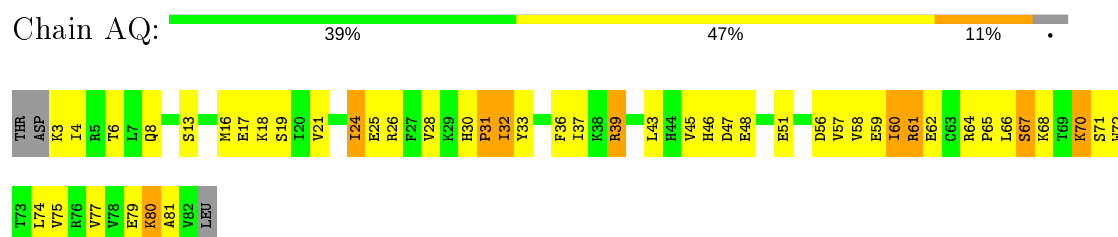
- Molecule 15: 30S ribosomal protein S16



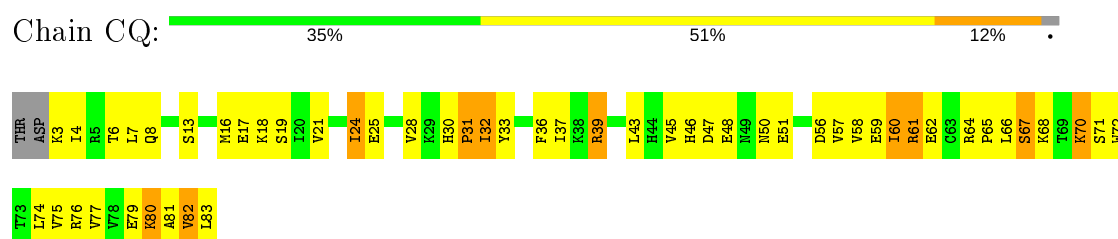
- Molecule 15: 30S ribosomal protein S16



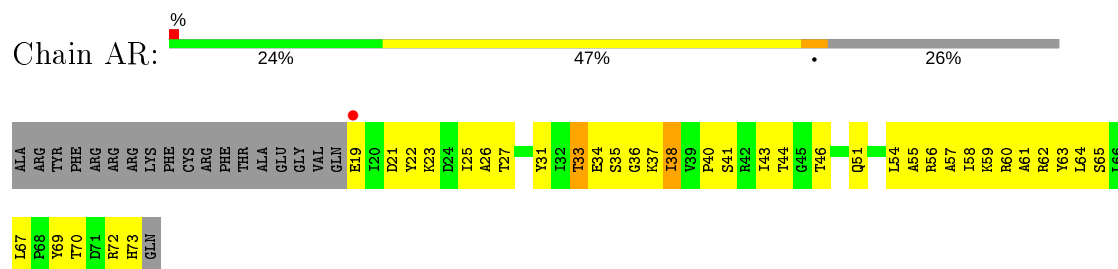
- Molecule 16: 30S ribosomal protein S17



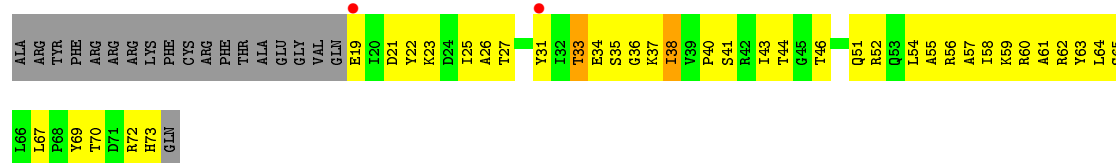
- Molecule 16: 30S ribosomal protein S17



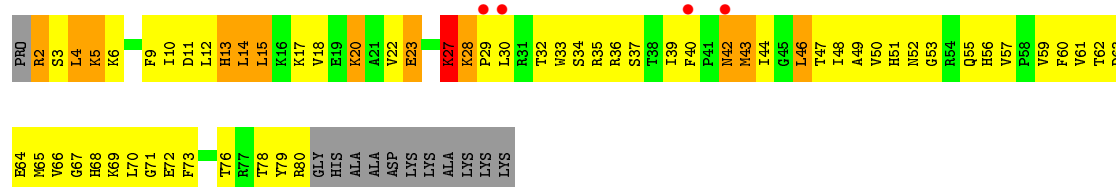
- Molecule 17: 30S ribosomal protein S18



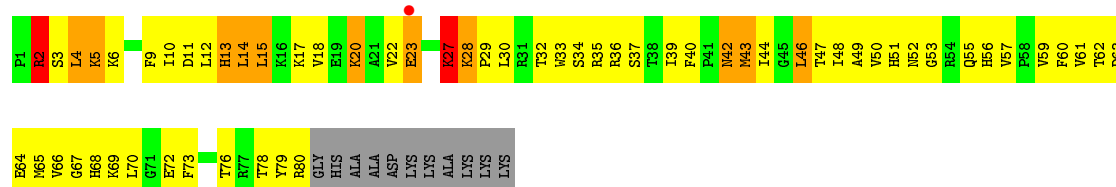
- Molecule 17: 30S ribosomal protein S18



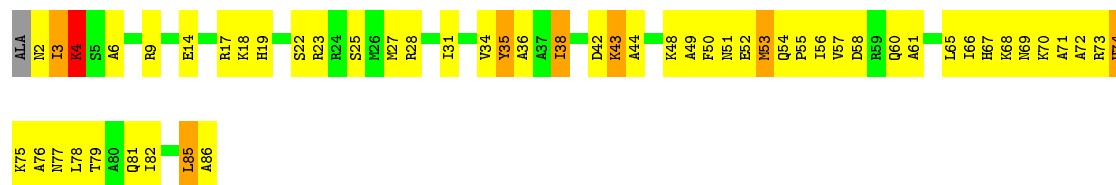
- Molecule 18: 30S ribosomal protein S19



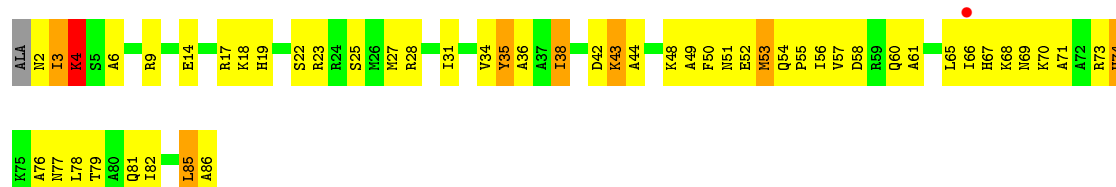
- Molecule 18: 30S ribosomal protein S19



- Molecule 19: 30S ribosomal protein S20

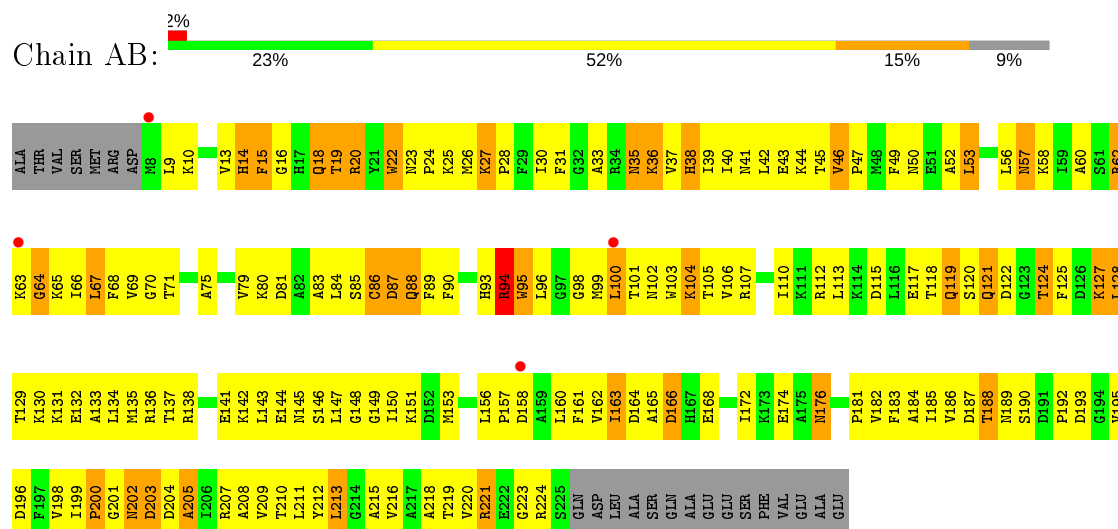


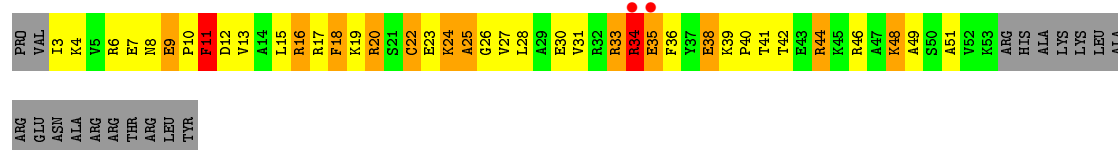
- Molecule 19: 30S ribosomal protein S20





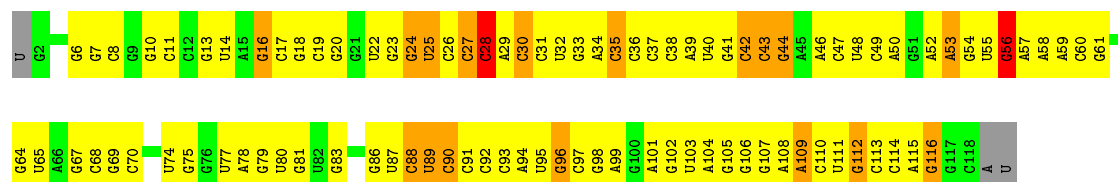
- Molecule 20: 30S ribosomal protein S2





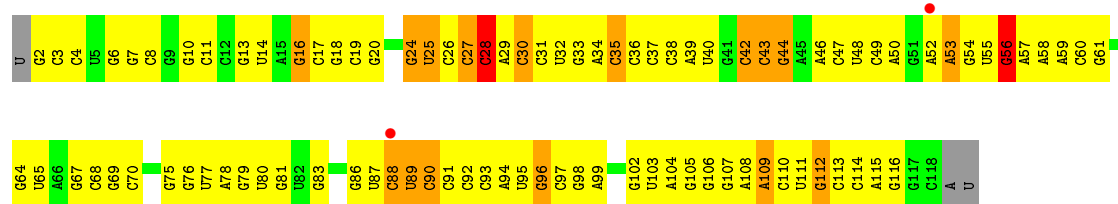
• Molecule 22: 5S rRNA

Chain BA: 19% 63% 14% . .



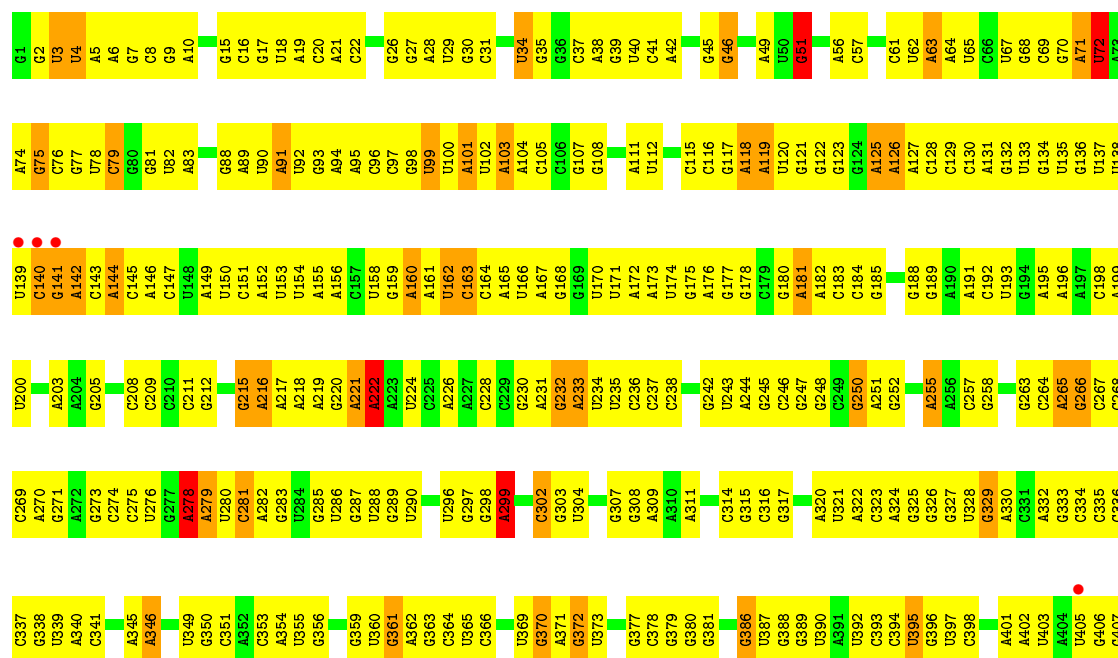
• Molecule 22: 5S rRNA

Chain DA: 2% 20% 63% 13% . .



• Molecule 23: 23S rRNA

Chain BB: % 23% 63% 11% . .



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A1260	A1194	A1133	A1069	A1009	G936	G874	C812	C740	C679	U615	G549	A481	G409
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	C1135	G1071	A1070	A1009	A941	G876	C814	A742	G681	G617	C551	A483	G411
G1266	G1197	G1136	G1072	G1011	A942	A877	C815	A743	G682	U618	C552	C484	G412
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A1268	G1199	G1138	G1074	U1013	G944	G	C817	G745	U684	G620	U554	C486	C414
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G1271	G1202	U1141	A1080	U1015	C947	G	A820		C687	G623	U558	C418	C417
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G1277	G1208	C1147	A1086	U1022		C	U826	G758	A693	G629	C564		A424
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	G1210	G1149	A1088	G1024	C956	C	A828	A764	G695	A631	U569	U499	C426
A1283	C1211	C1150	A1089	G1025	C957	G	A829	C765	G696	A632	G570	A501	U427
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G1299	U1231	C1166	C1104	A1040			A845	A783		U648	C586	C517	A443
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A1308	A1242	A1175	U1113	C1049	C986	A918	C854		A722	G659	C596	A526	C456
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	U1245	C1178	C1116	C1052	G989	C921	G857	C796	G725	G662	U598		U459
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	U1255	A1189	G1082	G1062	U999	A833		C806	A735		G611		
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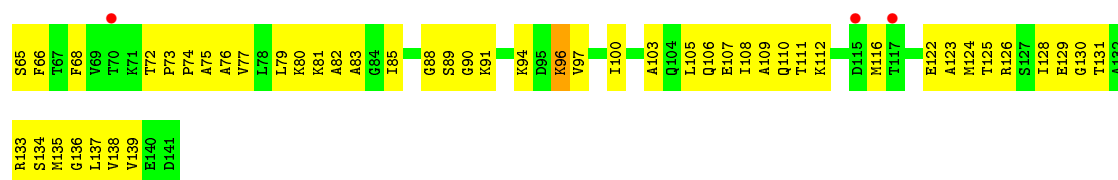
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• Molecule 24: 50S ribosomal protein L11

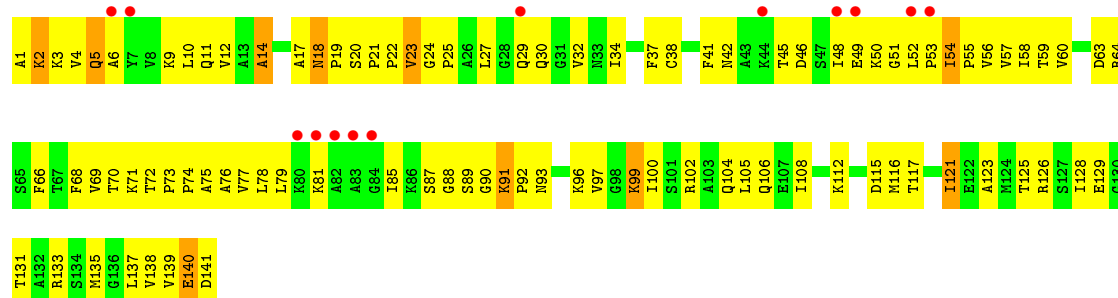


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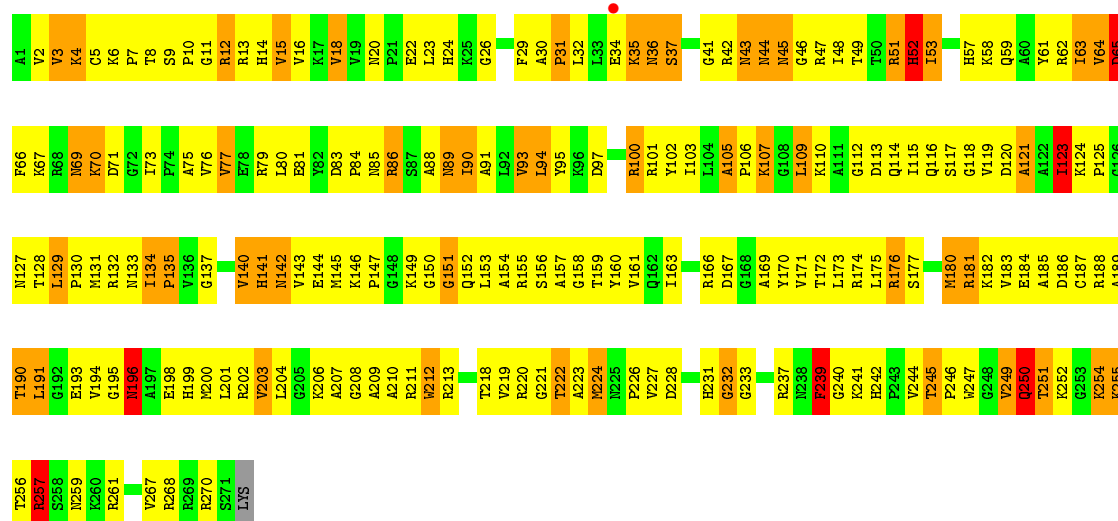




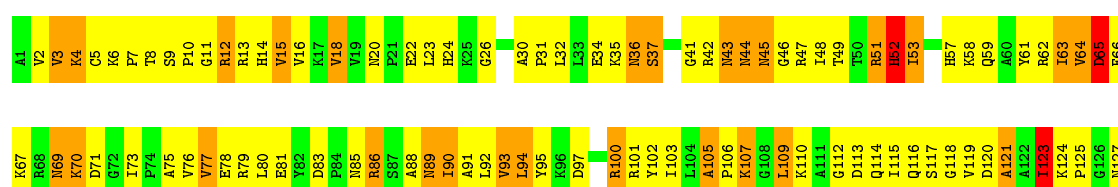
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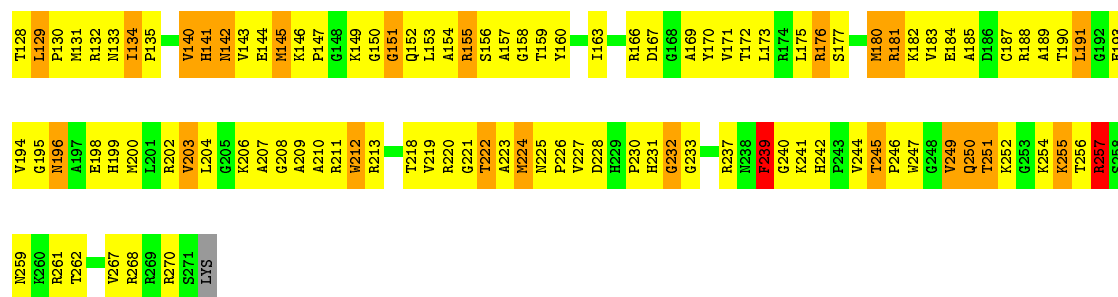


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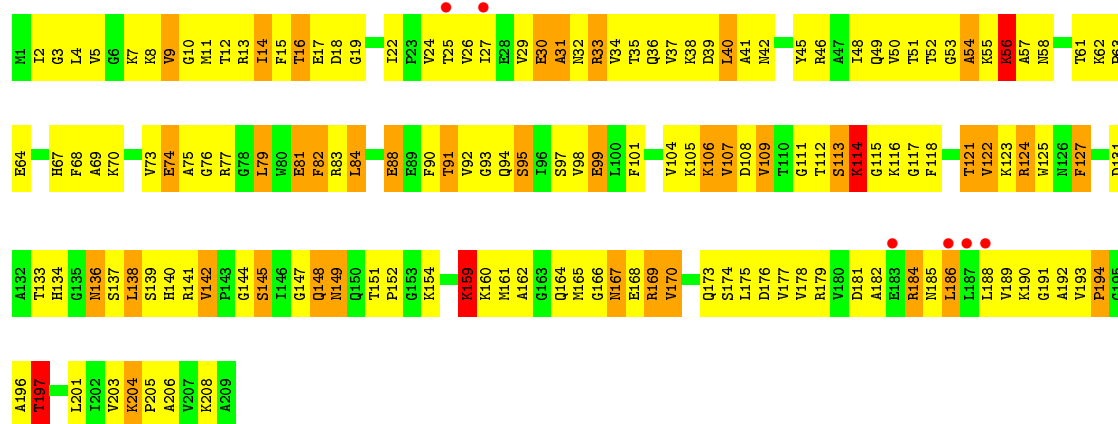


• Molecule 25: 50S ribosomal protein L2

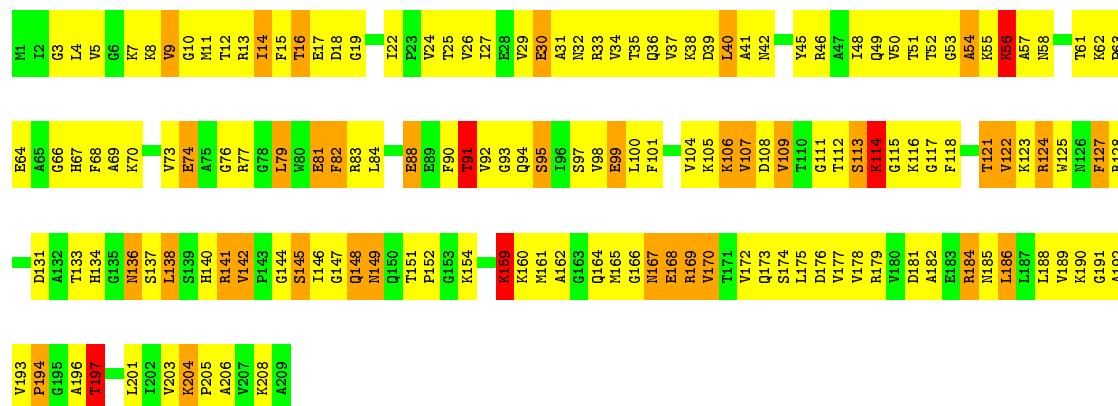




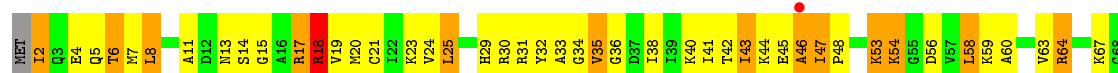
• Molecule 26: 50S ribosomal protein L3



• Molecule 26: 50S ribosomal protein L3

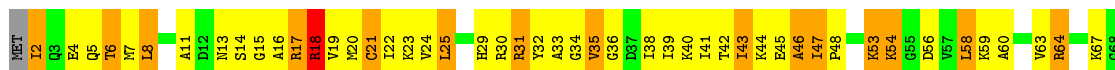


• Molecule 27: 50S ribosomal protein L14

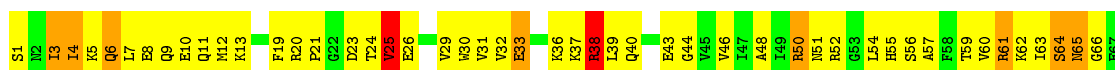




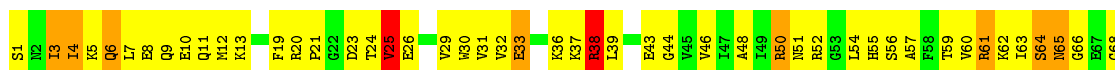
- Molecule 27: 50S ribosomal protein L14



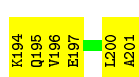
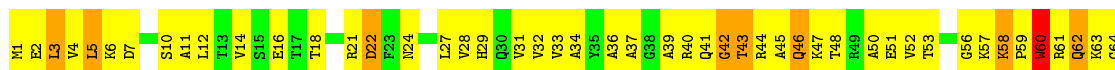
- Molecule 28: 50S ribosomal protein L19



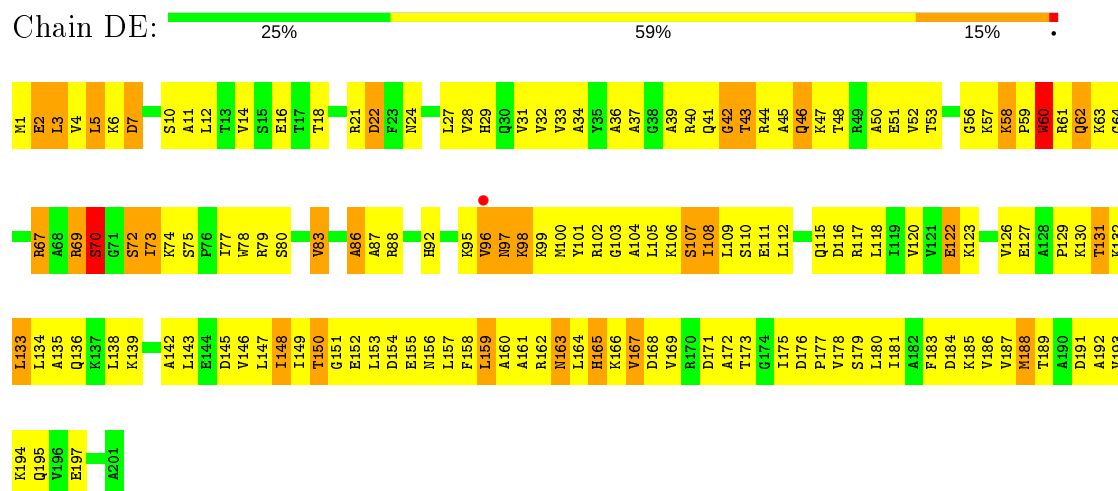
- Molecule 28: 50S ribosomal protein L19



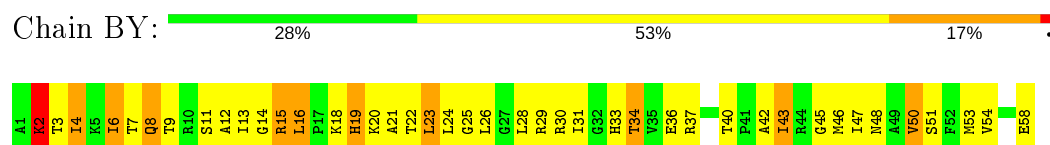
- Molecule 29: 50S ribosomal protein L4



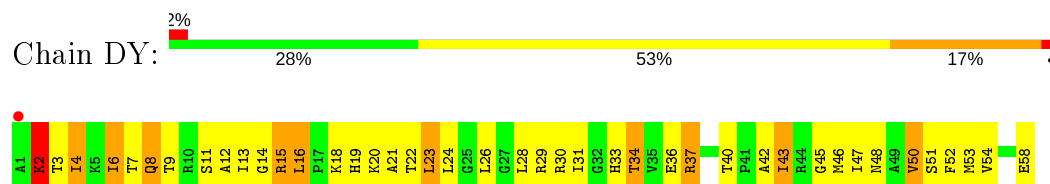
- Molecule 29: 50S ribosomal protein L4



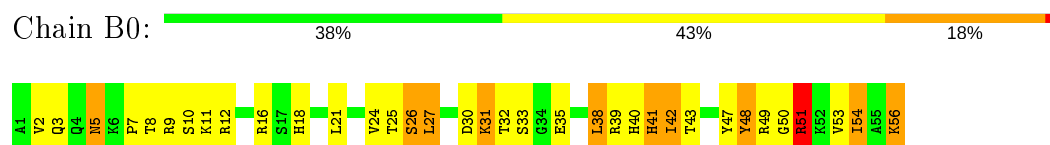
- Molecule 30: 50S ribosomal protein L30



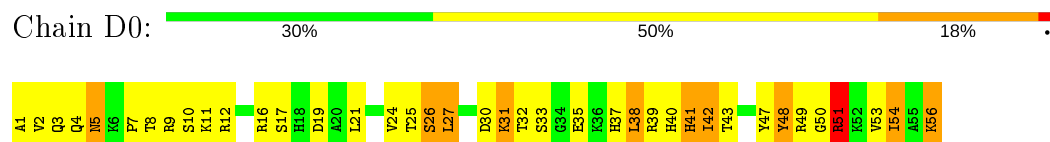
- Molecule 30: 50S ribosomal protein L30



- Molecule 31: 50S ribosomal protein L32

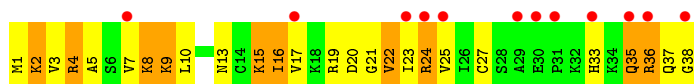


- Molecule 31: 50S ribosomal protein L32

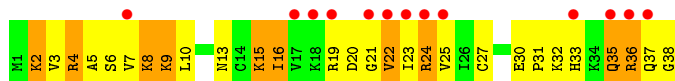


- Molecule 32: 50S ribosomal protein L36

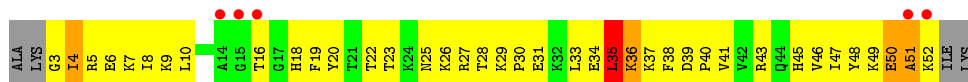




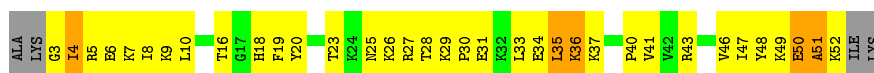
- Molecule 32: 50S ribosomal protein L36



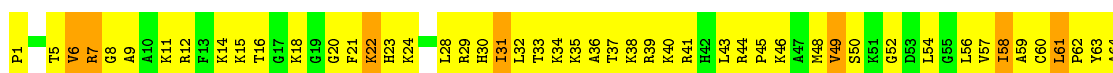
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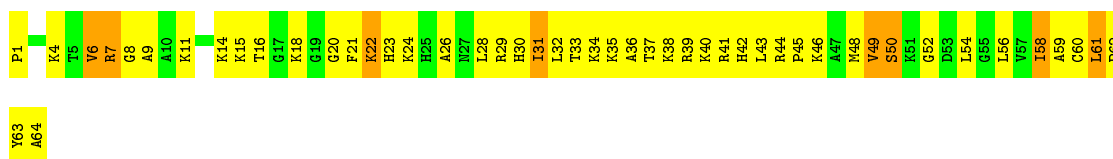
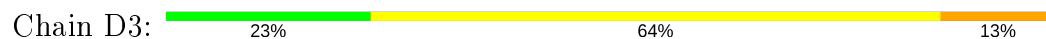
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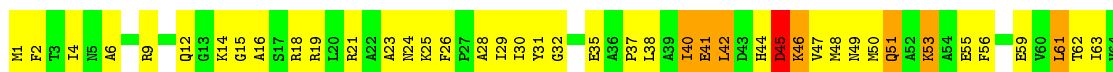
- Molecule 34: 50S ribosomal protein L35



- Molecule 34: 50S ribosomal protein L35

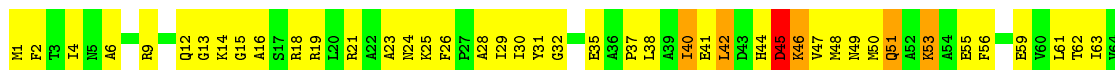


- Molecule 35: 50S ribosomal protein L25

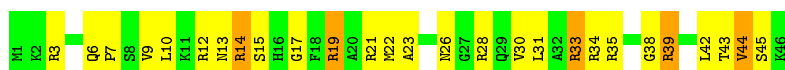




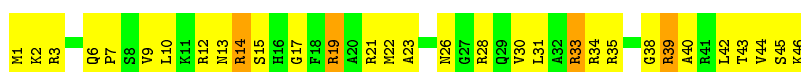
- Molecule 35: 50S ribosomal protein L25



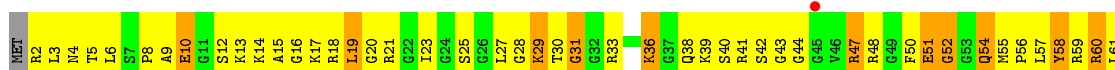
- Molecule 36: 50S ribosomal protein L34



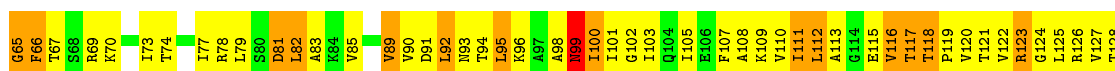
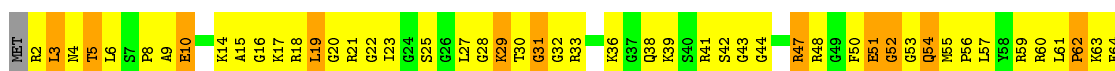
- Molecule 36: 50S ribosomal protein L34



- Molecule 37: 50S ribosomal protein L15

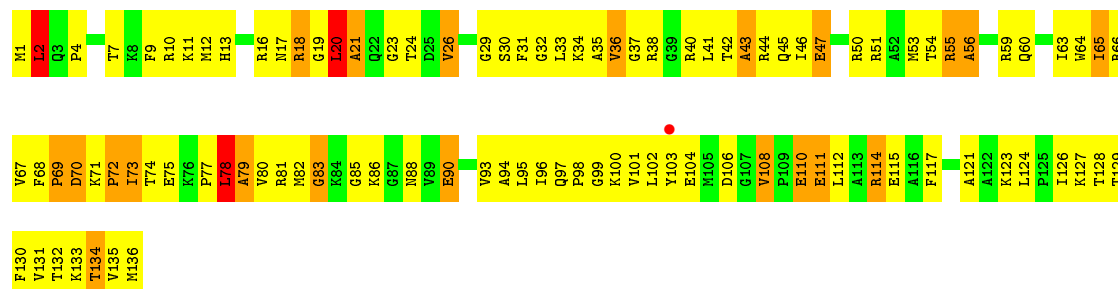


- Molecule 37: 50S ribosomal protein L15

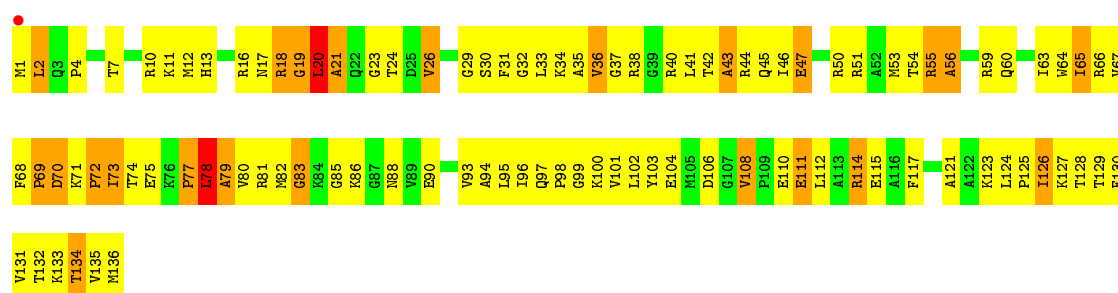




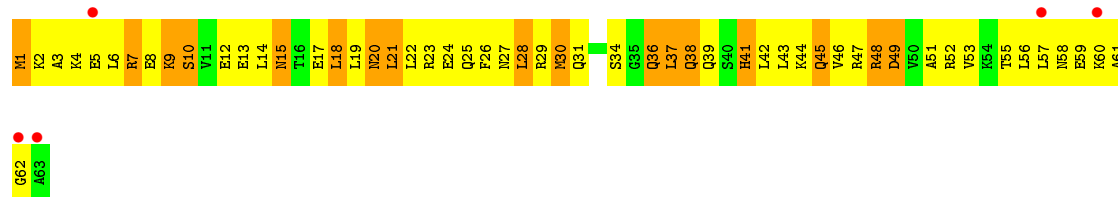
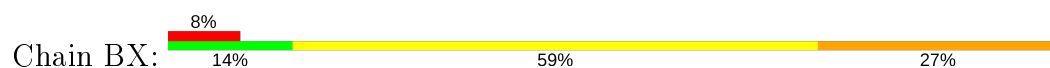
- Molecule 38: 50S ribosomal protein L16



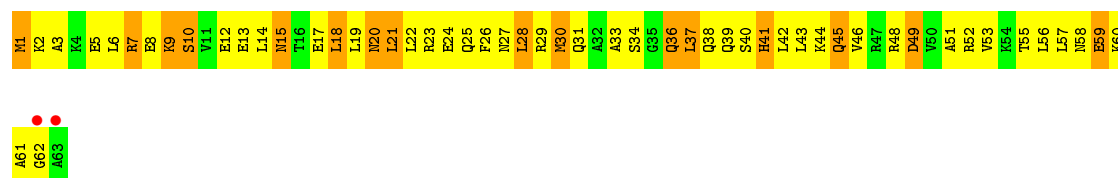
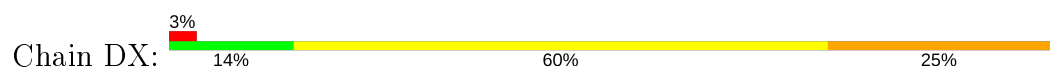
- Molecule 38: 50S ribosomal protein L16



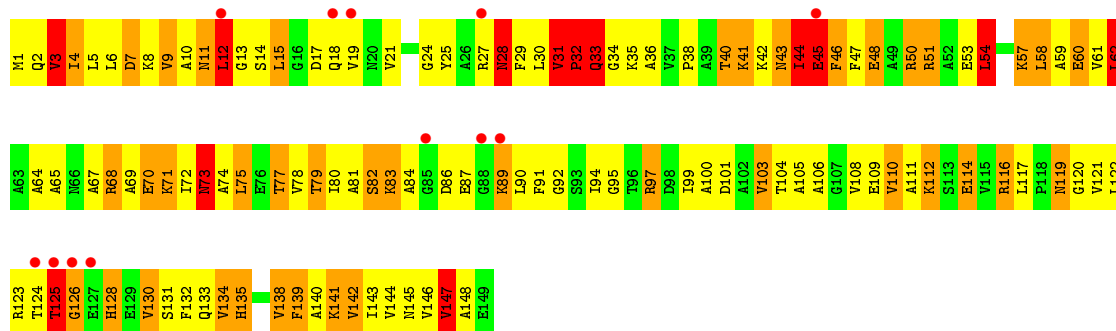
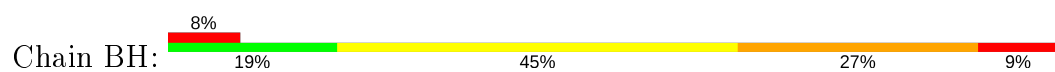
- Molecule 39: 50S ribosomal protein L29



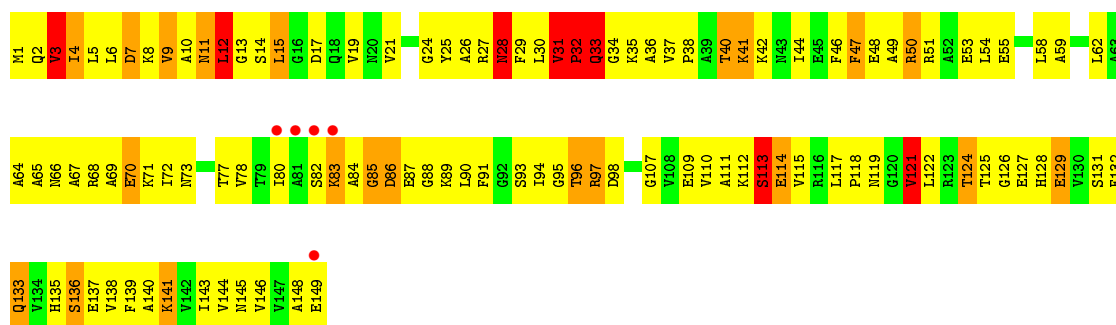
- Molecule 39: 50S ribosomal protein L29



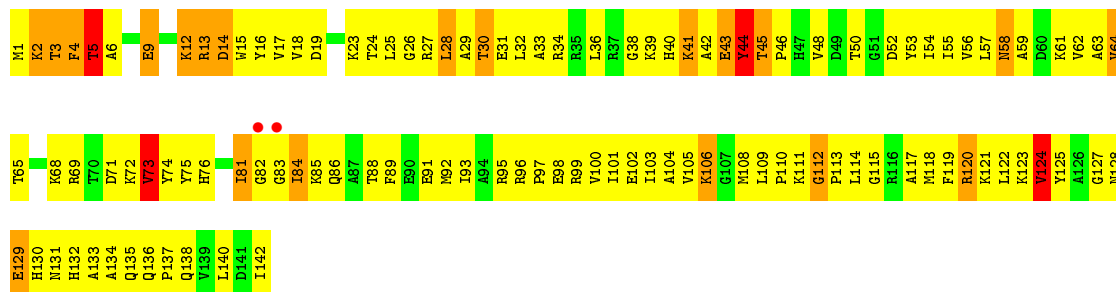
- Molecule 40: 50S ribosomal protein L9



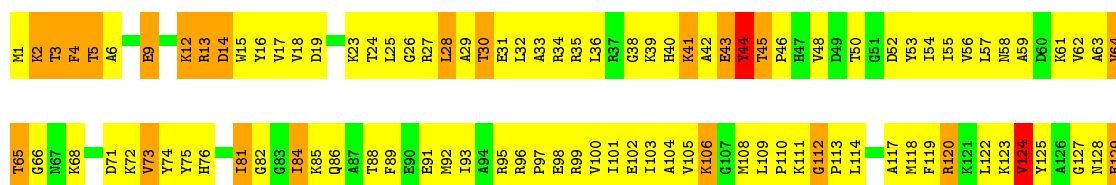
• Molecule 40: 50S ribosomal protein L9



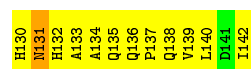
• Molecule 41: 50S ribosomal protein L13



• Molecule 41: 50S ribosomal protein L13

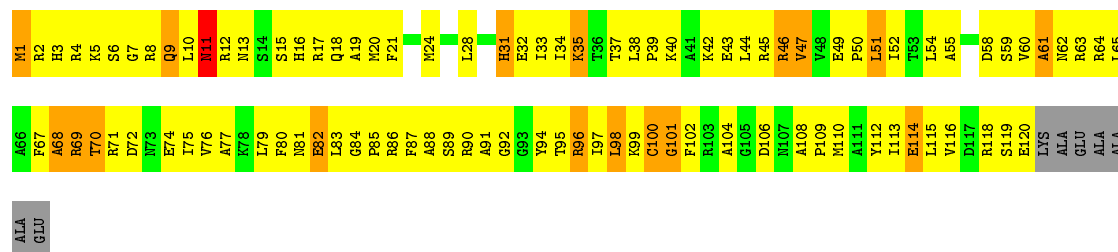






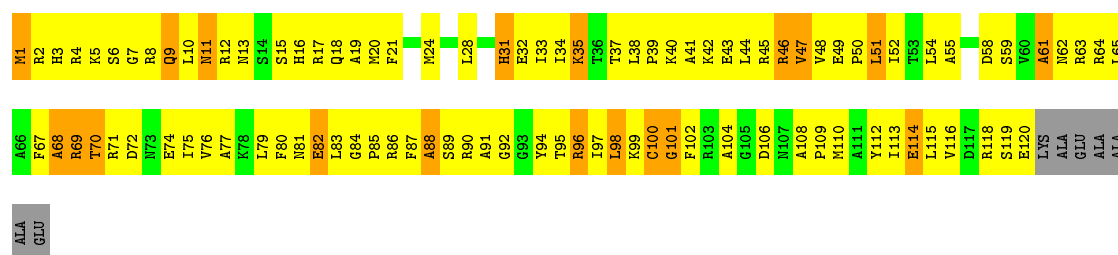
- Molecule 42: 50S ribosomal protein L17

Chain BN: 18% 62% 13% 6%



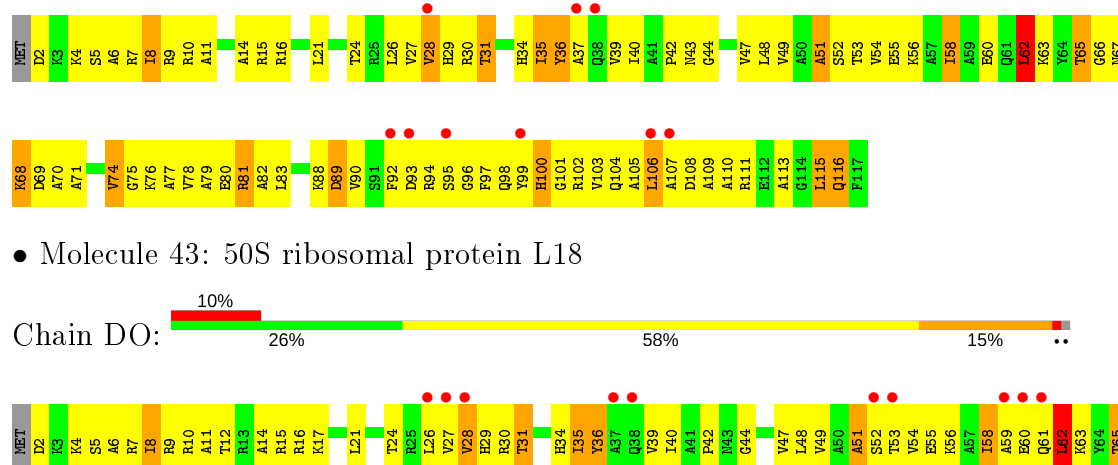
- Molecule 42: 50S ribosomal protein L17

Chain DN: 17% 62% 15% 6%



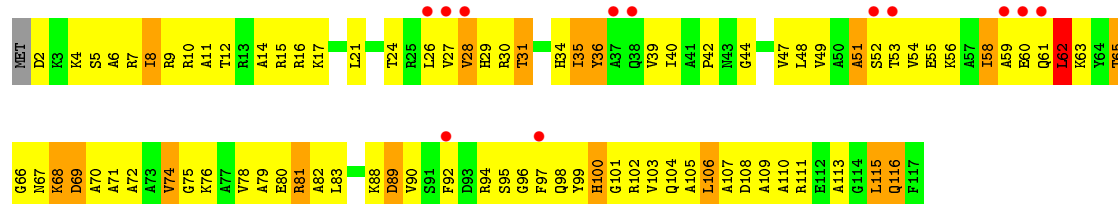
- Molecule 43: 50S ribosomal protein L18

Chain BO: 8% 26% 58% 14% ..



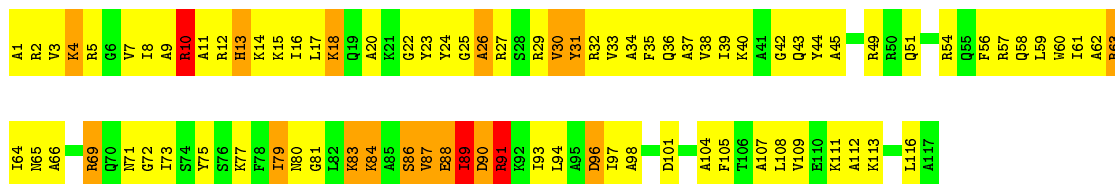
- Molecule 43: 50S ribosomal protein L18

Chain DO: 10% 26% 58% 15% ..



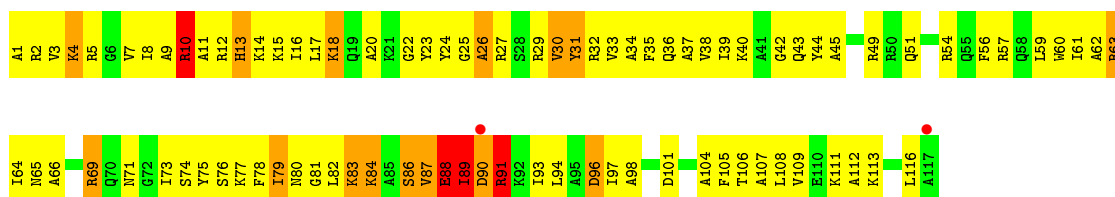
- Molecule 44: 50S ribosomal protein L20

Chain BQ: 



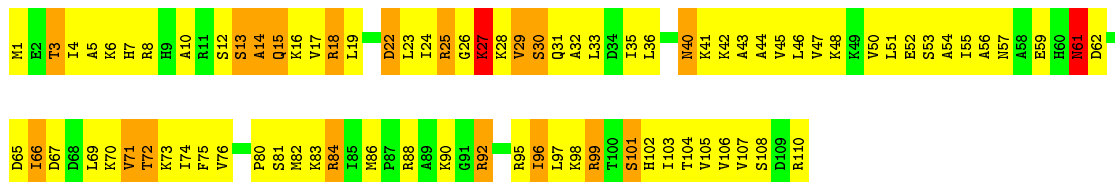
- Molecule 44: 50S ribosomal protein L20

Chain DQ: 



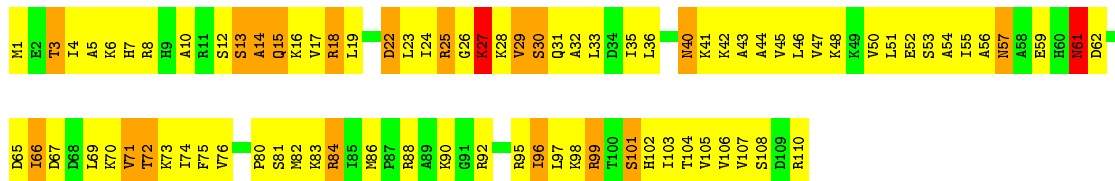
- Molecule 45: 50S ribosomal protein L22

Chain BS: 

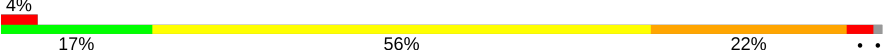


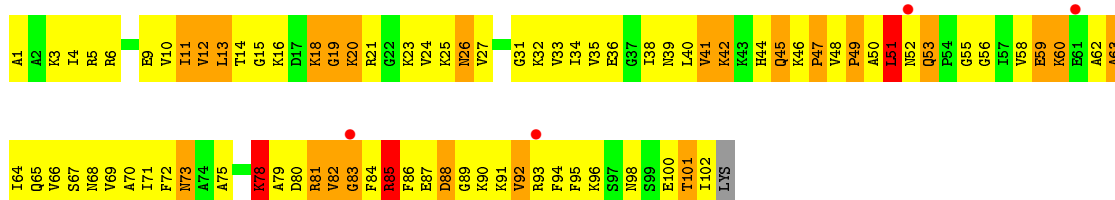
- Molecule 45: 50S ribosomal protein L22

Chain DS: 

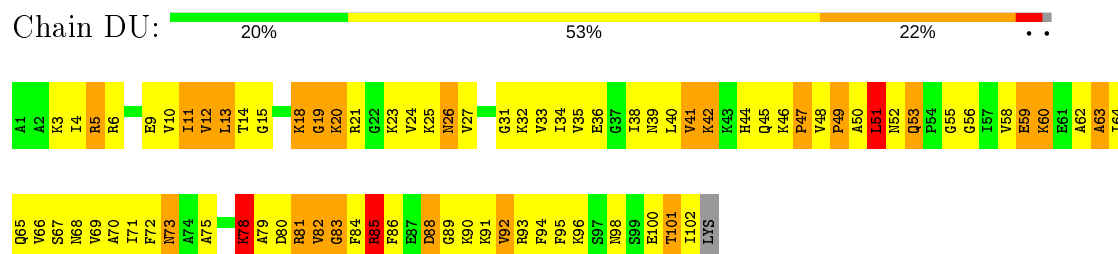


- Molecule 46: 50S ribosomal protein L24

Chain BU: 



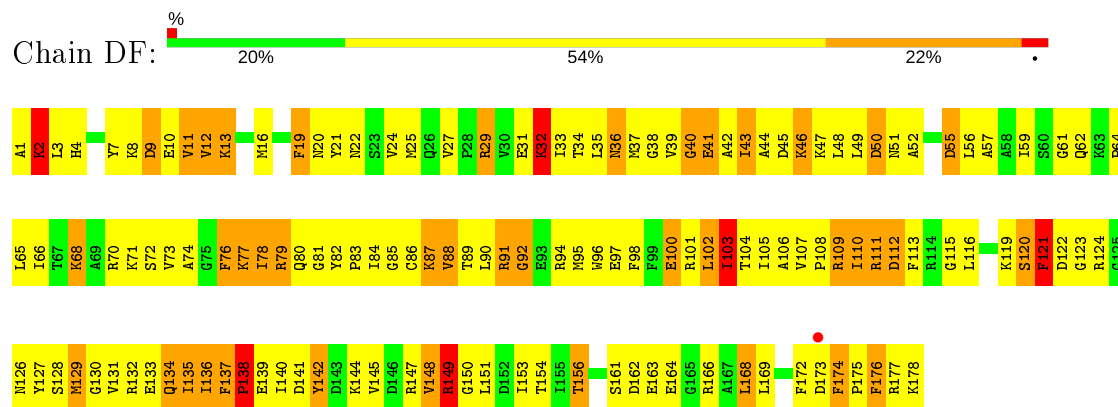
- Molecule 46: 50S ribosomal protein L24



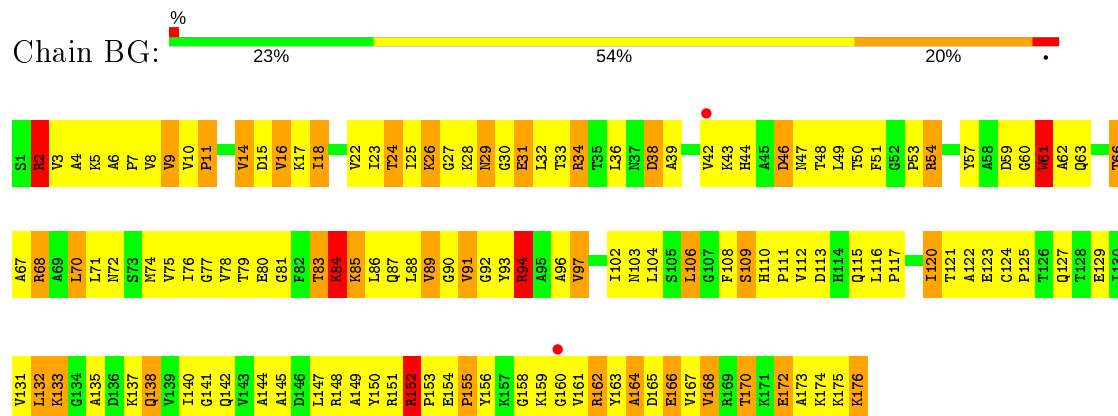
- Molecule 47: 50S ribosomal protein L5



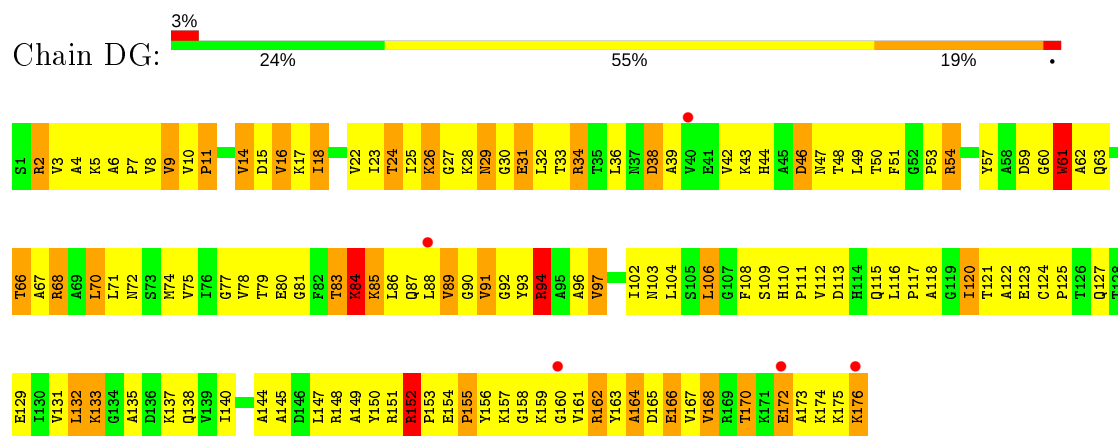
- Molecule 47: 50S ribosomal protein L5



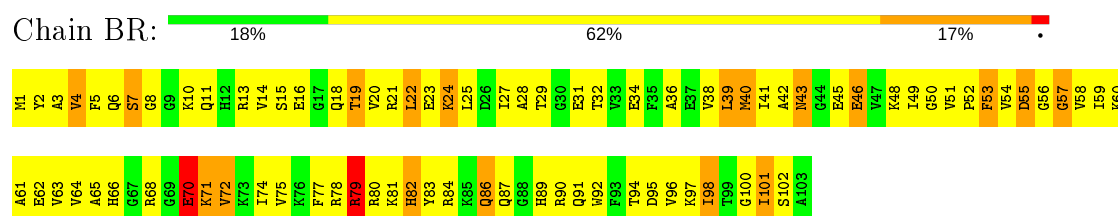
- Molecule 48: 50S ribosomal protein L6



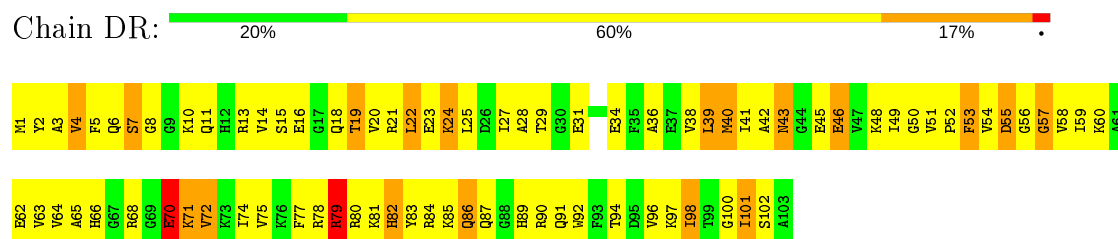
- Molecule 48: 50S ribosomal protein L6



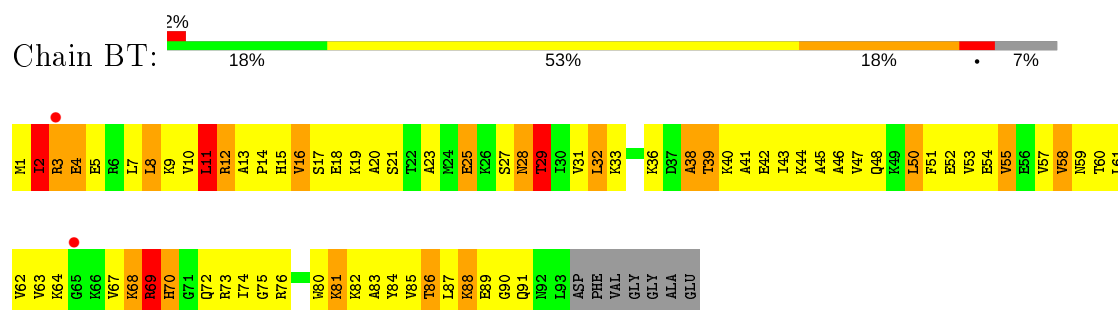
- Molecule 49: 50S ribosomal protein L21



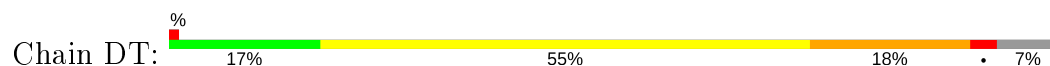
- Molecule 49: 50S ribosomal protein L21

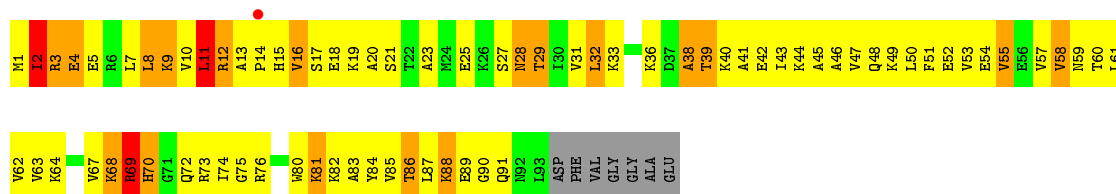


- Molecule 50: 50S ribosomal protein L23

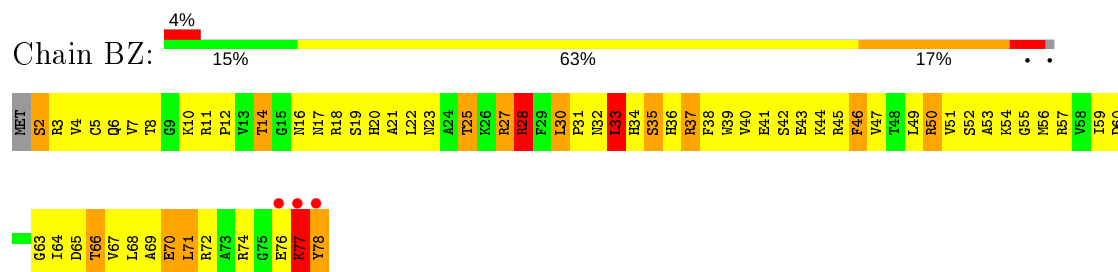


- Molecule 50: 50S ribosomal protein L23

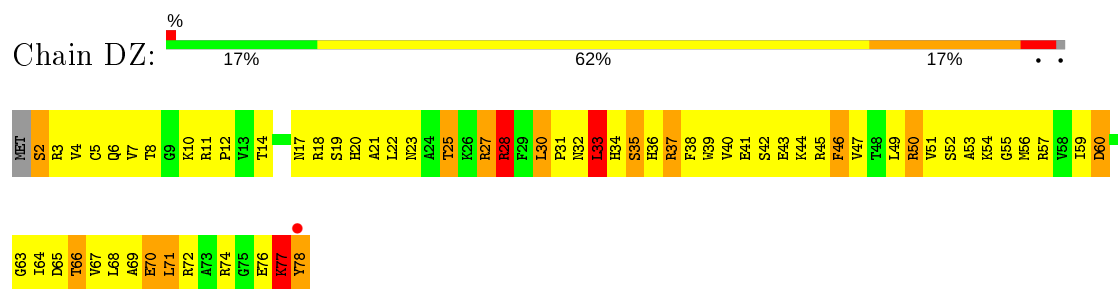




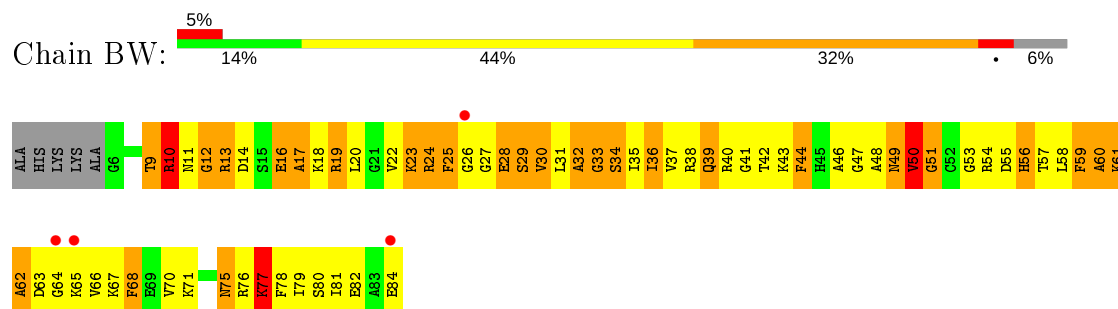
• Molecule 51: 50S ribosomal protein L28



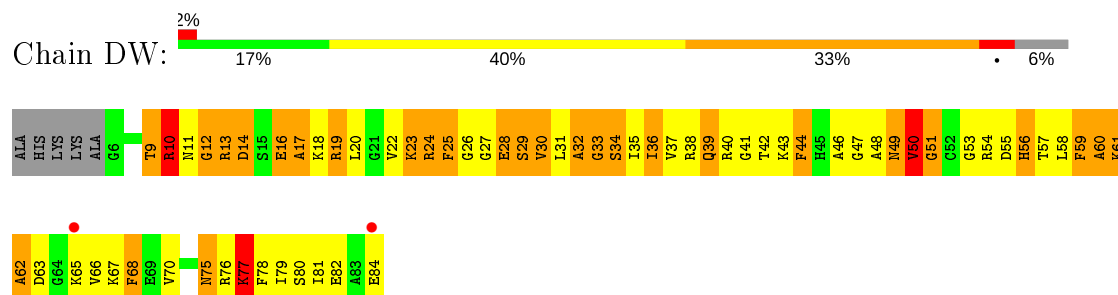
• Molecule 51: 50S ribosomal protein L28



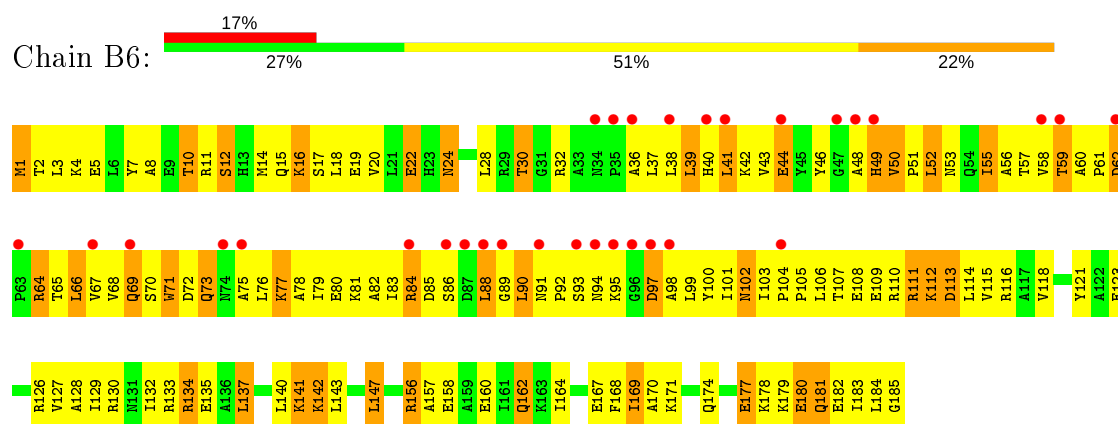
• Molecule 52: 50S ribosomal protein L27



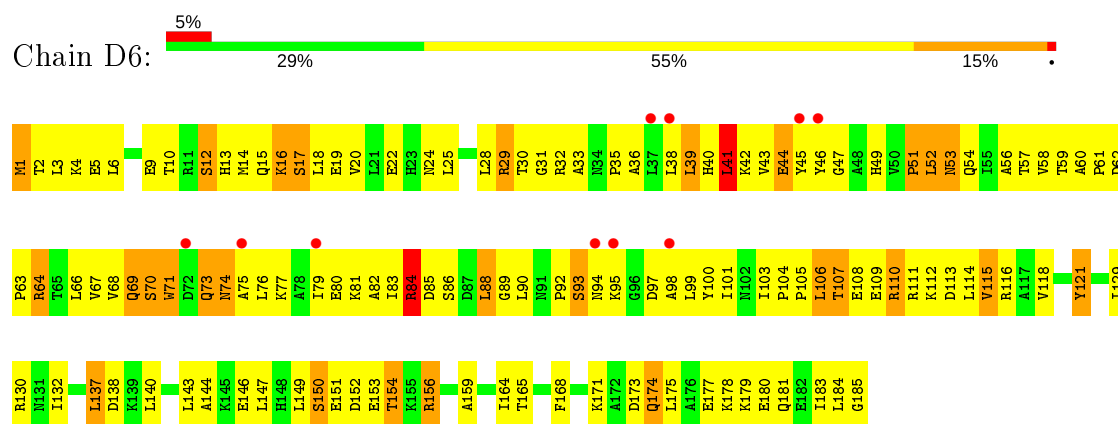
• Molecule 52: 50S ribosomal protein L27



• Molecule 53: 50S ribosomal protein RRF



● Molecule 53: 50S ribosomal protein RRF



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	208.87Å 378.75Å 738.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 4.45 69.15 – 4.45	Depositor EDS
% Data completeness (in resolution range)	95.7 (40.00-4.45) 95.6 (69.15-4.45)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.39 (at 4.46Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.263 , 0.309 0.235 , 0.273	Depositor DCC
$R_{free}$ test set	16978 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	150.5	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.17 , 59.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	287128	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.03% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.28	1/36762 (0.0%)	0.76	6/57350 (0.0%)
1	CA	0.28	1/36762 (0.0%)	0.76	10/57350 (0.0%)
2	AC	0.23	0/1651	0.44	0/2225
2	CC	0.23	0/1651	0.44	0/2225
3	AD	0.23	0/1665	0.44	0/2227
3	CD	0.23	0/1665	0.44	0/2227
4	AE	0.23	0/1118	0.45	0/1504
4	CE	0.24	0/1118	0.45	0/1504
5	AF	0.24	0/835	0.45	0/1128
5	CF	0.24	0/835	0.45	0/1128
6	AG	0.23	0/1187	0.45	0/1591
6	CG	0.23	0/1211	0.45	0/1624
7	AH	0.23	0/989	0.44	0/1326
7	CH	0.23	0/989	0.44	0/1326
8	AI	0.24	0/1034	0.45	0/1375
8	CI	0.24	0/1034	0.45	0/1375
9	AJ	0.22	0/796	0.49	0/1077
9	CJ	0.22	0/796	0.48	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	0.48	0/1300
11	CL	0.22	0/969	0.48	0/1300
12	AM	0.21	0/892	0.45	0/1193
12	CM	0.21	0/884	0.45	0/1181
13	AN	0.24	0/785	0.46	0/1043
13	CN	0.24	0/785	0.46	0/1043
14	AO	0.23	0/722	0.47	0/964
14	CO	0.23	0/722	0.47	0/964
15	AP	0.25	0/659	0.46	0/884
15	CP	0.25	0/648	0.46	0/870
16	AQ	0.23	0/657	0.47	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	0.46	0/877
18	CS	0.25	0/660	0.47	0/888
19	AT	0.24	0/671	0.40	0/888
19	CT	0.24	0/671	0.40	0/888
20	AB	0.25	0/1735	0.45	0/2338
20	CB	0.25	0/1735	0.45	0/2338
21	AU	0.26	0/430	0.48	0/570
21	CU	0.26	0/430	0.47	0/570
22	BA	0.55	6/2803 (0.2%)	0.83	7/4371 (0.2%)
22	DA	0.56	6/2803 (0.2%)	0.83	7/4371 (0.2%)
23	BB	0.31	8/68314 (0.0%)	0.79	41/106569 (0.0%)
23	DB	0.31	7/68314 (0.0%)	0.79	38/106569 (0.0%)
24	BI	0.24	0/1046	0.47	0/1410
24	DI	0.25	0/1046	0.48	0/1410
25	BC	0.22	0/2121	0.48	0/2852
25	DC	0.22	0/2121	0.48	0/2852
26	BD	0.24	0/1586	0.48	0/2134
26	DD	0.24	0/1586	0.48	0/2134
27	BK	0.24	0/939	0.55	0/1258
27	DK	0.24	0/939	0.55	0/1258
28	BP	0.24	0/929	0.51	0/1242
28	DP	0.24	0/929	0.51	0/1242
29	BE	0.24	0/1571	0.50	0/2113
29	DE	0.24	0/1571	0.50	0/2113
30	BY	0.23	0/453	0.49	0/605
30	DY	0.23	0/453	0.49	0/605
31	B0	0.22	0/450	0.55	0/599
31	D0	0.22	0/450	0.55	0/599
32	B4	0.23	0/303	0.47	0/397
32	D4	0.23	0/303	0.47	0/397
33	B1	0.27	0/416	0.49	0/554
33	D1	0.27	0/416	0.49	0/554
34	B3	0.24	0/513	0.48	0/676
34	D3	0.24	0/513	0.48	0/676
35	BV	0.25	0/766	0.43	0/1025
35	DV	0.25	0/766	0.42	0/1025
36	B2	0.26	0/380	0.46	0/498
36	D2	0.26	0/380	0.46	0/498
37	BL	0.24	0/1054	0.48	0/1403
37	DL	0.23	0/1054	0.48	0/1403
38	BM	0.25	0/1093	0.48	0/1460

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	DM	0.25	0/1093	0.48	0/1460
39	BX	0.24	0/510	0.54	0/677
39	DX	0.24	0/510	0.54	0/677
40	BH	0.25	0/1122	0.47	0/1515
40	DH	0.25	0/1122	0.49	0/1515
41	BJ	0.24	0/1152	0.48	0/1551
41	DJ	0.24	0/1152	0.48	0/1551
42	BN	0.24	0/973	0.52	0/1301
42	DN	0.24	0/973	0.52	0/1301
43	BO	0.23	0/902	0.48	0/1209
43	DO	0.23	0/902	0.48	0/1209
44	BQ	0.25	0/960	0.49	0/1278
44	DQ	0.25	0/960	0.49	0/1278
45	BS	0.22	0/864	0.52	0/1156
45	DS	0.22	0/864	0.52	0/1156
46	BU	0.25	0/787	0.47	0/1051
46	DU	0.25	0/787	0.47	0/1051
47	BF	0.26	0/1444	0.51	0/1937
47	DF	0.26	0/1444	0.52	0/1937
48	BG	0.23	0/1343	0.46	0/1816
48	DG	0.23	0/1343	0.46	0/1816
49	BR	0.25	0/829	0.48	0/1107
49	DR	0.25	0/829	0.48	0/1107
50	BT	0.23	0/744	0.55	0/994
50	DT	0.23	0/744	0.55	0/994
51	BZ	0.25	0/635	0.52	0/848
51	DZ	0.25	0/635	0.52	0/848
52	BW	0.28	0/603	0.51	0/797
52	DW	0.27	0/603	0.51	0/797
53	B6	0.23	0/1497	0.48	0/2017
53	D6	0.24	0/1497	0.47	0/2017
All	All	0.29	29/309354 (0.0%)	0.71	109/462003 (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	12
22	BA	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
22	DA	0	2
23	BB	0	50
23	DB	0	48
All	All	0	128

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	BB	1086	A	C5-C6	-16.24	1.26	1.41
23	DB	1086	A	C5-C6	-16.14	1.26	1.41
22	DA	28	C	C2-O2	-14.83	1.11	1.24
22	BA	28	C	C2-O2	-14.74	1.11	1.24
23	DB	2276	G	O3'-P	-14.11	1.44	1.61

The worst 5 of 109 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	DB	2204	G	O5'-P-OP1	-29.74	75.02	110.70
23	BB	2204	G	O5'-P-OP2	-28.61	76.37	110.70
23	BB	2791	G	O5'-P-OP1	-27.22	78.03	110.70
23	DB	2791	G	O5'-P-OP2	-26.58	78.80	110.70
23	BB	2791	G	O5'-P-OP2	18.87	133.34	110.70

There are no chirality outliers.

5 of 128 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	78	A	Sidechain
1	AA	86	G	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	1250	0
1	CA	32831	0	16521	1242	0
2	AC	1624	0	1699	139	0
2	CC	1624	0	1699	141	0
3	AD	1643	0	1710	173	0
3	CD	1643	0	1710	170	0
4	AE	1105	0	1148	99	0
4	CE	1105	0	1148	104	0
5	AF	817	0	808	83	0
5	CF	817	0	808	80	0
6	AG	1174	0	1230	115	0
6	CG	1196	0	1246	98	0
7	AH	979	0	1034	94	0
7	CH	979	0	1034	90	0
8	AI	1022	0	1070	142	0
8	CI	1022	0	1070	134	0
9	AJ	786	0	828	79	0
9	CJ	786	0	828	85	0
10	AK	877	0	887	108	0
10	CK	877	0	887	99	0
11	AL	955	0	1019	82	0
11	CL	955	0	1019	82	0
12	AM	883	0	944	105	0
12	CM	876	0	937	108	0
13	AN	774	0	827	113	0
13	CN	774	0	827	117	0
14	AO	714	0	734	47	0
14	CO	714	0	734	48	0
15	AP	649	0	666	51	0
15	CP	638	0	656	53	0
16	AQ	648	0	691	58	0
16	CQ	657	0	702	61	0
17	AR	455	0	478	45	0
17	CR	455	0	478	49	0
18	AS	637	0	665	89	0
18	CS	644	0	675	88	0
19	AT	665	0	714	58	0
19	CT	665	0	714	55	0
20	AB	1704	0	1732	189	0
20	CB	1704	0	1732	206	0
21	AU	425	0	449	77	0
21	CU	425	0	449	70	0
22	BA	2507	0	1270	119	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	DA	2507	0	1270	119	1
23	BB	60995	0	30679	2401	0
23	DB	60995	0	30677	2528	1
24	BI	1032	0	1088	117	0
24	DI	1032	0	1088	185	0
25	BC	2082	0	2157	254	0
25	DC	2082	0	2157	253	0
26	BD	1565	0	1616	196	0
26	DD	1565	0	1616	200	0
27	BK	930	0	1000	107	0
27	DK	930	0	1000	114	0
28	BP	917	0	965	102	0
28	DP	917	0	965	99	0
29	BE	1552	0	1619	211	0
29	DE	1552	0	1619	196	0
30	BY	449	0	491	51	0
30	DY	449	0	491	51	0
31	B0	444	0	461	56	0
31	D0	444	0	461	53	0
32	B4	302	0	340	34	0
32	D4	302	0	341	40	0
33	B1	409	0	440	48	0
33	D1	409	0	440	44	0
34	B3	504	0	574	51	0
34	D3	504	0	574	52	0
35	BV	753	0	780	90	0
35	DV	753	0	780	101	0
36	B2	377	0	418	36	0
36	D2	377	0	418	38	0
37	BL	1045	0	1117	163	0
37	DL	1045	0	1117	163	0
38	BM	1074	0	1157	117	0
38	DM	1074	0	1157	121	0
39	BX	509	0	543	70	0
39	DX	509	0	543	66	0
40	BH	1111	0	1148	207	0
40	DH	1111	0	1148	144	0
41	BJ	1129	0	1162	144	0
41	DJ	1129	0	1162	146	0
42	BN	960	0	1000	123	0
42	DN	960	0	1000	121	0
43	BO	892	0	923	104	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	DO	892	0	923	113	0
44	BQ	947	0	1022	156	0
44	DQ	947	0	1022	160	0
45	BS	857	0	922	106	0
45	DS	857	0	922	109	0
46	BU	779	0	834	117	0
46	DU	779	0	834	116	0
47	BF	1420	0	1460	236	0
47	DF	1420	0	1460	248	0
48	BG	1323	0	1374	200	0
48	DG	1323	0	1374	195	0
49	BR	816	0	839	124	0
49	DR	816	0	839	127	0
50	BT	738	0	807	120	0
50	DT	738	0	807	116	0
51	BZ	625	0	652	77	0
51	DZ	625	0	652	71	0
52	BW	596	0	610	124	0
52	DW	596	0	610	130	0
53	B6	1478	0	1526	187	0
53	D6	1478	0	1526	166	0
54	AA	60	0	0	0	0
54	BB	110	0	0	0	0
54	CA	61	0	0	0	0
54	CE	1	0	0	0	0
54	DB	111	0	0	0	0
55	AA	42	0	45	3	0
55	BB	42	0	45	1	0
55	CA	42	0	45	2	0
55	DB	42	0	45	1	0
56	B4	1	0	0	0	0
56	D4	1	0	0	0	0
57	AA	291	0	0	5	0
57	AL	3	0	0	0	0
57	AN	4	0	0	0	0
57	AT	2	0	0	0	0
57	BB	495	0	0	8	0
57	BC	6	0	0	0	0
57	BD	1	0	0	0	0
57	BE	2	0	0	0	0
57	BL	1	0	0	0	0
57	BT	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	CA	296	0	0	1	0
57	CE	3	0	0	0	0
57	CL	4	0	0	0	0
57	CN	4	0	0	0	0
57	CP	1	0	0	0	0
57	CT	1	0	0	0	0
57	DB	502	0	0	15	0
57	DC	4	0	0	0	0
57	DD	1	0	0	0	0
57	DE	1	0	0	0	0
57	DL	2	0	0	0	0
57	DQ	1	0	0	0	0
57	DR	1	0	0	0	0
All	All	287128	0	193895	17520	1

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 37.

The worst 5 of 17520 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:H8	24:DI:3:LYS:N	1.37	1.19
40:BH:31:VAL:HB	40:BH:32:PRO:HD2	1.28	1.15
49:DR:60:LYS:H	49:DR:100:GLY:HA3	1.08	1.15
2:CC:126:ARG:HH22	2:CC:190:THR:HG23	1.09	1.14
50:DT:5:GLU:HA	50:DT:8:LEU:HB2	1.30	1.13

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:DA:53:A:OP1	23:DB:1592:C:O2'[1_655]	2.08	0.12

## 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	204/232 (88%)	150 (74%)	41 (20%)	13 (6%)	1	19
2	CC	204/232 (88%)	154 (76%)	36 (18%)	14 (7%)	1	17
3	AD	203/205 (99%)	151 (74%)	41 (20%)	11 (5%)	2	22
3	CD	203/205 (99%)	150 (74%)	41 (20%)	12 (6%)	1	20
4	AE	148/166 (89%)	113 (76%)	32 (22%)	3 (2%)	7	40
4	CE	148/166 (89%)	116 (78%)	28 (19%)	4 (3%)	5	34
5	AF	98/135 (73%)	66 (67%)	25 (26%)	7 (7%)	1	16
5	CF	98/135 (73%)	67 (68%)	24 (24%)	7 (7%)	1	16
6	AG	148/178 (83%)	121 (82%)	23 (16%)	4 (3%)	5	34
6	CG	150/178 (84%)	123 (82%)	23 (15%)	4 (3%)	5	34
7	AH	127/129 (98%)	96 (76%)	27 (21%)	4 (3%)	4	31
7	CH	127/129 (98%)	96 (76%)	28 (22%)	3 (2%)	6	36
8	AI	125/129 (97%)	96 (77%)	23 (18%)	6 (5%)	2	23
8	CI	125/129 (97%)	96 (77%)	22 (18%)	7 (6%)	2	21
9	AJ	96/103 (93%)	72 (75%)	16 (17%)	8 (8%)	1	13
9	CJ	96/103 (93%)	71 (74%)	17 (18%)	8 (8%)	1	13
10	AK	115/128 (90%)	86 (75%)	22 (19%)	7 (6%)	1	19
10	CK	115/128 (90%)	85 (74%)	23 (20%)	7 (6%)	1	19
11	AL	121/123 (98%)	76 (63%)	34 (28%)	11 (9%)	1	12
11	CL	121/123 (98%)	74 (61%)	36 (30%)	11 (9%)	1	12
12	AM	112/117 (96%)	77 (69%)	28 (25%)	7 (6%)	1	19
12	CM	111/117 (95%)	79 (71%)	25 (22%)	7 (6%)	1	19
13	AN	92/100 (92%)	58 (63%)	21 (23%)	13 (14%)	0	4
13	CN	92/100 (92%)	59 (64%)	21 (23%)	12 (13%)	0	5
14	AO	86/89 (97%)	66 (77%)	17 (20%)	3 (4%)	3	29
14	CO	86/89 (97%)	67 (78%)	16 (19%)	3 (4%)	3	29
15	AP	80/82 (98%)	58 (72%)	18 (22%)	4 (5%)	2	23
15	CP	78/82 (95%)	56 (72%)	17 (22%)	5 (6%)	1	19
16	AQ	78/83 (94%)	58 (74%)	16 (20%)	4 (5%)	2	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	CQ	79/83 (95%)	59 (75%)	15 (19%)	5 (6%)	1	19
17	AR	53/74 (72%)	45 (85%)	8 (15%)	0	100	100
17	CR	53/74 (72%)	44 (83%)	9 (17%)	0	100	100
18	AS	77/91 (85%)	52 (68%)	24 (31%)	1 (1%)	12	48
18	CS	78/91 (86%)	53 (68%)	23 (30%)	2 (3%)	5	34
19	AT	83/86 (96%)	67 (81%)	13 (16%)	3 (4%)	3	28
19	CT	83/86 (96%)	67 (81%)	13 (16%)	3 (4%)	3	28
20	AB	216/240 (90%)	159 (74%)	36 (17%)	21 (10%)	0	11
20	CB	216/240 (90%)	156 (72%)	37 (17%)	23 (11%)	0	8
21	AU	49/70 (70%)	27 (55%)	14 (29%)	8 (16%)	0	3
21	CU	49/70 (70%)	26 (53%)	14 (29%)	9 (18%)	0	2
24	BI	139/141 (99%)	119 (86%)	15 (11%)	5 (4%)	3	28
24	DI	139/141 (99%)	114 (82%)	21 (15%)	4 (3%)	4	32
25	BC	269/272 (99%)	164 (61%)	63 (23%)	42 (16%)	0	4
25	DC	269/272 (99%)	161 (60%)	68 (25%)	40 (15%)	0	4
26	BD	207/209 (99%)	118 (57%)	55 (27%)	34 (16%)	0	3
26	DD	207/209 (99%)	115 (56%)	59 (28%)	33 (16%)	0	3
27	BK	119/123 (97%)	72 (60%)	30 (25%)	17 (14%)	0	4
27	DK	119/123 (97%)	71 (60%)	30 (25%)	18 (15%)	0	4
28	BP	112/114 (98%)	62 (55%)	37 (33%)	13 (12%)	0	6
28	DP	112/114 (98%)	63 (56%)	35 (31%)	14 (12%)	0	5
29	BE	199/201 (99%)	124 (62%)	56 (28%)	19 (10%)	0	11
29	DE	199/201 (99%)	121 (61%)	58 (29%)	20 (10%)	0	10
30	BY	56/58 (97%)	36 (64%)	15 (27%)	5 (9%)	1	13
30	DY	56/58 (97%)	37 (66%)	14 (25%)	5 (9%)	1	13
31	B0	54/56 (96%)	35 (65%)	13 (24%)	6 (11%)	0	8
31	D0	54/56 (96%)	36 (67%)	11 (20%)	7 (13%)	0	5
32	B4	36/38 (95%)	18 (50%)	11 (31%)	7 (19%)	0	2
32	D4	36/38 (95%)	18 (50%)	11 (31%)	7 (19%)	0	2
33	B1	48/54 (89%)	36 (75%)	7 (15%)	5 (10%)	0	9
33	D1	48/54 (89%)	36 (75%)	7 (15%)	5 (10%)	0	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	B3	62/64 (97%)	40 (64%)	16 (26%)	6 (10%)	0	11
34	D3	62/64 (97%)	41 (66%)	14 (23%)	7 (11%)	0	7
35	BV	92/94 (98%)	70 (76%)	16 (17%)	6 (6%)	1	18
35	DV	92/94 (98%)	69 (75%)	18 (20%)	5 (5%)	2	22
36	B2	44/46 (96%)	26 (59%)	15 (34%)	3 (7%)	1	17
36	D2	44/46 (96%)	26 (59%)	15 (34%)	3 (7%)	1	17
37	BL	141/144 (98%)	76 (54%)	42 (30%)	23 (16%)	0	3
37	DL	141/144 (98%)	76 (54%)	40 (28%)	25 (18%)	0	2
38	BM	134/136 (98%)	88 (66%)	31 (23%)	15 (11%)	0	8
38	DM	134/136 (98%)	89 (66%)	29 (22%)	16 (12%)	0	6
39	BX	61/63 (97%)	36 (59%)	18 (30%)	7 (12%)	0	7
39	DX	61/63 (97%)	37 (61%)	17 (28%)	7 (12%)	0	7
40	BH	147/149 (99%)	71 (48%)	49 (33%)	27 (18%)	0	2
40	DH	147/149 (99%)	96 (65%)	28 (19%)	23 (16%)	0	4
41	BJ	140/142 (99%)	89 (64%)	34 (24%)	17 (12%)	0	6
41	DJ	140/142 (99%)	88 (63%)	36 (26%)	16 (11%)	0	7
42	BN	118/127 (93%)	73 (62%)	34 (29%)	11 (9%)	0	12
42	DN	118/127 (93%)	71 (60%)	35 (30%)	12 (10%)	0	10
43	BO	114/117 (97%)	80 (70%)	25 (22%)	9 (8%)	1	14
43	DO	114/117 (97%)	79 (69%)	26 (23%)	9 (8%)	1	14
44	BQ	115/117 (98%)	70 (61%)	34 (30%)	11 (10%)	0	11
44	DQ	115/117 (98%)	69 (60%)	35 (30%)	11 (10%)	0	11
45	BS	108/110 (98%)	72 (67%)	22 (20%)	14 (13%)	0	5
45	DS	108/110 (98%)	70 (65%)	24 (22%)	14 (13%)	0	5
46	BU	100/103 (97%)	52 (52%)	28 (28%)	20 (20%)	0	2
46	DU	100/103 (97%)	50 (50%)	29 (29%)	21 (21%)	0	2
47	BF	176/178 (99%)	106 (60%)	43 (24%)	27 (15%)	0	4
47	DF	176/178 (99%)	107 (61%)	42 (24%)	27 (15%)	0	4
48	BG	174/176 (99%)	100 (58%)	49 (28%)	25 (14%)	0	4
48	DG	174/176 (99%)	99 (57%)	49 (28%)	26 (15%)	0	4
49	BR	101/103 (98%)	67 (66%)	21 (21%)	13 (13%)	0	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	DR	101/103 (98%)	68 (67%)	20 (20%)	13 (13%)	0	5
50	BT	91/100 (91%)	51 (56%)	26 (29%)	14 (15%)	0	4
50	DT	91/100 (91%)	50 (55%)	27 (30%)	14 (15%)	0	4
51	BZ	75/78 (96%)	51 (68%)	18 (24%)	6 (8%)	1	14
51	DZ	75/78 (96%)	51 (68%)	18 (24%)	6 (8%)	1	14
52	BW	77/84 (92%)	31 (40%)	21 (27%)	25 (32%)	0	0
52	DW	77/84 (92%)	31 (40%)	21 (27%)	25 (32%)	0	0
53	B6	183/185 (99%)	151 (82%)	25 (14%)	7 (4%)	3	27
53	D6	183/185 (99%)	132 (72%)	40 (22%)	11 (6%)	1	19
All	All	11607/12284 (94%)	7747 (67%)	2693 (23%)	1167 (10%)	0	10

5 of 1167 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AC	54	ILE
2	AC	205	GLU
6	AG	6	ILE
8	AI	8	THR
9	AJ	36	VAL

### 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	170/189 (90%)	142 (84%)	28 (16%)	2	14
2	CC	170/189 (90%)	142 (84%)	28 (16%)	2	14
3	AD	172/172 (100%)	147 (86%)	25 (14%)	3	17
3	CD	172/172 (100%)	148 (86%)	24 (14%)	3	19
4	AE	113/125 (90%)	96 (85%)	17 (15%)	3	17
4	CE	113/125 (90%)	96 (85%)	17 (15%)	3	17
5	AF	87/116 (75%)	71 (82%)	16 (18%)	1	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	CF	87/116 (75%)	70 (80%)	17 (20%)	1	9
6	AG	123/146 (84%)	106 (86%)	17 (14%)	3	19
6	CG	125/146 (86%)	109 (87%)	16 (13%)	4	21
7	AH	104/104 (100%)	96 (92%)	8 (8%)	13	39
7	CH	104/104 (100%)	96 (92%)	8 (8%)	13	39
8	AI	105/106 (99%)	88 (84%)	17 (16%)	2	15
8	CI	105/106 (99%)	88 (84%)	17 (16%)	2	15
9	AJ	86/90 (96%)	73 (85%)	13 (15%)	3	16
9	CJ	86/90 (96%)	73 (85%)	13 (15%)	3	16
10	AK	90/98 (92%)	76 (84%)	14 (16%)	2	16
10	CK	90/98 (92%)	76 (84%)	14 (16%)	2	16
11	AL	103/103 (100%)	92 (89%)	11 (11%)	6	26
11	CL	103/103 (100%)	91 (88%)	12 (12%)	5	23
12	AM	92/95 (97%)	78 (85%)	14 (15%)	3	16
12	CM	91/95 (96%)	77 (85%)	14 (15%)	2	16
13	AN	79/83 (95%)	66 (84%)	13 (16%)	2	14
13	CN	79/83 (95%)	66 (84%)	13 (16%)	2	14
14	AO	76/77 (99%)	64 (84%)	12 (16%)	2	15
14	CO	76/77 (99%)	64 (84%)	12 (16%)	2	15
15	AP	65/65 (100%)	60 (92%)	5 (8%)	13	39
15	CP	65/65 (100%)	60 (92%)	5 (8%)	13	39
16	AQ	74/77 (96%)	66 (89%)	8 (11%)	6	26
16	CQ	75/77 (97%)	67 (89%)	8 (11%)	6	26
17	AR	48/64 (75%)	45 (94%)	3 (6%)	18	44
17	CR	48/64 (75%)	45 (94%)	3 (6%)	18	44
18	AS	70/78 (90%)	54 (77%)	16 (23%)	1	5
18	CS	71/78 (91%)	55 (78%)	16 (22%)	1	6
19	AT	65/65 (100%)	56 (86%)	9 (14%)	3	19
19	CT	65/65 (100%)	56 (86%)	9 (14%)	3	19
20	AB	180/198 (91%)	150 (83%)	30 (17%)	2	14
20	CB	180/198 (91%)	149 (83%)	31 (17%)	2	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	AU	44/60 (73%)	31 (70%)	13 (30%)	0	2
21	CU	44/60 (73%)	31 (70%)	13 (30%)	0	2
24	BI	109/109 (100%)	107 (98%)	2 (2%)	59	77
24	DI	109/109 (100%)	103 (94%)	6 (6%)	21	49
25	BC	216/217 (100%)	178 (82%)	38 (18%)	2	12
25	DC	216/217 (100%)	179 (83%)	37 (17%)	2	13
26	BD	164/164 (100%)	142 (87%)	22 (13%)	4	20
26	DD	164/164 (100%)	140 (85%)	24 (15%)	3	17
27	BK	102/104 (98%)	75 (74%)	27 (26%)	0	4
27	DK	102/104 (98%)	75 (74%)	27 (26%)	0	4
28	BP	99/99 (100%)	82 (83%)	17 (17%)	2	13
28	DP	99/99 (100%)	82 (83%)	17 (17%)	2	13
29	BE	165/165 (100%)	141 (86%)	24 (14%)	3	17
29	DE	165/165 (100%)	140 (85%)	25 (15%)	3	16
30	BY	48/48 (100%)	38 (79%)	10 (21%)	1	7
30	DY	48/48 (100%)	38 (79%)	10 (21%)	1	7
31	B0	47/47 (100%)	39 (83%)	8 (17%)	2	13
31	D0	47/47 (100%)	39 (83%)	8 (17%)	2	13
32	B4	34/34 (100%)	28 (82%)	6 (18%)	2	12
32	D4	34/34 (100%)	28 (82%)	6 (18%)	2	12
33	B1	45/48 (94%)	42 (93%)	3 (7%)	16	43
33	D1	45/48 (94%)	42 (93%)	3 (7%)	16	43
34	B3	51/51 (100%)	47 (92%)	4 (8%)	12	38
34	D3	51/51 (100%)	47 (92%)	4 (8%)	12	38
35	BV	78/78 (100%)	66 (85%)	12 (15%)	2	16
35	DV	78/78 (100%)	67 (86%)	11 (14%)	3	19
36	B2	38/38 (100%)	34 (90%)	4 (10%)	7	26
36	D2	38/38 (100%)	34 (90%)	4 (10%)	7	26
37	BL	102/103 (99%)	87 (85%)	15 (15%)	3	17
37	DL	102/103 (99%)	88 (86%)	14 (14%)	3	19
38	BM	109/109 (100%)	88 (81%)	21 (19%)	1	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	DM	109/109 (100%)	89 (82%)	20 (18%)	1	11
39	BX	55/55 (100%)	40 (73%)	15 (27%)	0	3
39	DX	55/55 (100%)	42 (76%)	13 (24%)	1	5
40	BH	114/114 (100%)	68 (60%)	46 (40%)	0	0
40	DH	114/114 (100%)	91 (80%)	23 (20%)	1	8
41	BJ	116/116 (100%)	99 (85%)	17 (15%)	3	17
41	DJ	116/116 (100%)	99 (85%)	17 (15%)	3	17
42	BN	100/103 (97%)	86 (86%)	14 (14%)	3	19
42	DN	100/103 (97%)	86 (86%)	14 (14%)	3	19
43	BO	86/87 (99%)	73 (85%)	13 (15%)	3	16
43	DO	86/87 (99%)	74 (86%)	12 (14%)	3	19
44	BQ	89/89 (100%)	76 (85%)	13 (15%)	3	17
44	DQ	89/89 (100%)	75 (84%)	14 (16%)	2	16
45	BS	93/93 (100%)	79 (85%)	14 (15%)	3	16
45	DS	93/93 (100%)	80 (86%)	13 (14%)	3	19
46	BU	83/84 (99%)	69 (83%)	14 (17%)	2	13
46	DU	83/84 (99%)	69 (83%)	14 (17%)	2	13
47	BF	149/149 (100%)	114 (76%)	35 (24%)	1	5
47	DF	149/149 (100%)	116 (78%)	33 (22%)	1	6
48	BG	137/137 (100%)	114 (83%)	23 (17%)	2	13
48	DG	137/137 (100%)	115 (84%)	22 (16%)	2	15
49	BR	84/84 (100%)	72 (86%)	12 (14%)	3	18
49	DR	84/84 (100%)	72 (86%)	12 (14%)	3	18
50	BT	80/84 (95%)	65 (81%)	15 (19%)	1	10
50	DT	80/84 (95%)	68 (85%)	12 (15%)	3	17
51	BZ	67/68 (98%)	53 (79%)	14 (21%)	1	7
51	DZ	67/68 (98%)	54 (81%)	13 (19%)	1	9
52	BW	59/62 (95%)	47 (80%)	12 (20%)	1	8
52	DW	59/62 (95%)	46 (78%)	13 (22%)	1	6
53	B6	157/157 (100%)	119 (76%)	38 (24%)	0	5
53	D6	157/157 (100%)	123 (78%)	34 (22%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9647/10014 (96%)	8085 (84%)	1562 (16%)	<b>2</b> <b>15</b>

5 of 1562 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
49	BR	4	VAL
5	CF	61	LEU
47	DF	111	ARG
50	BT	50	LEU
53	B6	174	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 336 such sidechains are listed below:

Mol	Chain	Res	Type
49	BR	11	GLN
6	CG	67	ASN
46	DU	73	ASN
50	BT	91	GLN
2	CC	2	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1529/1542 (99%)	246 (16%)	16 (1%)
1	CA	1529/1542 (99%)	244 (15%)	16 (1%)
22	BA	116/120 (96%)	18 (15%)	0
22	DA	116/120 (96%)	18 (15%)	0
23	BB	2837/2904 (97%)	446 (15%)	14 (0%)
23	DB	2837/2904 (97%)	447 (15%)	16 (0%)
All	All	8964/9132 (98%)	1419 (15%)	62 (0%)

5 of 1419 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	7	A
1	AA	9	G
1	AA	14	U
1	AA	31	G
1	AA	32	A

5 of 62 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	BB	2832	U
1	CA	328	C
23	DB	2336	A
1	CA	239	U
1	CA	372	C

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 349 ligands modelled in this entry, 345 are monoatomic - leaving 4 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	$\# Z  > 2$
55	PAR	BB	3111	-	45,45,45	1.94	11 (24%)	64,67,67	1.13	6 (9%)
55	PAR	AA	1661	-	45,45,45	1.85	10 (22%)	64,67,67	1.14	5 (7%)
55	PAR	DB	3112	-	45,45,45	1.98	12 (26%)	64,67,67	1.18	6 (9%)
55	PAR	CA	1662	-	45,45,45	1.94	11 (24%)	64,67,67	1.16	5 (7%)

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
55	PAR	BB	3111	-	-	4/18/94/94	0/4/4/4
55	PAR	AA	1661	-	-	6/18/94/94	0/4/4/4
55	PAR	DB	3112	-	-	3/18/94/94	0/4/4/4
55	PAR	CA	1662	-	-	4/18/94/94	0/4/4/4

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	DB	3112	PAR	C64-C54	5.26	1.59	1.52
55	BB	3111	PAR	C64-C54	5.25	1.59	1.52
55	AA	1661	PAR	C64-C54	5.07	1.58	1.52
55	CA	1662	PAR	C64-C54	5.00	1.58	1.52
55	CA	1662	PAR	C31-C21	4.73	1.59	1.53

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	DB	3112	PAR	O33-C14-C24	3.65	114.50	108.22
55	BB	3111	PAR	O33-C14-C24	3.49	114.23	108.22
55	DB	3112	PAR	O52-C13-O43	3.33	115.04	111.43
55	CA	1662	PAR	O33-C14-C24	3.27	113.85	108.22
55	DB	3112	PAR	O54-C54-C64	3.23	112.02	106.01

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

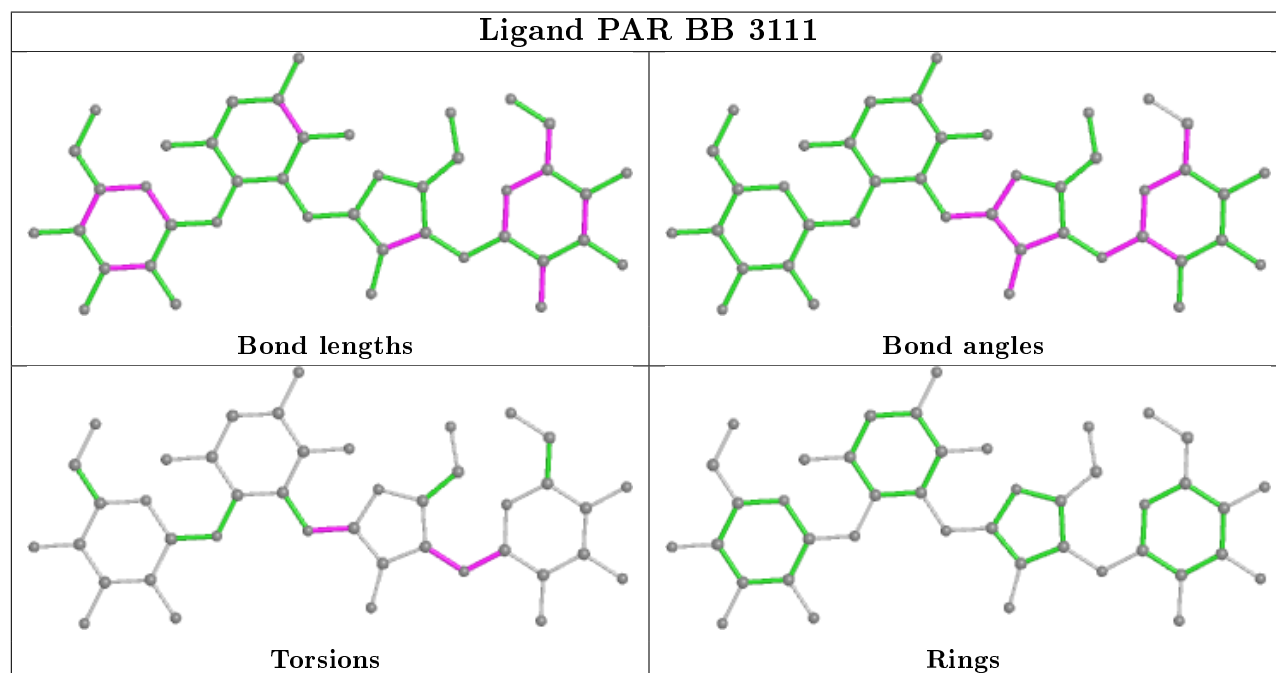
Mol	Chain	Res	Type	Atoms
55	DB	3112	PAR	C24-C14-O33-C33
55	CA	1662	PAR	C23-C13-O52-C52
55	CA	1662	PAR	O43-C13-O52-C52
55	AA	1661	PAR	C23-C13-O52-C52
55	BB	3111	PAR	C24-C14-O33-C33

There are no ring outliers.

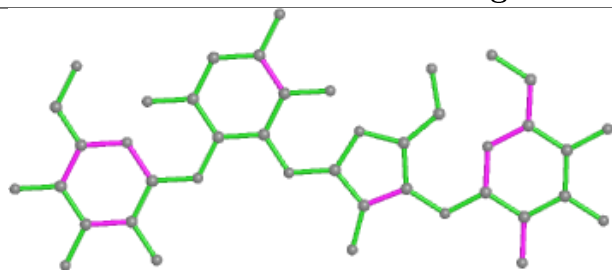
4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	BB	3111	PAR	1	0
55	AA	1661	PAR	3	0
55	DB	3112	PAR	1	0
55	CA	1662	PAR	2	0

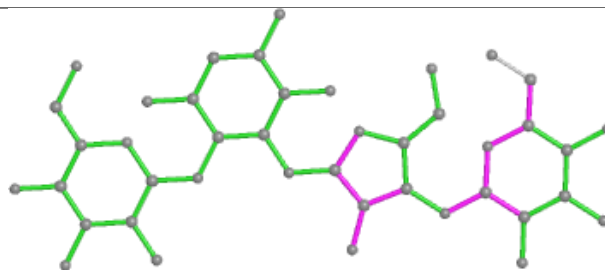
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



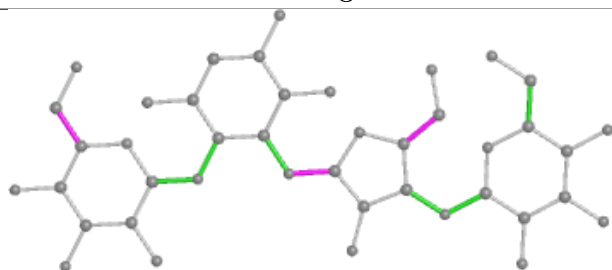
## Ligand PAR AA 1661



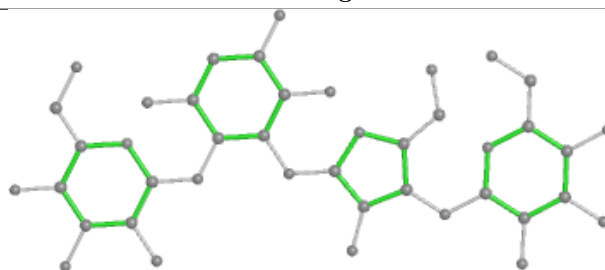
Bond lengths



Bond angles

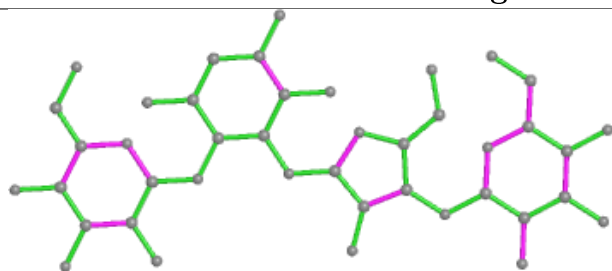


Torsions

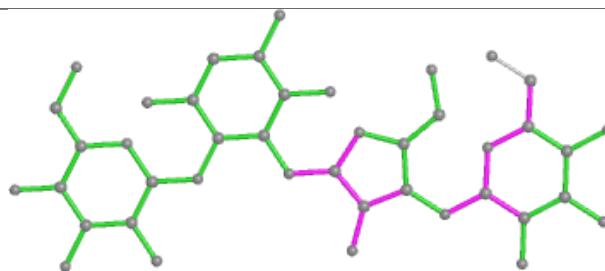


Rings

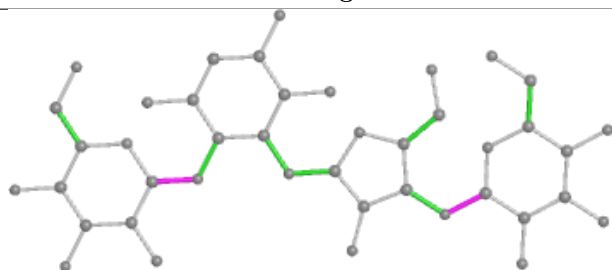
## Ligand PAR DB 3112



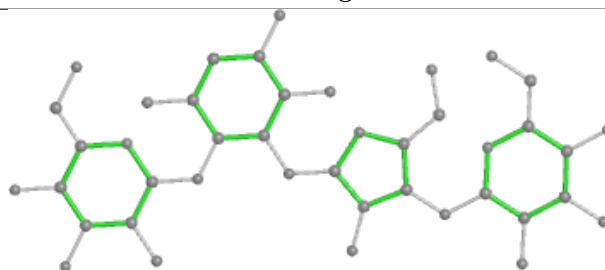
Bond lengths



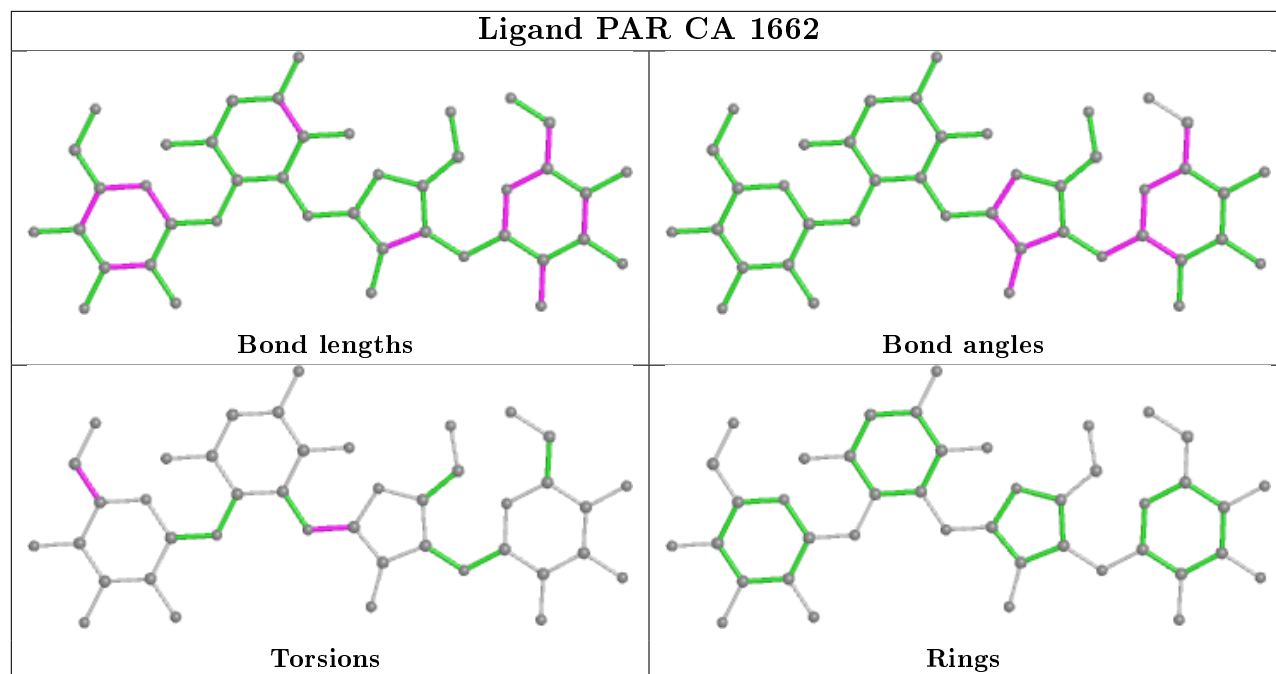
Bond angles



Torsions



Rings



## 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%)	0.03	16 (1%) 82 74	8, 88, 162, 180	0
1	CA	1530/1542 (99%)	-0.12	9 (0%) 89 84	5, 54, 146, 180	0
2	AC	206/232 (88%)	-0.03	5 (2%) 59 49	9, 89, 158, 180	0
2	CC	206/232 (88%)	-0.33	2 (0%) 82 74	9, 83, 141, 180	0
3	AD	205/205 (100%)	-0.10	3 (1%) 73 64	5, 97, 172, 180	0
3	CD	205/205 (100%)	-0.39	0 100 100	5, 59, 151, 180	0
4	AE	150/166 (90%)	-0.17	0 100 100	5, 85, 159, 180	0
4	CE	150/166 (90%)	-0.14	1 (0%) 87 82	5, 52, 137, 180	0
5	AF	100/135 (74%)	-0.15	1 (1%) 82 74	8, 73, 146, 172	0
5	CF	100/135 (74%)	-0.35	0 100 100	5, 84, 153, 180	0
6	AG	150/178 (84%)	-0.20	4 (2%) 54 45	10, 110, 170, 180	0
6	CG	152/178 (85%)	0.08	5 (3%) 46 37	28, 93, 162, 180	0
7	AH	129/129 (100%)	-0.04	3 (2%) 60 51	15, 85, 159, 180	0
7	CH	129/129 (100%)	-0.23	2 (1%) 72 63	5, 50, 128, 175	0
8	AI	127/129 (98%)	0.06	4 (3%) 49 39	5, 98, 163, 180	0
8	CI	127/129 (98%)	-0.22	1 (0%) 86 79	5, 102, 180, 180	0
9	AJ	98/103 (95%)	0.21	4 (4%) 37 30	5, 105, 174, 180	0
9	CJ	98/103 (95%)	0.30	5 (5%) 28 24	10, 93, 158, 180	0
10	AK	117/128 (91%)	-0.27	0 100 100	9, 67, 129, 146	0
10	CK	117/128 (91%)	-0.41	2 (1%) 70 61	5, 63, 134, 180	0
11	AL	123/123 (100%)	-0.01	1 (0%) 86 79	19, 84, 158, 180	0
11	CL	123/123 (100%)	-0.43	0 100 100	5, 54, 113, 180	0
12	AM	114/117 (97%)	0.08	3 (2%) 56 46	55, 122, 180, 180	0
12	CM	113/117 (96%)	0.15	4 (3%) 44 35	31, 114, 180, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AN	96/100 (96%)	0.32	8 (8%) 11 10	5, 108, 170, 180	0
13	CN	96/100 (96%)	0.16	5 (5%) 27 24	6, 99, 162, 180	0
14	AO	88/89 (98%)	-0.26	0 100 100	7, 86, 156, 180	0
14	CO	88/89 (98%)	-0.52	0 100 100	5, 60, 132, 175	0
15	AP	82/82 (100%)	0.26	3 (3%) 41 33	35, 106, 173, 180	0
15	CP	80/82 (97%)	0.27	5 (6%) 20 16	5, 47, 142, 180	0
16	AQ	80/83 (96%)	-0.13	0 100 100	48, 104, 180, 180	0
16	CQ	81/83 (97%)	-0.22	0 100 100	5, 53, 140, 173	0
17	AR	55/74 (74%)	-0.14	1 (1%) 68 59	5, 65, 143, 180	0
17	CR	55/74 (74%)	0.28	2 (3%) 42 34	13, 68, 130, 180	0
18	AS	79/91 (86%)	0.35	4 (5%) 28 24	55, 129, 180, 180	0
18	CS	80/91 (87%)	0.11	1 (1%) 77 68	46, 108, 180, 180	0
19	AT	85/86 (98%)	-0.19	0 100 100	44, 105, 154, 180	0
19	CT	85/86 (98%)	-0.20	1 (1%) 79 70	5, 56, 117, 161	0
20	AB	218/240 (90%)	-0.15	4 (1%) 68 59	7, 105, 171, 180	0
20	CB	218/240 (90%)	0.33	10 (4%) 32 27	23, 111, 172, 180	0
21	AU	51/70 (72%)	-0.03	1 (1%) 65 56	23, 104, 180, 180	0
21	CU	51/70 (72%)	-0.08	2 (3%) 39 31	24, 96, 173, 180	0
22	BA	117/120 (97%)	-0.27	0 100 100	37, 82, 145, 178	0
22	DA	117/120 (97%)	-0.02	2 (1%) 70 61	18, 84, 143, 180	0
23	BB	2841/2904 (97%)	-0.05	26 (0%) 84 77	6, 58, 150, 180	0
23	DB	2841/2904 (97%)	-0.15	9 (0%) 94 90	5, 38, 149, 180	0
24	BI	141/141 (100%)	0.61	9 (6%) 19 16	63, 161, 180, 180	0
24	DI	141/141 (100%)	0.48	13 (9%) 9 8	65, 157, 180, 180	0
25	BC	271/272 (99%)	-0.28	1 (0%) 92 87	5, 48, 108, 166	0
25	DC	271/272 (99%)	-0.26	0 100 100	5, 30, 102, 180	0
26	BD	209/209 (100%)	0.07	6 (2%) 51 41	5, 79, 148, 180	0
26	DD	209/209 (100%)	-0.38	0 100 100	5, 51, 123, 180	0
27	BK	121/123 (98%)	0.07	1 (0%) 86 79	5, 74, 149, 180	0
27	DK	121/123 (98%)	-0.32	0 100 100	5, 33, 106, 180	0
28	BP	114/114 (100%)	-0.08	0 100 100	18, 89, 153, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	DP	114/114 (100%)	-0.32	0 100 100	5, 48, 124, 180	0
29	BE	201/201 (100%)	-0.35	2 (0%) 82 74	5, 67, 146, 180	0
29	DE	201/201 (100%)	-0.28	1 (0%) 91 85	5, 67, 142, 177	0
30	BY	58/58 (100%)	-0.05	0 100 100	18, 82, 151, 171	0
30	DY	58/58 (100%)	-0.27	1 (1%) 70 61	5, 68, 126, 162	0
31	B0	56/56 (100%)	-0.21	0 100 100	5, 73, 153, 164	0
31	D0	56/56 (100%)	-0.22	0 100 100	5, 56, 147, 180	0
32	B4	38/38 (100%)	1.71	12 (31%) 0 1	45, 115, 169, 180	0
32	D4	38/38 (100%)	1.82	13 (34%) 0 0	36, 110, 169, 180	0
33	B1	50/54 (92%)	0.40	5 (10%) 7 7	22, 95, 157, 180	0
33	D1	50/54 (92%)	0.32	0 100 100	19, 73, 122, 161	0
34	B3	64/64 (100%)	-0.19	0 100 100	20, 63, 125, 145	0
34	D3	64/64 (100%)	-0.09	0 100 100	5, 35, 88, 129	0
35	BV	94/94 (100%)	-0.19	0 100 100	24, 96, 156, 180	0
35	DV	94/94 (100%)	-0.18	0 100 100	11, 93, 151, 180	0
36	B2	46/46 (100%)	-0.10	0 100 100	5, 75, 137, 180	0
36	D2	46/46 (100%)	-0.19	0 100 100	5, 44, 101, 180	0
37	BL	143/144 (99%)	-0.15	1 (0%) 87 82	5, 71, 133, 180	0
37	DL	143/144 (99%)	-0.25	0 100 100	5, 51, 116, 180	0
38	BM	136/136 (100%)	-0.12	1 (0%) 87 82	9, 70, 149, 180	0
38	DM	136/136 (100%)	-0.20	1 (0%) 87 82	5, 50, 131, 176	0
39	BX	63/63 (100%)	0.06	5 (7%) 12 11	7, 84, 165, 180	0
39	DX	63/63 (100%)	-0.03	2 (3%) 47 37	47, 108, 173, 180	0
40	BH	149/149 (100%)	0.49	12 (8%) 12 11	5, 130, 180, 180	0
40	DH	149/149 (100%)	0.08	5 (3%) 45 36	12, 97, 172, 180	0
41	BJ	142/142 (100%)	-0.14	2 (1%) 75 66	6, 81, 147, 180	0
41	DJ	142/142 (100%)	-0.26	0 100 100	5, 58, 135, 180	0
42	BN	120/127 (94%)	-0.15	0 100 100	5, 68, 139, 178	0
42	DN	120/127 (94%)	-0.46	0 100 100	5, 38, 101, 180	0
43	BO	116/117 (99%)	0.23	9 (7%) 13 11	21, 91, 147, 180	0
43	DO	116/117 (99%)	0.34	12 (10%) 6 7	8, 86, 164, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	BQ	117/117 (100%)	-0.40	0 100 100	5, 66, 135, 176	0
44	DQ	117/117 (100%)	-0.19	2 (1%) 70 61	5, 48, 134, 180	0
45	BS	110/110 (100%)	-0.11	0 100 100	6, 58, 139, 180	0
45	DS	110/110 (100%)	-0.33	0 100 100	5, 50, 121, 180	0
46	BU	102/103 (99%)	0.28	4 (3%) 39 31	5, 89, 144, 180	0
46	DU	102/103 (99%)	0.06	0 100 100	24, 99, 159, 180	0
47	BF	178/178 (100%)	-0.28	0 100 100	36, 111, 174, 180	0
47	DF	178/178 (100%)	-0.08	1 (0%) 89 84	8, 103, 177, 180	0
48	BG	176/176 (100%)	0.19	2 (1%) 80 72	9, 114, 179, 180	0
48	DG	176/176 (100%)	0.00	5 (2%) 53 43	15, 91, 167, 180	0
49	BR	103/103 (100%)	0.12	0 100 100	16, 93, 157, 180	0
49	DR	103/103 (100%)	0.07	0 100 100	5, 88, 145, 180	0
50	BT	93/100 (93%)	-0.10	2 (2%) 62 52	5, 88, 180, 180	0
50	DT	93/100 (93%)	0.07	1 (1%) 80 72	7, 90, 180, 180	0
51	BZ	77/78 (98%)	-0.03	3 (3%) 39 31	5, 52, 127, 154	0
51	DZ	77/78 (98%)	-0.21	1 (1%) 77 68	5, 43, 95, 135	0
52	BW	79/84 (94%)	0.25	4 (5%) 28 24	10, 85, 145, 179	0
52	DW	79/84 (94%)	0.26	2 (2%) 57 48	5, 66, 152, 180	0
53	B6	185/185 (100%)	0.56	31 (16%) 1 2	5, 125, 180, 180	0
53	D6	185/185 (100%)	0.03	10 (5%) 25 22	5, 90, 180, 180	0
All	All	20787/21416 (97%)	-0.07	341 (1%) 72 63	5, 70, 162, 180	0

The worst 5 of 341 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
39	DX	63	ALA	10.6
23	BB	2147	A	10.0
24	BI	1	ALA	7.5
24	BI	2	LYS	6.9
23	DB	1175	A	6.0

## 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(Å <sup>2</sup> )	Q<0.9
54	MG	AA	1625	1/1	0.01	0.18	144,144,144,144	1
54	MG	DB	3060	1/1	0.24	0.12	160,160,160,160	0
54	MG	DB	3059	1/1	0.41	0.13	152,152,152,152	0
54	MG	AA	1659	1/1	0.41	0.55	127,127,127,127	0
54	MG	AA	1608	1/1	0.55	0.52	136,136,136,136	0
54	MG	AA	1657	1/1	0.57	1.78	155,155,155,155	0
54	MG	AA	1626	1/1	0.57	0.63	28,28,28,28	1
54	MG	CE	201	1/1	0.61	0.91	145,145,145,145	0
54	MG	DB	3045	1/1	0.65	0.12	108,108,108,108	0
54	MG	CA	1608	1/1	0.66	0.57	178,178,178,178	0
54	MG	AA	1639	1/1	0.66	1.94	126,126,126,126	0
54	MG	CA	1657	1/1	0.68	0.57	97,97,97,97	0
54	MG	AA	1632	1/1	0.69	0.43	80,80,80,80	0
54	MG	CA	1616	1/1	0.70	0.24	94,94,94,94	0
54	MG	BB	3079	1/1	0.71	0.19	43,43,43,43	0
55	PAR	BB	3111	42/42	0.71	0.41	100,100,100,100	42
54	MG	AA	1650	1/1	0.73	0.17	116,116,116,116	0
54	MG	BB	3042	1/1	0.74	0.06	100,100,100,100	0
54	MG	AA	1613	1/1	0.75	0.30	82,82,82,82	0
54	MG	BB	3053	1/1	0.76	0.12	38,38,38,38	0
54	MG	AA	1658	1/1	0.77	0.11	97,97,97,97	0
54	MG	CA	1660	1/1	0.77	0.22	58,58,58,58	0
54	MG	CA	1623	1/1	0.77	0.36	180,180,180,180	0
54	MG	DB	3052	1/1	0.78	0.56	166,166,166,166	0
55	PAR	DB	3112	42/42	0.78	0.40	55,55,55,55	42
54	MG	BB	3064	1/1	0.78	0.19	78,78,78,78	0
54	MG	AA	1656	1/1	0.79	0.26	50,50,50,50	0
54	MG	AA	1603	1/1	0.80	0.17	38,38,38,38	0
54	MG	AA	1617	1/1	0.80	0.22	138,138,138,138	0
54	MG	CA	1649	1/1	0.81	0.34	134,134,134,134	0
54	MG	AA	1647	1/1	0.81	1.42	180,180,180,180	0
54	MG	BB	3108	1/1	0.81	0.30	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DB	3037	1/1	0.81	0.14	45,45,45,45	0
54	MG	CA	1619	1/1	0.82	0.24	78,78,78,78	0
54	MG	AA	1627	1/1	0.83	0.29	46,46,46,46	0
54	MG	AA	1637	1/1	0.83	1.21	146,146,146,146	0
54	MG	DB	3083	1/1	0.83	0.33	72,72,72,72	0
54	MG	AA	1660	1/1	0.83	0.21	75,75,75,75	0
54	MG	BB	3031	1/1	0.84	0.19	44,44,44,44	0
54	MG	CA	1629	1/1	0.84	0.49	96,96,96,96	1
54	MG	BB	3033	1/1	0.84	0.55	125,125,125,125	0
54	MG	CA	1622	1/1	0.84	0.18	38,38,38,38	0
54	MG	CA	1614	1/1	0.84	0.19	85,85,85,85	0
54	MG	CA	1606	1/1	0.85	0.22	103,103,103,103	0
54	MG	DB	3013	1/1	0.85	0.21	35,35,35,35	0
54	MG	AA	1601	1/1	0.85	0.22	10,10,10,10	0
54	MG	BB	3077	1/1	0.85	0.17	64,64,64,64	0
54	MG	BB	3093	1/1	0.85	0.44	98,98,98,98	0
54	MG	BB	3081	1/1	0.85	0.16	31,31,31,31	0
54	MG	CA	1648	1/1	0.85	0.20	17,17,17,17	0
54	MG	AA	1635	1/1	0.86	0.20	120,120,120,120	0
54	MG	BB	3097	1/1	0.86	0.33	95,95,95,95	0
54	MG	AA	1615	1/1	0.86	0.46	171,171,171,171	0
54	MG	DB	3072	1/1	0.86	0.09	48,48,48,48	0
54	MG	BB	3099	1/1	0.87	0.11	40,40,40,40	0
54	MG	AA	1651	1/1	0.87	0.19	55,55,55,55	0
54	MG	AA	1633	1/1	0.87	0.41	56,56,56,56	0
54	MG	BB	3047	1/1	0.87	0.18	92,92,92,92	0
54	MG	CA	1634	1/1	0.87	0.17	30,30,30,30	0
54	MG	BB	3010	1/1	0.88	0.12	38,38,38,38	0
54	MG	AA	1619	1/1	0.88	1.61	180,180,180,180	0
54	MG	DB	3035	1/1	0.88	0.23	52,52,52,52	0
54	MG	CA	1626	1/1	0.88	0.31	23,23,23,23	1
54	MG	BB	3049	1/1	0.88	0.27	25,25,25,25	0
54	MG	DB	3064	1/1	0.88	0.12	23,23,23,23	0
54	MG	DB	3026	1/1	0.88	0.20	54,54,54,54	0
54	MG	CA	1658	1/1	0.88	0.37	70,70,70,70	0
54	MG	AA	1602	1/1	0.88	0.18	105,105,105,105	0
54	MG	BB	3080	1/1	0.88	0.59	131,131,131,131	0
54	MG	AA	1652	1/1	0.89	0.22	126,126,126,126	0
54	MG	BB	3019	1/1	0.89	0.17	56,56,56,56	0
54	MG	BB	3012	1/1	0.89	0.16	71,71,71,71	0
54	MG	AA	1622	1/1	0.89	0.34	111,111,111,111	0
54	MG	DB	3058	1/1	0.89	0.56	157,157,157,157	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	0.89	0.19	5,5,5,5	0
55	PAR	AA	1661	42/42	0.89	0.22	62,62,62,62	0
54	MG	DB	3080	1/1	0.89	0.11	13,13,13,13	0
54	MG	BB	3051	1/1	0.89	0.37	75,75,75,75	0
54	MG	CA	1630	1/1	0.90	0.23	65,65,65,65	0
54	MG	CA	1609	1/1	0.90	0.16	81,81,81,81	0
54	MG	BB	3095	1/1	0.90	0.11	65,65,65,65	0
54	MG	AA	1621	1/1	0.90	0.26	27,27,27,27	0
54	MG	AA	1610	1/1	0.90	0.32	82,82,82,82	0
54	MG	AA	1623	1/1	0.90	0.63	33,33,33,33	1
54	MG	CA	1625	1/1	0.90	0.31	46,46,46,46	0
55	PAR	CA	1662	42/42	0.90	0.21	45,45,45,45	0
54	MG	BB	3013	1/1	0.90	0.28	86,86,86,86	0
54	MG	CA	1620	1/1	0.90	0.26	104,104,104,104	0
54	MG	AA	1620	1/1	0.90	0.06	95,95,95,95	0
54	MG	DB	3050	1/1	0.91	0.11	118,118,118,118	0
54	MG	BB	3043	1/1	0.91	0.23	97,97,97,97	0
56	ZN	D4	101	1/1	0.91	0.30	96,96,96,96	0
54	MG	BB	3063	1/1	0.91	0.09	5,5,5,5	0
54	MG	CA	1615	1/1	0.91	0.25	180,180,180,180	0
54	MG	DB	3054	1/1	0.91	0.12	69,69,69,69	0
54	MG	CA	1654	1/1	0.91	0.13	72,72,72,72	0
54	MG	DB	3100	1/1	0.92	0.13	22,22,22,22	0
54	MG	BB	3004	1/1	0.92	0.31	44,44,44,44	0
54	MG	DB	3094	1/1	0.92	0.10	81,81,81,81	0
54	MG	BB	3006	1/1	0.92	0.09	37,37,37,37	0
54	MG	DB	3022	1/1	0.92	0.17	85,85,85,85	0
54	MG	CA	1643	1/1	0.92	0.13	11,11,11,11	0
54	MG	DB	3053	1/1	0.92	0.26	65,65,65,65	0
54	MG	DB	3066	1/1	0.92	0.18	123,123,123,123	0
54	MG	DB	3016	1/1	0.92	0.12	5,5,5,5	0
54	MG	CA	1624	1/1	0.92	0.20	48,48,48,48	0
54	MG	CA	1652	1/1	0.93	0.22	58,58,58,58	0
54	MG	CA	1635	1/1	0.93	0.16	105,105,105,105	0
54	MG	DB	3015	1/1	0.93	0.10	39,39,39,39	0
54	MG	DB	3061	1/1	0.93	0.17	95,95,95,95	0
54	MG	CA	1637	1/1	0.93	0.13	116,116,116,116	0
54	MG	BB	3027	1/1	0.93	0.18	83,83,83,83	0
54	MG	DB	3073	1/1	0.93	0.12	25,25,25,25	0
54	MG	CA	1621	1/1	0.93	0.56	67,67,67,67	0
54	MG	BB	3078	1/1	0.93	0.33	92,92,92,92	0
54	MG	BB	3071	1/1	0.93	0.21	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BB	3026	1/1	0.93	0.23	44,44,44,44	0
54	MG	CA	1632	1/1	0.93	0.14	34,34,34,34	0
54	MG	AA	1606	1/1	0.93	0.04	73,73,73,73	0
54	MG	DB	3027	1/1	0.93	0.17	11,11,11,11	0
54	MG	BB	3083	1/1	0.94	0.14	51,51,51,51	0
54	MG	DB	3030	1/1	0.94	0.23	30,30,30,30	0
54	MG	BB	3091	1/1	0.94	0.11	81,81,81,81	0
54	MG	DB	3097	1/1	0.94	0.14	32,32,32,32	0
54	MG	DB	3008	1/1	0.94	0.19	11,11,11,11	0
54	MG	AA	1638	1/1	0.94	0.10	45,45,45,45	0
54	MG	AA	1624	1/1	0.94	0.20	76,76,76,76	0
54	MG	CA	1659	1/1	0.94	0.13	70,70,70,70	0
54	MG	CA	1607	1/1	0.94	0.11	20,20,20,20	0
54	MG	DB	3090	1/1	0.94	0.22	35,35,35,35	0
54	MG	BB	3037	1/1	0.94	0.15	63,63,63,63	0
54	MG	CA	1640	1/1	0.94	0.11	35,35,35,35	0
56	ZN	B4	101	1/1	0.94	0.20	68,68,68,68	0
54	MG	CA	1636	1/1	0.94	0.21	90,90,90,90	0
54	MG	DB	3065	1/1	0.94	0.32	68,68,68,68	0
54	MG	BB	3017	1/1	0.94	0.15	46,46,46,46	0
54	MG	AA	1634	1/1	0.94	0.11	79,79,79,79	0
54	MG	DB	3049	1/1	0.94	0.12	11,11,11,11	0
54	MG	BB	3066	1/1	0.94	0.05	34,34,34,34	0
54	MG	BB	3046	1/1	0.94	0.19	64,64,64,64	0
54	MG	DB	3051	1/1	0.94	0.15	20,20,20,20	0
54	MG	BB	3100	1/1	0.94	0.20	109,109,109,109	0
54	MG	CA	1661	1/1	0.94	0.12	40,40,40,40	0
54	MG	DB	3067	1/1	0.94	0.15	13,13,13,13	0
54	MG	BB	3054	1/1	0.94	0.10	55,55,55,55	0
54	MG	AA	1612	1/1	0.94	0.15	96,96,96,96	0
54	MG	BB	3020	1/1	0.94	0.48	23,23,23,23	0
54	MG	AA	1646	1/1	0.94	0.12	98,98,98,98	0
54	MG	AA	1644	1/1	0.94	0.22	69,69,69,69	0
54	MG	AA	1645	1/1	0.95	0.17	138,138,138,138	0
54	MG	BB	3009	1/1	0.95	0.11	76,76,76,76	0
54	MG	BB	3002	1/1	0.95	0.09	18,18,18,18	0
54	MG	DB	3010	1/1	0.95	0.14	5,5,5,5	0
54	MG	BB	3070	1/1	0.95	0.18	40,40,40,40	0
54	MG	BB	3041	1/1	0.95	0.12	15,15,15,15	0
54	MG	BB	3088	1/1	0.95	0.08	11,11,11,11	0
54	MG	BB	3059	1/1	0.95	0.16	39,39,39,39	0
54	MG	AA	1648	1/1	0.95	0.10	5,5,5,5	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DB	3108	1/1	0.95	0.24	13,13,13,13	0
54	MG	CA	1646	1/1	0.95	0.34	78,78,78,78	0
54	MG	AA	1642	1/1	0.95	0.20	63,63,63,63	0
54	MG	AA	1604	1/1	0.95	0.12	37,37,37,37	0
54	MG	DB	3075	1/1	0.95	0.16	10,10,10,10	0
54	MG	AA	1649	1/1	0.95	0.09	93,93,93,93	0
54	MG	BB	3008	1/1	0.95	0.13	81,81,81,81	0
54	MG	BB	3090	1/1	0.95	0.17	115,115,115,115	0
54	MG	DB	3017	1/1	0.95	0.13	23,23,23,23	0
54	MG	BB	3061	1/1	0.95	0.14	46,46,46,46	0
54	MG	AA	1605	1/1	0.95	0.09	54,54,54,54	0
54	MG	DB	3036	1/1	0.95	0.31	51,51,51,51	0
54	MG	BB	3029	1/1	0.95	0.10	12,12,12,12	0
54	MG	BB	3018	1/1	0.95	0.25	32,32,32,32	0
54	MG	DB	3029	1/1	0.95	0.16	70,70,70,70	0
54	MG	BB	3011	1/1	0.95	0.16	68,68,68,68	0
54	MG	CA	1604	1/1	0.95	0.28	11,11,11,11	0
54	MG	BB	3065	1/1	0.95	0.10	30,30,30,30	0
54	MG	AA	1655	1/1	0.95	0.22	83,83,83,83	0
54	MG	CA	1645	1/1	0.96	0.07	82,82,82,82	0
54	MG	BB	3057	1/1	0.96	0.72	65,65,65,65	0
54	MG	AA	1630	1/1	0.96	0.11	118,118,118,118	0
54	MG	AA	1640	1/1	0.96	0.09	77,77,77,77	0
54	MG	DB	3082	1/1	0.96	0.07	37,37,37,37	0
54	MG	DB	3007	1/1	0.96	0.15	27,27,27,27	0
54	MG	DB	3048	1/1	0.96	0.24	8,8,8,8	0
54	MG	BB	3040	1/1	0.96	0.12	47,47,47,47	0
54	MG	AA	1636	1/1	0.96	0.16	38,38,38,38	0
54	MG	CA	1628	1/1	0.96	0.21	82,82,82,82	0
54	MG	DB	3093	1/1	0.96	0.12	9,9,9,9	0
54	MG	DB	3014	1/1	0.96	0.33	39,39,39,39	0
54	MG	DB	3095	1/1	0.96	0.24	62,62,62,62	0
54	MG	DB	3110	1/1	0.96	0.14	44,44,44,44	0
54	MG	DB	3111	1/1	0.96	0.23	68,68,68,68	0
54	MG	CA	1627	1/1	0.96	0.20	35,35,35,35	1
54	MG	DB	3092	1/1	0.96	0.14	60,60,60,60	0
54	MG	CA	1638	1/1	0.96	0.06	56,56,56,56	0
54	MG	AA	1607	1/1	0.96	0.10	35,35,35,35	0
54	MG	DB	3041	1/1	0.96	0.12	9,9,9,9	0
54	MG	BB	3035	1/1	0.96	0.14	60,60,60,60	0
54	MG	AA	1631	1/1	0.96	0.08	61,61,61,61	0
54	MG	BB	3072	1/1	0.96	0.18	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DB	3009	1/1	0.96	0.09	22,22,22,22	0
54	MG	DB	3006	1/1	0.96	0.07	15,15,15,15	0
54	MG	BB	3068	1/1	0.96	0.14	102,102,102,102	0
54	MG	DB	3088	1/1	0.96	0.07	31,31,31,31	0
54	MG	BB	3003	1/1	0.96	0.21	60,60,60,60	0
54	MG	DB	3011	1/1	0.96	0.12	22,22,22,22	0
54	MG	DB	3102	1/1	0.96	0.17	20,20,20,20	0
54	MG	DB	3023	1/1	0.96	0.07	35,35,35,35	0
54	MG	DB	3046	1/1	0.96	0.14	38,38,38,38	0
54	MG	CA	1617	1/1	0.96	0.11	12,12,12,12	0
54	MG	AA	1614	1/1	0.96	0.54	131,131,131,131	0
54	MG	BB	3092	1/1	0.96	0.08	60,60,60,60	0
54	MG	BB	3001	1/1	0.96	0.08	14,14,14,14	0
54	MG	CA	1618	1/1	0.96	0.12	23,23,23,23	0
54	MG	BB	3069	1/1	0.96	0.11	5,5,5,5	0
54	MG	AA	1611	1/1	0.96	0.09	75,75,75,75	0
54	MG	BB	3044	1/1	0.97	0.09	29,29,29,29	0
54	MG	DB	3063	1/1	0.97	0.06	23,23,23,23	0
54	MG	DB	3034	1/1	0.97	0.11	52,52,52,52	0
54	MG	DB	3068	1/1	0.97	0.19	16,16,16,16	0
54	MG	DB	3076	1/1	0.97	0.15	27,27,27,27	0
54	MG	BB	3103	1/1	0.97	0.08	20,20,20,20	0
54	MG	DB	3002	1/1	0.97	0.09	14,14,14,14	0
54	MG	DB	3032	1/1	0.97	0.18	21,21,21,21	0
54	MG	CA	1653	1/1	0.97	0.05	43,43,43,43	0
54	MG	AA	1609	1/1	0.97	0.06	11,11,11,11	0
54	MG	CA	1633	1/1	0.97	0.17	106,106,106,106	0
54	MG	DB	3103	1/1	0.97	0.10	37,37,37,37	0
54	MG	AA	1618	1/1	0.97	0.04	105,105,105,105	0
54	MG	CA	1644	1/1	0.97	0.11	69,69,69,69	0
54	MG	DB	3038	1/1	0.97	0.09	23,23,23,23	0
54	MG	DB	3085	1/1	0.97	0.20	49,49,49,49	0
54	MG	AA	1654	1/1	0.97	0.08	52,52,52,52	0
54	MG	BB	3039	1/1	0.97	0.12	12,12,12,12	0
54	MG	DB	3081	1/1	0.97	0.09	20,20,20,20	0
54	MG	DB	3071	1/1	0.97	0.09	41,41,41,41	0
54	MG	BB	3024	1/1	0.97	0.08	76,76,76,76	0
54	MG	BB	3086	1/1	0.97	0.13	5,5,5,5	0
54	MG	BB	3038	1/1	0.97	0.12	157,157,157,157	0
54	MG	BB	3107	1/1	0.97	0.06	13,13,13,13	0
54	MG	AA	1653	1/1	0.97	0.10	51,51,51,51	0
54	MG	DB	3070	1/1	0.97	0.08	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	CA	1611	1/1	0.97	0.09	114,114,114,114	0
54	MG	BB	3032	1/1	0.97	0.12	31,31,31,31	0
54	MG	DB	3031	1/1	0.97	0.10	29,29,29,29	0
54	MG	BB	3048	1/1	0.97	0.18	8,8,8,8	0
54	MG	DB	3043	1/1	0.97	0.12	7,7,7,7	0
54	MG	BB	3098	1/1	0.97	0.14	10,10,10,10	0
54	MG	BB	3034	1/1	0.97	0.18	41,41,41,41	0
54	MG	CA	1642	1/1	0.97	0.08	85,85,85,85	0
54	MG	BB	3073	1/1	0.97	0.14	70,70,70,70	0
54	MG	DB	3078	1/1	0.97	0.11	31,31,31,31	0
54	MG	BB	3109	1/1	0.97	0.12	49,49,49,49	0
54	MG	CA	1601	1/1	0.97	0.15	9,9,9,9	0
54	MG	CA	1641	1/1	0.97	0.12	76,76,76,76	0
54	MG	BB	3106	1/1	0.97	0.10	45,45,45,45	0
54	MG	AA	1629	1/1	0.97	0.09	44,44,44,44	0
54	MG	BB	3110	1/1	0.97	0.17	41,41,41,41	0
54	MG	DB	3055	1/1	0.97	0.16	26,26,26,26	0
54	MG	CA	1610	1/1	0.97	0.11	65,65,65,65	0
54	MG	CA	1605	1/1	0.97	0.12	5,5,5,5	0
54	MG	DB	3069	1/1	0.97	0.19	5,5,5,5	0
54	MG	BB	3023	1/1	0.98	0.11	6,6,6,6	0
54	MG	CA	1647	1/1	0.98	0.12	58,58,58,58	0
54	MG	DB	3042	1/1	0.98	0.10	36,36,36,36	0
54	MG	BB	3028	1/1	0.98	0.23	95,95,95,95	0
54	MG	BB	3014	1/1	0.98	0.19	46,46,46,46	0
54	MG	DB	3019	1/1	0.98	0.07	8,8,8,8	0
54	MG	DB	3104	1/1	0.98	0.11	21,21,21,21	0
54	MG	BB	3050	1/1	0.98	0.09	16,16,16,16	0
54	MG	CA	1602	1/1	0.98	0.21	16,16,16,16	0
54	MG	DB	3039	1/1	0.98	0.09	34,34,34,34	0
54	MG	BB	3096	1/1	0.98	0.13	69,69,69,69	0
54	MG	AA	1628	1/1	0.98	0.22	49,49,49,49	0
54	MG	AA	1616	1/1	0.98	0.12	15,15,15,15	0
54	MG	CA	1651	1/1	0.98	0.09	37,37,37,37	0
54	MG	CA	1639	1/1	0.98	0.15	5,5,5,5	0
54	MG	DB	3044	1/1	0.98	0.10	16,16,16,16	0
54	MG	BB	3055	1/1	0.98	0.26	78,78,78,78	0
54	MG	CA	1631	1/1	0.98	0.14	55,55,55,55	0
54	MG	DB	3107	1/1	0.98	0.08	51,51,51,51	0
54	MG	DB	3106	1/1	0.98	0.11	17,17,17,17	0
54	MG	DB	3057	1/1	0.98	0.05	17,17,17,17	0
54	MG	DB	3020	1/1	0.98	0.14	5,5,5,5	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	0.98	0.09	59,59,59,59	0
54	MG	DB	3004	1/1	0.98	0.26	40,40,40,40	0
54	MG	BB	3016	1/1	0.98	0.17	94,94,94,94	0
54	MG	BB	3045	1/1	0.98	0.12	32,32,32,32	0
54	MG	DB	3018	1/1	0.98	0.15	17,17,17,17	0
54	MG	DB	3012	1/1	0.98	0.12	8,8,8,8	0
54	MG	DB	3028	1/1	0.98	0.30	33,33,33,33	0
54	MG	DB	3086	1/1	0.98	0.19	25,25,25,25	0
54	MG	BB	3105	1/1	0.98	0.10	21,21,21,21	0
54	MG	DB	3096	1/1	0.98	0.15	37,37,37,37	0
54	MG	DB	3089	1/1	0.98	0.22	75,75,75,75	0
54	MG	DB	3062	1/1	0.98	0.04	44,44,44,44	0
54	MG	DB	3105	1/1	0.98	0.06	24,24,24,24	0
54	MG	BB	3102	1/1	0.98	0.13	76,76,76,76	0
54	MG	BB	3087	1/1	0.98	0.18	102,102,102,102	0
54	MG	BB	3060	1/1	0.98	0.15	43,43,43,43	0
54	MG	BB	3075	1/1	0.98	0.12	55,55,55,55	0
54	MG	DB	3101	1/1	0.98	0.25	7,7,7,7	0
54	MG	DB	3098	1/1	0.98	0.07	69,69,69,69	0
54	MG	BB	3076	1/1	0.98	0.09	48,48,48,48	0
54	MG	DB	3025	1/1	0.98	0.09	18,18,18,18	0
54	MG	DB	3047	1/1	0.98	0.17	31,31,31,31	0
54	MG	BB	3030	1/1	0.98	0.05	83,83,83,83	0
54	MG	BB	3007	1/1	0.98	0.21	103,103,103,103	0
54	MG	DB	3033	1/1	0.98	0.16	20,20,20,20	0
54	MG	AA	1641	1/1	0.98	0.05	32,32,32,32	0
54	MG	DB	3005	1/1	0.98	0.06	52,52,52,52	0
54	MG	BB	3005	1/1	0.98	0.11	9,9,9,9	0
54	MG	BB	3067	1/1	0.98	0.07	25,25,25,25	0
54	MG	DB	3099	1/1	0.98	0.15	21,21,21,21	0
54	MG	DB	3024	1/1	0.98	0.14	47,47,47,47	0
54	MG	AA	1643	1/1	0.99	0.18	118,118,118,118	0
54	MG	CA	1656	1/1	0.99	0.06	7,7,7,7	0
54	MG	DB	3079	1/1	0.99	0.16	30,30,30,30	0
54	MG	CA	1613	1/1	0.99	0.12	24,24,24,24	0
54	MG	DB	3021	1/1	0.99	0.11	18,18,18,18	0
54	MG	DB	3001	1/1	0.99	0.10	5,5,5,5	0
54	MG	BB	3085	1/1	0.99	0.10	76,76,76,76	0
54	MG	BB	3058	1/1	0.99	0.09	17,17,17,17	0
54	MG	DB	3087	1/1	0.99	0.22	67,67,67,67	0
54	MG	DB	3074	1/1	0.99	0.15	17,17,17,17	0
54	MG	DB	3056	1/1	0.99	0.16	16,16,16,16	0

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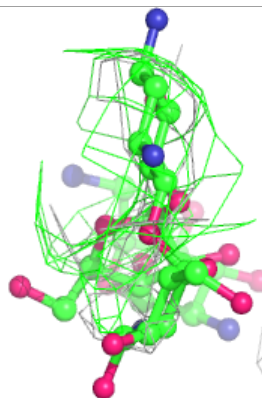
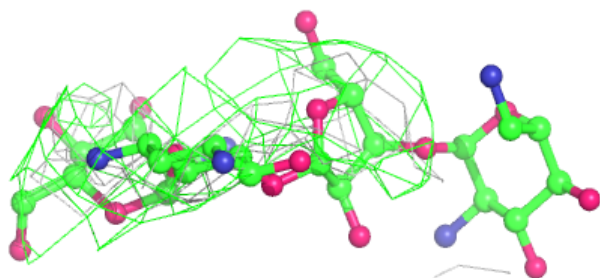
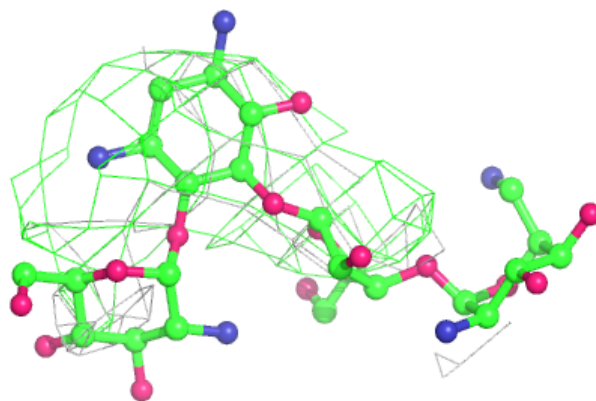
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BB	3074	1/1	0.99	0.08	7,7,7,7	0
54	MG	BB	3094	1/1	0.99	0.12	55,55,55,55	0
54	MG	BB	3036	1/1	0.99	0.22	68,68,68,68	0
54	MG	BB	3056	1/1	0.99	0.05	61,61,61,61	0
54	MG	BB	3015	1/1	0.99	0.05	9,9,9,9	0
54	MG	CA	1650	1/1	0.99	0.05	5,5,5,5	0
54	MG	DB	3040	1/1	0.99	0.10	5,5,5,5	0
54	MG	DB	3109	1/1	0.99	0.20	27,27,27,27	0
54	MG	BB	3084	1/1	0.99	0.14	60,60,60,60	0
54	MG	BB	3082	1/1	0.99	0.33	22,22,22,22	0
54	MG	BB	3022	1/1	0.99	0.03	34,34,34,34	0
54	MG	CA	1612	1/1	0.99	0.11	97,97,97,97	0
54	MG	BB	3021	1/1	0.99	0.12	62,62,62,62	0
54	MG	CA	1655	1/1	0.99	0.06	22,22,22,22	0
54	MG	BB	3104	1/1	0.99	0.13	43,43,43,43	0
54	MG	BB	3062	1/1	0.99	0.15	5,5,5,5	0
54	MG	BB	3025	1/1	0.99	0.07	22,22,22,22	0
54	MG	CA	1603	1/1	0.99	0.12	37,37,37,37	0
54	MG	BB	3089	1/1	0.99	0.06	30,30,30,30	0
54	MG	DB	3091	1/1	0.99	0.09	11,11,11,11	0
54	MG	DB	3077	1/1	0.99	0.11	17,17,17,17	0
54	MG	DB	3084	1/1	1.00	0.16	14,14,14,14	0
54	MG	BB	3101	1/1	1.00	0.23	64,64,64,64	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.

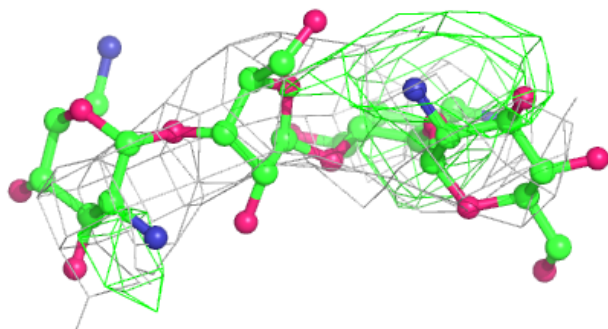
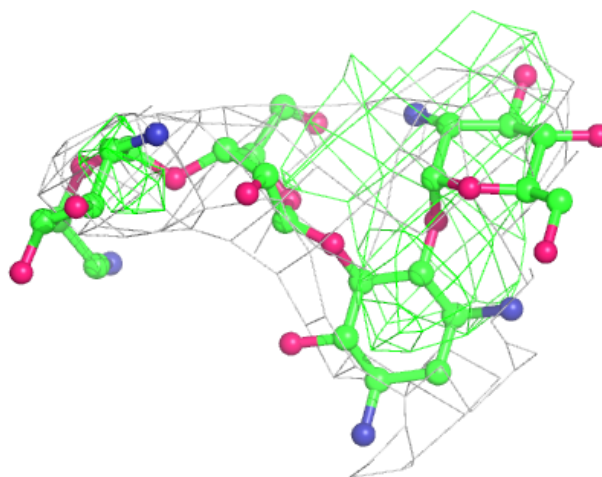
**Electron density around PAR BB 3111:**

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



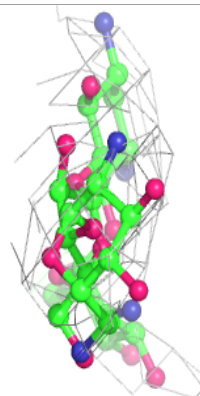
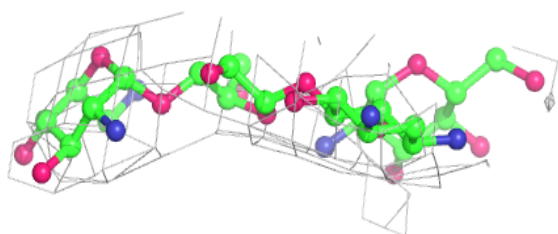
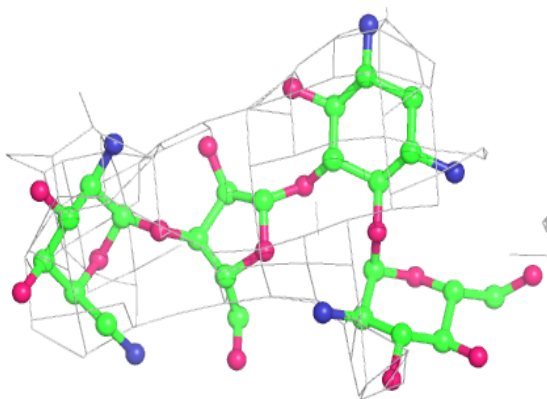
**Electron density around PAR DB 3112:**

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

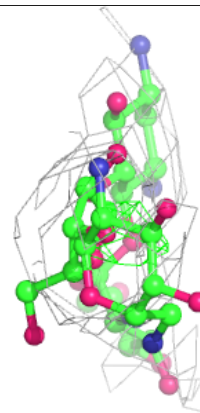
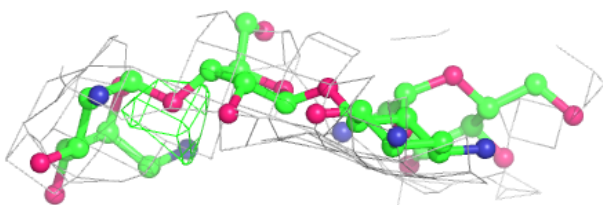
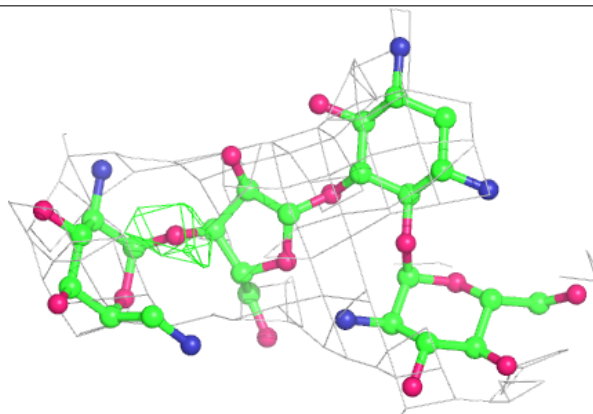


**Electron density around PAR AA 1661:**

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

**Electron density around PAR CA 1662:**

$2mF_o-DF_c$  (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.