



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 05:21 am BST

PDB ID : 4V50  
Title : Crystal Structure of Ribosome with messenger RNA and the Anticodon stem-loop of P-site tRNA.  
Authors : Berk, V.; Zhang, W.; Pai, R.D.; Cate, J.H.D.  
Deposited on : 2006-08-16  
Resolution : 3.22 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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11



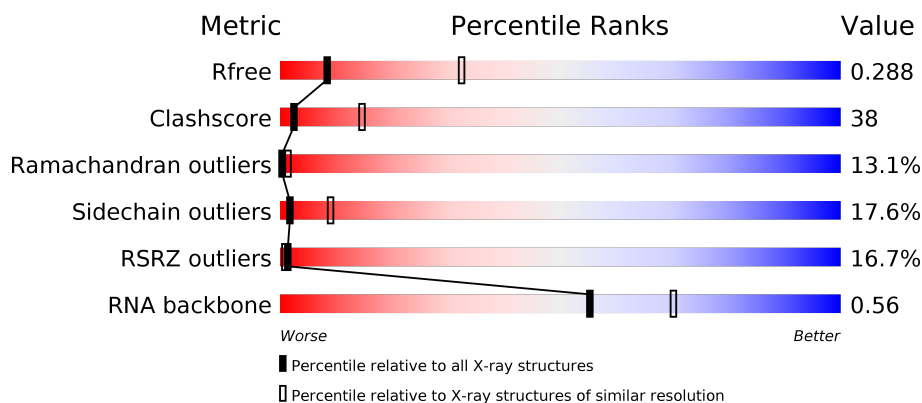
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.22 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	1335 (3.24-3.20)
Clashscore	141614	1460 (3.24-3.20)
Ramachandran outliers	138981	1437 (3.24-3.20)
Sidechain outliers	138945	1436 (3.24-3.20)
RSRZ outliers	127900	1291 (3.24-3.20)
RNA backbone	3102	1023 (3.54-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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>10%</div> <div>19%</div> <div>65%</div> <div>15%</div> <div>..</div> </div>
1	CA	1542	<div> <div>%</div> <div>20%</div> <div>64%</div> <div>15%</div> <div>.</div> </div>
2	AW	17	<div> <div>59%</div> <div>47%</div> <div>53%</div> </div>
2	CW	17	<div> <div>6%</div> <div>47%</div> <div>53%</div> </div>

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Mol	Chain	Length	Quality of chain
3	AX	6	
3	CX	6	
4	AB	240	
4	CB	240	
5	AC	232	
5	CC	232	
6	AD	205	
6	CD	205	
7	AE	166	
7	CE	166	
8	AF	135	
8	CF	135	
9	AG	178	
9	CG	178	
10	AH	129	
10	CH	129	
11	AI	129	
11	CI	129	
12	AJ	103	
12	CJ	103	
13	AK	128	
13	CK	128	
14	AL	123	
14	CL	123	
15	AM	117	

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Mol	Chain	Length	Quality of chain
15	CM	117	
16	AN	100	
16	CN	100	
17	AO	88	
17	CO	88	
18	AP	82	
18	CP	82	
19	AQ	83	
19	CQ	83	
20	AR	74	
20	CR	74	
21	AS	91	
21	CS	91	
22	AT	86	
22	CT	86	
23	AU	70	
23	CU	70	
24	BA	120	
24	DA	120	
25	BB	2904	
25	DB	2904	
26	BC	272	
26	DC	272	
27	BD	209	
27	DD	209	

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Mol	Chain	Length	Quality of chain
28	BE	201	
28	DE	201	
29	BF	178	
29	DF	178	
30	BG	176	
30	DG	176	
31	BH	149	
31	DH	149	
32	BI	141	
32	DI	141	
33	BJ	142	
33	DJ	142	
34	BK	123	
34	DK	123	
35	BL	144	
35	DL	144	
36	BM	136	
36	DM	136	
37	BN	127	
37	DN	127	
38	BO	117	
38	DO	117	
39	BP	114	
39	DP	114	
40	BQ	117	

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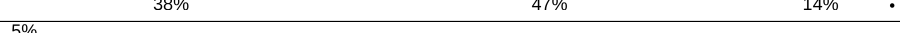
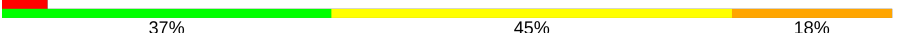
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Mol	Chain	Length	Quality of chain
40	DQ	117	
41	BR	103	
41	DR	103	
42	BS	110	
42	DS	110	
43	BT	100	
43	DT	100	
44	BU	103	
44	DU	103	
45	BV	94	
45	DV	94	
46	BW	84	
46	DW	84	
47	BX	77	
47	DX	77	
48	BY	63	
48	DY	63	
49	BZ	58	
49	DZ	58	
50	B0	56	
50	D0	56	
51	B1	54	
51	D1	54	
52	B2	46	
52	D2	46	

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Mol	Chain	Length	Quality of chain
53	B3	64	
53	D3	64	
54	B4	38	
54	D4	38	

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
55	MG	AA	1611	-	-	-	X
55	MG	AA	1614	-	-	-	X
55	MG	AA	1626	-	-	-	X
55	MG	AA	1637	-	-	-	X
55	MG	AA	1643	-	-	-	X
55	MG	AA	1658	-	-	-	X
55	MG	BB	3057	-	-	-	X
55	MG	BB	3093	-	-	-	X
55	MG	CA	1640	-	-	-	X
55	MG	CA	1646	-	-	-	X
55	MG	DB	3052	-	-	-	X



## 2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 285033 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

- Molecule 2 is a RNA chain called PHE tRNA (UNMODIFIED BASES).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AW	17	Total	C	N	O	P	0	0	0
			360	161	64	118	17			
2	CW	17	Total	C	N	O	P	0	0	0
			360	161	64	118	17			

- Molecule 3 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AX	6	Total	C	N	O	P	0	0	0
			125	56	18	45	6			
3	CX	6	Total	C	N	O	P	0	0	0
			125	56	18	45	6			

- Molecule 4 is a protein called 30S ribosomal protein S2.

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

- Molecule 5 is a protein called 30S ribosomal protein S3.



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

- Molecule 6 is a protein called 30S ribosomal protein S4.

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

- Molecule 7 is a protein called 30S ribosomal protein S5.

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

- Molecule 8 is a protein called 30S ribosomal protein S6.

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

- Molecule 9 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AG	150	Total	C	N	O	S	0	0	0
			1174	730	226	214	4			
9	CG	150	Total	C	N	O	S	0	0	0
			1174	730	226	214	4			

- Molecule 10 is a protein called 30S ribosomal protein S8.

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

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

- Molecule 11 is a protein called 30S ribosomal protein S9.

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

- Molecule 12 is a protein called 30S ribosomal protein S10.

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

- Molecule 13 is a protein called 30S ribosomal protein S11.

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

- Molecule 14 is a protein called 30S ribosomal protein S12.

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

- Molecule 15 is a protein called 30S ribosomal protein S13.

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



- Molecule 16 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			
16	CN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			

- Molecule 17 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AO	88	Total	C	N	O	S	0	0	0
			716	440	146	129	1			
17	CO	88	Total	C	N	O	S	0	0	0
			716	440	146	129	1			

- Molecule 18 is a protein called 30S ribosomal protein S16.

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

- Molecule 19 is a protein called 30S ribosomal protein S17.

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

- Molecule 20 is a protein called 30S ribosomal protein S18.

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

- Molecule 21 is a protein called 30S ribosomal protein S19.



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

- Molecule 22 is a protein called 30S ribosomal protein S20.

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

- Molecule 23 is a protein called 30S ribosomal protein S21.

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

- Molecule 24 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 25 is a RNA chain called 23S ribosomal RNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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



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

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

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

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	BB	118	Total	Mg	0	0
			118	118		
55	CN	1	Total	Mg	0	0
			1	1		
55	CA	56	Total	Mg	0	0
			56	56		
55	AA	60	Total	Mg	0	0
			60	60		
55	AX	2	Total	Mg	0	0
			2	2		
55	BJ	1	Total	Mg	0	0
			1	1		
55	CX	1	Total	Mg	0	0
			1	1		
55	DB	119	Total	Mg	0	0
			119	119		

- 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	287	Total O 287 287	0	0
57	AX	9	Total O 9 9	0	0
57	AE	3	Total O 3 3	0	0
57	AI	1	Total O 1 1	0	0
57	AK	2	Total O 2 2	0	0
57	AL	2	Total O 2 2	0	0
57	AN	1	Total O 1 1	0	0
57	AP	1	Total O 1 1	0	0
57	AT	2	Total O 2 2	0	0
57	BB	532	Total O 532 532	0	0
57	BC	7	Total O 7 7	0	0
57	BE	3	Total O 3 3	0	0
57	BH	3	Total O 3 3	0	0
57	BJ	3	Total O 3 3	0	0
57	BL	2	Total O 2 2	0	0
57	BN	3	Total O 3 3	0	0
57	B2	1	Total O 1 1	0	0
57	B4	5	Total O 5 5	0	0
57	CA	264	Total O 264 264	0	0
57	CX	6	Total O 6 6	0	0
57	CE	2	Total O 2 2	0	0
57	CI	3	Total O 3 3	0	0

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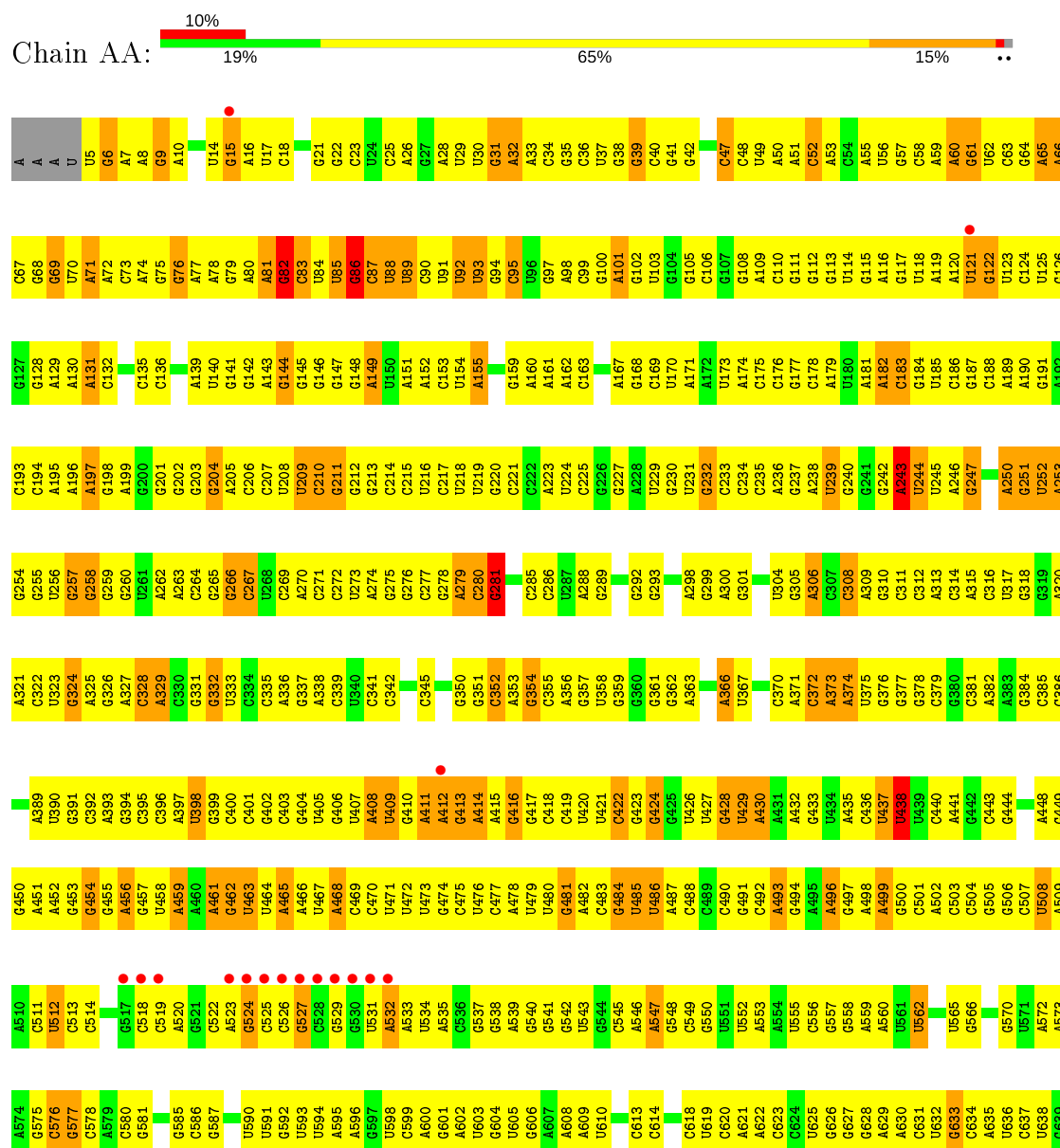
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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57	CP	1	Total 1	O 1	0	0
57	CT	3	Total 3	O 3	0	0
57	CU	1	Total 1	O 1	0	0
57	DB	531	Total 531	O 531	0	0
57	DC	7	Total 7	O 7	0	0
57	DD	1	Total 1	O 1	0	0
57	DE	3	Total 3	O 3	0	0
57	DJ	2	Total 2	O 2	0	0
57	DL	3	Total 3	O 3	0	0
57	DN	3	Total 3	O 3	0	0
57	DT	1	Total 1	O 1	0	0
57	D2	1	Total 1	O 1	0	0
57	D4	4	Total 4	O 4	0	0



### 3 Residue-property plots

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

- Molecule 1: 16S ribosomal RNA



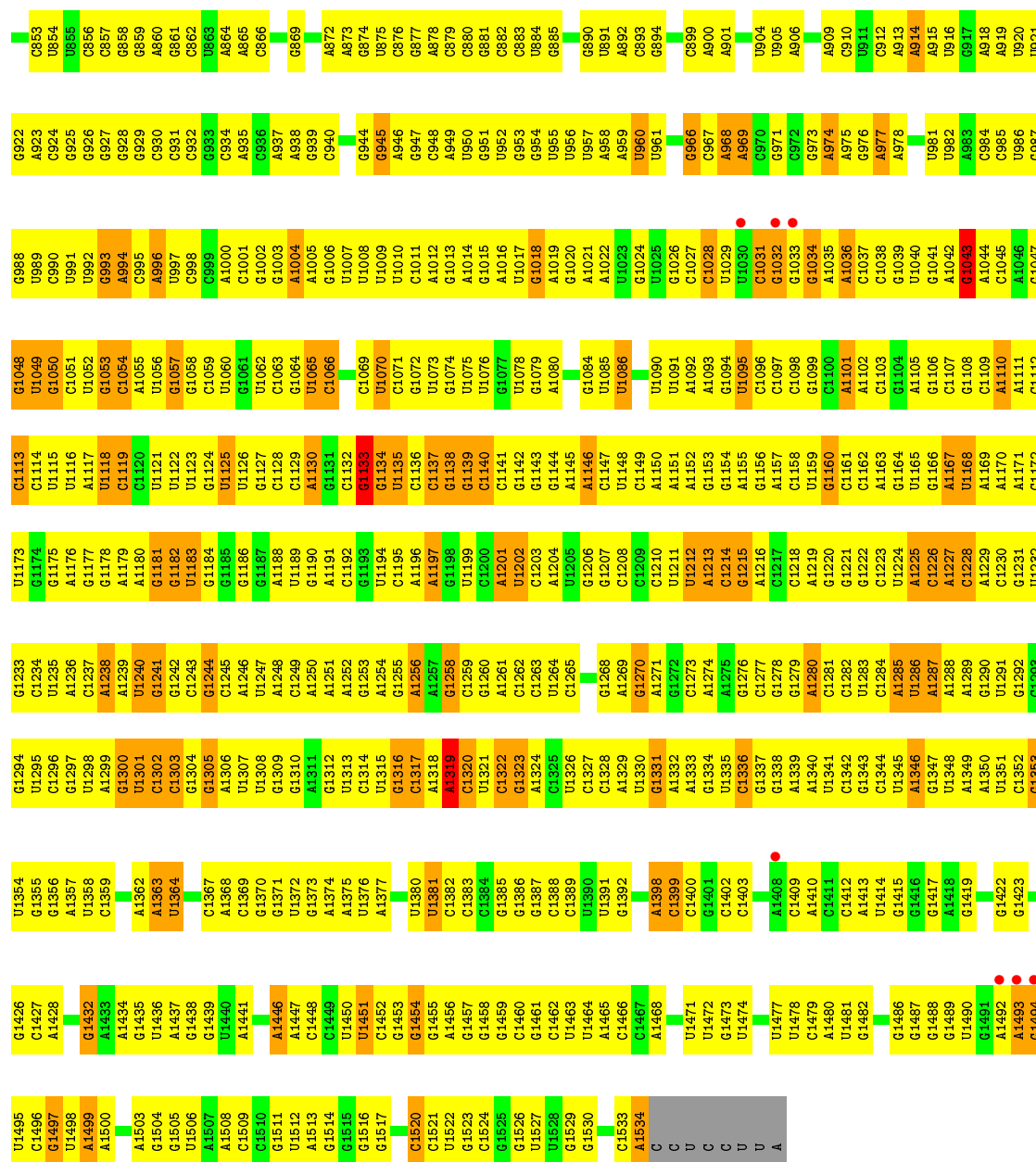








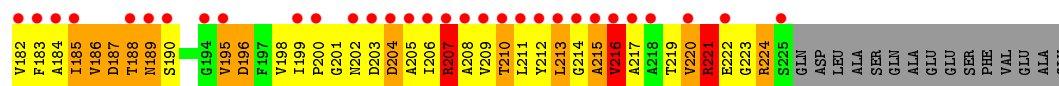




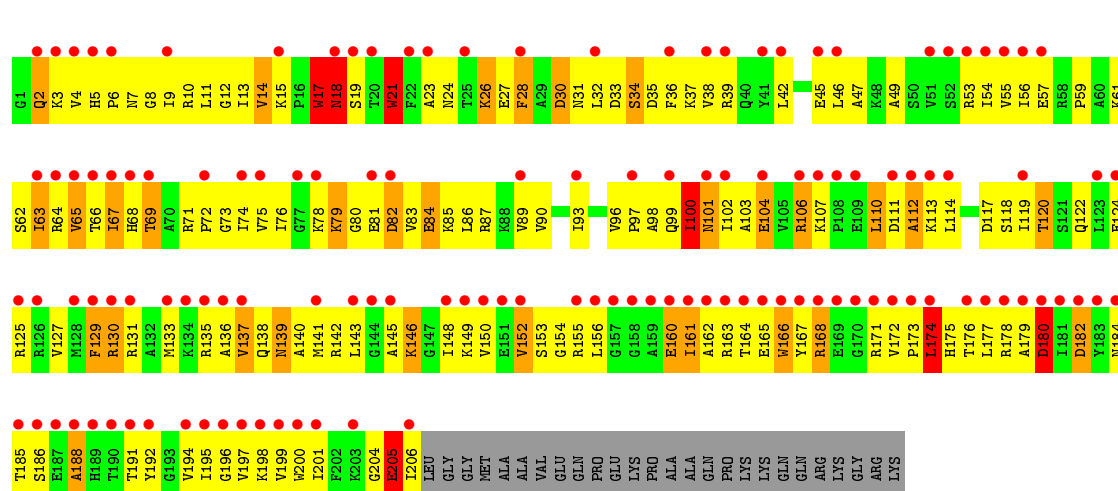




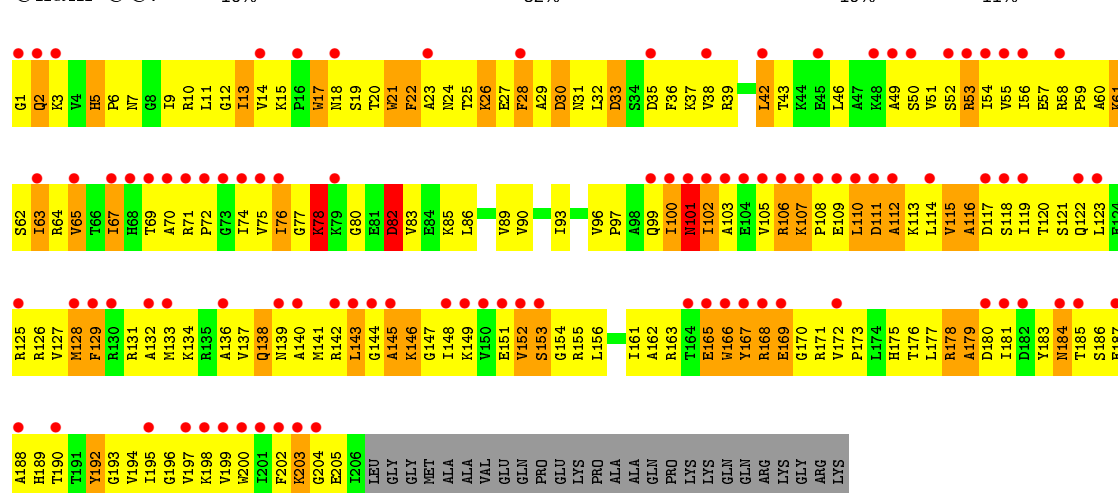
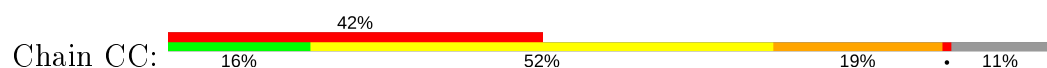




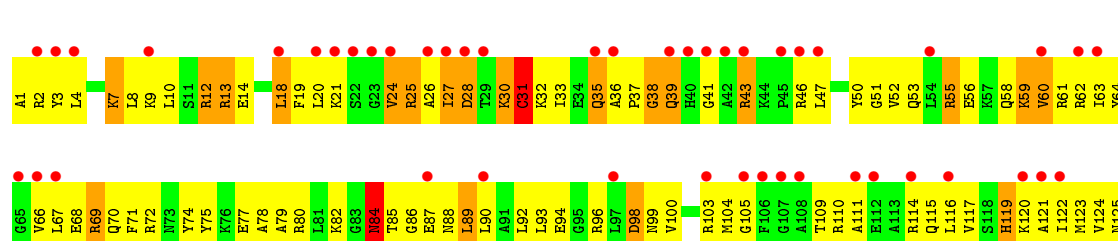
• Molecule 5: 30S ribosomal protein S3



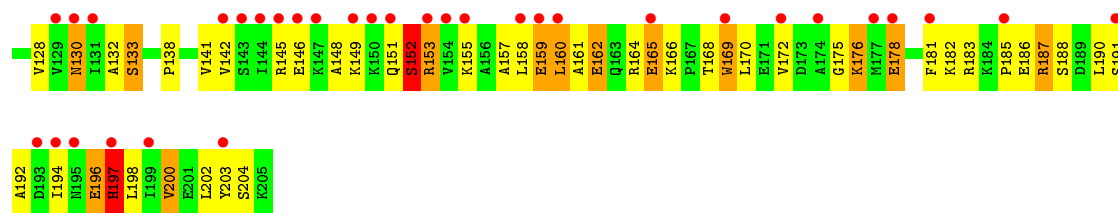
• Molecule 5: 30S ribosomal protein S3



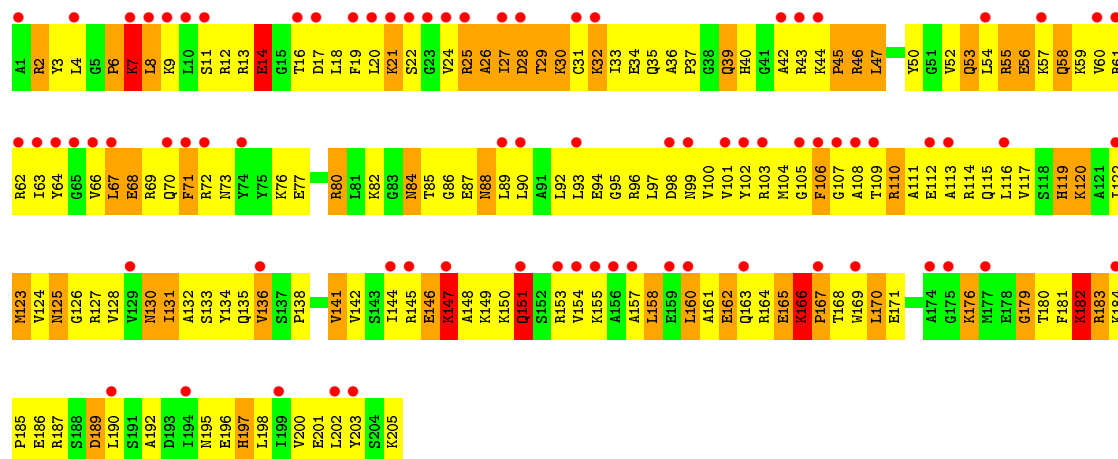
• Molecule 6: 30S ribosomal protein S4



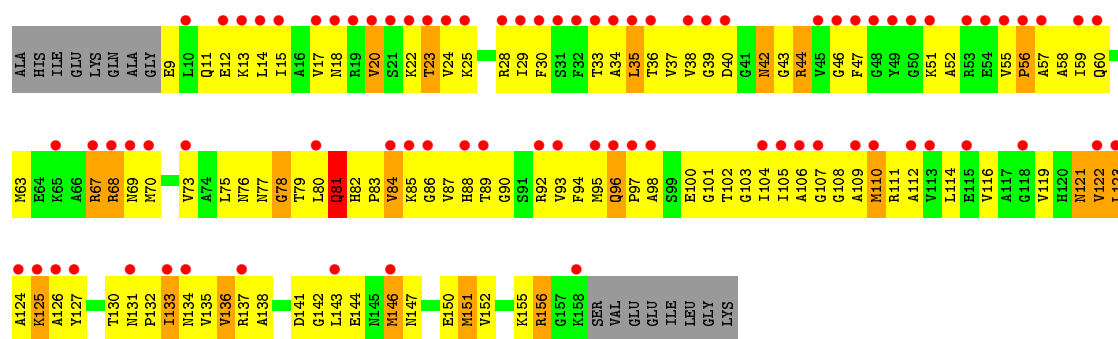




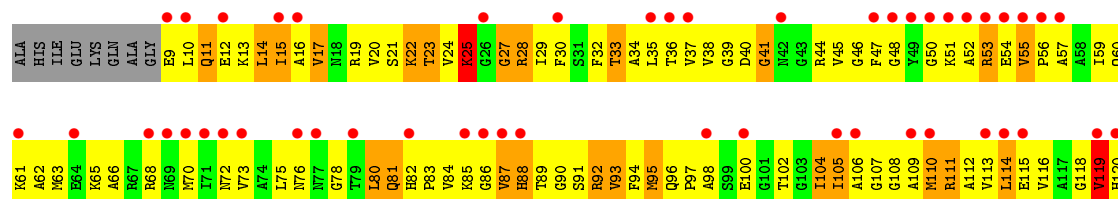
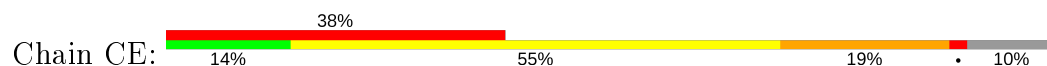
• Molecule 6: 30S ribosomal protein S4



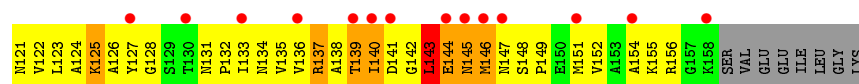
• Molecule 7: 30S ribosomal protein S5



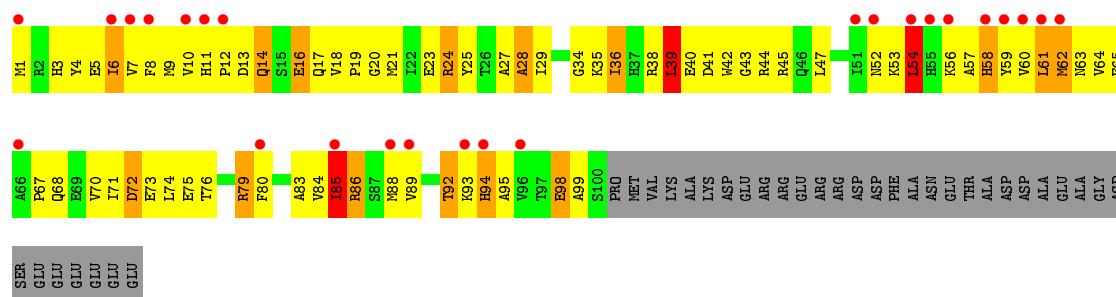
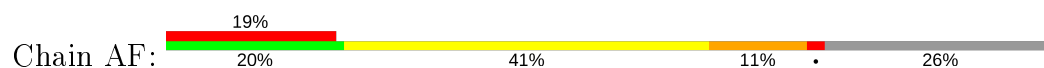
• Molecule 7: 30S ribosomal protein S5



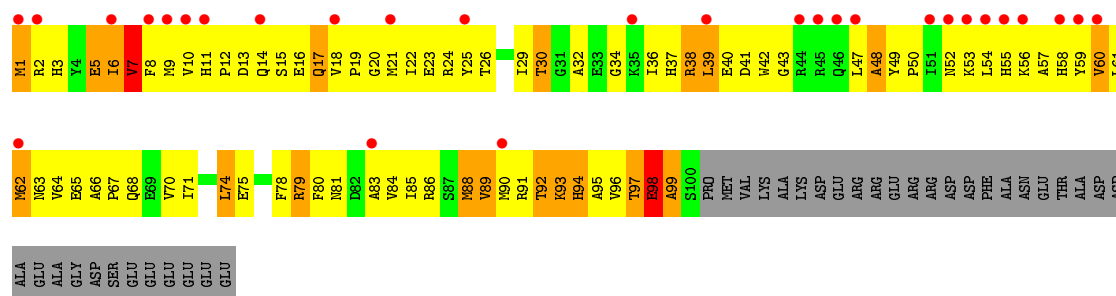
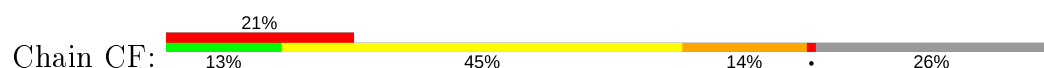




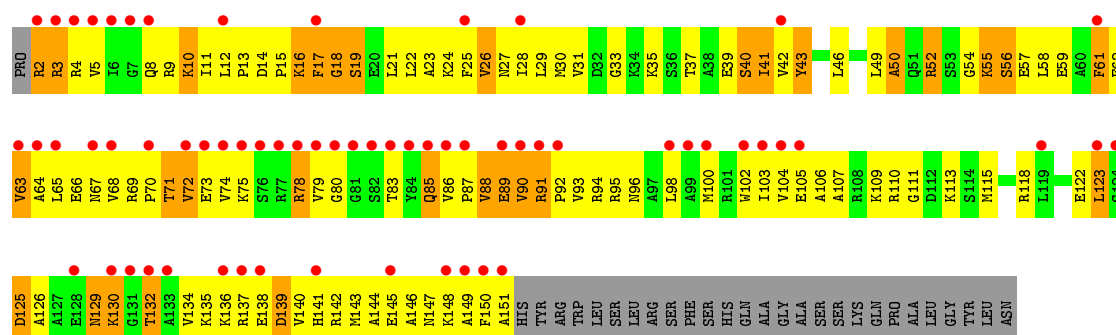
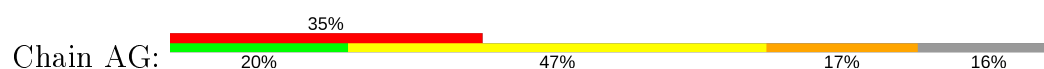
• Molecule 8: 30S ribosomal protein S6



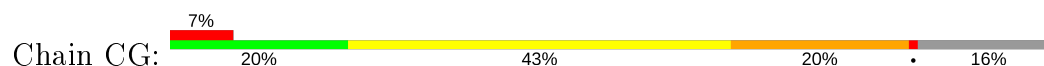
• Molecule 8: 30S ribosomal protein S6



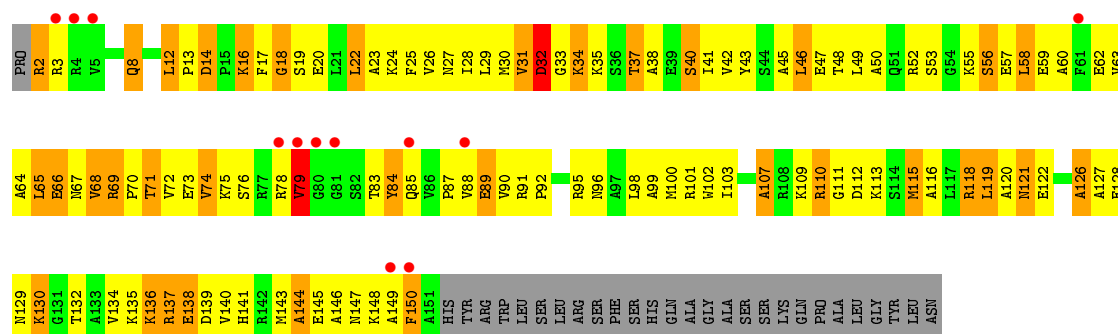
• Molecule 9: 30S ribosomal protein S7



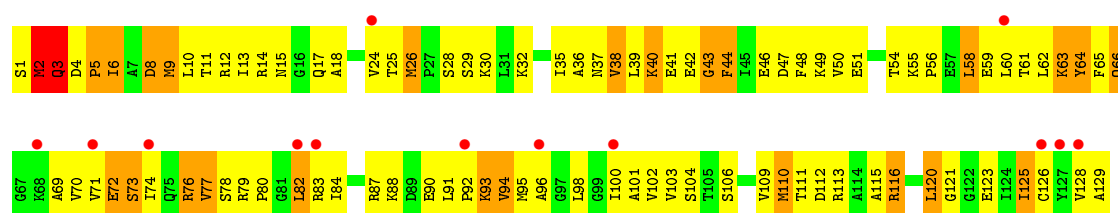
• Molecule 9: 30S ribosomal protein S7



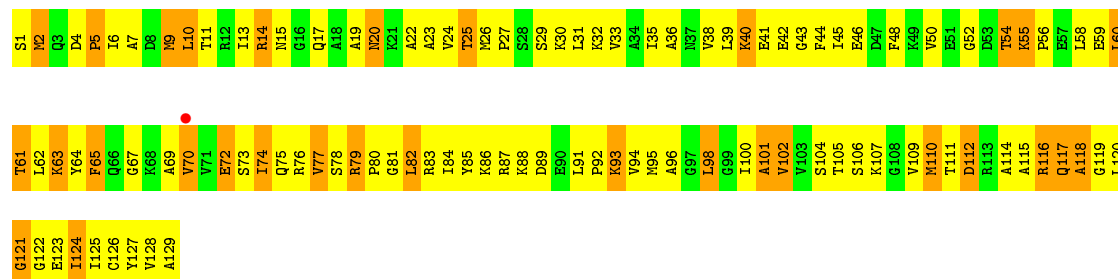




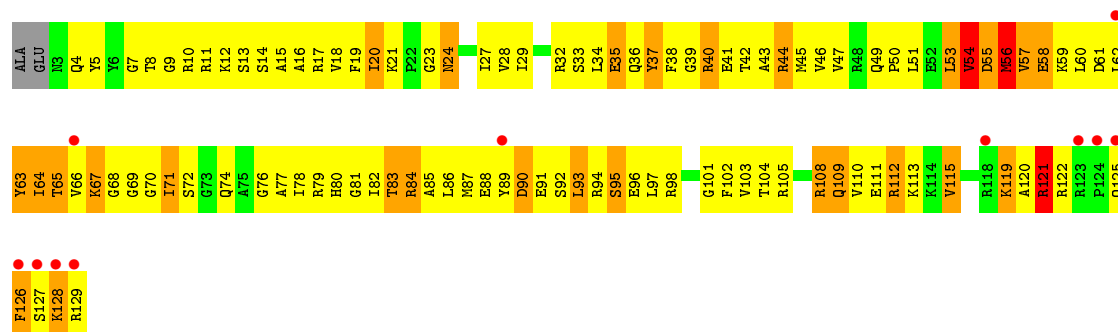
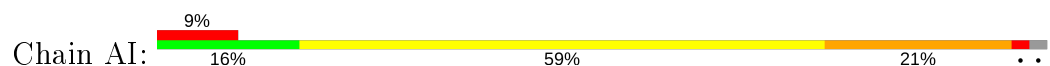
• Molecule 10: 30S ribosomal protein S8



• Molecule 10: 30S ribosomal protein S8



• Molecule 11: 30S ribosomal protein S9

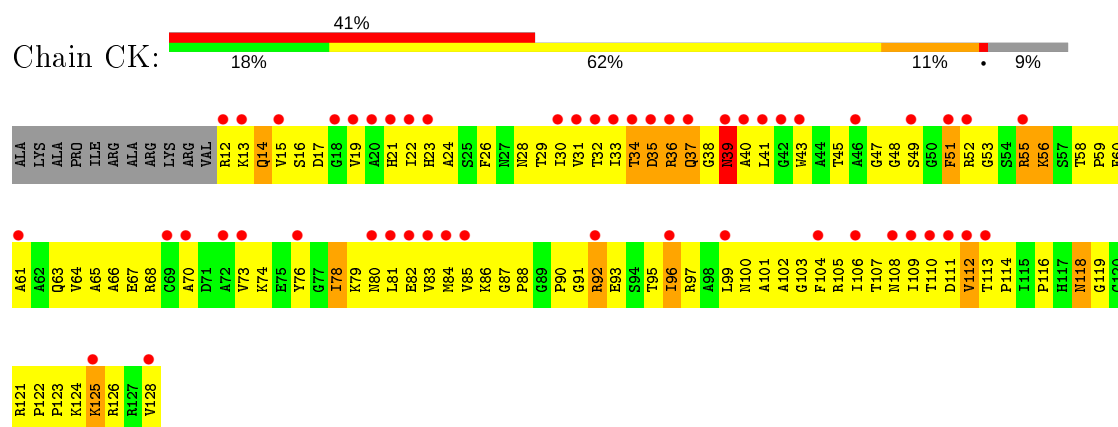


• Molecule 11: 30S ribosomal protein S9

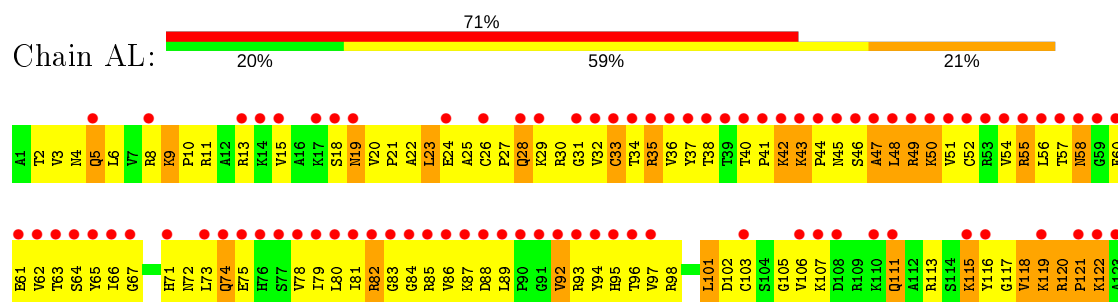




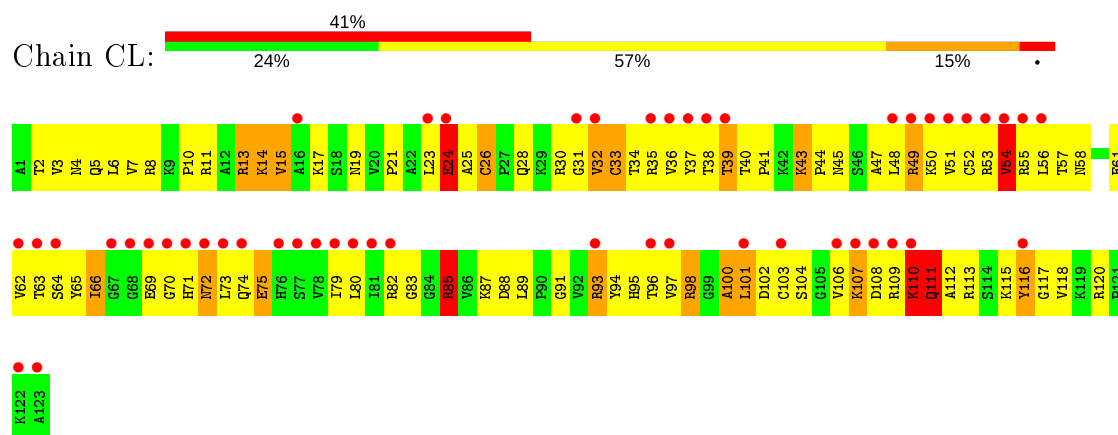




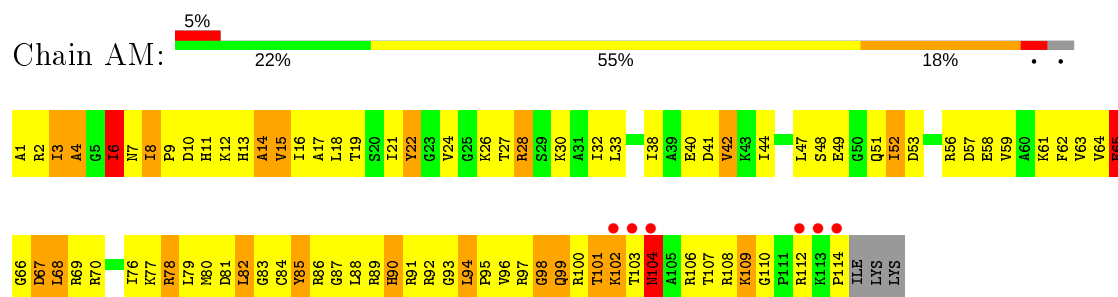
• Molecule 14: 30S ribosomal protein S12



• Molecule 14: 30S ribosomal protein S12

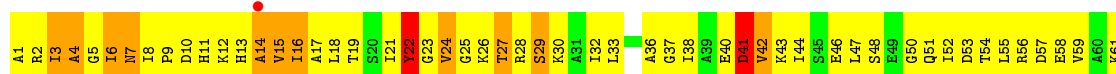
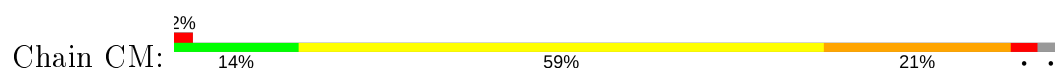


• Molecule 15: 30S ribosomal protein S13



• Molecule 15: 30S ribosomal protein S13

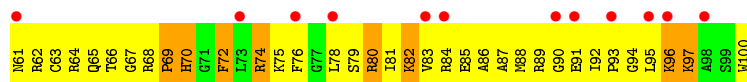
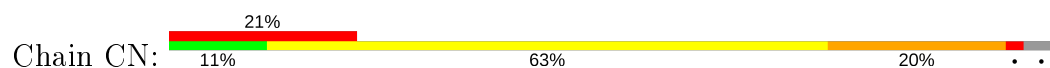




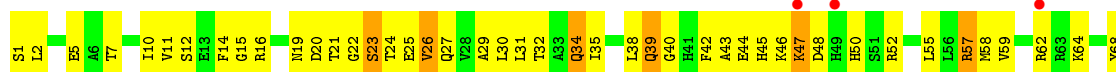
• Molecule 16: 30S ribosomal protein S14



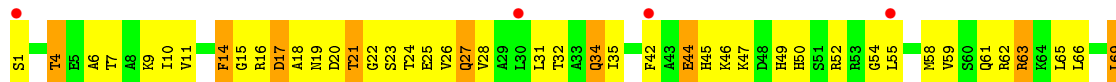
• Molecule 16: 30S ribosomal protein S14



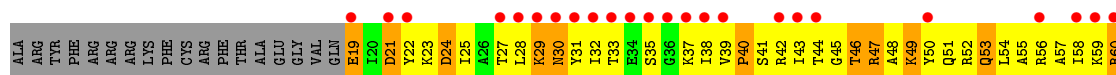
• Molecule 17: 30S ribosomal protein S15



• Molecule 17: 30S ribosomal protein S15



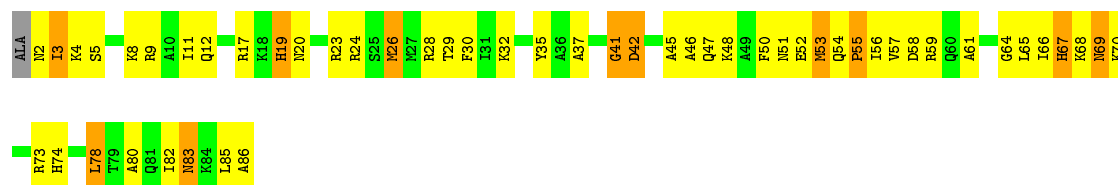




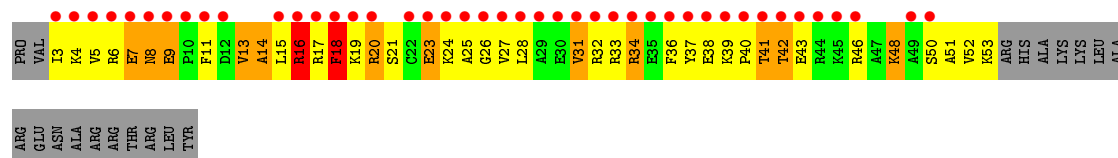




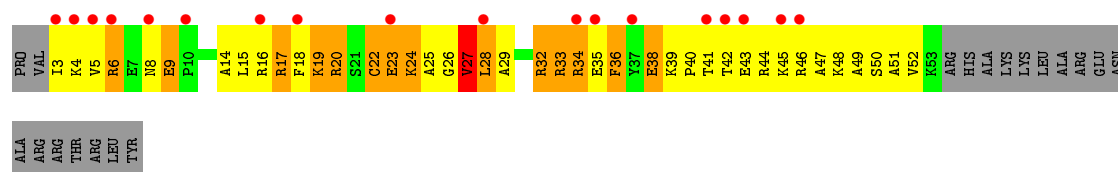




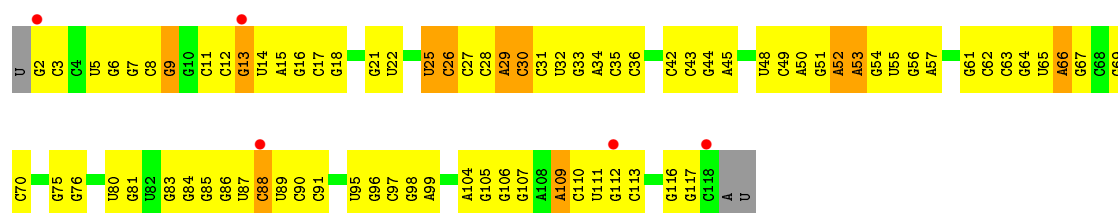
• Molecule 23: 30S ribosomal protein S21



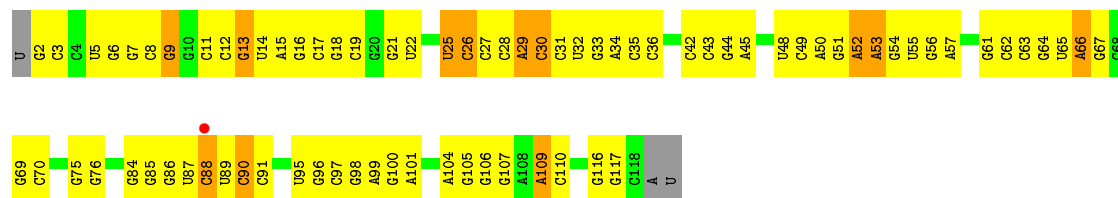
• Molecule 23: 30S ribosomal protein S21



• Molecule 24: 5S ribosomal RNA



• Molecule 24: 5S ribosomal RNA



• Molecule 25: 23S ribosomal RNA









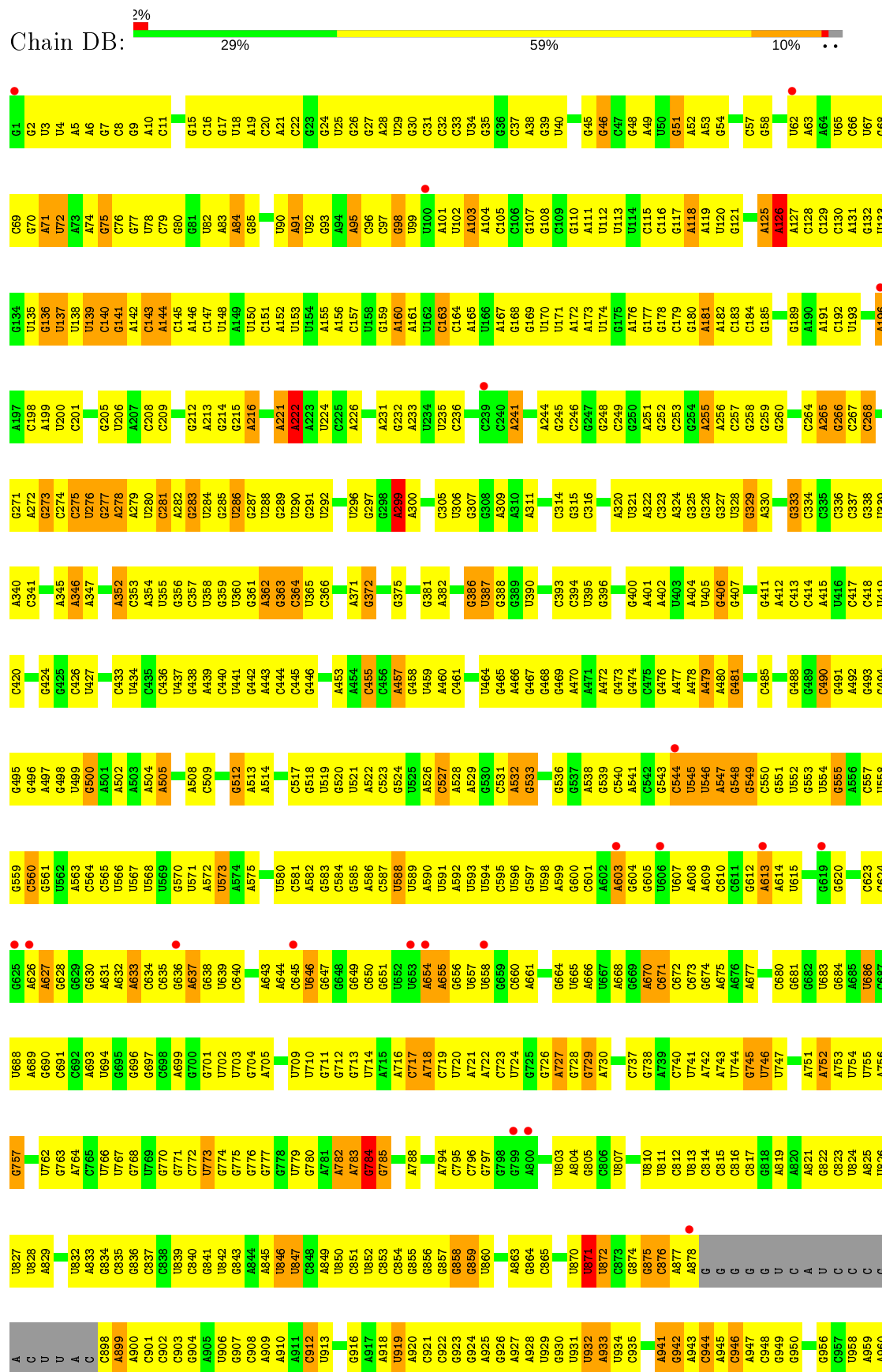
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G1934	G1873	A1808	U1747	C1585	C1585	G1516	G1447		G1310	G1239		G1099	G1036
G1935	C1874	A1809	C1748	A1586	G1517	G1517			G1311	U1240		U1101	G1037
A1936	G1875	A1810	A1749	G1587	U1523	U1523	G1450	G1380	U1313	U1241	A1169	G1104	G1038
A1937	G1811	G1811	G1750		G1524	G1524	G1451	G1381	G1312	A1242	C1170	U1105	A1039
A1938	U1812	G1813	U1751		A1525	A1525	G1452	G1382	C1314	C1243	C1171	U1106	A1040
U1939	G1814	G1814			C1526	C1526	A1453	A1383	C1315	A1244	C1172	G1107	G1041
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U1943	C1881	G1816	G1756	C1685	U1594		C1455	A1386	U1318		U1174	G1109	
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G1945	U1818	G1818	U1758	U1599	U1533	U1533	G1459		C1320	U1249	G1177	G1110	A1046
U1946	A1885	A1819	A1759	U1589	U1534	U1534	G1460	U1394	A1321	G1250	C1178	G1047	
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G1967	C1902	C1837	U1776	A1634	A1551	A1551	G1477	U1411		U1273	C1064	U1132	C1064
C1968	G1903	G1838	U1777	A1635	A1552	A1552	G1478	U1412	U1344	A1274	U1065	A1133	U1065
A1969	G1904	C1839	U1778	U1636	A1553	A1553		A1413	G1345	A1275	U1066	A1134	U1066
A1970	C1905	G1842	U1779	A1637	C1556	C1556	G1482	C1414	G1346	A1276	G1068	C1135	G1068
U1971	U1971		A1780	G1638	C1557	C1557	U1484	G1416	A1347	U1279	A1069	G1137	A1069
G1972	G1907	C1843	U1781	C1639	U1558	U1558	U1485	G1417	G1348	G1280	A1070	G1138	A1070
G1973	C1908	G1844	A1783	C1639	U1559	U1559	U1486	G1418	C1349	G1281	G1071	G1139	G1071
C1974	C1909	G1845	A1784	A1640	G1560	G1560	U1487	A1419	C1350	U1282	C1140	C1140	C1072
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A1981	A1912	A1848	U1787	U1647	U1563	U1563	A1490		A1353	A1285	C1211	A1143	G1076
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G1983	C1914	G1850	C1727	U1648	G1492	G1492	G1492	A1427	G1355	A1287	A1213	C1145	
C1984	U1915		G1728	G1653	C1567	C1567	C1493	C1428	C1357	G1288		C1146	A1080
C1985	A1916	A1853	U1729	G1653	G1568	G1568	A1494	G1429		C1289	U1219	A1147	U1081
C1986	U1917	A1854	C1730	A1654	A1568	A1568	U1495	G1430		C1290	G1220	U1148	U1082
A1987	A1918	U1855	G1731	A1655	A1569	A1569	A1496	A1431	G1360	C1291	U1083	G1149	U1083
G1988	A1919	U1856	C1732	C1656	A1570	A1570	U1497	G1432	G1361	G1292	A1084	C1150	A1084
	C1920	G1857	G1733	U1657	A1571	A1571	G1497	G1433	C1362	C1293	A1085	C1151	A1085
U1991	G1921	A1858	G1734	C1658	A1572	A1572	C1498	A1434	G1363		A1086	C1152	A1086
G1992	U1922		A1735	G1661	G1573	G1573	A1504	C1437	G1364	G1296	G1087	C1153	G1087
U1993	U1923	G1862	U1736	U1662	C1574	C1574	A1505	C1437	A1365	C1297	A1088	C1156	A1088
C1994	C1924	G1863	G1737	U1662	C1575	C1575	U1506	U1438	A1366	G1228	A1089	A1157	A1089
U1995	G1925	U1864	G1738	U1665	U1576	U1576	C1507	A1439	G1367	G1300	G1157	G1157	A1090
C1996	U1926	U1865	A1739	G1666	U1577	U1577	U1440	U1440	A1368	A1301	G1158	U1158	G1091
C1997	A1801	A1866	G1740	G1667	U1578	U1578	G1441	G1441	G1369	A1302	U1231	U1159	G1092
	A1802	G1867	C1741	G1667	A1579	A1579	U1442	U1442	C1370	C1306	G1232	G1160	
U1929	G1929	C1968	U1742	A1668	A1580	A1580	G1510	U1443	G1371		A1095		A1095
C2000	C2001		G1743	A1669	C1582	C1582	U1513	G1444	U1372	A1307		G1163	A1096
			A1744										



U2866	A2800	G2794	G2670	G2529	A2459	G2391	G2323	C2260	G2193	U	C2008
G2867	G2801	G2795	G2671	A2590	U2460	A2392	U2324	C2261	U2194	G2193	A2009
G2868	G2802	U2796	G2672	A2591	A2461	U2393	G2325	U2262	C2072	A2134	A2010
G2869	G2803	U2797	G2673	G2592	C2462	C2394	G2326	G2263	C2073	A2135	U2011
G2870	U2804	A2740	G2674	G2593	G2463	G2395	A2327	C2264	U2074	G2136	G2012
G2805	G2805	A2741	G2675	A2594	G2464	G2396	A2328	U2265	U2075	A2013	A2013
G2806	U2806	G2742	G2676	G2595	G2465	U2400	U2329	U2266	U2076	U2014	U2014
U2807	G2743	U2807	G2677	G2596	C2466	G2401	G2330	A2267	A2077	G2140	A2015
G2808	G2744	U2808	G2678	U2597	C2467	U2402	G2331	A2268	C2078	G2141	U2016
G2809	G2745	G2809	G2679	C2538	A2468	U2403	G2332	G2269	U2079	A2142	U2017
A2810	G2810	G2746	U2680	C2539	A2469	G2403	A2333	A2270	U2018	G2143	G2018
G2811	G2811	G2747	C2681	C2540	G2470	U2404	U2334	G2271	A2082	G2144	A2019
G2812	A2682	A2748	G2682	U2610	G2471	U2405	U2335	U2272	A2083	G2145	G2020
A2813	G2683	U2749	G2683	G2543	G2472	A2406	A2336	A2273	C2084	C2146	C2021
A2814	U2684	G2751	U2684	G2544	U2473	A2407	G2337	A2274	U2085	A2147	U2022
G2815	G2685	C2752	G2685	U2545	C2475	U2408	G2338	U2275	U2086	U2148	C2023
G2816	U2686	U2753	G2686	U2546	U2476	G2409	C2339	A2276	G2087	U2149	C2024
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U2819	U2689	U2756	U2689	U2552	U2479	G2412	C2342	U2281	C2091	G2152	C2027
G2820	G2690	U2757	G2690	U2553	U2480	A2413	U2343	U2282	U2092	C2153	U2028
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A2833	C2703	G2770	G2703	A2566	C2493	A2426	G2358	G2295	U2106	U	U2041
U2834	U2704	A2705	A2705	G2567	C2494	G2427	G2359	U2296	G2107	U	A2042
G2835	U2706	U2707	U2707	G2568	C2495	G2428	G2360	G2297	A2108	G	G2043
G2836	G2707	G2708	G2708	U2569	U2500	A2430	G2361	A2297	C2044	A	C2044
G2709	G2638	G2709	G2638	G2570	G2501	U2431	G2362	U2298	U2109	A	G2045
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U2713	G2640	U2713	G2640	U2572	A2503	A2434	G2364	C2301	U	A	C2047
G2714	U2645	G2714	U2645	U2573	U2504	A2435	G2365	G2302	G	C	G2048
C2715	G2646	C2715	G2646	A2574	G2505	G2436	G2366	U2303	U	C	G2049
C2716	U2648	C2716	U2648	U2575	U2506	G2437	G2367	U2304	A	C	A2050
C2717	G2649	C2717	G2649	G2576	C2507	U2438	G2368	C2305	A	C	A2051
G2718	U2650	U2718	U2650	G2577	G2508	A2439	A2369	C2306	G	C	A2052
G2719	G2651	U2719	G2651	U2578	U2509	G2440	G2370	G2307	U	C	A2053
A2721	G2655	A2721	G2655	U2579	U2510	U2441	G2371	G2308	A	A	C2054
G2722	U2656	U2722	U2656	U2580	C2511	G2442	C2372	A2309	U	U	C2055
C2723	G2657	U2723	U2657	U2581	A2512	C2443	C2373	U2243	A	A	G2056
U2724	U2659	U2724	U2659	U2582	U2513	G2444	A2377	G2244	G	U2181	G2057
A2725	G2661	A2725	G2661	U2583	U2514	G2445	G2378	U2245	U	U2182	A2058
A2726	U2662	A2726	U2662	U2584	G2515	G2446	G2379	G2246	A2059	A2183	A2059
G2727	G2663	G2727	G2663	U2585	A2516	G2447	C2380	A2247	G	A2184	A2060
U2728	G2664	U2728	G2664	U2586	A2517	A2448	C2381	G2248	G	U2185	G2061
G2729	U2665	G2729	U2665	C2591	U2518	U2449	G2382	G2249	G	U2186	A2062
C2730	G2666	C2730	G2666	U2592	G2519	A2450	G2383	G2250	A	G2187	C2063
G2731	G2667	G2731	G2667	U2593	C2520	U2451	U2384	A2317	G	U2188	C2064
G2732	U2668	U2732	U2668	C2594	U2521	G2452	G2385	G2319	G	U2189	C2065
A2733	G2669	A2733	G2669	U2595	U2522	G2453	A2386	U2320	C	G2190	C2066
U2799	G2670	U2799	G2670	U2596	G2523	U2454	U2387	U2321	U	A2191	U2067
G2794	G2671	G2794	G2671	U2597	G2524	G2455	G2388	A2322	U	U2192	G2068



● Molecule 25: 23S ribosomal RNA





U1880	C1881	G1814	C1748	G1667	A1590	G1524	G1450	A1383	U1316	A1244	G1171	A1103	C961
C1882	U1882	A1815	A1749	A1668	A1591	A1525	A1451	A1384	G1317	G1246	C1172	C1104	G962
U1883	G1816	G1817	U1751	A1669	A1592	A1526	A1452	A1385	U1318	G1248	U1173	U1105	G963
A1884	U1818	G1752	G1753	G1674	A1593	G1527	A1454	C1386	C1319	U1249	U1175	G1106	C964
A1885	A1819	G1763	A1754	A1677	A1594	G1595	G1455	A1387	C1320	G1250	U1176	U1107	U967
U1886	U1820	A1755	A1756	A1677	C1595		U1458	A1392	A1322	A1253	G1177	C1109	C968
C1887	A1821	G1756	A1757	U1680	U1599	C1533	G1459	A1393	C1323	A1254	G1178	G1110	C969
A1888	G1822	A1758	A1759	G1681	C1600	A1534	A1460	U1394	G1324	A1255	U1179	A1111	U970
A1889	G1823	U1758	A1758	G1682	A1595	A1535	A1461	A1395	U1325	U1256	U1180	U1112	A973
G1890	U1824	A1759	A1759	U1683	A1602	G1537	A1462	U1396	U1326	G1257	U1181	U1113	G974
G1891	U1825	C1760	A1760	G1684	A1603	G1538	C1463	U1397	A1327	U1258	U1182	G1114	A975
C1892	G1826	C1761	A1761	C1685	C1604	U1539	G1464	C1398	G1331	G1259	U1183	G1115	
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C1894	G1828	G1763	G1763	C1687	C1606	C1541	G1466	U1400	G1333	G1266	U1188	G1120	A981
C1895	A1829	C1764	C1764	C1688	C1607	C1542	U1467	U1401	G1334	A1267	U1189	A1054	C982
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G1897	U1833	G1766	G1766	A1609	A1609	A1545	A1471	A1403	A1336	A1269	G1191	G1057	A984
U1898	U1834	G1767	G1767	C1691	A1610	A1546	A1472	U1404	G1337	G1270	G1192	U1058	C985
A1899		A1773	A1773	G1695	G1613	G1546	C1473	U1405	G1338	A1271	G1193	U1059	C986
C1902	C1837	G1776	G1776	A1700	A1616	C1547	U1474	U1406	U1340	A1272	U1194	U1060	C987
G1903	G1838	U1777	U1777	U1709	C1617	A1549	U1475	U1409	G1339	A1273	G1195	G1061	A988
G1904	G1839	U1778	U1778	G1710	A1618	A1551	A1477	U1410	U1341	A1274	G1196	G1062	A989
C1905		U1779	U1779	G1711	G1623	A1553	G1478	U1411	U1344	A1275	U1198	C1064	C991
G1906	G1842	U1780	U1780	U1712	U1624	C1556	G1482	U1412	G1345	A1276	C1200	U1066	C992
G1907	C1843	U1781	U1781	U1713	C1625	C1557	U1483	A1413	G1346	G1279	U1203	G1137	C995
C1908	G1844	U1782	U1782	U1714	A1634	C1558	U1484	U1414	A1347	G1280	U1204	A1067	A996
C1909	G1845	A1783	A1783	U1715	A1635	C1559	U1485	U1415	C1348	G1281	A1205	G1068	C997
A1913	G1846	U1784	U1784	U1716	U1636	C1560	U1486	A1416	C1349	G1282	G1206	A1069	C998
G1914	A1848	A1785	A1785	U1717	U1637	G1561	U1487	G1418	C1350	U1283	U1141	A1070	U999
U1915	G1849	A1786	A1786	A1717	U1638	C1562	U1488	U1419	U1352	A1284	G1210	G1071	A1000
A1916	G1850	C1787	C1787	U1720	C1639	C1563	U1489	A1420	A1353	A1285	C1211	C1072	A1001
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A1918	A1853	U1789	U1789	A1722	A1641	C1565	G1492	G1426	C1357	G1288	U1219	A1143	
C1921	U1855	C1790	C1790	G1723	A1642	C1566	U1493	A1427	G1360	G1292	G1220	A1144	A1010
U1922	G1857	A1791	A1791	G1724	G1643	C1567	A1494	C1428	G1361	U1293	U1221	A1145	G1011
C1923	A1858	A1794	A1794	U1725	G1643	C1568	A1495	G1429	G1362	U1294	C1221	C1146	U1012
C1925		C1795	C1795	G1726	U1647	C1569	U1496	G1430	C1363	G1295	U1224	U1147	C1013
U1926	G1862	U1796	U1796	C1727	G1649	A1570	U1497	G1431	G1364	G1296	G1225	G1149	C1014
A1927	G1863	U1797	U1797	U1728	A1650	A1571	C1498	G1432	G1365	C1297	A1226	A1150	U1015
U1928	U1864	G1799	G1799	U1729	A1651	C1572	A1504	A1433	A1366	C1298	G1227	C1151	G1016
G1929	A1865	C1800	C1800	C1730	G1652	C1573	U1506	C1437	A1367	G1300	A1230	A1152	G1017
G1930	G1866	A1801	A1801	G1731	A1653	C1574	A1507	U1438	G1368	A1301	G1228	C1153	A1086
U1931	G1867	G1802	G1802	G1732	G1654	C1575	U1508	A1439	A1369	A1302	A1231	G1157	G1087
C1935	G1868	A1803	A1803	G1733	A1655	C1576	A1509	A1440	G1370	C1306	G1232	A1158	U1018
A1936	C1870	C1804	C1804	G1734	A1656	C1577	U1509	A1441	G1371	G1309	U1236	G1159	U1019
A1937	A1871	A1805	A1805	U1735	C1656	C1578	A1509	U1442	U1372	G1310	G1237	C1163	A1020
U1938	G1872	C1806	C1806	U1736	C1657	C1579	G1510	U1443	A1373	G1311	G1238	A1165	G1088
U1939	G1873	A1807	A1807	G1738	C1658	C1580	G1511	G1444	G1374	G1312	U1240	G1166	A1028
U1940	C1874	A1808	A1808	A1739	G1659	C1581	C1512	G1445		U1313	U1241	G1167	A1029
	G1875	A1809	A1809	G1740	G1661	C1582	U1513	G1446	U1379	U1314	U1242	C1168	C1030
U1943	A1876	A1810	A1810	U1745	U1662	A1583	G1514	C1447	G1380	G1315	C1243	C1169	G1031
U1944	A1877	U1811	U1811	A1746	A1665	C1584	A1515	G1448	G1381			U1101	C1102
U1946	G1878	G1813	G1813	U1747	G1666	A1586	G1517	G1449					

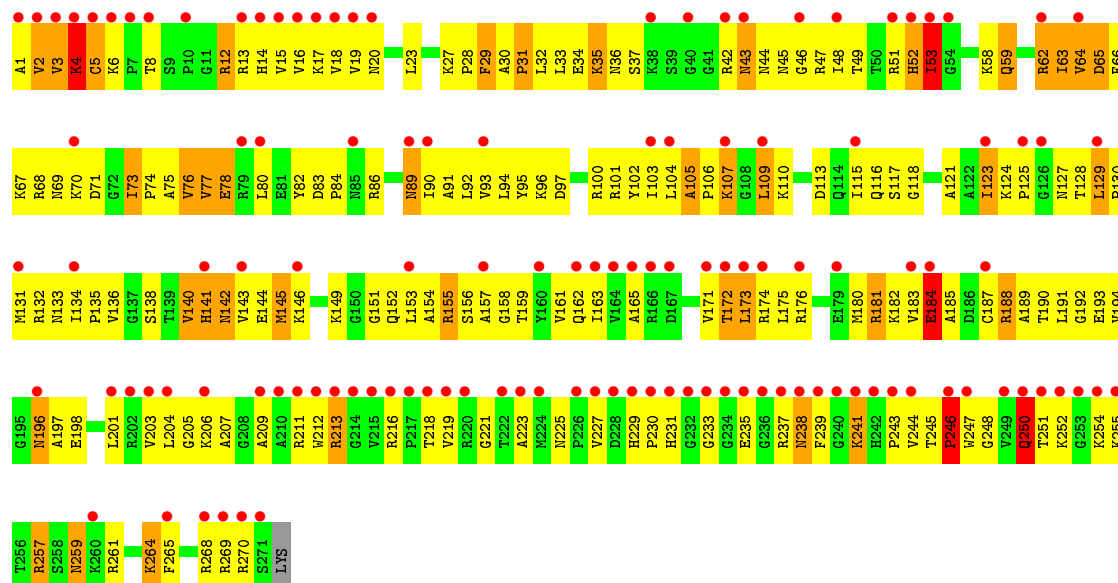




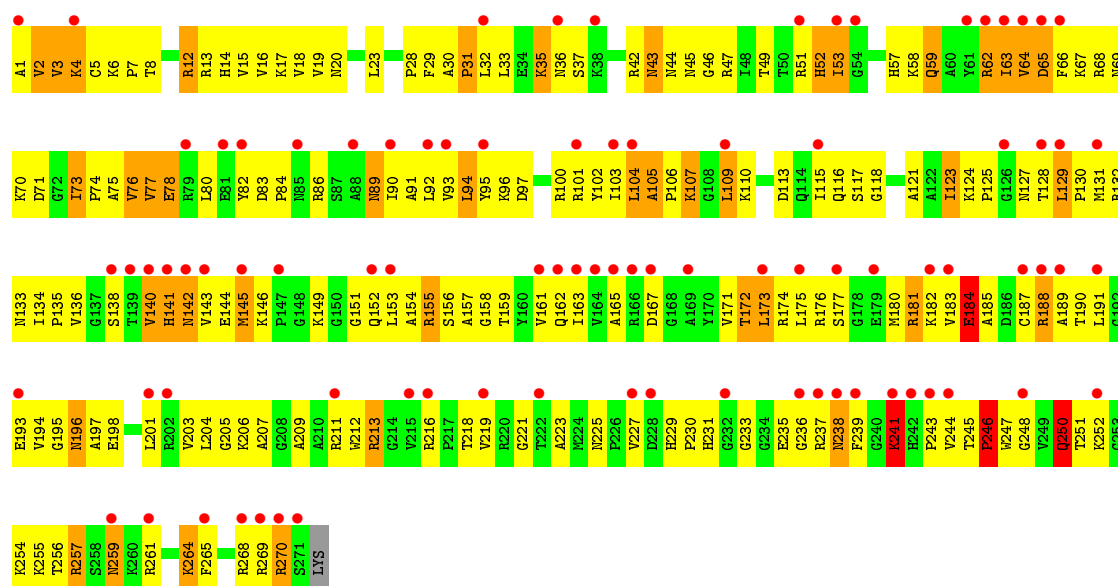




- Molecule 26: 50S ribosomal protein L2



- Molecule 26: 50S ribosomal protein L2



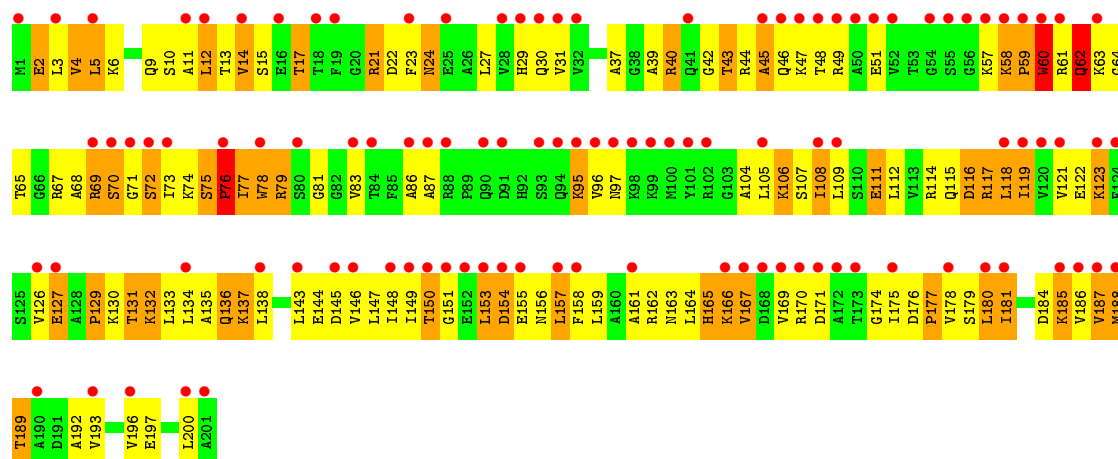
- Molecule 27: 50S ribosomal protein L3



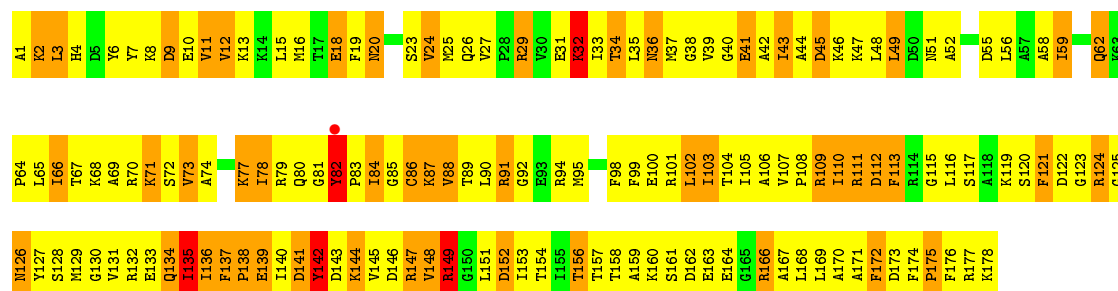
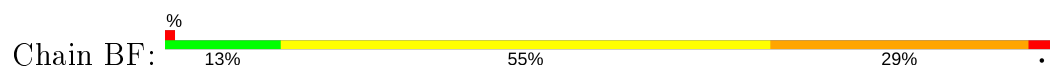




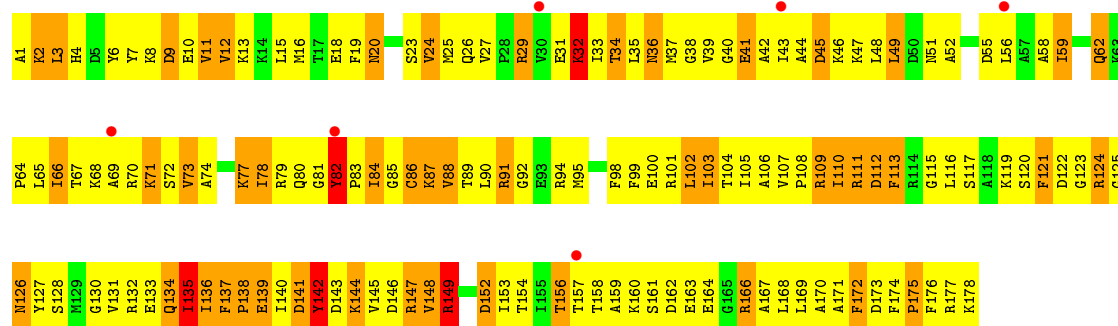
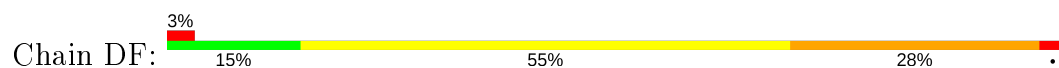




• Molecule 29: 50S ribosomal protein L5



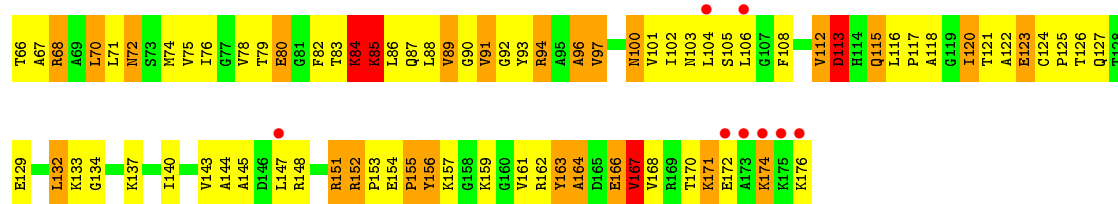
• Molecule 29: 50S ribosomal protein L5



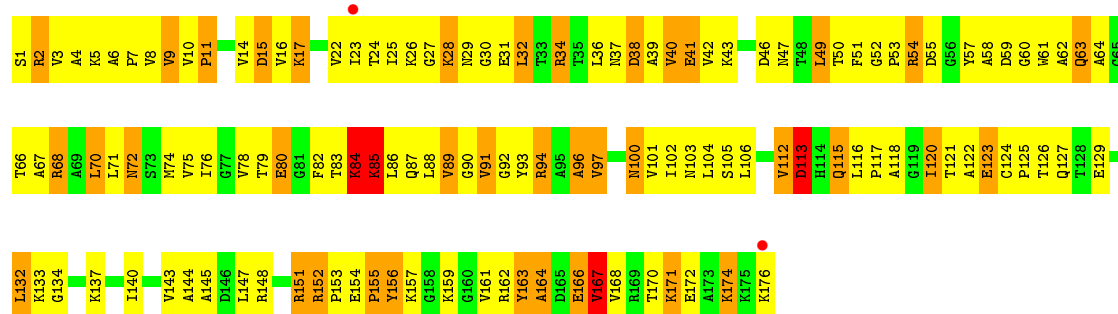
• Molecule 30: 50S ribosomal protein L6



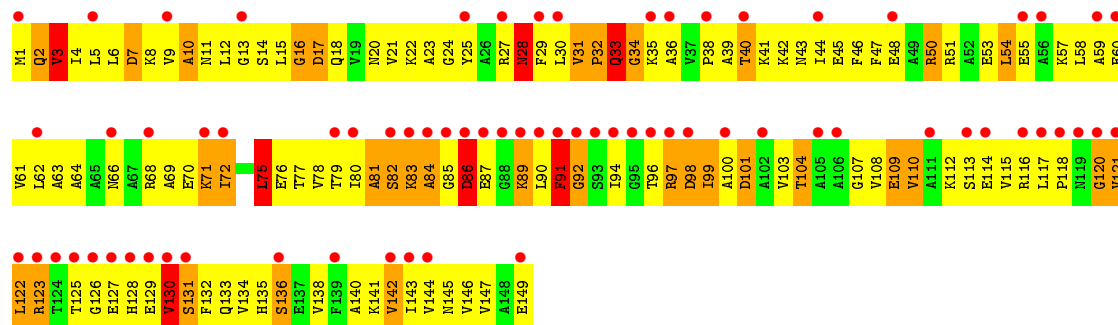
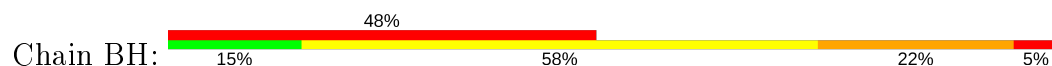




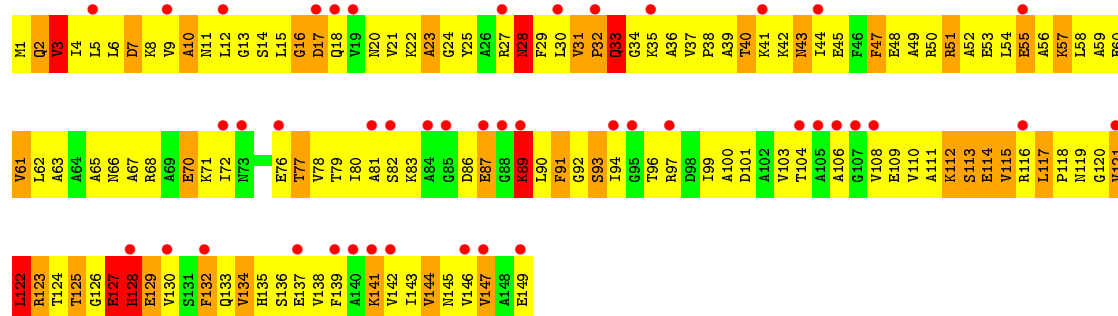
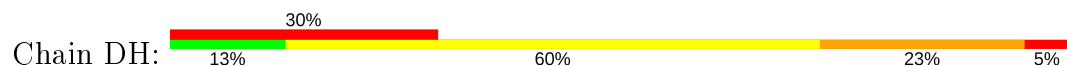
• Molecule 30: 50S ribosomal protein L6



• Molecule 31: 50S ribosomal protein L9

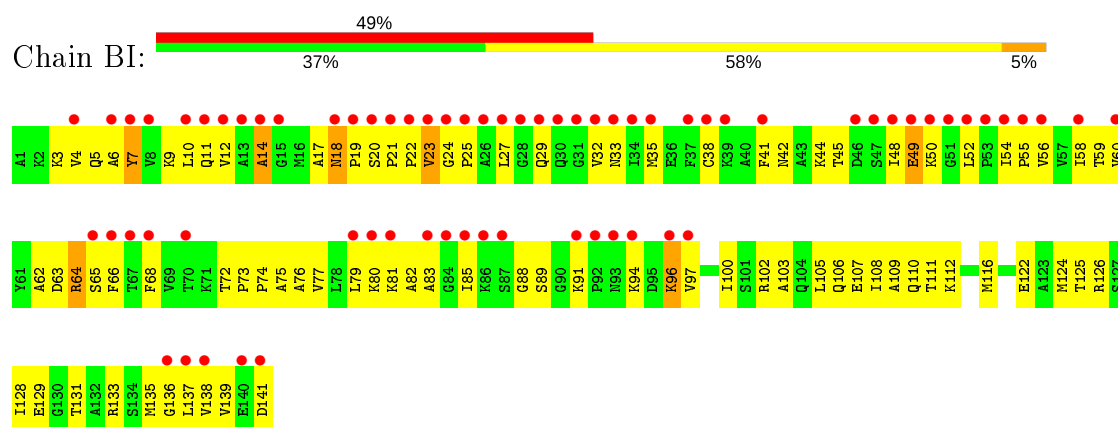


• Molecule 31: 50S ribosomal protein L9

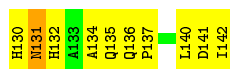


• Molecule 32: 50S ribosomal protein L11

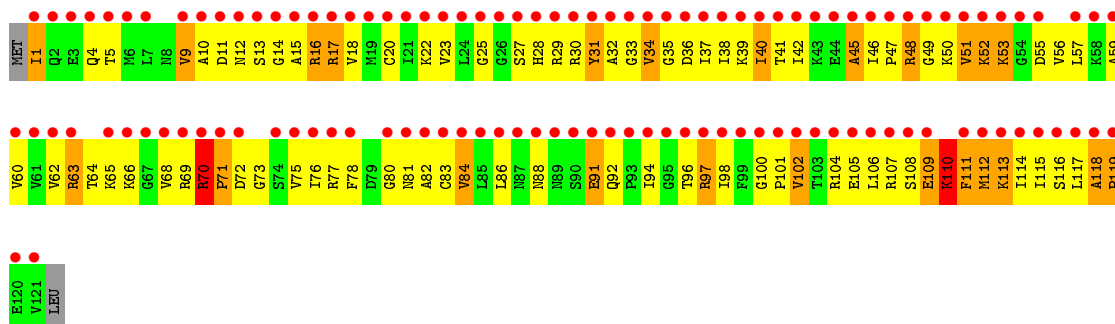




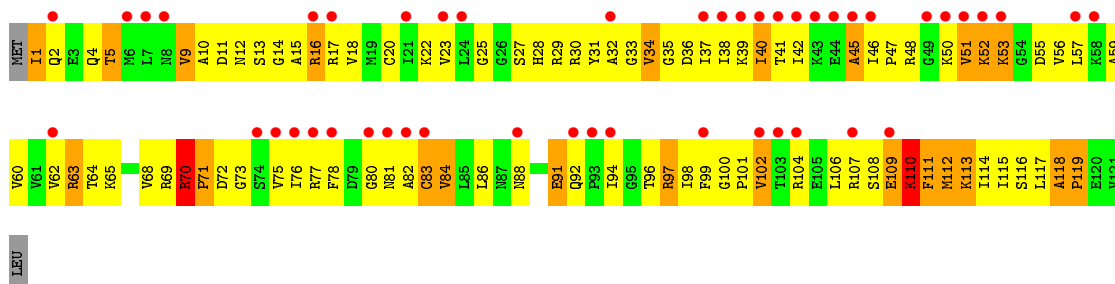




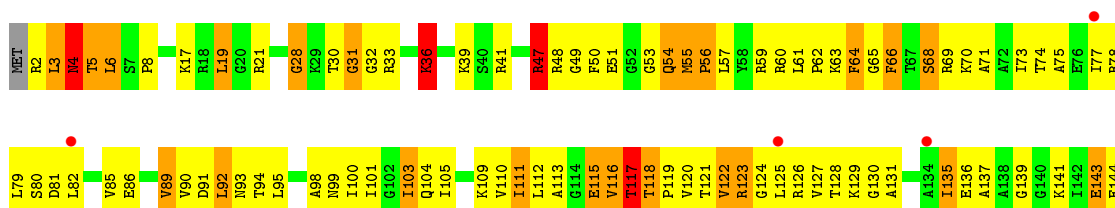
- Molecule 34: 50S ribosomal protein L14



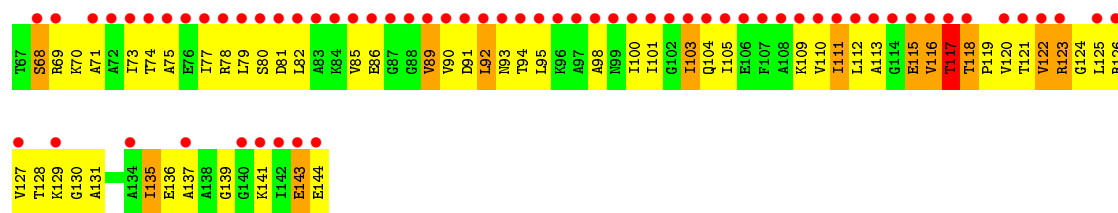
- Molecule 34: 50S ribosomal protein L14



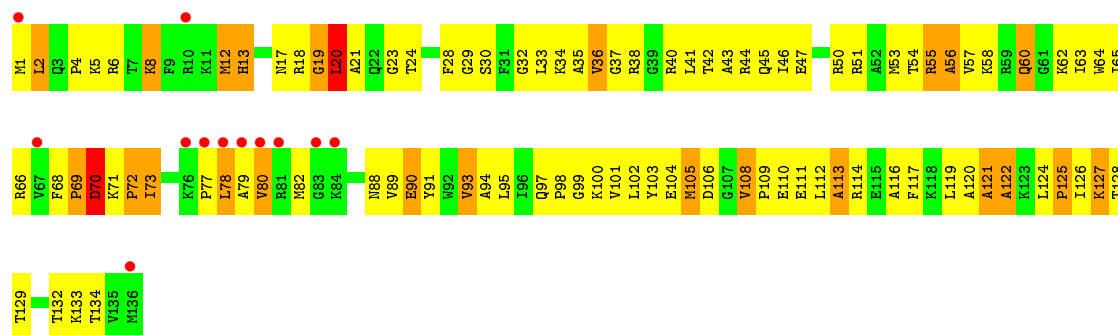
- Molecule 35: 50S ribosomal protein L15



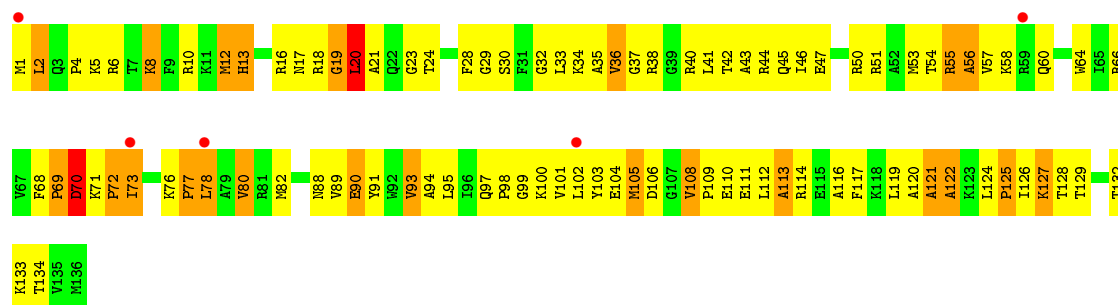




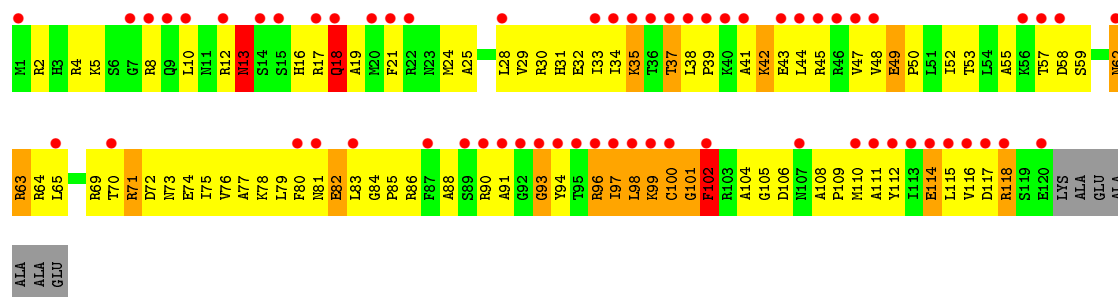
• Molecule 36: 50S ribosomal protein L16



• Molecule 36: 50S ribosomal protein L16

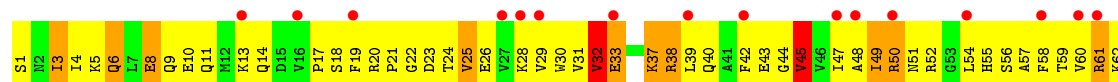


• Molecule 37: 50S ribosomal protein L17

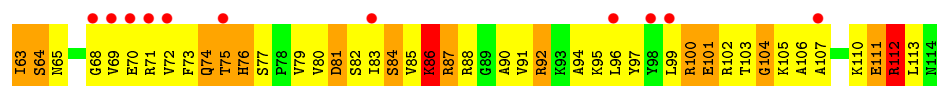


• Molecule 37: 50S ribosomal protein L17

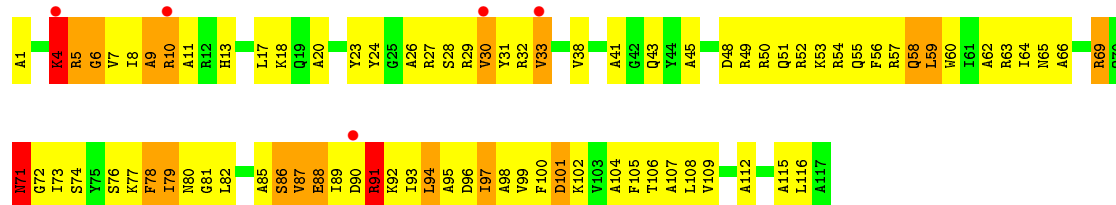




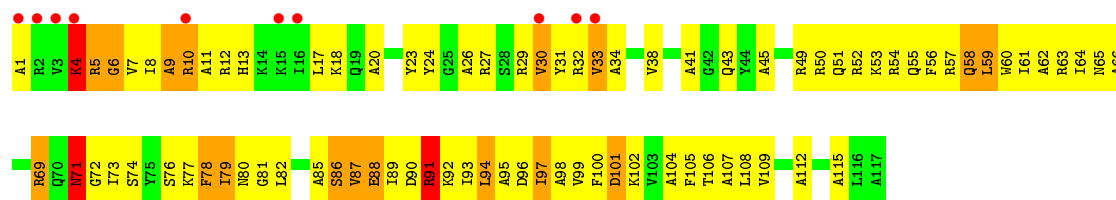




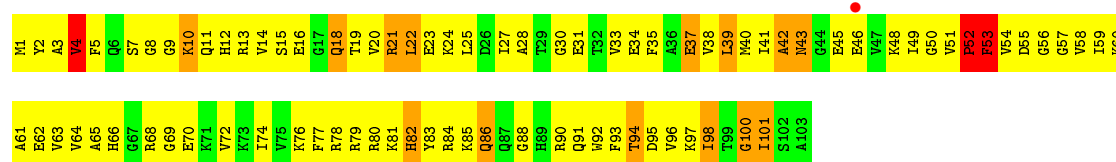
- Molecule 40: 50S ribosomal protein L20



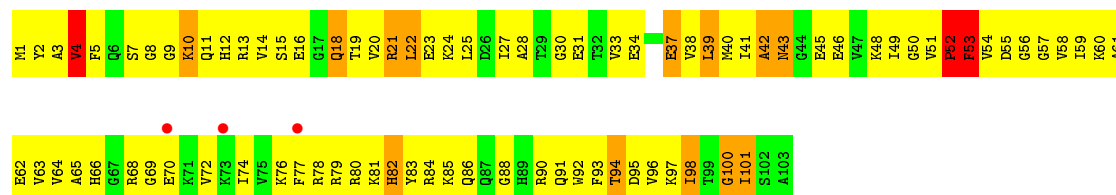
- Molecule 40: 50S ribosomal protein L20



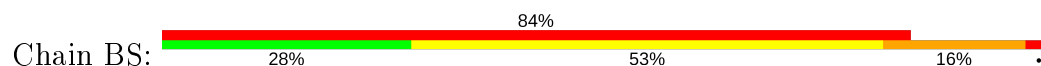
- Molecule 41: 50S ribosomal protein L21



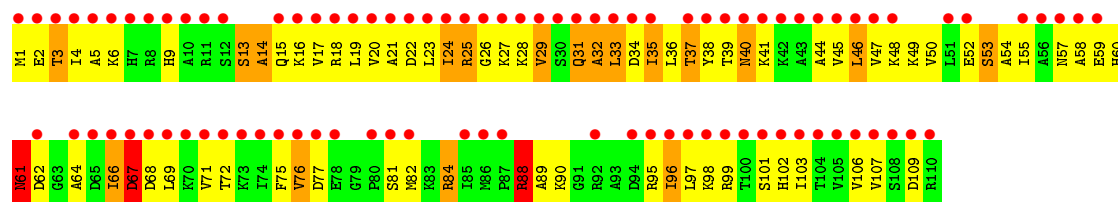
- Molecule 41: 50S ribosomal protein L21



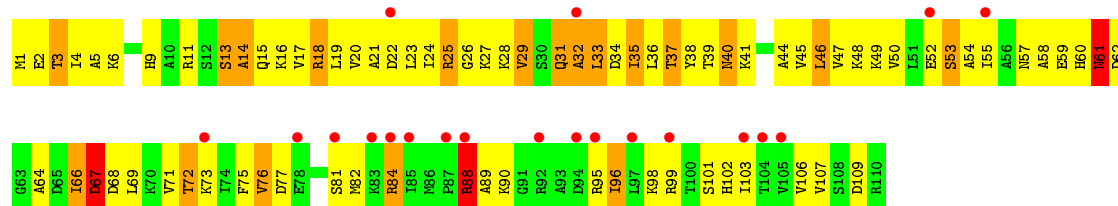
- Molecule 42: 50S ribosomal protein L22



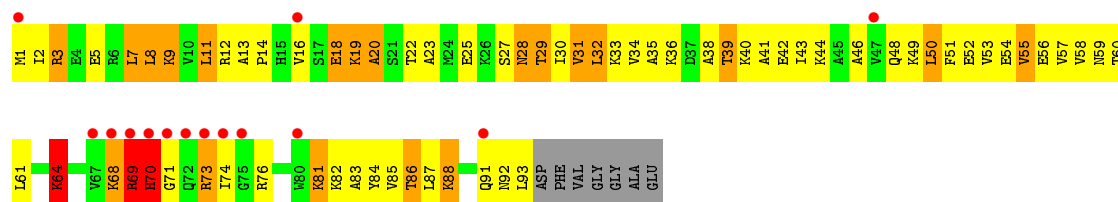




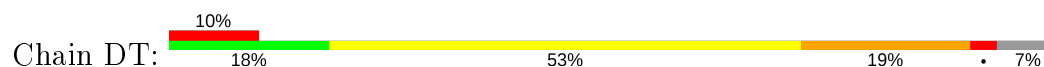
• Molecule 42: 50S ribosomal protein L22



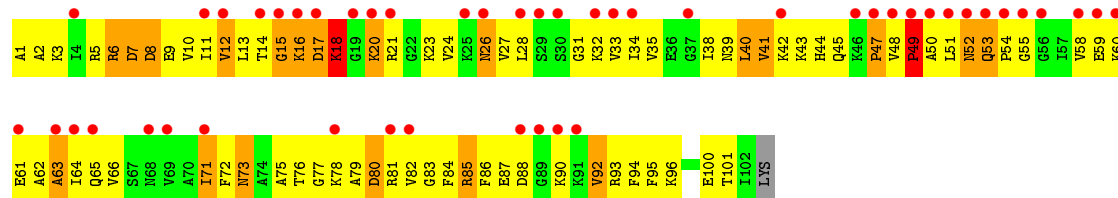
• Molecule 43: 50S ribosomal protein L23



• Molecule 43: 50S ribosomal protein L23

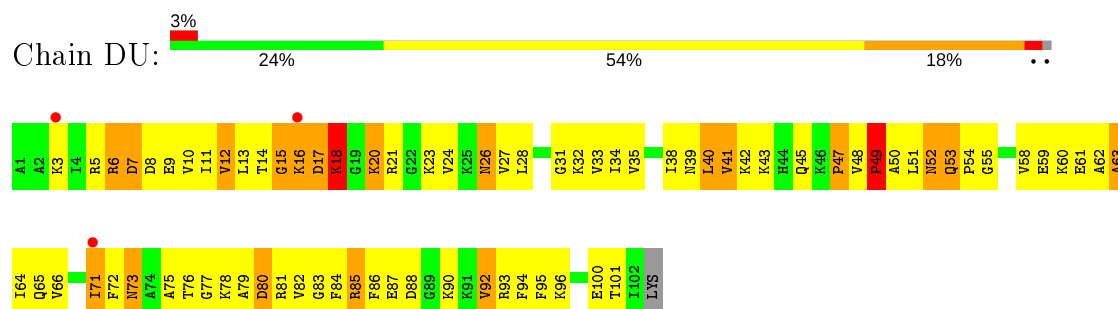


• Molecule 44: 50S ribosomal protein L24

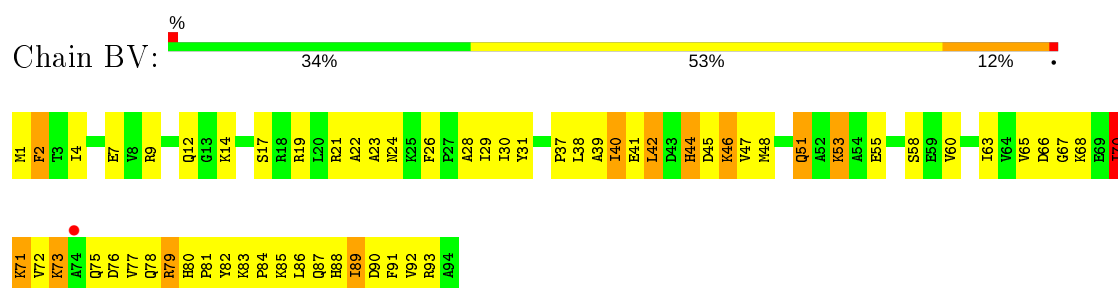




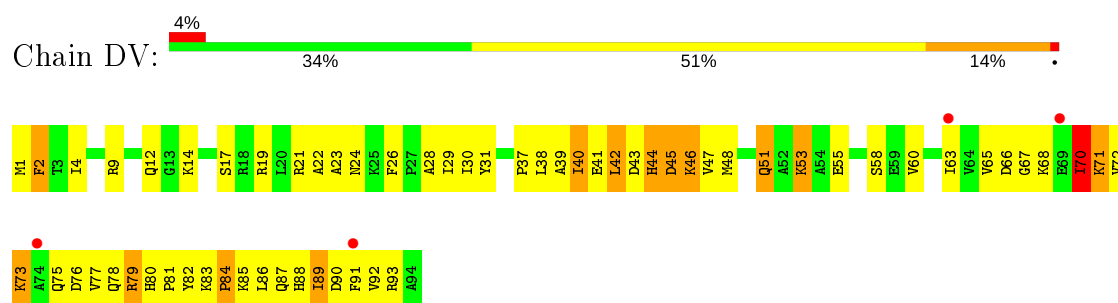
- Molecule 44: 50S ribosomal protein L24



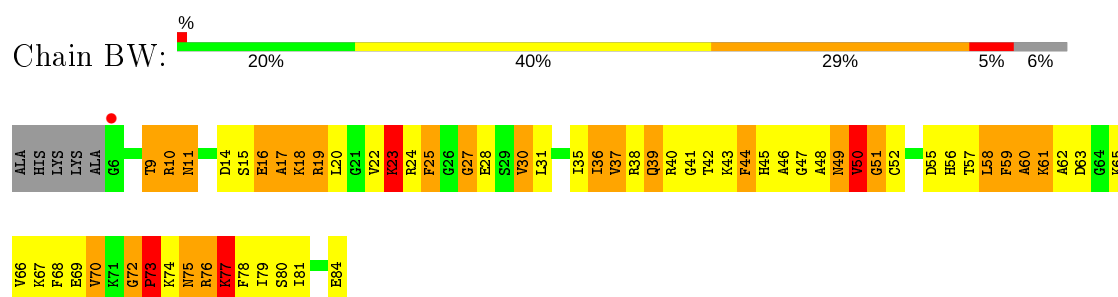
- Molecule 45: 50S ribosomal protein L25



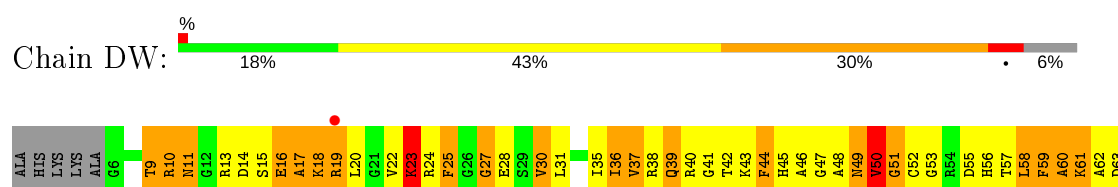
- Molecule 45: 50S ribosomal protein L25



- Molecule 46: 50S ribosomal protein L27



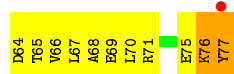
- Molecule 46: 50S ribosomal protein L27



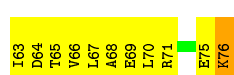
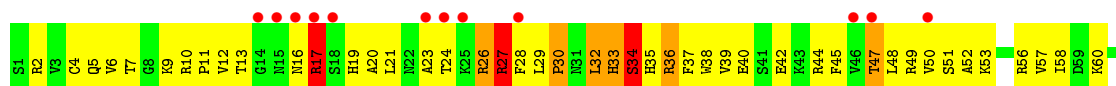




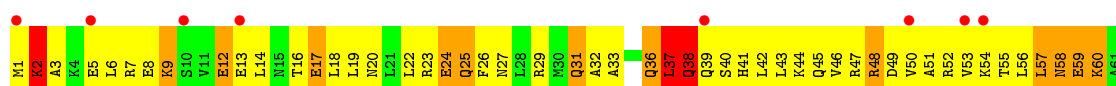
- Molecule 47: 50S ribosomal protein L28



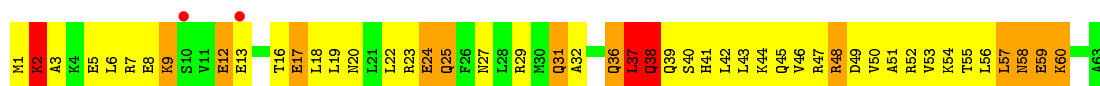
- Molecule 47: 50S ribosomal protein L28



- Molecule 48: 50S ribosomal protein L29



- Molecule 48: 50S ribosomal protein L29



- Molecule 49: 50S ribosomal protein L30





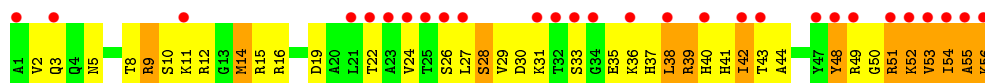
- Molecule 49: 50S ribosomal protein L30

Chain DZ: 



- Molecule 50: 50S ribosomal protein L32

Chain B0: 



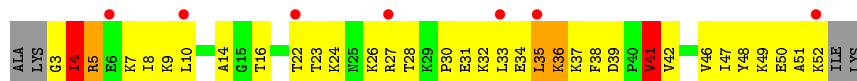
- Molecule 50: 50S ribosomal protein L32

Chain D0: 



- Molecule 51: 50S ribosomal protein L33

Chain B1: 



- Molecule 51: 50S ribosomal protein L33

Chain D1: 



- Molecule 52: 50S ribosomal protein L34

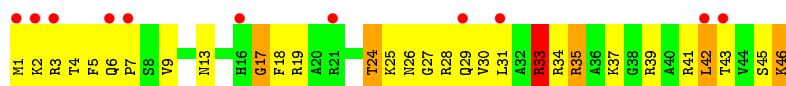
Chain B2: 



- Molecule 52: 50S ribosomal protein L34

Chain D2: 

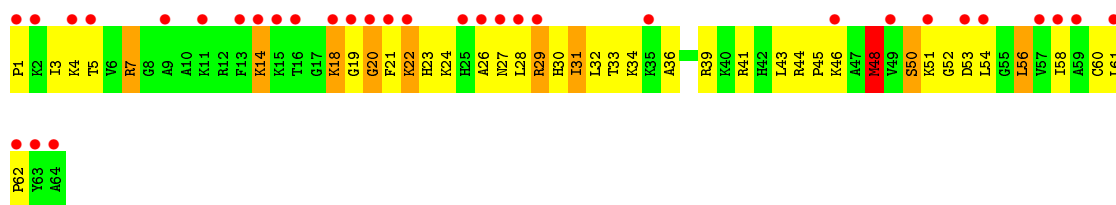




- Molecule 53: 50S ribosomal protein L35



- Molecule 53: 50S ribosomal protein L35



- Molecule 54: 50S ribosomal protein L36



- Molecule 54: 50S ribosomal protein L36





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.78Å 395.22Å 744.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.00 – 3.22 184.07 – 3.22	Depositor EDS
% Data completeness (in resolution range)	(Not available) (70.00-3.22) 75.6 (184.07-3.22)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.11 (at 3.19Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.287 , 0.320 0.260 , 0.288	Depositor DCC
$R_{free}$ test set	37294 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	80.0	Xtriage
Anisotropy	0.720	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.22 , 62.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	285033	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% 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

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	0.25	0/36762	0.74	11/57350 (0.0%)
1	CA	0.25	0/36762	0.73	7/57350 (0.0%)
2	AW	0.32	0/401	0.75	0/622
2	CW	0.31	0/401	0.74	0/622
3	AX	0.48	0/138	0.88	0/212
3	CX	0.49	0/138	0.88	0/212
4	AB	0.25	0/1735	0.44	0/2338
4	CB	0.25	0/1735	0.45	0/2338
5	AC	0.23	0/1651	0.44	0/2225
5	CC	0.23	0/1651	0.44	0/2225
6	AD	0.23	0/1665	0.44	0/2227
6	CD	0.23	0/1665	0.45	0/2227
7	AE	0.23	0/1118	0.45	0/1504
7	CE	0.23	0/1118	0.47	0/1504
8	AF	0.24	0/835	0.44	0/1128
8	CF	0.24	0/835	0.45	0/1128
9	AG	0.23	0/1187	0.43	0/1591
9	CG	0.23	0/1187	0.44	0/1591
10	AH	0.23	0/989	0.47	0/1326
10	CH	0.23	0/989	0.46	0/1326
11	AI	0.24	0/1034	0.45	0/1375
11	CI	0.24	0/1034	0.44	0/1375
12	AJ	0.22	0/796	0.47	0/1077
12	CJ	0.22	0/796	0.47	0/1077
13	AK	0.24	0/893	0.46	0/1205
13	CK	0.24	0/893	0.45	0/1205
14	AL	0.22	0/969	0.46	0/1300
14	CL	0.22	0/969	0.46	0/1300
15	AM	0.21	0/892	0.46	0/1193
15	CM	0.22	0/884	0.46	0/1181
16	AN	0.24	0/785	0.43	0/1043
16	CN	0.24	0/786	0.44	0/1046



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AO	0.23	0/724	0.44	0/966
17	CO	0.23	0/724	0.44	0/966
18	AP	0.25	0/659	0.45	0/884
18	CP	0.25	0/648	0.43	0/870
19	AQ	0.23	0/657	0.46	0/881
19	CQ	0.24	0/657	0.46	0/881
20	AR	0.23	0/462	0.45	0/621
20	CR	0.23	0/462	0.46	0/621
21	AS	0.25	0/652	0.43	0/877
21	CS	0.25	0/652	0.45	0/877
22	AT	0.23	0/671	0.42	0/888
22	CT	0.23	0/671	0.41	0/888
23	AU	0.26	0/430	0.45	0/570
23	CU	0.26	0/430	0.44	0/570
24	BA	0.24	0/2803	0.72	0/4371
24	DA	0.24	0/2803	0.73	0/4371
25	BB	0.27	7/68314 (0.0%)	0.77	53/106569 (0.0%)
25	DB	0.28	7/68314 (0.0%)	0.77	62/106569 (0.1%)
26	BC	0.22	0/2121	0.52	0/2852
26	DC	0.22	0/2121	0.52	0/2852
27	BD	0.25	0/1586	0.60	0/2134
27	DD	0.25	0/1586	0.60	0/2134
28	BE	0.24	0/1571	0.61	2/2113 (0.1%)
28	DE	0.24	0/1571	0.61	2/2113 (0.1%)
29	BF	0.26	0/1444	0.59	0/1937
29	DF	0.27	0/1444	0.59	0/1937
30	BG	0.23	0/1343	0.52	0/1816
30	DG	0.23	0/1343	0.52	0/1816
31	BH	0.28	0/1122	0.56	1/1515 (0.1%)
31	DH	0.26	0/1122	0.52	0/1515
32	BI	0.24	0/1046	0.46	0/1410
32	DI	0.24	0/1046	0.46	0/1410
33	BJ	0.24	0/1152	0.59	0/1551
33	DJ	0.24	0/1152	0.59	0/1551
34	BK	0.25	0/939	0.81	2/1258 (0.2%)
34	DK	0.25	0/939	0.81	2/1258 (0.2%)
35	BL	0.23	0/1054	0.58	0/1403
35	DL	0.23	0/1054	0.58	0/1403
36	BM	0.26	0/1093	0.56	0/1460
36	DM	0.26	0/1093	0.56	0/1460
37	BN	0.25	0/973	0.62	0/1301
37	DN	0.25	0/973	0.62	0/1301
38	BO	0.24	0/902	0.55	0/1209



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	DO	0.23	0/902	0.55	0/1209
39	BP	0.25	0/929	0.60	0/1242
39	DP	0.25	0/929	0.60	0/1242
40	BQ	0.26	0/960	0.65	0/1278
40	DQ	0.26	0/960	0.65	0/1278
41	BR	0.26	0/829	0.58	0/1107
41	DR	0.26	0/829	0.58	0/1107
42	BS	0.23	0/864	0.61	1/1156 (0.1%)
42	DS	0.23	0/864	0.61	1/1156 (0.1%)
43	BT	0.23	0/744	0.73	2/994 (0.2%)
43	DT	0.23	0/744	0.73	2/994 (0.2%)
44	BU	0.26	0/787	0.56	0/1051
44	DU	0.26	0/787	0.56	0/1051
45	BV	0.25	0/766	0.46	0/1025
45	DV	0.25	0/766	0.46	0/1025
46	BW	0.31	0/603	0.65	0/797
46	DW	0.31	0/603	0.65	0/797
47	BX	0.25	0/635	0.58	0/848
47	DX	0.25	0/635	0.58	0/848
48	BY	0.24	0/510	0.64	0/677
48	DY	0.25	0/510	0.64	0/677
49	BZ	0.24	0/453	0.55	0/605
49	DZ	0.23	0/453	0.55	0/605
50	B0	0.23	0/450	0.65	0/599
50	D0	0.22	0/450	0.65	0/599
51	B1	0.27	0/416	0.55	0/554
51	D1	0.27	0/416	0.55	0/554
52	B2	0.26	0/380	0.58	0/498
52	D2	0.26	0/380	0.58	0/498
53	B3	0.26	0/513	0.66	2/676 (0.3%)
53	D3	0.26	0/513	0.66	2/676 (0.3%)
54	B4	0.24	0/303	0.54	0/397
54	D4	0.23	0/303	0.54	0/397
All	All	0.26	14/307402 (0.0%)	0.70	152/459589 (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	16

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	CA	0	15
25	BB	0	37
25	DB	0	36
All	All	0	104

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BB	1086	A	C5-C6	-16.31	1.26	1.41
25	DB	1086	A	C5-C6	-16.20	1.26	1.41
25	DB	1088	A	C6-N1	-10.54	1.28	1.35
25	BB	1088	A	C6-N1	-10.43	1.28	1.35
25	DB	1060	U	C2-N3	7.83	1.43	1.37

The worst 5 of 152 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	DB	2204	G	O5'-P-OP1	-29.28	75.56	110.70
25	DB	2791	G	O5'-P-OP2	-29.23	75.63	110.70
25	BB	2791	G	O5'-P-OP1	-28.43	76.59	110.70
25	BB	2204	G	O5'-P-OP2	-27.54	77.65	110.70
25	DB	2204	G	O5'-P-OP2	18.17	132.50	110.70

There are no chirality outliers.

5 of 104 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	187	G	Sidechain
1	AA	281	G	Sidechain
1	AA	324	G	Sidechain
1	AA	437	U	Sidechain
1	AA	82	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	1479	0
1	CA	32831	0	16521	1483	0
2	AW	360	0	185	9	0
2	CW	360	0	185	9	0
3	AX	125	0	63	6	0
3	CX	125	0	63	5	0
4	AB	1704	0	1732	269	0
4	CB	1704	0	1732	320	0
5	AC	1624	0	1699	212	0
5	CC	1624	0	1699	251	0
6	AD	1643	0	1710	195	0
6	CD	1643	0	1710	260	0
7	AE	1105	0	1148	159	0
7	CE	1105	0	1148	217	0
8	AF	817	0	808	94	0
8	CF	817	0	808	123	0
9	AG	1174	0	1230	146	0
9	CG	1174	0	1230	167	0
10	AH	979	0	1034	120	0
10	CH	979	0	1034	166	0
11	AI	1022	0	1070	188	0
11	CI	1022	0	1070	193	0
12	AJ	786	0	828	125	0
12	CJ	786	0	828	121	0
13	AK	877	0	887	117	0
13	CK	877	0	887	141	0
14	AL	955	0	1019	139	0
14	CL	955	0	1019	119	0
15	AM	883	0	944	127	0
15	CM	876	0	937	165	0
16	AN	774	0	827	128	0
16	CN	774	0	828	133	0
17	AO	716	0	742	62	0
17	CO	716	0	742	70	0
18	AP	649	0	666	101	0
18	CP	638	0	656	103	0
19	AQ	648	0	691	97	0
19	CQ	648	0	691	75	0
20	AR	455	0	478	76	0
20	CR	455	0	478	54	0
21	AS	637	0	665	83	0
21	CS	637	0	665	109	0
22	AT	665	0	714	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	CT	665	0	714	60	0
23	AU	425	0	449	77	0
23	CU	425	0	449	88	0
24	BA	2507	0	1270	87	0
24	DA	2507	0	1270	76	0
25	BB	60995	0	30678	2083	0
25	DB	60995	0	30678	2153	0
26	BC	2082	0	2157	218	0
26	DC	2082	0	2157	215	0
27	BD	1565	0	1616	219	0
27	DD	1565	0	1616	215	0
28	BE	1552	0	1619	163	0
28	DE	1552	0	1619	165	0
29	BF	1420	0	1460	254	0
29	DF	1420	0	1460	241	0
30	BG	1323	0	1374	181	0
30	DG	1323	0	1374	175	0
31	BH	1111	0	1148	203	0
31	DH	1111	0	1148	174	0
32	BI	1032	0	1088	108	0
32	DI	1032	0	1088	184	0
33	BJ	1129	0	1162	155	0
33	DJ	1129	0	1162	167	0
34	BK	930	0	1003	99	0
34	DK	930	0	1003	96	0
35	BL	1045	0	1117	123	0
35	DL	1045	0	1117	123	0
36	BM	1074	0	1157	109	0
36	DM	1074	0	1157	105	0
37	BN	960	0	1000	103	0
37	DN	960	0	1000	102	0
38	BO	892	0	923	77	0
38	DO	892	0	923	73	0
39	BP	917	0	965	118	0
39	DP	917	0	965	111	0
40	BQ	947	0	1022	133	0
40	DQ	947	0	1022	140	0
41	BR	816	0	839	111	0
41	DR	816	0	839	114	0
42	BS	857	0	922	95	0
42	DS	857	0	922	96	0
43	BT	738	0	807	109	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	DT	738	0	807	118	0
44	BU	779	0	834	111	0
44	DU	779	0	834	105	0
45	BV	753	0	780	75	0
45	DV	753	0	780	71	0
46	BW	596	0	610	149	0
46	DW	596	0	610	146	0
47	BX	625	0	655	79	0
47	DX	625	0	655	78	0
48	BY	509	0	543	84	0
48	DY	509	0	543	75	0
49	BZ	449	0	491	47	0
49	DZ	449	0	491	40	0
50	B0	444	0	461	45	0
50	D0	444	0	461	48	0
51	B1	409	0	440	31	0
51	D1	409	0	440	32	0
52	B2	377	0	418	32	0
52	D2	377	0	418	29	0
53	B3	504	0	574	49	0
53	D3	504	0	574	48	0
54	B4	302	0	340	27	0
54	D4	302	0	340	28	0
55	AA	60	0	0	0	0
55	AX	2	0	0	0	0
55	BB	118	0	0	0	0
55	BJ	1	0	0	0	0
55	CA	56	0	0	0	0
55	CN	1	0	0	0	0
55	CX	1	0	0	0	0
55	DB	119	0	0	0	0
56	B4	1	0	0	0	0
56	D4	1	0	0	0	0
57	AA	287	0	0	5	0
57	AE	3	0	0	0	0
57	AI	1	0	0	0	0
57	AK	2	0	0	0	0
57	AL	2	0	0	0	0
57	AN	1	0	0	0	0
57	AP	1	0	0	0	0
57	AT	2	0	0	0	0
57	AX	9	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	B2	1	0	0	0	0
57	B4	5	0	0	0	0
57	BB	532	0	0	7	0
57	BC	7	0	0	0	0
57	BE	3	0	0	0	0
57	BH	3	0	0	0	0
57	BJ	3	0	0	0	0
57	BL	2	0	0	1	0
57	BN	3	0	0	0	0
57	CA	264	0	0	4	0
57	CE	2	0	0	0	0
57	CI	3	0	0	1	0
57	CL	1	0	0	0	0
57	CN	1	0	0	0	0
57	CP	1	0	0	0	0
57	CT	3	0	0	0	0
57	CU	1	0	0	0	0
57	CX	6	0	0	1	0
57	D2	1	0	0	0	0
57	D4	4	0	0	0	0
57	DB	531	0	0	5	0
57	DC	7	0	0	0	0
57	DD	1	0	0	0	0
57	DE	3	0	0	0	0
57	DJ	2	0	0	0	0
57	DL	3	0	0	0	0
57	DN	3	0	0	0	0
57	DT	1	0	0	0	0
All	All	285033	0	191150	17782	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 38.

The worst 5 of 17782 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)
37:DN:101:GLY:HA2	37:DN:110:MET:H	1.04	1.18
27:BD:148:GLN:HG3	27:BD:152:PRO:HG2	1.29	1.15
34:BK:70:ARG:HB3	34:BK:71:PRO:CD	1.76	1.14
37:BN:101:GLY:HA2	37:BN:110:MET:H	1.06	1.13
28:DE:46:GLN:HG3	28:DE:87:ALA:HB3	1.31	1.12



There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	AB	216/240 (90%)	133 (62%)	59 (27%)	24 (11%)	0	2
4	CB	216/240 (90%)	106 (49%)	71 (33%)	39 (18%)	0	0
5	AC	204/232 (88%)	134 (66%)	50 (24%)	20 (10%)	0	3
5	CC	204/232 (88%)	119 (58%)	57 (28%)	28 (14%)	0	1
6	AD	203/205 (99%)	123 (61%)	56 (28%)	24 (12%)	0	2
6	CD	203/205 (99%)	122 (60%)	54 (27%)	27 (13%)	0	1
7	AE	148/166 (89%)	101 (68%)	38 (26%)	9 (6%)	1	11
7	CE	148/166 (89%)	78 (53%)	50 (34%)	20 (14%)	0	1
8	AF	98/135 (73%)	63 (64%)	24 (24%)	11 (11%)	0	2
8	CF	98/135 (73%)	52 (53%)	30 (31%)	16 (16%)	0	1
9	AG	148/178 (83%)	107 (72%)	31 (21%)	10 (7%)	1	8
9	CG	148/178 (83%)	89 (60%)	40 (27%)	19 (13%)	0	1
10	AH	127/129 (98%)	83 (65%)	31 (24%)	13 (10%)	0	3
10	CH	127/129 (98%)	78 (61%)	35 (28%)	14 (11%)	0	2
11	AI	125/129 (97%)	78 (62%)	33 (26%)	14 (11%)	0	2
11	CI	125/129 (97%)	74 (59%)	44 (35%)	7 (6%)	2	13
12	AJ	96/103 (93%)	55 (57%)	27 (28%)	14 (15%)	0	1
12	CJ	96/103 (93%)	60 (62%)	22 (23%)	14 (15%)	0	1
13	AK	115/128 (90%)	75 (65%)	30 (26%)	10 (9%)	1	4
13	CK	115/128 (90%)	82 (71%)	25 (22%)	8 (7%)	1	7
14	AL	121/123 (98%)	80 (66%)	30 (25%)	11 (9%)	1	3
14	CL	121/123 (98%)	80 (66%)	24 (20%)	17 (14%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	AM	112/117 (96%)	75 (67%)	22 (20%)	15 (13%)	0	1
15	CM	111/117 (95%)	66 (60%)	29 (26%)	16 (14%)	0	1
16	AN	92/100 (92%)	61 (66%)	25 (27%)	6 (6%)	1	9
16	CN	94/100 (94%)	46 (49%)	29 (31%)	19 (20%)	0	0
17	AO	86/88 (98%)	69 (80%)	14 (16%)	3 (4%)	3	23
17	CO	86/88 (98%)	70 (81%)	14 (16%)	2 (2%)	6	33
18	AP	80/82 (98%)	46 (58%)	26 (32%)	8 (10%)	0	3
18	CP	78/82 (95%)	53 (68%)	17 (22%)	8 (10%)	0	3
19	AQ	78/83 (94%)	51 (65%)	16 (20%)	11 (14%)	0	1
19	CQ	78/83 (94%)	51 (65%)	20 (26%)	7 (9%)	1	4
20	AR	53/74 (72%)	39 (74%)	9 (17%)	5 (9%)	0	3
20	CR	53/74 (72%)	37 (70%)	12 (23%)	4 (8%)	1	6
21	AS	77/91 (85%)	53 (69%)	19 (25%)	5 (6%)	1	9
21	CS	77/91 (85%)	55 (71%)	18 (23%)	4 (5%)	2	14
22	AT	83/86 (96%)	63 (76%)	11 (13%)	9 (11%)	0	2
22	CT	83/86 (96%)	59 (71%)	20 (24%)	4 (5%)	2	16
23	AU	49/70 (70%)	21 (43%)	17 (35%)	11 (22%)	0	0
23	CU	49/70 (70%)	27 (55%)	16 (33%)	6 (12%)	0	2
26	BC	269/272 (99%)	166 (62%)	68 (25%)	35 (13%)	0	1
26	DC	269/272 (99%)	168 (62%)	63 (23%)	38 (14%)	0	1
27	BD	207/209 (99%)	113 (55%)	56 (27%)	38 (18%)	0	0
27	DD	207/209 (99%)	110 (53%)	56 (27%)	41 (20%)	0	0
28	BE	199/201 (99%)	126 (63%)	43 (22%)	30 (15%)	0	1
28	DE	199/201 (99%)	127 (64%)	42 (21%)	30 (15%)	0	1
29	BF	176/178 (99%)	97 (55%)	40 (23%)	39 (22%)	0	0
29	DF	176/178 (99%)	95 (54%)	43 (24%)	38 (22%)	0	0
30	BG	174/176 (99%)	94 (54%)	54 (31%)	26 (15%)	0	1
30	DG	174/176 (99%)	93 (53%)	55 (32%)	26 (15%)	0	1
31	BH	147/149 (99%)	69 (47%)	50 (34%)	28 (19%)	0	0
31	DH	147/149 (99%)	68 (46%)	54 (37%)	25 (17%)	0	0
32	BI	139/141 (99%)	118 (85%)	16 (12%)	5 (4%)	3	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	DI	139/141 (99%)	114 (82%)	21 (15%)	4 (3%)	4	27
33	BJ	140/142 (99%)	88 (63%)	30 (21%)	22 (16%)	0	1
33	DJ	140/142 (99%)	88 (63%)	30 (21%)	22 (16%)	0	1
34	BK	119/123 (97%)	75 (63%)	26 (22%)	18 (15%)	0	1
34	DK	119/123 (97%)	75 (63%)	26 (22%)	18 (15%)	0	1
35	BL	141/144 (98%)	81 (57%)	37 (26%)	23 (16%)	0	1
35	DL	141/144 (98%)	81 (57%)	37 (26%)	23 (16%)	0	1
36	BM	134/136 (98%)	77 (58%)	32 (24%)	25 (19%)	0	0
36	DM	134/136 (98%)	77 (58%)	33 (25%)	24 (18%)	0	0
37	BN	118/127 (93%)	75 (64%)	27 (23%)	16 (14%)	0	1
37	DN	118/127 (93%)	75 (64%)	27 (23%)	16 (14%)	0	1
38	BO	114/117 (97%)	85 (75%)	24 (21%)	5 (4%)	2	18
38	DO	114/117 (97%)	85 (75%)	24 (21%)	5 (4%)	2	18
39	BP	112/114 (98%)	71 (63%)	20 (18%)	21 (19%)	0	0
39	DP	112/114 (98%)	71 (63%)	20 (18%)	21 (19%)	0	0
40	BQ	115/117 (98%)	74 (64%)	28 (24%)	13 (11%)	0	2
40	DQ	115/117 (98%)	74 (64%)	28 (24%)	13 (11%)	0	2
41	BR	101/103 (98%)	64 (63%)	24 (24%)	13 (13%)	0	1
41	DR	101/103 (98%)	64 (63%)	24 (24%)	13 (13%)	0	1
42	BS	108/110 (98%)	66 (61%)	26 (24%)	16 (15%)	0	1
42	DS	108/110 (98%)	66 (61%)	26 (24%)	16 (15%)	0	1
43	BT	91/100 (91%)	54 (59%)	23 (25%)	14 (15%)	0	1
43	DT	91/100 (91%)	52 (57%)	25 (28%)	14 (15%)	0	1
44	BU	100/103 (97%)	58 (58%)	27 (27%)	15 (15%)	0	1
44	DU	100/103 (97%)	57 (57%)	28 (28%)	15 (15%)	0	1
45	BV	92/94 (98%)	74 (80%)	11 (12%)	7 (8%)	1	6
45	DV	92/94 (98%)	73 (79%)	12 (13%)	7 (8%)	1	6
46	BW	77/84 (92%)	29 (38%)	23 (30%)	25 (32%)	0	0
46	DW	77/84 (92%)	29 (38%)	22 (29%)	26 (34%)	0	0
47	BX	75/77 (97%)	43 (57%)	26 (35%)	6 (8%)	1	5
47	DX	75/77 (97%)	41 (55%)	27 (36%)	7 (9%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	BY	61/63 (97%)	37 (61%)	18 (30%)	6 (10%)	0	3
48	DY	61/63 (97%)	34 (56%)	21 (34%)	6 (10%)	0	3
49	BZ	56/58 (97%)	42 (75%)	11 (20%)	3 (5%)	2	13
49	DZ	56/58 (97%)	42 (75%)	11 (20%)	3 (5%)	2	13
50	B0	54/56 (96%)	35 (65%)	8 (15%)	11 (20%)	0	0
50	D0	54/56 (96%)	34 (63%)	10 (18%)	10 (18%)	0	0
51	B1	48/54 (89%)	33 (69%)	7 (15%)	8 (17%)	0	1
51	D1	48/54 (89%)	33 (69%)	6 (12%)	9 (19%)	0	0
52	B2	44/46 (96%)	26 (59%)	13 (30%)	5 (11%)	0	2
52	D2	44/46 (96%)	26 (59%)	14 (32%)	4 (9%)	1	3
53	B3	62/64 (97%)	42 (68%)	15 (24%)	5 (8%)	1	5
53	D3	62/64 (97%)	41 (66%)	17 (27%)	4 (6%)	1	9
54	B4	36/38 (95%)	21 (58%)	11 (31%)	4 (11%)	0	2
54	D4	36/38 (95%)	21 (58%)	11 (31%)	4 (11%)	0	2
All	All	11239/11910 (94%)	6961 (62%)	2802 (25%)	1476 (13%)	0	1

5 of 1476 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AB	19	THR
4	AB	22	TRP
4	AB	75	ALA
4	AB	76	SER
4	AB	91	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	
4	AB	180/198 (91%)	140 (78%)	40 (22%)	1	4
4	CB	180/198 (91%)	143 (79%)	37 (21%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	AC	170/189 (90%)	134 (79%)	36 (21%)	1	5
5	CC	170/189 (90%)	138 (81%)	32 (19%)	1	8
6	AD	172/172 (100%)	146 (85%)	26 (15%)	3	13
6	CD	172/172 (100%)	130 (76%)	42 (24%)	0	2
7	AE	113/125 (90%)	95 (84%)	18 (16%)	2	11
7	CE	113/125 (90%)	87 (77%)	26 (23%)	1	3
8	AF	87/116 (75%)	74 (85%)	13 (15%)	3	13
8	CF	87/116 (75%)	76 (87%)	11 (13%)	4	20
9	AG	123/146 (84%)	99 (80%)	24 (20%)	1	7
9	CG	123/146 (84%)	100 (81%)	23 (19%)	1	8
10	AH	104/104 (100%)	89 (86%)	15 (14%)	3	14
10	CH	104/104 (100%)	81 (78%)	23 (22%)	1	4
11	AI	105/106 (99%)	83 (79%)	22 (21%)	1	5
11	CI	105/106 (99%)	83 (79%)	22 (21%)	1	5
12	AJ	86/90 (96%)	75 (87%)	11 (13%)	4	19
12	CJ	86/90 (96%)	71 (83%)	15 (17%)	2	9
13	AK	90/98 (92%)	75 (83%)	15 (17%)	2	10
13	CK	90/98 (92%)	77 (86%)	13 (14%)	3	14
14	AL	103/103 (100%)	83 (81%)	20 (19%)	1	7
14	CL	103/103 (100%)	80 (78%)	23 (22%)	1	4
15	AM	92/95 (97%)	75 (82%)	17 (18%)	1	8
15	CM	91/95 (96%)	71 (78%)	20 (22%)	1	4
16	AN	79/83 (95%)	60 (76%)	19 (24%)	0	3
16	CN	79/83 (95%)	66 (84%)	13 (16%)	2	10
17	AO	76/76 (100%)	65 (86%)	11 (14%)	3	14
17	CO	76/76 (100%)	67 (88%)	9 (12%)	5	22
18	AP	65/65 (100%)	52 (80%)	13 (20%)	1	6
18	CP	65/65 (100%)	58 (89%)	7 (11%)	6	26
19	AQ	74/77 (96%)	60 (81%)	14 (19%)	1	8
19	CQ	74/77 (96%)	66 (89%)	8 (11%)	6	26
20	AR	48/64 (75%)	37 (77%)	11 (23%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	CR	48/64 (75%)	43 (90%)	5 (10%)	7	28
21	AS	70/78 (90%)	55 (79%)	15 (21%)	1	5
21	CS	70/78 (90%)	51 (73%)	19 (27%)	0	1
22	AT	65/65 (100%)	56 (86%)	9 (14%)	3	16
22	CT	65/65 (100%)	55 (85%)	10 (15%)	2	12
23	AU	44/60 (73%)	37 (84%)	7 (16%)	2	11
23	CU	44/60 (73%)	32 (73%)	12 (27%)	0	1
26	BC	216/217 (100%)	182 (84%)	34 (16%)	2	11
26	DC	216/217 (100%)	182 (84%)	34 (16%)	2	11
27	BD	164/164 (100%)	136 (83%)	28 (17%)	2	9
27	DD	164/164 (100%)	137 (84%)	27 (16%)	2	10
28	BE	165/165 (100%)	130 (79%)	35 (21%)	1	5
28	DE	165/165 (100%)	130 (79%)	35 (21%)	1	5
29	BF	149/149 (100%)	116 (78%)	33 (22%)	1	4
29	DF	149/149 (100%)	117 (78%)	32 (22%)	1	5
30	BG	137/137 (100%)	110 (80%)	27 (20%)	1	6
30	DG	137/137 (100%)	110 (80%)	27 (20%)	1	6
31	BH	114/114 (100%)	85 (75%)	29 (25%)	0	2
31	DH	114/114 (100%)	86 (75%)	28 (25%)	0	2
32	BI	109/109 (100%)	107 (98%)	2 (2%)	59	81
32	DI	109/109 (100%)	104 (95%)	5 (5%)	27	62
33	BJ	116/116 (100%)	100 (86%)	16 (14%)	3	16
33	DJ	116/116 (100%)	100 (86%)	16 (14%)	3	16
34	BK	102/104 (98%)	84 (82%)	18 (18%)	2	9
34	DK	102/104 (98%)	83 (81%)	19 (19%)	1	8
35	BL	102/103 (99%)	87 (85%)	15 (15%)	3	14
35	DL	102/103 (99%)	88 (86%)	14 (14%)	3	16
36	BM	109/109 (100%)	93 (85%)	16 (15%)	3	14
36	DM	109/109 (100%)	93 (85%)	16 (15%)	3	14
37	BN	100/103 (97%)	85 (85%)	15 (15%)	3	13
37	DN	100/103 (97%)	84 (84%)	16 (16%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	BO	86/87 (99%)	76 (88%)	10 (12%)	5	23
38	DO	86/87 (99%)	76 (88%)	10 (12%)	5	23
39	BP	99/99 (100%)	76 (77%)	23 (23%)	1	3
39	DP	99/99 (100%)	77 (78%)	22 (22%)	1	4
40	BQ	89/89 (100%)	73 (82%)	16 (18%)	1	8
40	DQ	89/89 (100%)	73 (82%)	16 (18%)	1	8
41	BR	84/84 (100%)	67 (80%)	17 (20%)	1	6
41	DR	84/84 (100%)	67 (80%)	17 (20%)	1	6
42	BS	93/93 (100%)	79 (85%)	14 (15%)	3	13
42	DS	93/93 (100%)	79 (85%)	14 (15%)	3	13
43	BT	80/84 (95%)	65 (81%)	15 (19%)	1	8
43	DT	80/84 (95%)	64 (80%)	16 (20%)	1	6
44	BU	83/84 (99%)	69 (83%)	14 (17%)	2	10
44	DU	83/84 (99%)	70 (84%)	13 (16%)	2	11
45	BV	78/78 (100%)	67 (86%)	11 (14%)	3	15
45	DV	78/78 (100%)	67 (86%)	11 (14%)	3	15
46	BW	59/62 (95%)	49 (83%)	10 (17%)	2	10
46	DW	59/62 (95%)	48 (81%)	11 (19%)	1	8
47	BX	67/67 (100%)	56 (84%)	11 (16%)	2	10
47	DX	67/67 (100%)	57 (85%)	10 (15%)	3	13
48	BY	55/55 (100%)	43 (78%)	12 (22%)	1	5
48	DY	55/55 (100%)	43 (78%)	12 (22%)	1	5
49	BZ	48/48 (100%)	43 (90%)	5 (10%)	7	28
49	DZ	48/48 (100%)	43 (90%)	5 (10%)	7	28
50	B0	47/47 (100%)	40 (85%)	7 (15%)	3	13
50	D0	47/47 (100%)	40 (85%)	7 (15%)	3	13
51	B1	45/48 (94%)	38 (84%)	7 (16%)	2	11
51	D1	45/48 (94%)	38 (84%)	7 (16%)	2	11
52	B2	38/38 (100%)	33 (87%)	5 (13%)	4	18
52	D2	38/38 (100%)	33 (87%)	5 (13%)	4	18
53	B3	51/51 (100%)	44 (86%)	7 (14%)	3	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	D3	51/51 (100%)	43 (84%)	8 (16%)	2	11
54	B4	34/34 (100%)	29 (85%)	5 (15%)	3	14
54	D4	34/34 (100%)	29 (85%)	5 (15%)	3	14
All	All	9329/9696 (96%)	7688 (82%)	1641 (18%)	2	9

5 of 1641 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
45	BV	79	ARG
6	CD	170	LEU
41	DR	95	ASP
47	BX	77	TYR
4	CB	122	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 364 such sidechains are listed below:

Mol	Chain	Res	Type
45	BV	88	HIS
7	CE	11	GLN
42	DS	57	ASN
48	BY	25	GLN
4	CB	121	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1529/1542 (99%)	278 (18%)	20 (1%)
1	CA	1529/1542 (99%)	272 (17%)	19 (1%)
2	AW	16/17 (94%)	0	0
2	CW	16/17 (94%)	0	0
24	BA	116/120 (96%)	19 (16%)	2 (1%)
24	DA	116/120 (96%)	19 (16%)	2 (1%)
25	BB	2837/2904 (97%)	416 (14%)	13 (0%)
25	DB	2837/2904 (97%)	420 (14%)	17 (0%)
3	AX	5/6 (83%)	3 (60%)	0
3	CX	5/6 (83%)	3 (60%)	0
All	All	9006/9178 (98%)	1430 (15%)	73 (0%)

5 of 1430 RNA backbone outliers are listed below:



Mol	Chain	Res	Type
1	AA	6	G
1	AA	8	A
1	AA	9	G
1	AA	14	U
1	AA	15	G

5 of 73 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	BB	2756	U
1	CA	366	A
25	DB	2308	G
1	CA	243	A
1	CA	428	G

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 360 ligands modelled in this entry, 360 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.



## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.



## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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%)	0.16	153 (10%) 7 4	41, 98, 164, 180	0
1	CA	1530/1542 (99%)	-0.34	14 (0%) 84 76	41, 109, 167, 180	0
2	AW	17/17 (100%)	2.89	10 (58%) 0 0	73, 87, 132, 177	0
2	CW	17/17 (100%)	0.22	1 (5%) 22 13	63, 86, 126, 150	0
3	AX	6/6 (100%)	6.38	6 (100%) 0 0	63, 78, 113, 127	0
3	CX	6/6 (100%)	1.48	3 (50%) 0 0	76, 83, 113, 115	0
4	AB	218/240 (90%)	2.82	129 (59%) 0 0	59, 127, 169, 180	0
4	CB	218/240 (90%)	3.74	136 (62%) 0 0	67, 141, 180, 180	0
5	AC	206/232 (88%)	2.89	128 (62%) 0 0	61, 104, 153, 180	0
5	CC	206/232 (88%)	2.29	97 (47%) 0 0	69, 121, 161, 180	0
6	AD	205/205 (100%)	1.85	79 (38%) 0 0	44, 106, 149, 180	0
6	CD	205/205 (100%)	1.93	79 (38%) 0 0	67, 120, 164, 180	0
7	AE	150/166 (90%)	2.31	81 (54%) 0 0	39, 98, 148, 180	0
7	CE	150/166 (90%)	2.52	63 (42%) 0 0	46, 129, 180, 180	0
8	AF	100/135 (74%)	1.21	25 (25%) 0 0	52, 100, 148, 180	0
8	CF	100/135 (74%)	1.47	29 (29%) 0 0	33, 101, 144, 165	0
9	AG	150/178 (84%)	2.10	63 (42%) 0 0	55, 113, 167, 180	0
9	CG	150/178 (84%)	-0.09	12 (8%) 12 7	71, 122, 165, 180	0
10	AH	129/129 (100%)	0.34	13 (10%) 7 4	51, 100, 143, 179	0
10	CH	129/129 (100%)	-0.46	1 (0%) 86 79	37, 106, 149, 176	0
11	AI	127/129 (98%)	0.35	11 (8%) 10 6	84, 120, 166, 180	0
11	CI	127/129 (98%)	-0.56	2 (1%) 72 60	68, 128, 167, 180	0
12	AJ	98/103 (95%)	1.73	47 (47%) 0 0	56, 124, 172, 180	0
12	CJ	98/103 (95%)	1.63	28 (28%) 0 0	76, 131, 164, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AK	117/128 (91%)	5.16	107 (91%) 0 0	36, 91, 142, 180	0
13	CK	117/128 (91%)	2.09	52 (44%) 0 0	48, 91, 131, 159	0
14	AL	123/123 (100%)	3.68	87 (70%) 0 0	31, 80, 130, 169	0
14	CL	123/123 (100%)	1.70	50 (40%) 0 0	42, 91, 138, 172	0
15	AM	114/117 (97%)	-0.06	6 (5%) 26 15	63, 119, 165, 180	0
15	CM	113/117 (96%)	-0.46	2 (1%) 68 56	58, 121, 165, 176	0
16	AN	96/100 (96%)	0.70	19 (19%) 1 0	56, 112, 155, 180	0
16	CN	96/100 (96%)	1.06	21 (21%) 0 0	65, 124, 154, 180	0
17	AO	88/88 (100%)	0.07	4 (4%) 33 21	54, 91, 138, 180	0
17	CO	88/88 (100%)	0.22	4 (4%) 33 21	37, 96, 143, 160	0
18	AP	82/82 (100%)	-0.52	0 100 100	49, 95, 163, 180	0
18	CP	80/82 (97%)	-0.52	0 100 100	68, 113, 155, 180	0
19	AQ	80/83 (96%)	-0.10	1 (1%) 77 66	54, 107, 155, 169	0
19	CQ	80/83 (96%)	-0.50	0 100 100	50, 104, 145, 155	0
20	AR	55/74 (74%)	2.82	35 (63%) 0 0	52, 98, 134, 158	0
20	CR	55/74 (74%)	2.03	24 (43%) 0 0	46, 101, 144, 157	0
21	AS	79/91 (86%)	0.27	8 (10%) 7 4	80, 133, 169, 180	0
21	CS	79/91 (86%)	0.02	4 (5%) 28 17	75, 128, 160, 180	0
22	AT	85/86 (98%)	-0.77	0 100 100	62, 101, 151, 162	0
22	CT	85/86 (98%)	-0.44	0 100 100	65, 104, 154, 180	0
23	AU	51/70 (72%)	5.08	43 (84%) 0 0	54, 110, 154, 180	0
23	CU	51/70 (72%)	1.88	18 (35%) 0 0	63, 125, 169, 180	0
24	BA	117/120 (97%)	0.93	5 (4%) 35 23	44, 75, 109, 180	0
24	DA	117/120 (97%)	-0.31	1 (0%) 84 76	33, 66, 105, 180	0
25	BB	2841/2904 (97%)	0.15	119 (4%) 36 24	13, 70, 147, 180	0
25	DB	2841/2904 (97%)	0.04	53 (1%) 66 54	12, 55, 149, 180	0
26	BC	271/272 (99%)	1.98	123 (45%) 0 0	16, 66, 111, 151	0
26	DC	271/272 (99%)	1.61	88 (32%) 0 0	9, 52, 97, 153	0
27	BD	209/209 (100%)	1.96	95 (45%) 0 0	25, 83, 146, 180	0
27	DD	209/209 (100%)	0.56	10 (4%) 30 19	20, 59, 119, 166	0
28	BE	201/201 (100%)	0.66	27 (13%) 3 2	22, 78, 139, 172	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	DE	201/201 (100%)	2.42	107 (53%) 0 0	11, 76, 143, 178	0
29	BF	178/178 (100%)	-0.27	1 (0%) 89 84	49, 111, 174, 180	0
29	DF	178/178 (100%)	0.09	6 (3%) 45 31	49, 110, 166, 180	0
30	BG	176/176 (100%)	-0.19	8 (4%) 33 21	47, 112, 165, 176	0
30	DG	176/176 (100%)	-0.36	2 (1%) 80 70	38, 88, 155, 174	0
31	BH	149/149 (100%)	3.61	71 (47%) 0 0	52, 131, 180, 180	0
31	DH	149/149 (100%)	1.54	44 (29%) 0 0	35, 109, 150, 180	0
32	BI	141/141 (100%)	2.74	69 (48%) 0 0	110, 167, 180, 180	0
32	DI	141/141 (100%)	3.53	84 (59%) 0 0	105, 179, 180, 180	0
33	BJ	142/142 (100%)	-0.00	4 (2%) 53 39	32, 86, 133, 180	0
33	DJ	142/142 (100%)	-0.16	0 100 100	19, 53, 108, 175	0
34	BK	121/123 (98%)	4.14	115 (95%) 0 0	32, 74, 148, 180	0
34	DK	121/123 (98%)	1.91	47 (38%) 0 0	27, 64, 130, 163	0
35	BL	143/144 (99%)	0.13	4 (2%) 53 39	27, 69, 121, 180	0
35	DL	143/144 (99%)	3.19	93 (65%) 0 0	17, 64, 115, 180	0
36	BM	136/136 (100%)	0.39	12 (8%) 10 6	33, 65, 132, 168	0
36	DM	136/136 (100%)	0.28	5 (3%) 41 28	11, 56, 109, 176	0
37	BN	120/127 (94%)	2.29	63 (52%) 0 0	43, 88, 131, 169	0
37	DN	120/127 (94%)	0.39	2 (1%) 70 58	19, 57, 97, 180	0
38	BO	116/117 (99%)	-0.14	0 100 100	34, 77, 118, 138	0
38	DO	116/117 (99%)	-0.39	0 100 100	28, 71, 129, 157	0
39	BP	114/114 (100%)	2.68	73 (64%) 0 0	43, 84, 145, 164	0
39	DP	114/114 (100%)	1.38	27 (23%) 0 0	26, 73, 123, 174	0
40	BQ	117/117 (100%)	-0.16	5 (4%) 35 23	34, 73, 135, 149	0
40	DQ	117/117 (100%)	0.36	10 (8%) 10 6	22, 53, 104, 158	0
41	BR	103/103 (100%)	-0.53	1 (0%) 82 73	44, 95, 146, 177	0
41	DR	103/103 (100%)	-0.09	3 (2%) 51 37	23, 72, 131, 156	0
42	BS	110/110 (100%)	3.74	92 (83%) 0 0	47, 84, 138, 180	0
42	DS	110/110 (100%)	1.16	20 (18%) 1 1	18, 53, 108, 152	0
43	BT	93/100 (93%)	0.93	14 (15%) 2 1	44, 93, 163, 180	0
43	DT	93/100 (93%)	0.65	10 (10%) 5 4	35, 72, 141, 178	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	BU	102/103 (99%)	1.83	48 (47%) 0 0	48, 106, 162, 175	0
44	DU	102/103 (99%)	0.15	3 (2%) 51 37	41, 94, 154, 180	0
45	BV	94/94 (100%)	-0.08	1 (1%) 80 70	37, 84, 140, 180	0
45	DV	94/94 (100%)	0.27	4 (4%) 35 23	31, 70, 138, 156	0
46	BW	79/84 (94%)	0.14	1 (1%) 77 66	6, 53, 116, 154	0
46	DW	79/84 (94%)	0.05	1 (1%) 77 66	7, 42, 103, 180	0
47	BX	77/77 (100%)	1.02	11 (14%) 2 2	24, 63, 107, 157	0
47	DX	77/77 (100%)	0.98	13 (16%) 1 1	23, 60, 112, 152	0
48	BY	63/63 (100%)	0.89	10 (15%) 1 1	47, 108, 165, 180	0
48	DY	63/63 (100%)	-0.04	2 (3%) 47 33	34, 92, 158, 180	0
49	BZ	58/58 (100%)	-0.21	0 100 100	40, 74, 124, 150	0
49	DZ	58/58 (100%)	-0.44	0 100 100	22, 58, 110, 114	0
50	B0	56/56 (100%)	2.75	28 (50%) 0 0	35, 87, 152, 180	0
50	D0	56/56 (100%)	0.50	1 (1%) 68 56	19, 56, 118, 135	0
51	B1	50/54 (92%)	0.68	7 (14%) 2 2	43, 72, 122, 140	0
51	D1	50/54 (92%)	0.77	6 (12%) 4 3	26, 76, 119, 163	0
52	B2	46/46 (100%)	1.56	18 (39%) 0 0	42, 61, 97, 162	0
52	D2	46/46 (100%)	1.34	11 (23%) 0 0	17, 47, 97, 131	0
53	B3	64/64 (100%)	0.08	0 100 100	21, 56, 99, 136	0
53	D3	64/64 (100%)	2.28	33 (51%) 0 0	27, 49, 85, 105	0
54	B4	38/38 (100%)	0.27	2 (5%) 26 15	36, 86, 126, 146	0
54	D4	38/38 (100%)	-0.20	0 100 100	44, 68, 126, 165	0
All	All	20459/21088 (97%)	0.71	3408 (16%) 1 1	6, 86, 162, 180	0

The worst 5 of 3408 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	DI	82	ALA	27.6
31	BH	88	GLY	27.1
7	CE	114	LEU	26.5
32	DI	138	VAL	19.9
15	AM	114	PRO	19.3



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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	1614	1/1	-0.08	0.74	174,174,174,174	0
55	MG	AA	1635	1/1	0.16	0.12	129,129,129,129	0
55	MG	AA	1658	1/1	0.23	0.53	147,147,147,147	0
55	MG	AA	1630	1/1	0.34	0.18	114,114,114,114	0
55	MG	DB	3115	1/1	0.34	0.25	132,132,132,132	0
55	MG	CA	1632	1/1	0.44	0.17	154,154,154,154	0
55	MG	AA	1626	1/1	0.54	0.75	139,139,139,139	0
55	MG	CA	1646	1/1	0.55	0.52	155,155,155,155	0
55	MG	CA	1610	1/1	0.56	0.17	130,130,130,130	0
55	MG	CA	1649	1/1	0.58	0.08	100,100,100,100	0
55	MG	BB	3010	1/1	0.60	0.17	95,95,95,95	0
55	MG	AA	1641	1/1	0.61	0.09	111,111,111,111	0
55	MG	CA	1629	1/1	0.61	0.09	94,94,94,94	0
55	MG	CA	1640	1/1	0.62	0.49	138,138,138,138	0
55	MG	BB	3019	1/1	0.62	0.10	62,62,62,62	0
55	MG	AA	1625	1/1	0.63	0.19	145,145,145,145	0
55	MG	CA	1618	1/1	0.63	0.12	87,87,87,87	0
55	MG	AA	1637	1/1	0.64	2.75	134,134,134,134	0
55	MG	CA	1627	1/1	0.64	0.13	122,122,122,122	0
55	MG	CA	1635	1/1	0.65	0.20	129,129,129,129	0
55	MG	DB	3052	1/1	0.68	0.68	137,137,137,137	0
55	MG	AA	1618	1/1	0.69	0.12	92,92,92,92	0
55	MG	AA	1643	1/1	0.69	0.52	112,112,112,112	0
55	MG	CA	1622	1/1	0.69	0.09	98,98,98,98	0
55	MG	CA	1607	1/1	0.70	0.09	108,108,108,108	0
55	MG	BB	3076	1/1	0.70	0.20	56,56,56,56	0
55	MG	AA	1619	1/1	0.71	0.36	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	CA	1643	1/1	0.71	0.09	138,138,138,138	0
55	MG	CA	1653	1/1	0.71	0.12	149,149,149,149	0
55	MG	AA	1611	1/1	0.72	3.92	148,148,148,148	0
55	MG	AA	1639	1/1	0.72	0.11	126,126,126,126	0
55	MG	DB	3059	1/1	0.73	0.13	110,110,110,110	0
55	MG	BB	3046	1/1	0.73	0.10	90,90,90,90	0
55	MG	CA	1614	1/1	0.73	0.33	171,171,171,171	0
55	MG	AA	1652	1/1	0.73	0.39	103,103,103,103	0
55	MG	BB	3014	1/1	0.74	0.31	76,76,76,76	0
55	MG	AA	1608	1/1	0.75	0.28	113,113,113,113	0
55	MG	CA	1625	1/1	0.76	0.07	54,54,54,54	0
55	MG	CA	1644	1/1	0.76	0.11	131,131,131,131	0
55	MG	DB	3013	1/1	0.76	0.10	62,62,62,62	0
55	MG	AA	1621	1/1	0.76	0.28	36,36,36,36	0
55	MG	DB	3065	1/1	0.77	0.29	67,67,67,67	0
55	MG	BB	3057	1/1	0.77	0.76	100,100,100,100	0
55	MG	CA	1631	1/1	0.77	0.09	91,91,91,91	0
55	MG	AA	1613	1/1	0.77	0.09	106,106,106,106	0
55	MG	AA	1647	1/1	0.77	0.39	79,79,79,79	0
55	MG	BB	3115	1/1	0.77	0.18	106,106,106,106	0
55	MG	CA	1650	1/1	0.77	0.06	103,103,103,103	0
55	MG	DB	3082	1/1	0.78	0.22	104,104,104,104	0
55	MG	BB	3093	1/1	0.78	0.69	120,120,120,120	0
55	MG	AA	1628	1/1	0.79	0.32	100,100,100,100	0
55	MG	CA	1606	1/1	0.79	0.13	139,139,139,139	0
55	MG	CA	1636	1/1	0.79	0.06	127,127,127,127	0
55	MG	BB	3097	1/1	0.79	0.08	112,112,112,112	0
55	MG	BB	3051	1/1	0.79	0.14	94,94,94,94	0
55	MG	AA	1653	1/1	0.80	0.13	84,84,84,84	0
55	MG	CA	1654	1/1	0.80	0.31	78,78,78,78	0
55	MG	CN	201	1/1	0.80	0.10	104,104,104,104	0
55	MG	AA	1642	1/1	0.81	0.10	63,63,63,63	0
55	MG	CA	1603	1/1	0.81	0.12	124,124,124,124	0
55	MG	CA	1641	1/1	0.82	0.12	123,123,123,123	0
55	MG	CA	1637	1/1	0.82	0.17	81,81,81,81	0
55	MG	CA	1615	1/1	0.82	0.10	156,156,156,156	0
55	MG	BB	3068	1/1	0.82	0.10	40,40,40,40	0
55	MG	CA	1655	1/1	0.83	0.20	153,153,153,153	0
55	MG	AA	1657	1/1	0.83	0.10	85,85,85,85	0
55	MG	CA	1656	1/1	0.83	0.41	97,97,97,97	0
55	MG	CA	1634	1/1	0.84	0.20	80,80,80,80	0
55	MG	CA	1609	1/1	0.84	0.09	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DB	3119	1/1	0.84	0.19	64,64,64,64	0
55	MG	DB	3058	1/1	0.84	0.60	136,136,136,136	0
55	MG	CA	1652	1/1	0.84	0.09	117,117,117,117	0
55	MG	DB	3068	1/1	0.84	0.08	35,35,35,35	0
55	MG	DB	3107	1/1	0.84	0.11	24,24,24,24	0
55	MG	DB	3034	1/1	0.84	0.34	87,87,87,87	0
55	MG	CA	1621	1/1	0.85	0.15	161,161,161,161	0
55	MG	DB	3087	1/1	0.85	0.10	28,28,28,28	0
55	MG	AA	1615	1/1	0.85	0.08	85,85,85,85	0
55	MG	AA	1640	1/1	0.85	0.09	99,99,99,99	0
55	MG	AA	1623	1/1	0.85	0.18	115,115,115,115	0
55	MG	CA	1605	1/1	0.85	0.08	98,98,98,98	0
55	MG	CA	1617	1/1	0.85	0.11	149,149,149,149	0
55	MG	BB	3118	1/1	0.85	0.36	113,113,113,113	0
55	MG	DB	3005	1/1	0.85	0.17	66,66,66,66	0
55	MG	AA	1648	1/1	0.85	0.11	67,67,67,67	0
55	MG	BB	3090	1/1	0.86	0.11	71,71,71,71	0
55	MG	DB	3070	1/1	0.86	0.18	61,61,61,61	0
55	MG	DB	3032	1/1	0.86	0.43	111,111,111,111	0
55	MG	CA	1639	1/1	0.86	0.37	99,99,99,99	0
55	MG	AA	1638	1/1	0.86	0.09	95,95,95,95	0
55	MG	AA	1606	1/1	0.86	0.09	114,114,114,114	0
55	MG	BB	3107	1/1	0.86	0.09	86,86,86,86	0
55	MG	AA	1605	1/1	0.86	0.06	87,87,87,87	0
55	MG	AA	1644	1/1	0.86	0.10	99,99,99,99	0
55	MG	DB	3045	1/1	0.86	0.08	140,140,140,140	0
55	MG	BB	3042	1/1	0.87	0.08	90,90,90,90	0
55	MG	AA	1633	1/1	0.87	0.06	85,85,85,85	0
55	MG	CA	1642	1/1	0.87	0.10	110,110,110,110	0
55	MG	CA	1608	1/1	0.87	0.08	82,82,82,82	0
55	MG	BB	3033	1/1	0.87	0.07	86,86,86,86	0
55	MG	AA	1617	1/1	0.87	0.42	123,123,123,123	0
55	MG	CA	1613	1/1	0.87	0.10	140,140,140,140	0
55	MG	CA	1620	1/1	0.88	0.12	103,103,103,103	0
55	MG	BB	3050	1/1	0.88	0.09	54,54,54,54	0
55	MG	AA	1632	1/1	0.88	0.54	106,106,106,106	0
55	MG	CA	1628	1/1	0.88	0.06	106,106,106,106	0
55	MG	DB	3044	1/1	0.88	0.08	20,20,20,20	0
55	MG	DB	3026	1/1	0.88	0.08	38,38,38,38	0
55	MG	BB	3047	1/1	0.88	0.08	131,131,131,131	0
55	MG	BB	3096	1/1	0.89	0.17	49,49,49,49	0
55	MG	BB	3073	1/1	0.89	0.06	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	1612	1/1	0.89	0.09	117,117,117,117	0
55	MG	DB	3027	1/1	0.89	0.13	43,43,43,43	0
55	MG	DB	3030	1/1	0.89	0.16	46,46,46,46	0
55	MG	DB	3067	1/1	0.89	0.15	33,33,33,33	0
55	MG	BB	3100	1/1	0.89	0.21	128,128,128,128	0
55	MG	DB	3029	1/1	0.89	0.84	92,92,92,92	0
55	MG	DB	3024	1/1	0.89	0.06	22,22,22,22	0
55	MG	CA	1647	1/1	0.89	0.08	109,109,109,109	0
55	MG	BB	3074	1/1	0.89	0.07	25,25,25,25	0
55	MG	AA	1624	1/1	0.89	0.05	88,88,88,88	0
55	MG	DB	3033	1/1	0.89	0.11	43,43,43,43	0
55	MG	DB	3037	1/1	0.89	0.09	32,32,32,32	0
55	MG	BB	3108	1/1	0.90	0.09	30,30,30,30	0
55	MG	AA	1660	1/1	0.90	0.54	95,95,95,95	0
55	MG	BB	3028	1/1	0.90	0.15	54,54,54,54	0
55	MG	DB	3064	1/1	0.90	0.12	32,32,32,32	0
55	MG	AA	1655	1/1	0.90	0.17	82,82,82,82	0
55	MG	DB	3091	1/1	0.90	0.20	39,39,39,39	0
55	MG	BB	3039	1/1	0.90	0.07	55,55,55,55	0
55	MG	AA	1656	1/1	0.90	1.00	101,101,101,101	0
55	MG	CX	101	1/1	0.90	0.12	73,73,73,73	0
55	MG	BB	3081	1/1	0.91	0.09	85,85,85,85	0
55	MG	BB	3087	1/1	0.91	0.17	63,63,63,63	0
55	MG	BB	3083	1/1	0.91	0.19	47,47,47,47	0
55	MG	BB	3112	1/1	0.91	0.32	27,27,27,27	0
55	MG	BB	3070	1/1	0.91	0.08	52,52,52,52	0
55	MG	BB	3059	1/1	0.91	0.07	37,37,37,37	0
55	MG	DB	3047	1/1	0.91	0.10	36,36,36,36	0
55	MG	DB	3041	1/1	0.91	0.08	32,32,32,32	0
55	MG	CA	1604	1/1	0.91	0.09	58,58,58,58	0
55	MG	BB	3011	1/1	0.91	0.10	45,45,45,45	0
55	MG	BB	3048	1/1	0.91	0.08	38,38,38,38	0
55	MG	DB	3028	1/1	0.91	0.06	42,42,42,42	0
55	MG	BB	3063	1/1	0.91	0.46	95,95,95,95	0
55	MG	CA	1623	1/1	0.91	0.16	136,136,136,136	0
55	MG	CA	1624	1/1	0.91	0.07	103,103,103,103	0
55	MG	BJ	201	1/1	0.91	0.47	160,160,160,160	0
55	MG	BB	3101	1/1	0.91	0.10	50,50,50,50	0
55	MG	BB	3029	1/1	0.91	0.09	81,81,81,81	0
55	MG	AA	1601	1/1	0.91	0.04	62,62,62,62	0
55	MG	BB	3031	1/1	0.91	0.28	83,83,83,83	0
55	MG	CA	1611	1/1	0.91	0.11	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	1603	1/1	0.91	0.10	55,55,55,55	0
55	MG	BB	3094	1/1	0.91	0.17	81,81,81,81	0
55	MG	BB	3077	1/1	0.92	0.17	50,50,50,50	0
55	MG	BB	3032	1/1	0.92	0.07	53,53,53,53	0
55	MG	AA	1646	1/1	0.92	0.39	74,74,74,74	0
55	MG	DB	3023	1/1	0.92	0.12	46,46,46,46	0
55	MG	CA	1645	1/1	0.92	0.12	119,119,119,119	0
55	MG	DB	3071	1/1	0.92	0.08	30,30,30,30	0
55	MG	DB	3088	1/1	0.92	0.16	83,83,83,83	0
55	MG	BB	3045	1/1	0.92	0.10	60,60,60,60	0
55	MG	AA	1616	1/1	0.92	0.18	104,104,104,104	0
55	MG	DB	3104	1/1	0.92	0.09	50,50,50,50	0
55	MG	BB	3082	1/1	0.92	0.16	80,80,80,80	0
55	MG	DB	3050	1/1	0.92	0.07	51,51,51,51	0
55	MG	BB	3054	1/1	0.92	0.13	56,56,56,56	0
55	MG	BB	3056	1/1	0.92	0.07	49,49,49,49	0
55	MG	DB	3061	1/1	0.92	0.14	97,97,97,97	0
55	MG	CA	1633	1/1	0.92	0.09	136,136,136,136	0
55	MG	AX	101	1/1	0.92	1.02	84,84,84,84	0
55	MG	AA	1602	1/1	0.93	0.28	83,83,83,83	0
55	MG	AA	1629	1/1	0.93	0.08	53,53,53,53	0
55	MG	BB	3034	1/1	0.93	0.22	70,70,70,70	0
55	MG	BB	3016	1/1	0.93	1.04	91,91,91,91	0
55	MG	BB	3040	1/1	0.93	0.12	64,64,64,64	0
55	MG	BB	3008	1/1	0.93	0.10	63,63,63,63	0
55	MG	BB	3060	1/1	0.93	0.17	33,33,33,33	0
55	MG	DB	3062	1/1	0.93	0.11	54,54,54,54	0
55	MG	BB	3009	1/1	0.93	0.06	92,92,92,92	0
55	MG	DB	3053	1/1	0.93	0.07	37,37,37,37	0
55	MG	BB	3117	1/1	0.93	0.18	82,82,82,82	0
55	MG	BB	3078	1/1	0.93	0.11	71,71,71,71	0
55	MG	BB	3084	1/1	0.93	0.09	61,61,61,61	0
55	MG	AA	1645	1/1	0.93	0.19	127,127,127,127	0
55	MG	AA	1649	1/1	0.93	0.12	84,84,84,84	0
55	MG	DB	3060	1/1	0.93	0.07	35,35,35,35	0
55	MG	BB	3099	1/1	0.93	0.23	41,41,41,41	0
55	MG	DB	3075	1/1	0.93	0.07	46,46,46,46	0
55	MG	AA	1659	1/1	0.93	0.19	86,86,86,86	0
55	MG	BB	3092	1/1	0.93	0.14	62,62,62,62	0
55	MG	BB	3088	1/1	0.93	0.08	76,76,76,76	0
55	MG	AA	1604	1/1	0.93	0.07	45,45,45,45	0
55	MG	DB	3063	1/1	0.93	0.10	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BB	3036	1/1	0.93	0.08	52,52,52,52	0
55	MG	DB	3036	1/1	0.93	0.09	36,36,36,36	0
55	MG	AA	1622	1/1	0.94	0.28	87,87,87,87	0
55	MG	BB	3064	1/1	0.94	0.08	63,63,63,63	0
55	MG	AA	1631	1/1	0.94	0.10	91,91,91,91	0
55	MG	DB	3089	1/1	0.94	0.17	51,51,51,51	0
55	MG	DB	3004	1/1	0.94	0.07	21,21,21,21	0
55	MG	DB	3046	1/1	0.94	0.09	47,47,47,47	0
55	MG	BB	3044	1/1	0.94	0.13	62,62,62,62	0
55	MG	DB	3057	1/1	0.94	0.16	63,63,63,63	0
55	MG	BB	3102	1/1	0.94	0.14	71,71,71,71	0
55	MG	DB	3002	1/1	0.94	0.09	44,44,44,44	0
55	MG	AA	1607	1/1	0.94	0.09	93,93,93,93	0
55	MG	DB	3048	1/1	0.94	0.07	45,45,45,45	0
55	MG	DB	3108	1/1	0.94	0.08	36,36,36,36	0
55	MG	BB	3024	1/1	0.94	0.14	47,47,47,47	0
55	MG	DB	3072	1/1	0.94	0.15	39,39,39,39	0
55	MG	AA	1651	1/1	0.94	0.13	83,83,83,83	0
55	MG	DB	3101	1/1	0.94	0.08	44,44,44,44	0
55	MG	DB	3114	1/1	0.94	0.27	43,43,43,43	0
55	MG	BB	3041	1/1	0.94	0.15	28,28,28,28	0
55	MG	BB	3038	1/1	0.94	0.08	125,125,125,125	0
55	MG	CA	1612	1/1	0.94	0.16	95,95,95,95	0
55	MG	BB	3030	1/1	0.94	0.08	111,111,111,111	0
55	MG	DB	3112	1/1	0.94	0.14	52,52,52,52	0
55	MG	BB	3069	1/1	0.94	0.14	28,28,28,28	0
55	MG	DB	3007	1/1	0.94	0.08	49,49,49,49	0
55	MG	BB	3015	1/1	0.94	0.10	69,69,69,69	0
55	MG	DB	3096	1/1	0.94	0.09	46,46,46,46	0
55	MG	CA	1648	1/1	0.94	0.10	119,119,119,119	0
55	MG	AA	1634	1/1	0.94	0.14	55,55,55,55	0
55	MG	DB	3100	1/1	0.95	0.09	10,10,10,10	0
55	MG	DB	3116	1/1	0.95	0.04	54,54,54,54	0
55	MG	DB	3093	1/1	0.95	0.12	54,54,54,54	0
55	MG	DB	3090	1/1	0.95	0.12	62,62,62,62	0
55	MG	DB	3039	1/1	0.95	0.08	95,95,95,95	0
55	MG	DB	3054	1/1	0.95	0.22	53,53,53,53	0
55	MG	DB	3043	1/1	0.95	0.20	49,49,49,49	0
55	MG	AA	1650	1/1	0.95	0.09	92,92,92,92	0
55	MG	BB	3110	1/1	0.95	0.15	56,56,56,56	0
55	MG	BB	3106	1/1	0.95	0.24	53,53,53,53	0
55	MG	BB	3013	1/1	0.95	0.05	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BB	3017	1/1	0.95	0.04	35,35,35,35	0
55	MG	BB	3012	1/1	0.95	0.10	32,32,32,32	0
55	MG	BB	3095	1/1	0.95	0.17	48,48,48,48	0
55	MG	BB	3005	1/1	0.95	0.16	52,52,52,52	0
55	MG	BB	3058	1/1	0.95	0.09	62,62,62,62	0
55	MG	DB	3077	1/1	0.95	0.15	57,57,57,57	0
55	MG	BB	3007	1/1	0.95	0.15	115,115,115,115	0
55	MG	DB	3040	1/1	0.95	0.05	41,41,41,41	0
55	MG	DB	3117	1/1	0.95	0.06	26,26,26,26	0
55	MG	DB	3018	1/1	0.95	0.15	32,32,32,32	0
55	MG	BB	3037	1/1	0.95	0.09	56,56,56,56	0
55	MG	DB	3110	1/1	0.95	0.09	41,41,41,41	0
55	MG	AA	1627	1/1	0.95	0.40	91,91,91,91	0
55	MG	DB	3111	1/1	0.95	0.08	38,38,38,38	0
55	MG	DB	3020	1/1	0.95	0.08	25,25,25,25	0
55	MG	BB	3001	1/1	0.95	0.10	57,57,57,57	0
55	MG	DB	3055	1/1	0.95	0.05	30,30,30,30	0
55	MG	CA	1601	1/1	0.95	0.09	48,48,48,48	0
55	MG	BB	3080	1/1	0.96	0.20	65,65,65,65	0
55	MG	BB	3061	1/1	0.96	0.12	57,57,57,57	0
55	MG	CA	1626	1/1	0.96	0.07	154,154,154,154	0
55	MG	DB	3105	1/1	0.96	0.06	18,18,18,18	0
55	MG	BB	3023	1/1	0.96	0.06	15,15,15,15	0
55	MG	BB	3066	1/1	0.96	0.16	51,51,51,51	0
55	MG	BB	3104	1/1	0.96	0.08	38,38,38,38	0
55	MG	DB	3010	1/1	0.96	0.09	20,20,20,20	0
55	MG	BB	3053	1/1	0.96	0.05	43,43,43,43	0
55	MG	CA	1602	1/1	0.96	0.12	87,87,87,87	0
55	MG	AA	1636	1/1	0.96	0.07	61,61,61,61	0
55	MG	BB	3022	1/1	0.96	0.16	56,56,56,56	0
55	MG	CA	1619	1/1	0.96	0.07	79,79,79,79	0
55	MG	BB	3049	1/1	0.96	0.09	40,40,40,40	0
55	MG	DB	3017	1/1	0.96	0.10	34,34,34,34	0
55	MG	BB	3067	1/1	0.96	0.09	39,39,39,39	0
55	MG	DB	3083	1/1	0.96	0.12	31,31,31,31	0
55	MG	AA	1609	1/1	0.96	0.07	67,67,67,67	0
55	MG	DB	3051	1/1	0.96	0.09	48,48,48,48	0
55	MG	BB	3091	1/1	0.96	0.19	44,44,44,44	0
56	ZN	B4	101	1/1	0.96	0.04	72,72,72,72	0
55	MG	BB	3018	1/1	0.96	0.07	42,42,42,42	0
55	MG	CA	1630	1/1	0.96	0.08	97,97,97,97	0
55	MG	DB	3095	1/1	0.96	0.11	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DB	3076	1/1	0.96	0.07	49,49,49,49	0
55	MG	DB	3092	1/1	0.96	0.16	44,44,44,44	0
55	MG	DB	3025	1/1	0.96	0.10	40,40,40,40	0
55	MG	BB	3020	1/1	0.96	0.22	45,45,45,45	0
55	MG	DB	3056	1/1	0.96	0.13	28,28,28,28	0
55	MG	DB	3012	1/1	0.96	0.18	37,37,37,37	0
55	MG	DB	3099	1/1	0.97	0.06	19,19,19,19	0
55	MG	DB	3078	1/1	0.97	0.05	28,28,28,28	0
55	MG	DB	3106	1/1	0.97	0.06	29,29,29,29	0
55	MG	DB	3118	1/1	0.97	0.06	35,35,35,35	0
55	MG	AX	102	1/1	0.97	0.41	66,66,66,66	0
55	MG	BB	3025	1/1	0.97	0.11	63,63,63,63	0
55	MG	BB	3027	1/1	0.97	0.44	40,40,40,40	0
55	MG	DB	3080	1/1	0.97	0.12	29,29,29,29	0
55	MG	DB	3074	1/1	0.97	0.08	9,9,9,9	0
55	MG	AA	1610	1/1	0.97	0.05	61,61,61,61	0
55	MG	DB	3011	1/1	0.97	0.05	16,16,16,16	0
55	MG	CA	1651	1/1	0.97	0.16	66,66,66,66	0
55	MG	DB	3006	1/1	0.97	0.15	38,38,38,38	0
55	MG	DB	3109	1/1	0.97	0.26	28,28,28,28	0
55	MG	DB	3098	1/1	0.97	0.09	42,42,42,42	0
55	MG	BB	3065	1/1	0.97	0.06	46,46,46,46	0
55	MG	DB	3022	1/1	0.97	0.09	42,42,42,42	0
55	MG	DB	3015	1/1	0.97	0.10	49,49,49,49	0
55	MG	DB	3038	1/1	0.97	0.11	19,19,19,19	0
55	MG	BB	3111	1/1	0.97	0.09	43,43,43,43	0
55	MG	DB	3003	1/1	0.97	0.06	24,24,24,24	0
55	MG	CA	1638	1/1	0.97	0.57	102,102,102,102	0
56	ZN	D4	401	1/1	0.97	0.17	72,72,72,72	0
55	MG	BB	3113	1/1	0.97	0.19	41,41,41,41	0
55	MG	AA	1654	1/1	0.97	0.05	49,49,49,49	0
55	MG	DB	3001	1/1	0.97	0.06	14,14,14,14	0
55	MG	BB	3086	1/1	0.97	0.11	50,50,50,50	0
55	MG	DB	3021	1/1	0.97	0.09	50,50,50,50	0
55	MG	BB	3072	1/1	0.98	0.11	58,58,58,58	0
55	MG	BB	3003	1/1	0.98	0.10	20,20,20,20	0
55	MG	DB	3014	1/1	0.98	0.05	32,32,32,32	0
55	MG	DB	3042	1/1	0.98	0.06	56,56,56,56	0
55	MG	BB	3043	1/1	0.98	0.14	107,107,107,107	0
55	MG	DB	3031	1/1	0.98	0.05	16,16,16,16	0
55	MG	DB	3085	1/1	0.98	0.09	21,21,21,21	0
55	MG	BB	3075	1/1	0.98	0.10	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DB	3019	1/1	0.98	0.08	43,43,43,43	0
55	MG	DB	3113	1/1	0.98	0.17	27,27,27,27	0
55	MG	BB	3055	1/1	0.98	0.09	72,72,72,72	0
55	MG	BB	3026	1/1	0.98	0.09	26,26,26,26	0
55	MG	CA	1616	1/1	0.98	0.08	80,80,80,80	0
55	MG	DB	3069	1/1	0.98	0.24	48,48,48,48	0
55	MG	BB	3052	1/1	0.98	0.07	33,33,33,33	0
55	MG	DB	3084	1/1	0.98	0.12	26,26,26,26	0
55	MG	BB	3105	1/1	0.98	0.13	64,64,64,64	0
55	MG	BB	3103	1/1	0.98	0.10	38,38,38,38	0
55	MG	DB	3094	1/1	0.98	0.21	77,77,77,77	0
55	MG	DB	3103	1/1	0.98	0.05	46,46,46,46	0
55	MG	BB	3098	1/1	0.98	0.11	73,73,73,73	0
55	MG	DB	3073	1/1	0.98	0.12	7,7,7,7	0
55	MG	DB	3035	1/1	0.98	0.18	27,27,27,27	0
55	MG	BB	3002	1/1	0.98	0.16	31,31,31,31	0
55	MG	BB	3035	1/1	0.98	0.14	40,40,40,40	0
55	MG	DB	3016	1/1	0.98	0.07	43,43,43,43	0
55	MG	BB	3021	1/1	0.98	0.13	45,45,45,45	0
55	MG	BB	3004	1/1	0.98	0.09	65,65,65,65	0
55	MG	BB	3109	1/1	0.98	0.13	52,52,52,52	0
55	MG	DB	3049	1/1	0.98	0.10	42,42,42,42	0
55	MG	BB	3006	1/1	0.98	0.11	35,35,35,35	0
55	MG	BB	3062	1/1	0.98	0.06	42,42,42,42	0
55	MG	DB	3081	1/1	0.98	0.07	36,36,36,36	0
55	MG	DB	3079	1/1	0.98	0.08	18,18,18,18	0
55	MG	AA	1620	1/1	0.98	0.10	74,74,74,74	0
55	MG	BB	3114	1/1	0.98	0.21	57,57,57,57	0
55	MG	DB	3097	1/1	0.98	0.11	39,39,39,39	0
55	MG	DB	3009	1/1	0.99	0.05	48,48,48,48	0
55	MG	DB	3008	1/1	0.99	0.11	55,55,55,55	0
55	MG	DB	3086	1/1	0.99	0.13	57,57,57,57	0
55	MG	BB	3089	1/1	0.99	0.06	51,51,51,51	0
55	MG	BB	3116	1/1	0.99	0.08	24,24,24,24	0
55	MG	DB	3102	1/1	0.99	0.09	67,67,67,67	0
55	MG	BB	3085	1/1	0.99	0.05	57,57,57,57	0
55	MG	BB	3071	1/1	0.99	0.10	41,41,41,41	0
55	MG	DB	3066	1/1	0.99	0.11	30,30,30,30	0
55	MG	BB	3079	1/1	0.99	0.14	46,46,46,46	0



## 6.5 Other polymers [i](#)

There are no such residues in this entry.