



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:40 PM GMT

PDB ID : 4V5B  
Title : Structure of PDF binding helix in complex with the ribosome  
Authors : Bingel-Erlenmeyer, R.; Kohler, R.; Kramer, G.; Sandikci, A.; Antolic, S.;  
Maier, T.; Schaffitzel, C.; Wiedmann, B.; Bukau, B.; Ban, N.  
Deposited on : 2007-11-22  
Resolution : 3.74 Å(reported)

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

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

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

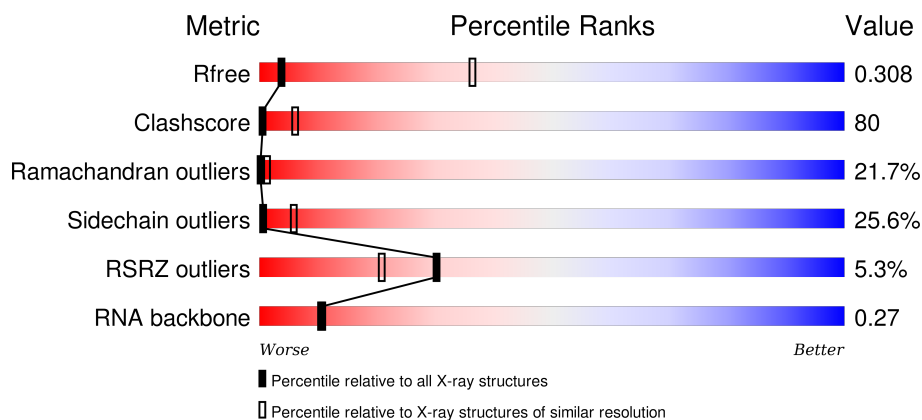
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.74 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1154 (3.98-3.50)
Clashscore	102246	1279 (3.98-3.50)
Ramachandran outliers	100387	1226 (3.98-3.50)
Sidechain outliers	100360	1224 (3.98-3.50)
RSRZ outliers	91569	1161 (3.98-3.50)
RNA backbone	2183	1068 (4.68-2.80)

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

Mol	Chain	Length	Quality of chain
1	A0	56	<div> <div>9%</div> <div>16%</div> <div>43%</div> <div>38%</div> <div>.</div> </div>
1	C0	56	<div> <div>9%</div> <div>13%</div> <div>41%</div> <div>46%</div> </div>
2	A1	54	<div> <div>17%</div> <div>15%</div> <div>48%</div> <div>33%</div> <div>.</div> </div>
2	C1	54	<div> <div>20%</div> <div>11%</div> <div>44%</div> <div>39%</div> <div>6%</div> </div>

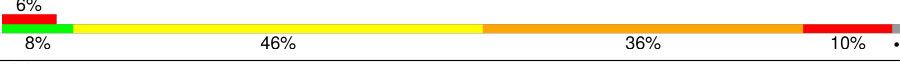
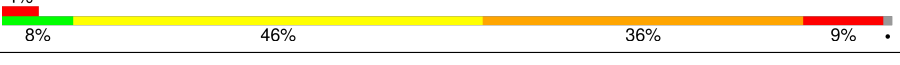
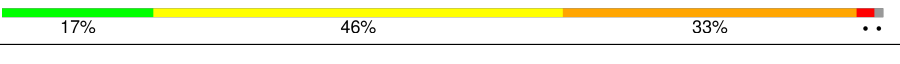
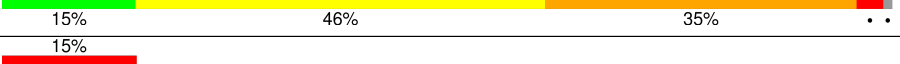


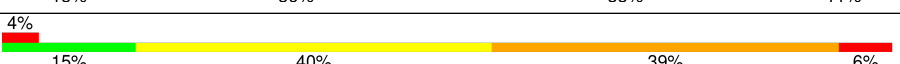
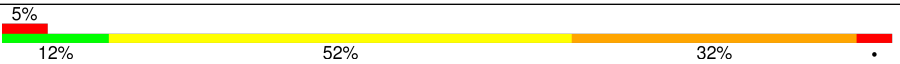

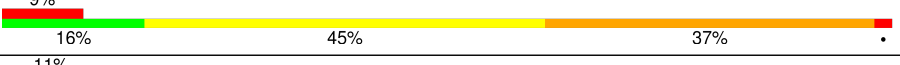
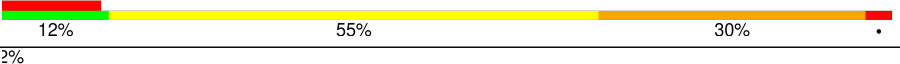
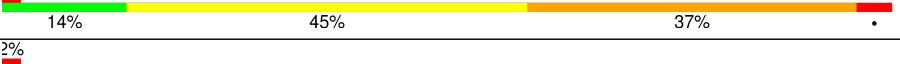

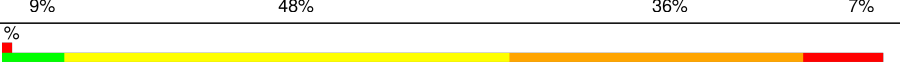
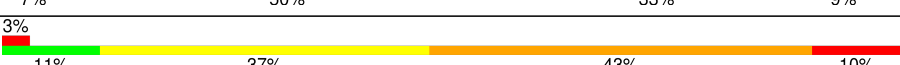
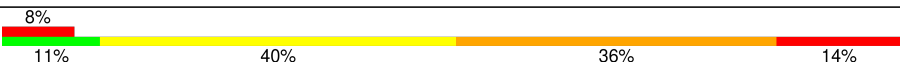

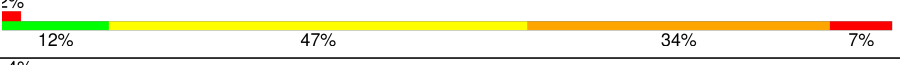
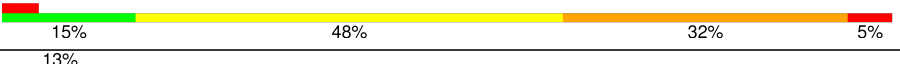


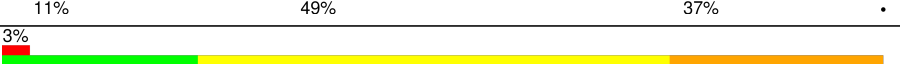
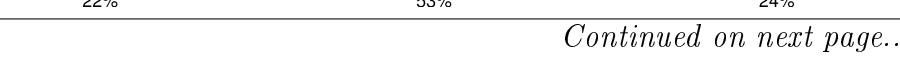


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Mol	Chain	Length	Quality of chain
3	A2	46	
3	C2	46	
4	A3	64	
4	C3	64	
5	A4	38	
5	C4	38	
6	A5	16	
7	AA	120	
7	CA	120	
8	AB	2904	
8	CB	2904	
9	AC	273	
9	CC	273	
10	AD	209	
10	CD	209	
11	AE	201	
11	CE	201	
12	AF	178	
12	CF	178	
13	AG	176	
13	CG	176	
14	AH	149	
14	CH	149	
15	AI	141	
15	CI	141	

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Mol	Chain	Length	Quality of chain
16	AJ	142	
16	CJ	142	
17	AK	123	
17	CK	123	
18	AL	144	
18	CL	144	
19	AM	136	
19	CM	136	
20	AN	127	
20	CN	127	
21	AO	117	
21	CO	117	
22	AP	114	
22	CP	114	
23	AQ	117	
23	CQ	117	
24	AR	103	
24	CR	103	
25	AS	110	
25	CS	110	
26	AT	100	
26	CT	100	
27	AU	103	
27	CU	103	
28	AV	94	

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Mol	Chain	Length	Quality of chain
28	CV	94	
29	AW	84	
29	CW	84	
30	AX	63	
30	CX	63	
31	AY	58	
31	CY	58	
32	AZ	70	
32	CZ	70	
33	BA	1542	
33	DA	1542	
34	BB	240	
34	DB	240	
35	BC	232	
35	DC	232	
36	BD	205	
36	DD	205	
37	BE	166	
37	DE	166	
38	BF	135	
38	DF	135	
39	BG	178	
39	DG	178	
40	BH	129	
40	DH	129	

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Mol	Chain	Length	Quality of chain
41	BI	129	
41	DI	129	
42	BJ	103	
42	DJ	103	
43	BK	128	
43	DK	128	
44	BL	123	
44	DL	123	
45	BM	117	
45	DM	117	
46	BN	100	
46	DN	100	
47	BO	89	
47	DO	89	
48	BP	82	
48	DP	82	
49	BQ	83	
49	DQ	83	
50	BR	74	
50	DR	74	
51	BS	91	
51	DS	91	
52	BT	86	
52	DT	86	
53	BU	71	

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Mol	Chain	Length	Quality of chain
53	DU	71	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	AB	4050	-	-	-	X
54	MG	AB	4057	-	-	-	X
54	MG	AB	4061	-	-	-	X
54	MG	AB	4082	-	-	-	X
54	MG	AB	4085	-	-	-	X
54	MG	AB	4091	-	-	-	X
54	MG	BA	4001	-	-	-	X
54	MG	BA	4002	-	-	-	X
54	MG	BA	4017	-	-	-	X
54	MG	BA	4027	-	-	-	X
54	MG	CB	3028	-	-	-	X
54	MG	CB	3041	-	-	-	X
54	MG	CB	3044	-	-	-	X
54	MG	CB	3070	-	-	-	X
54	MG	CB	3077	-	-	-	X
54	MG	CB	3080	-	-	-	X
54	MG	DA	1644	-	-	-	X

## 2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 284264 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			
1	C0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			

- Molecule 2 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	A1	54	Total	C	N	O	0	0	0
			441	284	81	76			
2	C1	54	Total	C	N	O	0	0	0
			441	284	81	76			

- Molecule 3 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			
3	C2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

- Molecule 4 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			
4	C3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

- Molecule 5 is a protein called 50S RIBOSOMAL PROTEIN L36.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	A4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			
5	C4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

- Molecule 6 is a protein called C-TERM HELIX PDF.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	A5	16	Total	C	N	O	0	0	0
			134	84	28	22			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A5	146	ALA	LEU	ENGINEERED MUTATION	UNP P0A6K3

- Molecule 7 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AA	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			
7	CA	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			

- Molecule 8 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AB	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			
8	CB	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			

- Molecule 9 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AC	268	Total	C	N	O	S	0	0	1
			2054	1271	417	359	7			
9	CC	268	Total	C	N	O	S	0	0	1
			2054	1271	417	359	7			

- Molecule 10 is a protein called 50S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			
10	CD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			
11	CE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			

- Molecule 12 is a protein called 50S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AF	178	Total	C	N	O	S	0	0	0
			1420	905	251	258	6			
12	CF	178	Total	C	N	O	S	0	0	0
			1420	905	251	258	6			

- Molecule 13 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			
13	CG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			

- Molecule 14 is a protein called 50S RIBOSOMAL PROTEIN L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AH	149	Total	C	N	O	S	0	0	0
			1111	699	197	214	1			
14	CH	149	Total	C	N	O	S	0	0	0
			1111	699	197	214	1			

- Molecule 15 is a protein called 50S RIBOSOMAL PROTEIN L11.

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

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

- Molecule 16 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AJ	141	Total	C	N	O	S	0	0	1
			1113	704	211	194	4			
16	CJ	141	Total	C	N	O	S	0	0	1
			1113	704	211	194	4			

- Molecule 17 is a protein called 50S RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AK	122	Total	C	N	O	S	0	0	1
			931	582	180	164	5			
17	CK	122	Total	C	N	O	S	0	0	1
			931	582	180	164	5			

- Molecule 18 is a protein called 50S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AL	144	Total	C	N	O	S	0	0	0
			1053	654	207	190	2			
18	CL	144	Total	C	N	O	S	0	0	0
			1053	654	207	190	2			

- Molecule 19 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AM	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			
19	CM	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			

- Molecule 20 is a protein called 50S RIBOSOMAL PROTEIN L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AN	127	Total	C	N	O	S	0	0	0
			1008	621	204	178	5			
20	CN	127	Total	C	N	O	S	0	0	0
			1008	621	204	178	5			

- Molecule 21 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AO	117	Total	C	N	O	S	0	0	0
			900	557	179	163	1			
21	CO	117	Total	C	N	O	S	0	0	0
			900	557	179	163	1			

- Molecule 22 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AP	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			
22	CP	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			

- Molecule 23 is a protein called 50S RIBOSOMAL PROTEIN L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AQ	117	Total	C	N	O		0	0	0
			947	604	192	151				
23	CQ	117	Total	C	N	O		0	0	0
			947	604	192	151				

- Molecule 24 is a protein called 50S RIBOSOMAL PROTEIN L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AR	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			
24	CR	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	AS	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			
25	CS	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	AT	100	Total	C	N	O	S	0	0	1
			778	491	146	139	2			
26	CT	100	Total	C	N	O	S	0	0	1
			778	491	146	139	2			

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	AU	103	Total	C	N	O	S	0	0	1
			780	492	147	141				
27	CU	103	Total	C	N	O	S	0	0	1
			780	492	147	141				

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	AV	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			
28	CV	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	AW	84	Total	C	N	O	S	0	0	0
			634	391	129	113	1			
29	CW	84	Total	C	N	O	S	0	0	0
			634	391	129	113	1			

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	AX	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			
30	CX	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	AY	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	CY	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	AZ	70	Total	C	N	O	S	0	0	0
			549	339	104	100	6			
32	CZ	70	Total	C	N	O	S	0	0	0
			549	339	104	100	6			

- Molecule 33 is a RNA chain called 16S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BA	1530	Total	C	N	O	P	0	0	0
			32831	14642	6024	10635	1530			
33	DA	1530	Total	C	N	O	P	0	0	0
			32831	14642	6024	10635	1530			

- Molecule 34 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BB	219	Total	C	N	O	S	0	0	1
			1705	1081	306	311	7			
34	DB	219	Total	C	N	O	S	0	0	1
			1705	1081	306	311	7			

- Molecule 35 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BC	207	Total	C	N	O	S	0	0	1
			1625	1028	306	288	3			
35	DC	207	Total	C	N	O	S	0	0	1
			1625	1028	306	288	3			

- Molecule 36 is a protein called 30S RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			
36	DD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			

- Molecule 37 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BE	151	Total	C	N	O	S	0	0	1
			1106	687	212	201	6			
37	DE	151	Total	C	N	O	S	0	0	1
			1106	687	212	201	6			

- Molecule 38 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BF	101	Total	C	N	O	S	0	0	1
			818	515	149	148	6			
38	DF	101	Total	C	N	O	S	0	0	1
			818	515	149	148	6			

- Molecule 39 is a protein called 30S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BG	151	Total	C	N	O	S	0	0	1
			1175	730	227	214	4			
39	DG	153	Total	C	N	O	S	0	0	1
			1197	745	231	217	4			

- Molecule 40 is a protein called 30S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			
40	DH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			

- Molecule 41 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			
41	DI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			

- Molecule 42 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BJ	99	Total	C	N	O	S	0	0	1
			787	493	151	142	1			
42	DJ	99	Total	C	N	O	S	0	0	1
			787	493	151	142	1			

- Molecule 43 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			
43	DK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			

- Molecule 44 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			
44	DL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			

- Molecule 45 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BM	115	Total	C	N	O	S	0	0	1
			884	546	179	156	3			
45	DM	114	Total	C	N	O	S	0	0	1
			877	541	178	155	3			

- Molecule 46 is a protein called 30S RIBOSOMAL PROTEIN S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			
46	DN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			

- Molecule 47 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BO	88	Total	C	N	O	S	0	0	0
			716	440	146	129	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	DO	88	Total	C	N	O	S	0	0	0
			716	440	146	129	1			

- Molecule 48 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			
48	DP	81	Total	C	N	O	S	0	0	1
			639	400	127	111	1			

- Molecule 49 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BQ	81	Total	C	N	O	S	0	0	1
			649	411	122	113	3			
49	DQ	81	Total	C	N	O	S	0	0	0
			657	417	122	115	3			

- Molecule 50 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
50	BR	56	Total	C	N	O	0	0	1
			456	288	87	81			
50	DR	56	Total	C	N	O	0	0	1
			456	288	87	81			

- Molecule 51 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BS	80	Total	C	N	O	S	0	0	1
			638	408	121	107	2			
51	DS	81	Total	C	N	O	S	0	0	1
			645	413	122	108	2			

- Molecule 52 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			
52	DT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			

- Molecule 53 is a protein called 30S RIBOSOMAL PROTEIN S21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BU	52	Total	C	N	O	S	0	0	1
			426	265	87	73	1			
53	DU	52	Total	C	N	O	S	0	0	1
			426	265	87	73	1			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	BT	1	Total	Mg	0	0
			1	1		
54	BA	58	Total	Mg	0	0
			58	58		
54	BN	1	Total	Mg	0	0
			1	1		
54	AE	1	Total	Mg	0	0
			1	1		
54	CB	109	Total	Mg	0	0
			109	109		
54	AB	109	Total	Mg	0	0
			109	109		
54	CC	1	Total	Mg	0	0
			1	1		
54	DN	1	Total	Mg	0	0
			1	1		
54	DA	61	Total	Mg	0	0
			61	61		
54	CL	1	Total	Mg	0	0
			1	1		

- Molecule 55 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	A2	2	Total	O	0	0
			2	2		
55	AB	489	Total	O	0	0
			489	489		
55	AC	3	Total	O	0	0
			3	3		
55	AD	1	Total	O	0	0
			1	1		
55	AE	3	Total	O	0	0
			3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	AJ	2	Total O 2 2	0	0
55	AL	3	Total O 3 3	0	0
55	BA	284	Total O 284 284	0	0
55	BE	3	Total O 3 3	0	0
55	BI	2	Total O 2 2	0	0
55	BK	1	Total O 1 1	0	0
55	BL	2	Total O 2 2	0	0
55	BN	3	Total O 3 3	0	0
55	BP	1	Total O 1 1	0	0
55	BT	2	Total O 2 2	0	0
55	C0	1	Total O 1 1	0	0
55	C2	2	Total O 2 2	0	0
55	CB	485	Total O 485 485	0	0
55	CC	3	Total O 3 3	0	0
55	CD	1	Total O 1 1	0	0
55	CE	1	Total O 1 1	0	0
55	CJ	2	Total O 2 2	0	0
55	CK	1	Total O 1 1	0	0
55	CL	5	Total O 5 5	0	0
55	CN	3	Total O 3 3	0	0
55	CP	1	Total O 1 1	0	0

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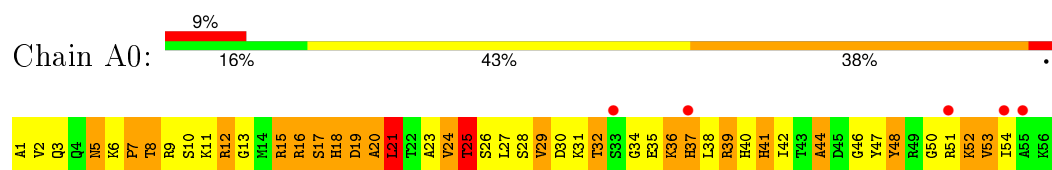
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	CQ	1	Total 1	O 1	0	0
55	CT	2	Total 2	O 2	0	0
55	CU	1	Total 1	O 1	0	0
55	DA	293	Total 293	O 293	0	0
55	DD	1	Total 1	O 1	0	0
55	DE	2	Total 2	O 2	0	0
55	DG	1	Total 1	O 1	0	0
55	DL	4	Total 4	O 4	0	0
55	DN	2	Total 2	O 2	0	0
55	DP	1	Total 1	O 1	0	0
55	DT	3	Total 3	O 3	0	0

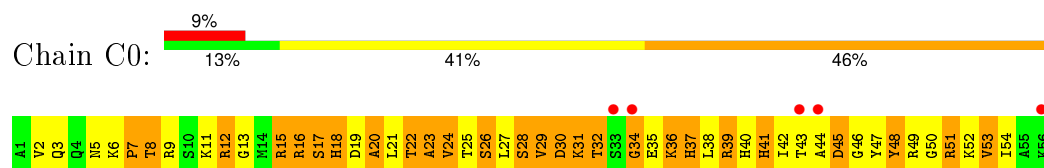
### 3 Residue-property plots [i](#)

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

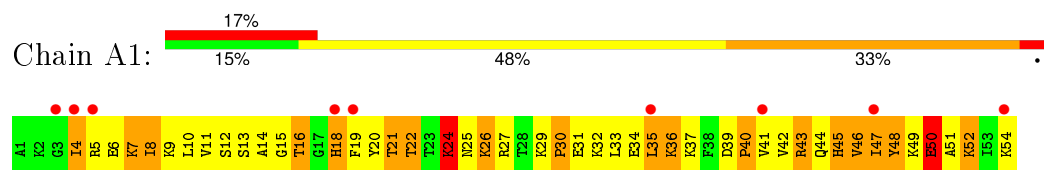
- Molecule 1: 50S RIBOSOMAL PROTEIN L32



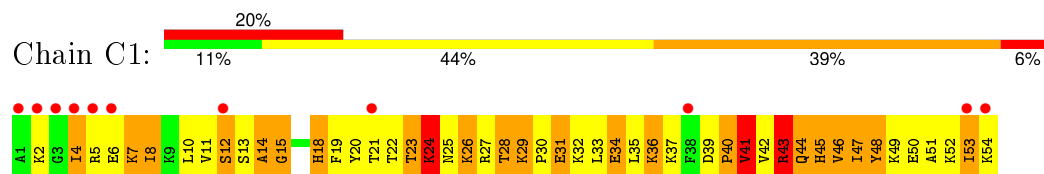
- Molecule 1: 50S RIBOSOMAL PROTEIN L32



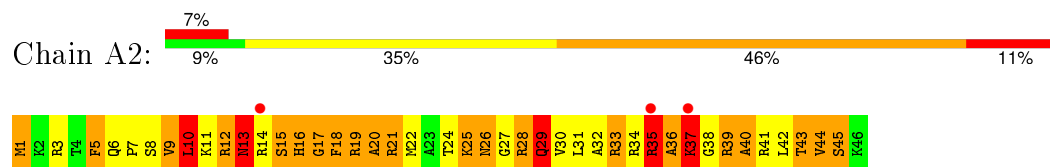
- Molecule 2: 50S RIBOSOMAL PROTEIN L33



- Molecule 2: 50S RIBOSOMAL PROTEIN L33



- Molecule 3: 50S RIBOSOMAL PROTEIN L34

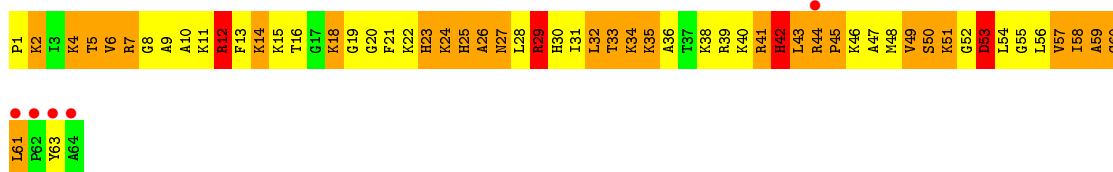


- Molecule 3: 50S RIBOSOMAL PROTEIN L34

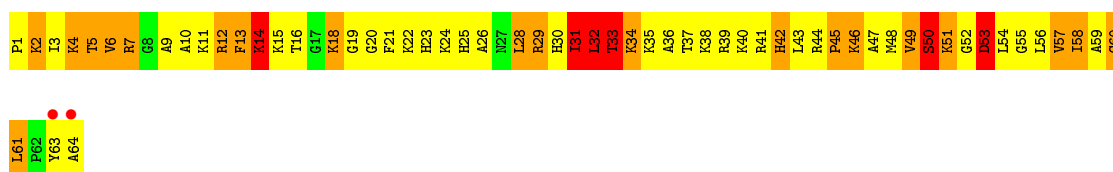




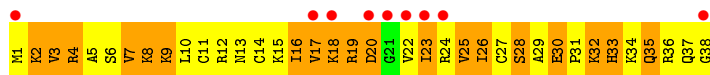
• Molecule 4: 50S RIBOSOMAL PROTEIN L35



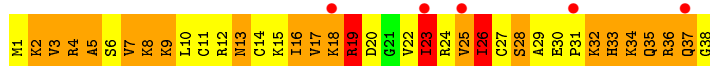
• Molecule 4: 50S RIBOSOMAL PROTEIN L35



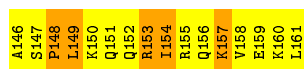
• Molecule 5: 50S RIBOSOMAL PROTEIN L36



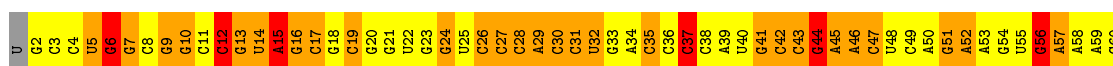
• Molecule 5: 50S RIBOSOMAL PROTEIN L36

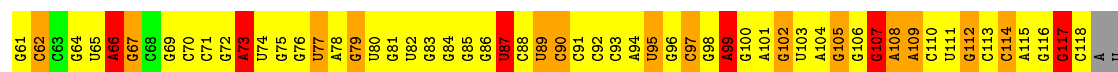


• Molecule 6: C-TERM HELIX PDF

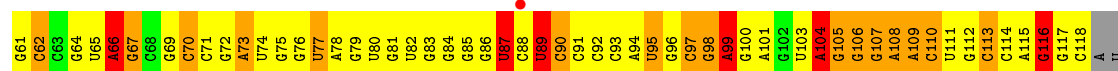
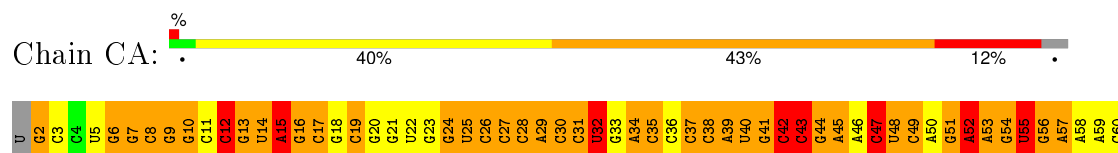


• Molecule 7: 5S RIBOSOMAL RNA

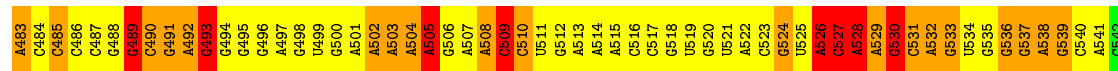
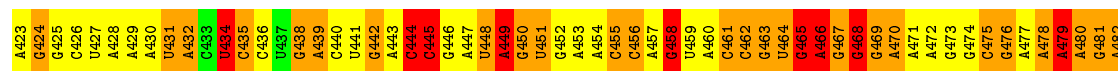
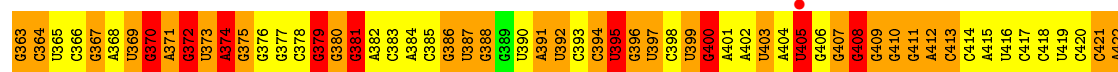
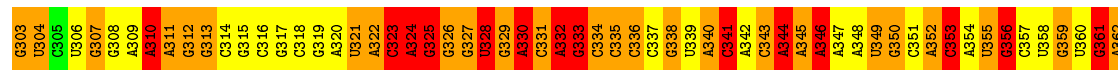
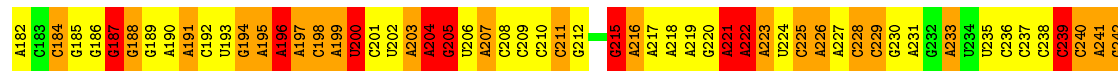
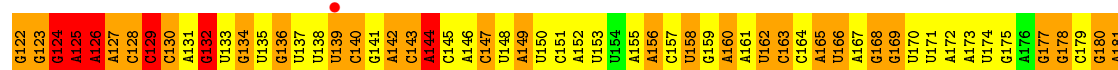
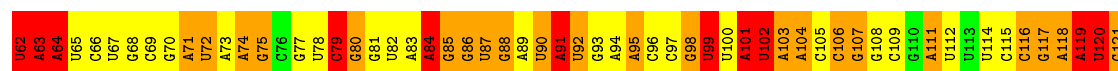




• Molecule 7: 5S RIBOSOMAL RNA



• Molecule 8: 23S RIBOSOMAL RNA



WORLDWIDE  
**PDB**  
PROTEIN DATA BANK

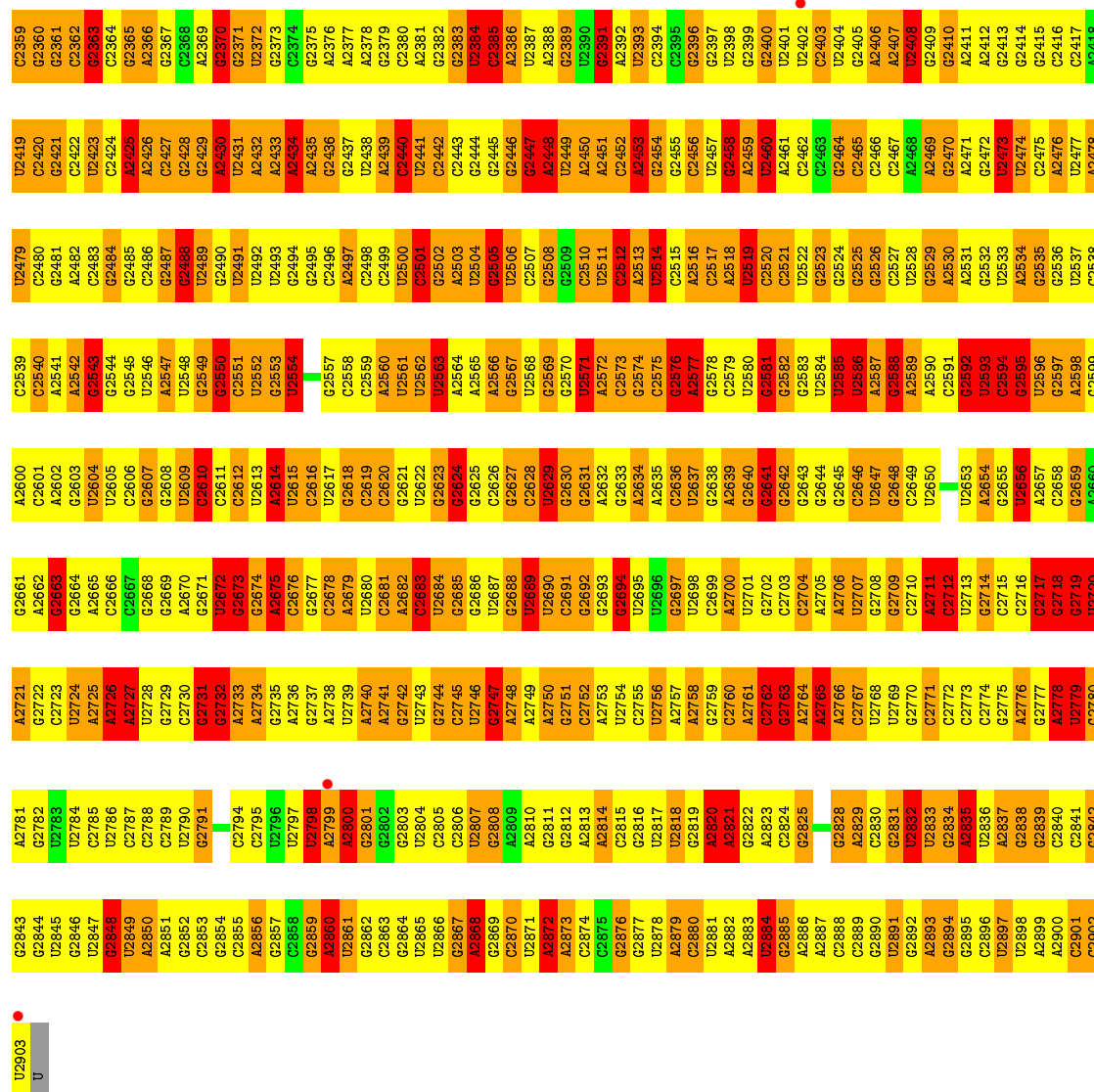


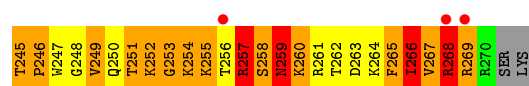
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G2481	G2421	G2361	C2301	A2241	U2181	U	G2061	C2001	C1941	A1819	A1759	A1699	
A2482	C2422	G2362	U2302	G2242	U2182	U	A2062	G2002	C1942	U1820	C1760	A1700	C1639
C2483	C2423	G2363	G2303	U2243	A2183	G	C2063	A2003	U1943	A1821	C1761	A1701	A1640
G2484	C2424	C2364	G2304	U2244	A2184	G	C2064	G2004	U1944	U1822	A1762	G1702	A1641
G2485	A2425	G2365	U2305	U2245	U2185	G	C2065	A2005	G1945	G1823	G1763	G1703	G1642
C2486	A2426	A2366	C2306	G2246	G2186	A	C2066	C2006	U1946	U1824	C1764	C1704	G1643
C2487	C2427	G2367	G2307	A2247	U2187	G	G2067	U2007	C1947	U1825	U1765	A1705	G1644
G2488	G2428	G2368	G2308	C2248	U2188	G	U2068	C2008	G1948	G1826	G1766	G1706	G1645
G2489	G2429	A2369	A2309	U2249	U2189	C	G2069	A2009	G1949	U1827	G1767	G1707	G1646
G2490	G2430	G2370	C2310	G2250	G2190	U	A2070	G2010	G1950	G1828	G1768	G1708	U1647
G2491	A2431	G2371	A2311	A2191	A2071	U	A2071	U2011	U1951	A1829	U1769	U1709	U1648
U2492	A2432	U2372	U2312	U2192	A2072	U	C2072	G2012	A1952	C1830	G1770	G1710	G1649
U2493	A2433	G2373	C2313	G2253	G2193	G2133	C2073	A2013	A1953	G1831	C1771	A1711	A1650
G2494	A2434	C2374	A2314	U2194	U2194	A2134	U2074	A2014	G1954	C1832	U1772	U1712	G1651
G2495	A2435	G2375	G2315	G2255	U2195	A2135	U2075	A2015	U1955	G1833	A1773	A1713	A1652
C2496	G2436	A2376	G2316	G2256	U2196	A2136	U2076	U2016	U1956	U1834	A1774	U1714	G1653
A2497	A2437	A2377	A2317	U2197	U2197	U2137	A2077	U2017	C1957	G1835	U1775	G1715	A1654
C2498	U2438	A2378	G2318	G2258	A2198	G2138	U2078	G2018	C1958	C1836	G1776	U1716	A1655
C2499	A2439	G2379	G2319	U2259	A2199	U2139	U2079	A2019	G1959	C1837	U1777	A1717	C1656
U2500	C2440	C2380	U2320	C2260	G2200	G2140	A2080	A2020	A1960	C1838	U1778	G1718	U1657
C2501	U2441	A2381	U2321	C2261	G2201	G2141	U2081	G2021	C1961	G1839	U1779	G1719	C1658
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A2503	C2443	G2383	G2323	C2263	U2203	C2143	G2083	C2023	U1963	U1841	U1781	G1721	G1660
U2504	G2444	U2384	U2324	G2264	G2204	G2144	C2084	G2024	G1964	G1842	U1782	A1722	G1661
G2505	G2445	C2385	G2325	U2265	A2205	G2145	U2085	C2025	C1965	C1843	A1783	G1723	U1662
U2506	A2446	A2386	C2326	A2266	C2206	C2146	U2086	U2026	A1966	G1844	A1784	G1724	G1663
G2507	G2447	A2387	A2327	A2267	C2207	A2147	G2087	G2027	G1967	G1845	A1785	C1725	A1664
C2508	A2448	G2388	A2328	C2268	C2208	G2148	A2088	U2028	G1968	G1846	A1786	U1726	A1665
G2509	U2449	G2389	U2329	G2269	G2209	U2149	C2089	G2029	A1969	A1847	A1787	C1727	G1666
C2510	A2450	U2390	G2330	A2270	U2210	C2150	A2090	A2030	A1970	A1848	C1788	U1728	G1667
A2511	A2451	G2391	G2331	G2271	A2211	U2151	C2091	A2031	U1971	G1849	A1789	U1729	A1668
C2512	C2452	A2392	U2332	U2272	U2212	C2152	U2092	G2032	G1972	A1850	C1790	G1731	A1669
A2513	A2453	A2393	A2333	A2273	U2213	C2153	G2093	A2033	G1973	U1851	A1791	G1732	C1670
U2514	G2454	C2394	U2334	A2274	C2214	A2154	A2094	C1974	C1974	U1852	G1792	G1733	U1671
G2515	G2455	C2395	A2335	G2275	C2215	U2155	A2095	G2035	G1975	A1853	C1793	G1733	A1672
A2516	C2456	G2396	A2336	G2276	G2216	G2156	C2096	C2036	U1976	A1854	A1794	G1734	G1673
U2517	U2457	G2397	G2337	G2277	G2217	G2157	A2097	A2037	A1977	U1855	C1795	A1735	G1674
A2518	G2458	U2398	C2338	A2278	G2218	A	U2098	U2038	A1978	U1856	U1796	U1736	C1675
U2519	A2459	G2399	G2339	G2279	U2219	G	U2099	U2039	U1979	G1857	G1797	G1737	A1676
C2520	U2460	G2400	A2340	G2280	U2220	C	G2100	G2040	G1980	U1987	U1798	G1738	A1677
U2521	A2461	U2401	G2341	A2281	G2221	C	A2101	U2041	A1981	G1921	G1799	A1739	A1678
U2522	C2462	U2402	C2342	C2282	C2222	G	G2102	A2042	U1982	G1861	C1800	G1740	A1679
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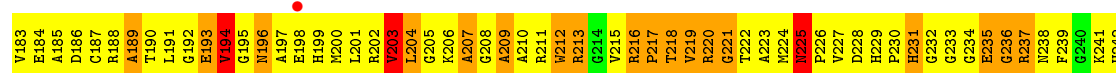
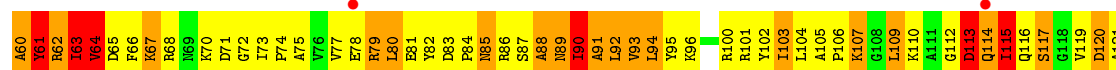
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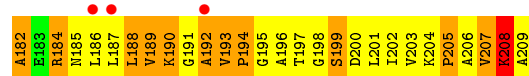
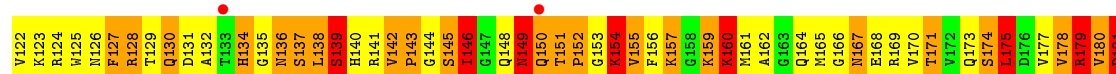
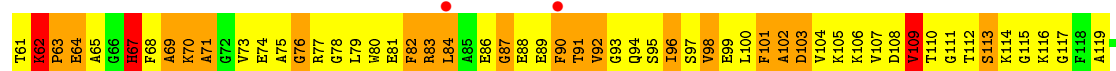




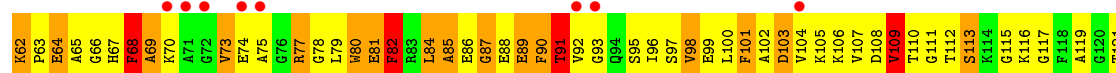
## ● Molecule 9: 50S RIBOSOMAL PROTEIN L2



## ● Molecule 10: 50S RIBOSOMAL PROTEIN L3



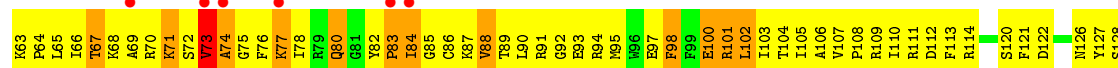
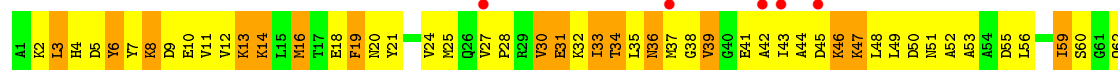
## ● Molecule 10: 50S RIBOSOMAL PROTEIN L3



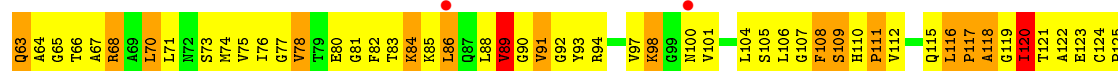
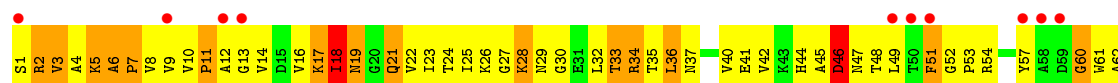
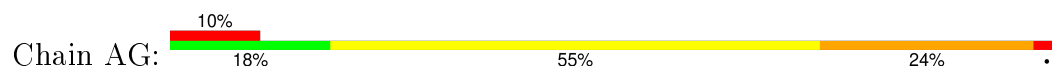




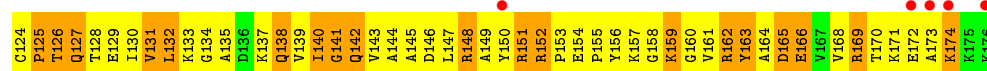
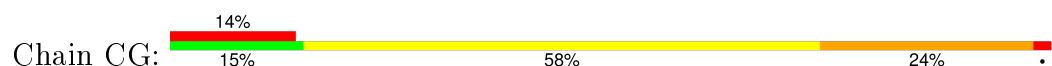
• Molecule 12: 50S RIBOSOMAL PROTEIN L5



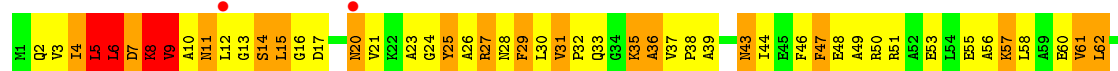
• Molecule 13: 50S RIBOSOMAL PROTEIN L6



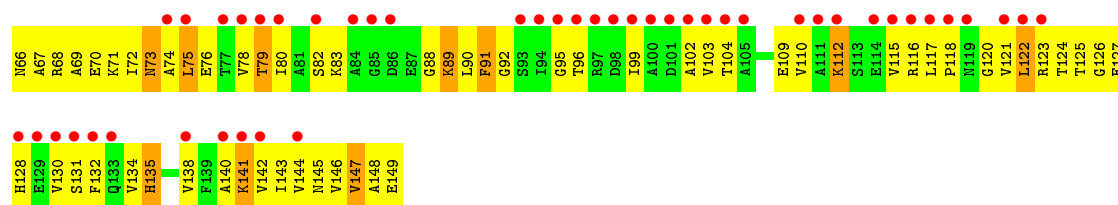
• Molecule 13: 50S RIBOSOMAL PROTEIN L6



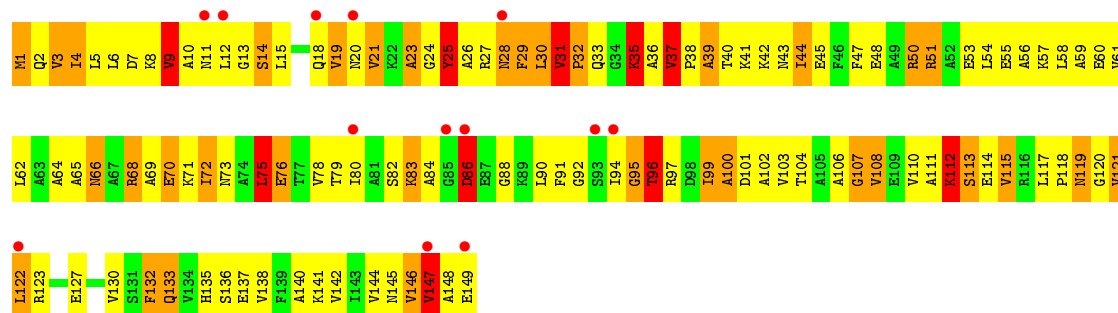
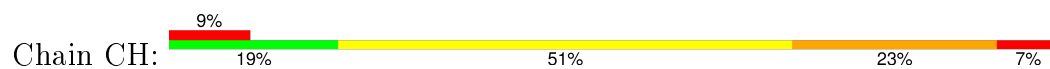
• Molecule 14: 50S RIBOSOMAL PROTEIN L9



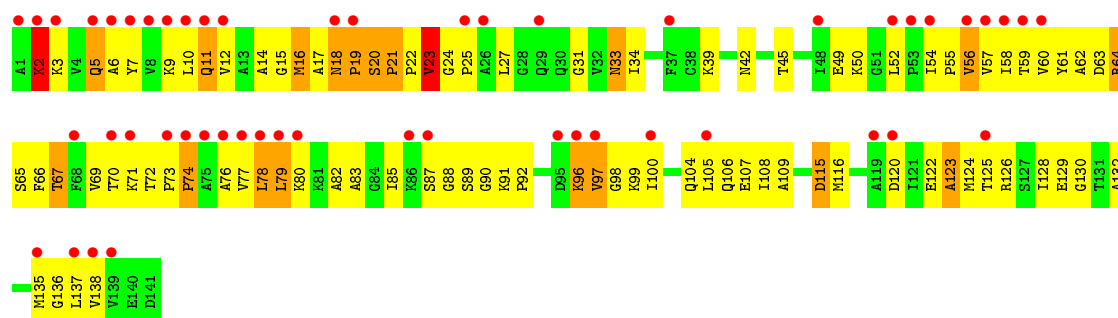




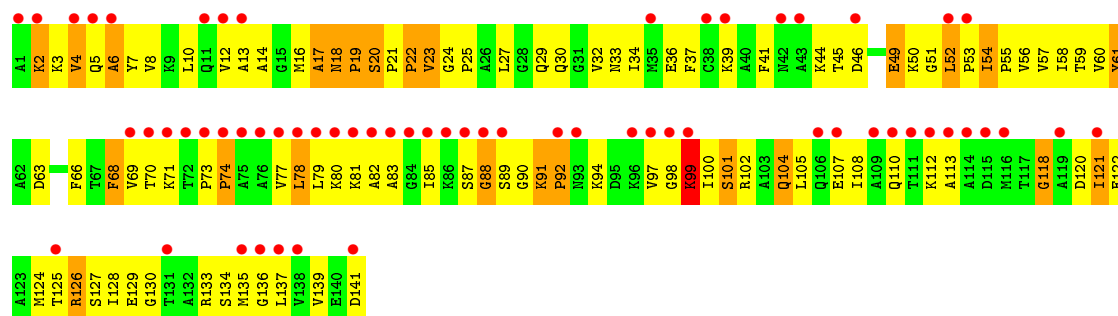
• Molecule 14: 50S RIBOSOMAL PROTEIN L9



• Molecule 15: 50S RIBOSOMAL PROTEIN L11

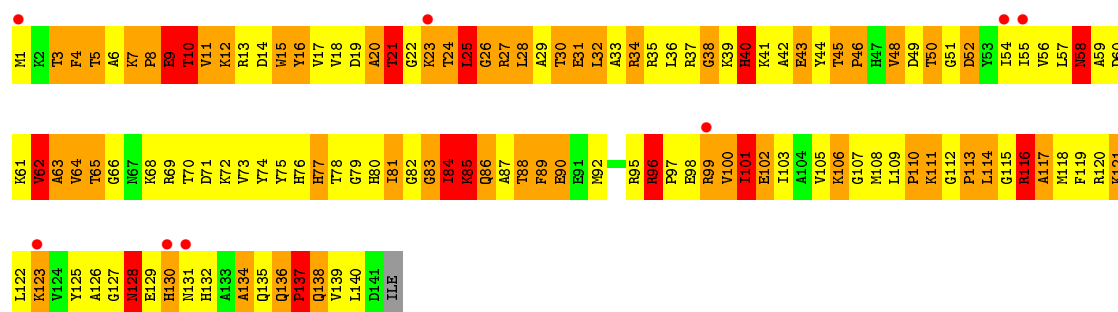


• Molecule 15: 50S RIBOSOMAL PROTEIN L11

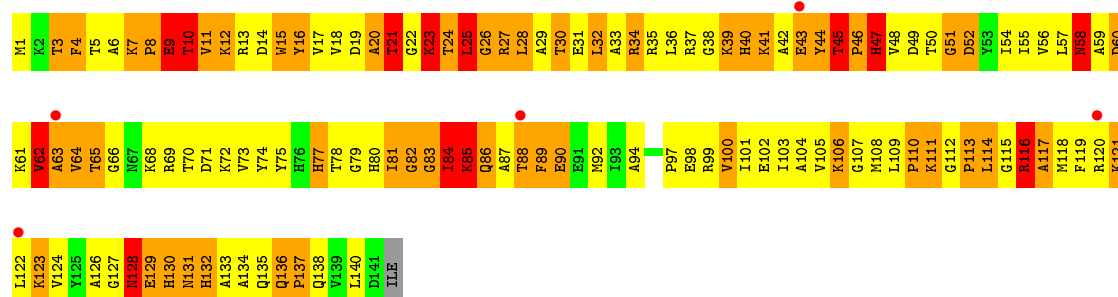


• Molecule 16: 50S RIBOSOMAL PROTEIN L13

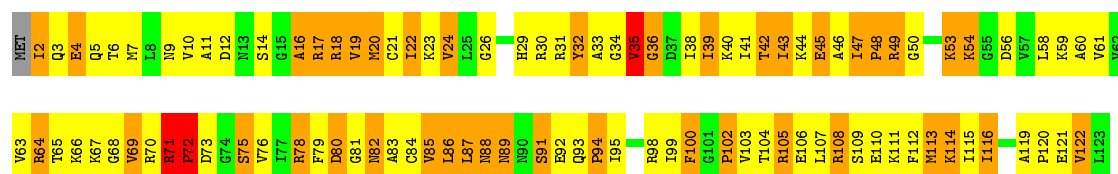
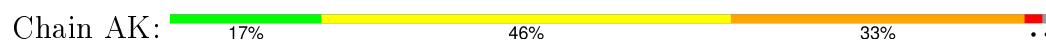




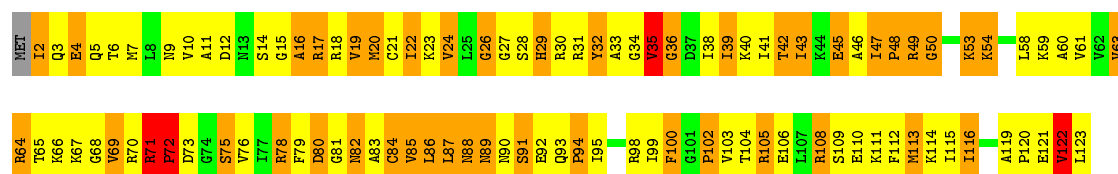
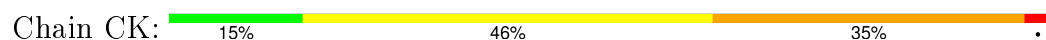
• Molecule 16: 50S RIBOSOMAL PROTEIN L13



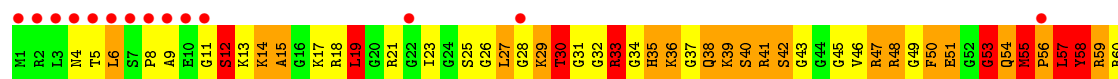
• Molecule 17: 50S RIBOSOMAL PROTEIN L14

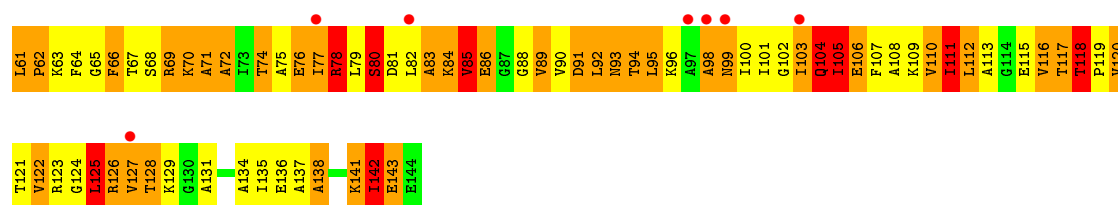


• Molecule 17: 50S RIBOSOMAL PROTEIN L14

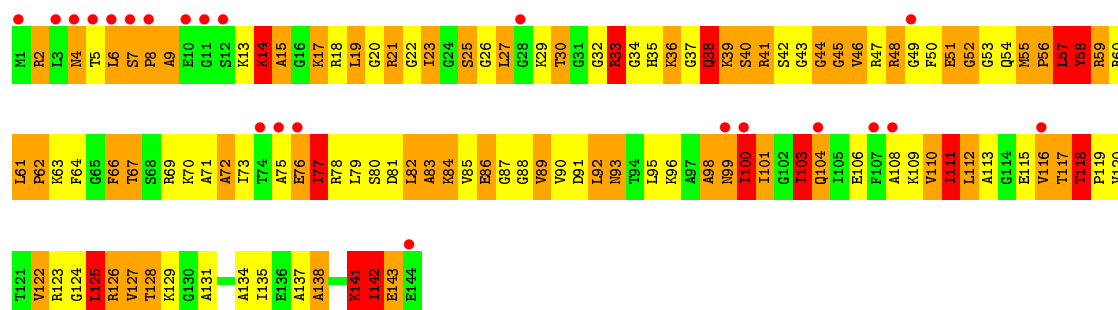
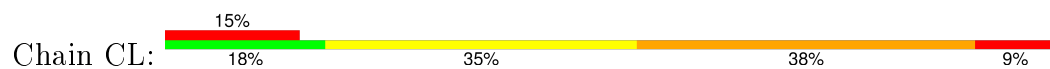


• Molecule 18: 50S RIBOSOMAL PROTEIN L15

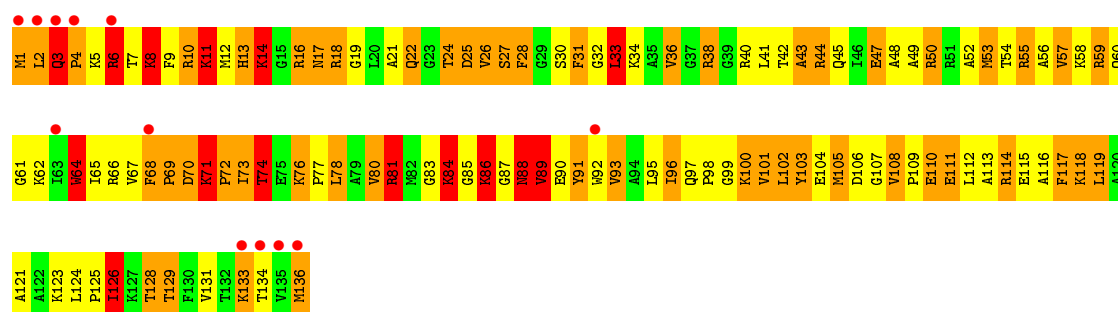




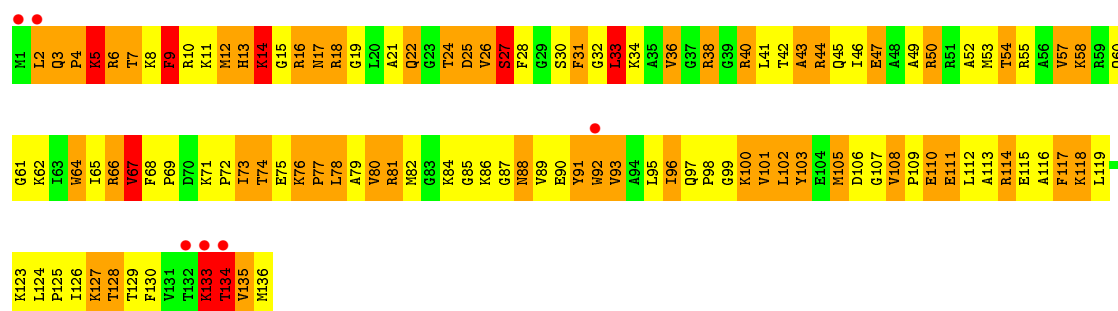
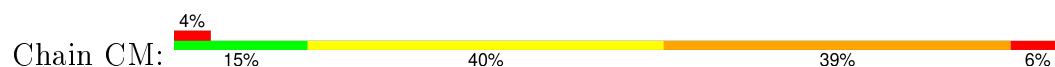
• Molecule 18: 50S RIBOSOMAL PROTEIN L15



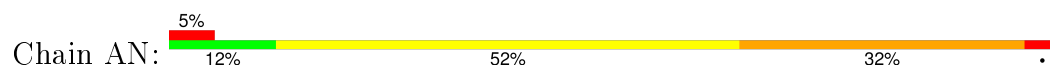
• Molecule 19: 50S RIBOSOMAL PROTEIN L16

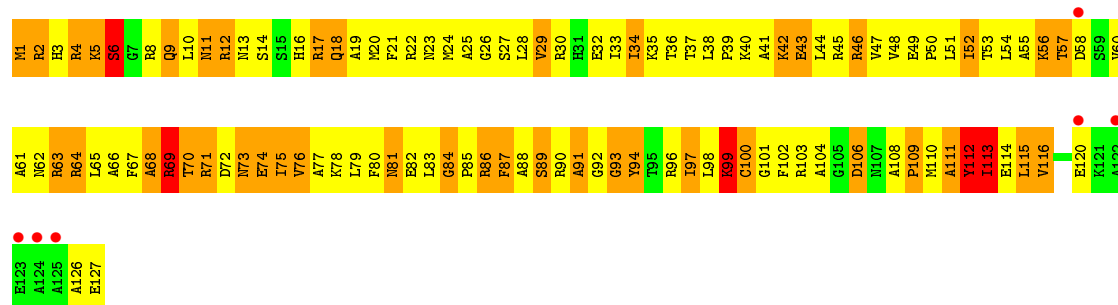


• Molecule 19: 50S RIBOSOMAL PROTEIN L16

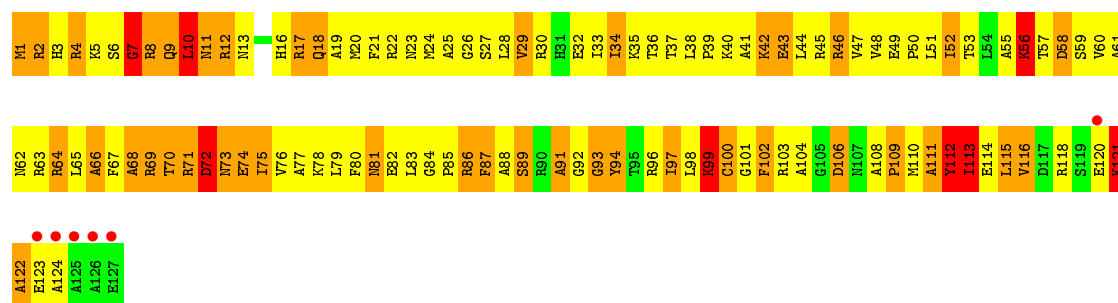
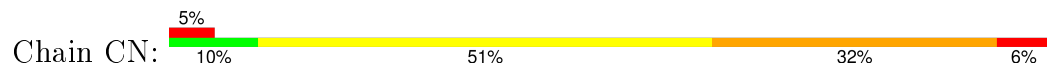


• Molecule 20: 50S RIBOSOMAL PROTEIN L17

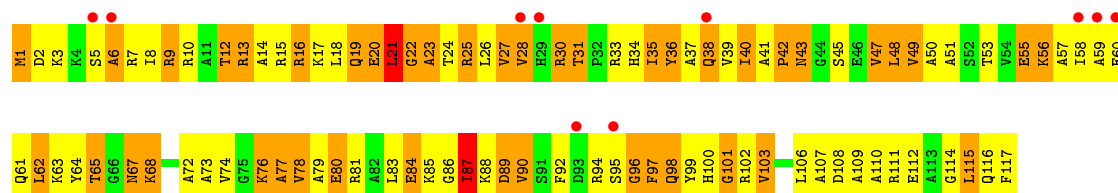
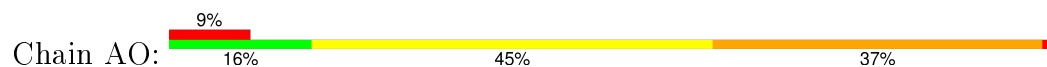




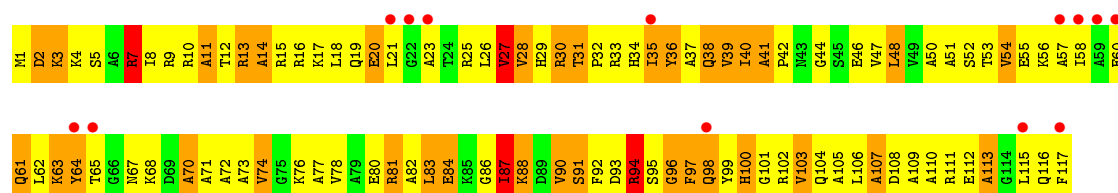
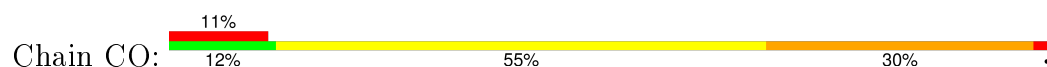
• Molecule 20: 50S RIBOSOMAL PROTEIN L17



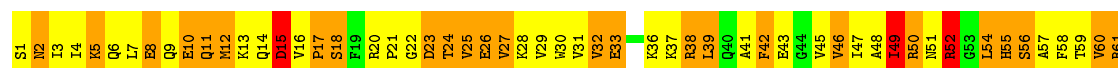
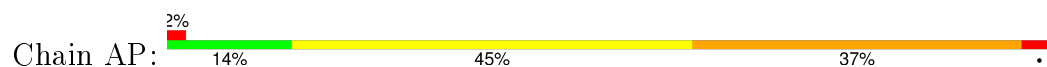
• Molecule 21: 50S RIBOSOMAL PROTEIN L18



• Molecule 21: 50S RIBOSOMAL PROTEIN L18

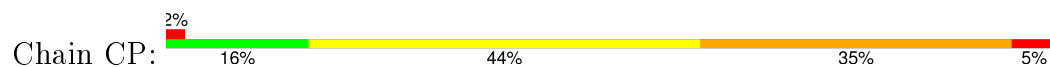


• Molecule 22: 50S RIBOSOMAL PROTEIN L19





• Molecule 22: 50S RIBOSOMAL PROTEIN L19



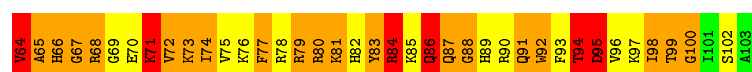
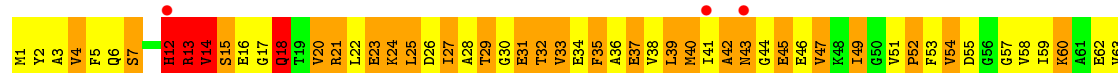
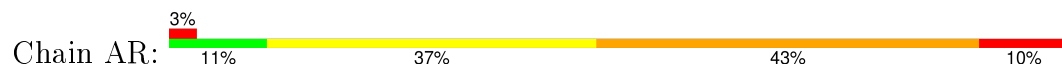
• Molecule 23: 50S RIBOSOMAL PROTEIN L20



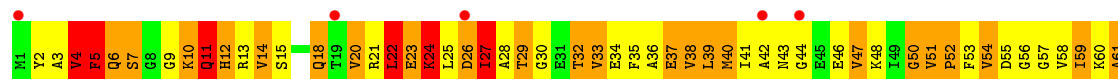
• Molecule 23: 50S RIBOSOMAL PROTEIN L20



• Molecule 24: 50S RIBOSOMAL PROTEIN L21

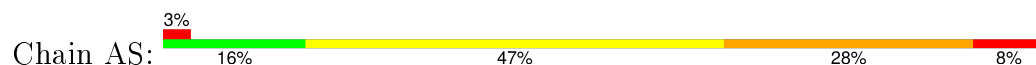


• Molecule 24: 50S RIBOSOMAL PROTEIN L21

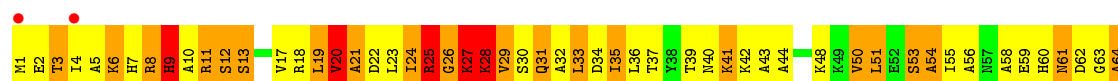
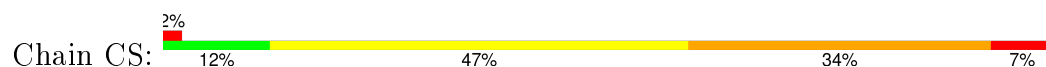




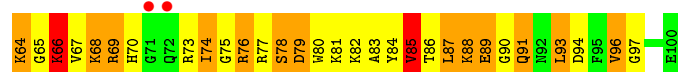
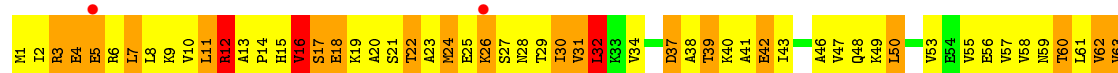
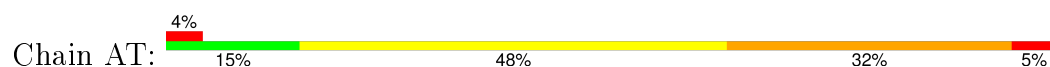
## ● Molecule 25: 50S RIBOSOMAL PROTEIN L22



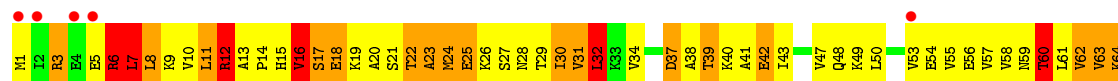
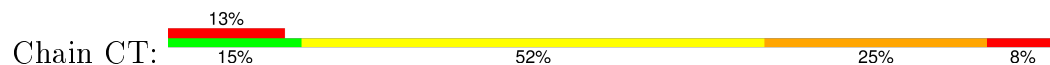
## ● Molecule 25: 50S RIBOSOMAL PROTEIN L22



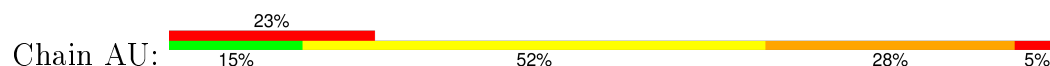
## ● Molecule 26: 50S RIBOSOMAL PROTEIN L23

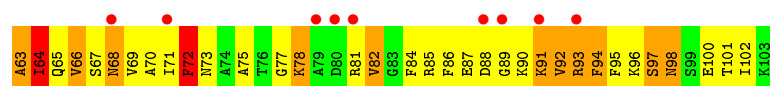


## ● Molecule 26: 50S RIBOSOMAL PROTEIN L23

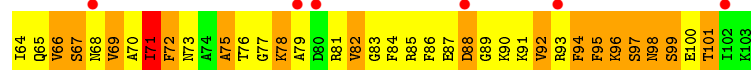
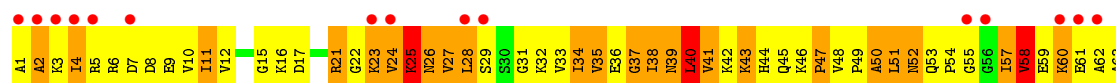
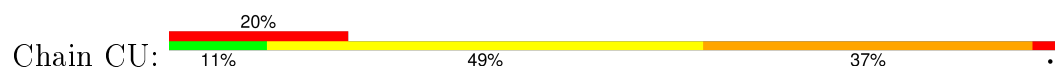


## ● Molecule 27: 50S RIBOSOMAL PROTEIN L24

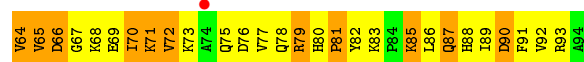




● Molecule 27: 50S RIBOSOMAL PROTEIN L24



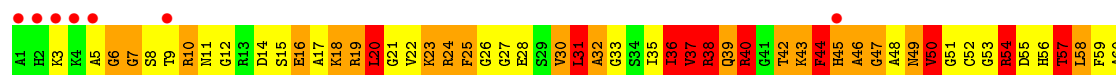
● Molecule 28: 50S RIBOSOMAL PROTEIN L25



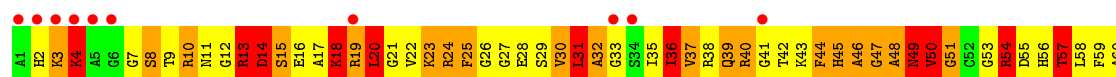
● Molecule 28: 50S RIBOSOMAL PROTEIN L25



● Molecule 29: 50S RIBOSOMAL PROTEIN L27

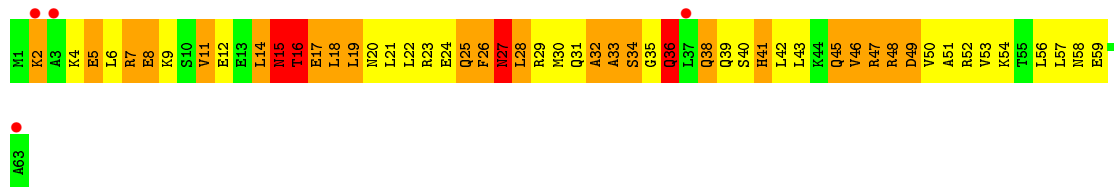
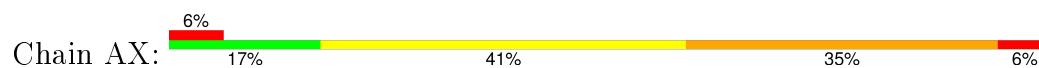


● Molecule 29: 50S RIBOSOMAL PROTEIN L27

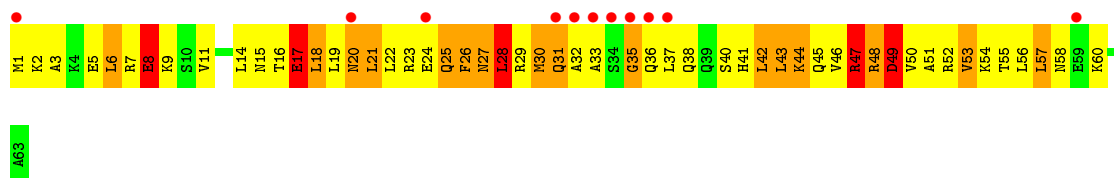
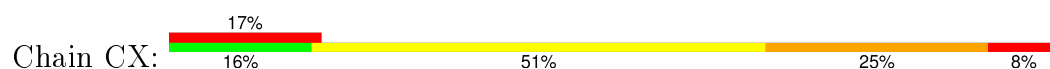




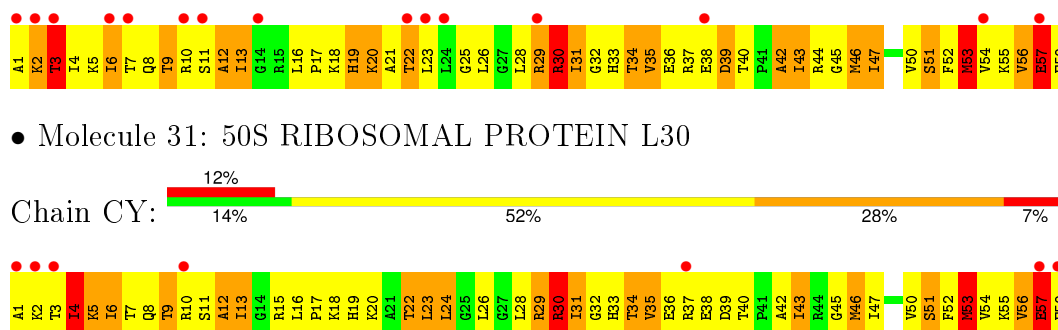
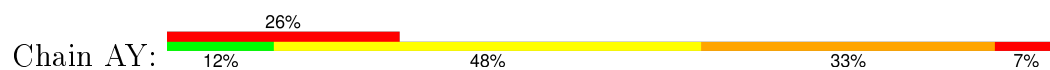
• Molecule 30: 50S RIBOSOMAL PROTEIN L29



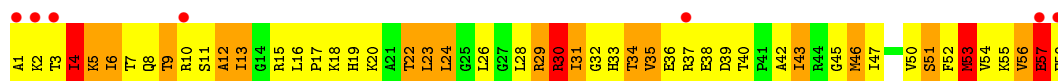
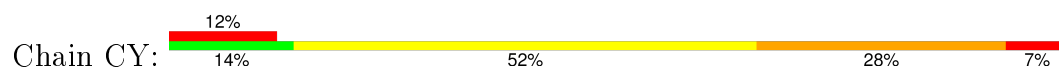
• Molecule 30: 50S RIBOSOMAL PROTEIN L29



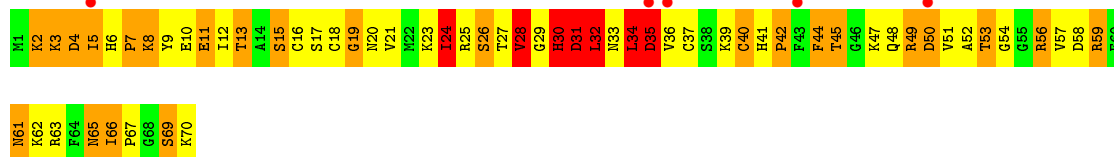
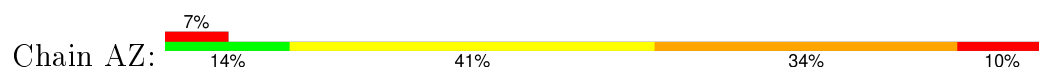
• Molecule 31: 50S RIBOSOMAL PROTEIN L30



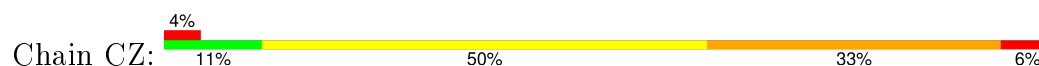
• Molecule 31: 50S RIBOSOMAL PROTEIN L30



• Molecule 32: 50S RIBOSOMAL PROTEIN L31



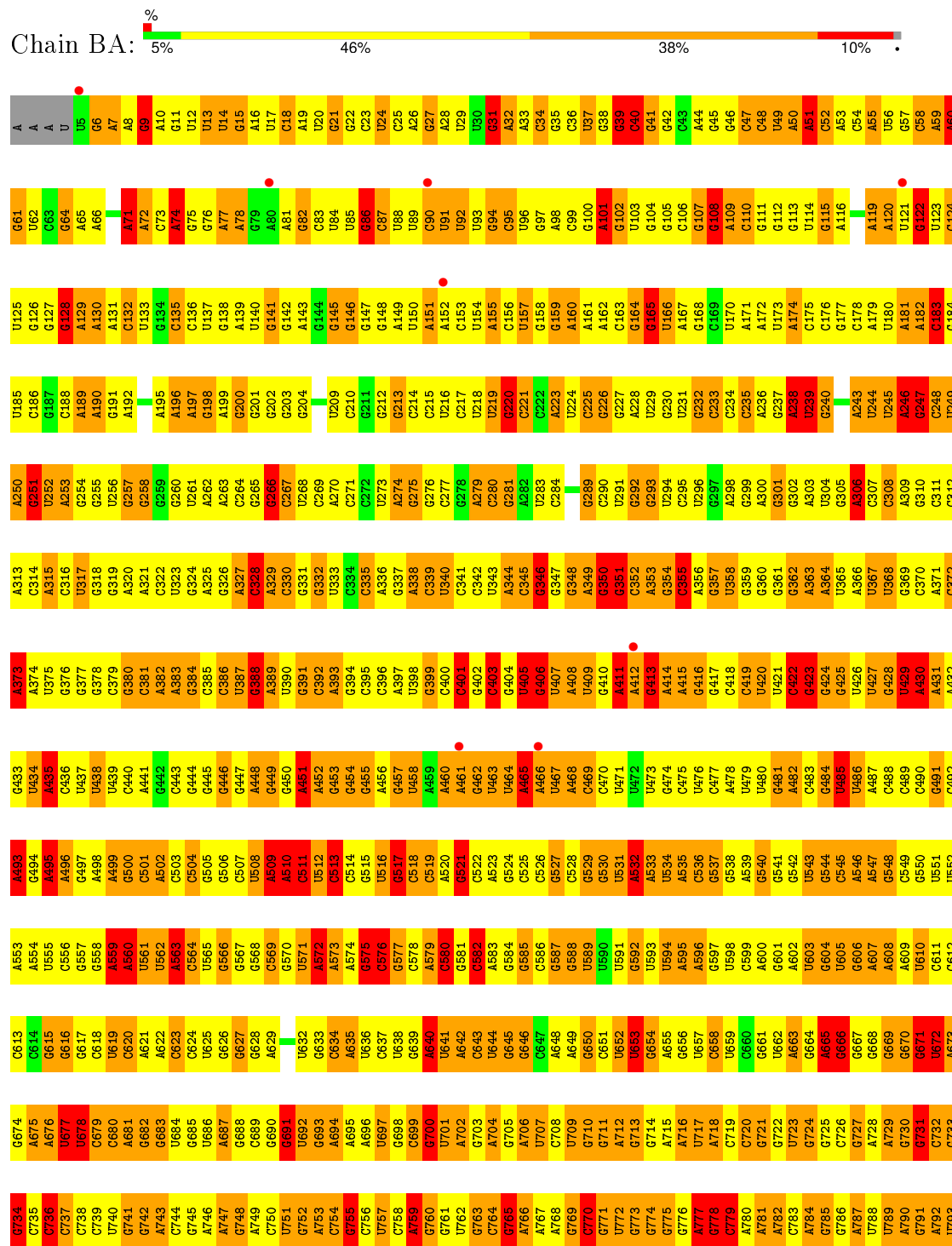
• Molecule 32: 50S RIBOSOMAL PROTEIN L31





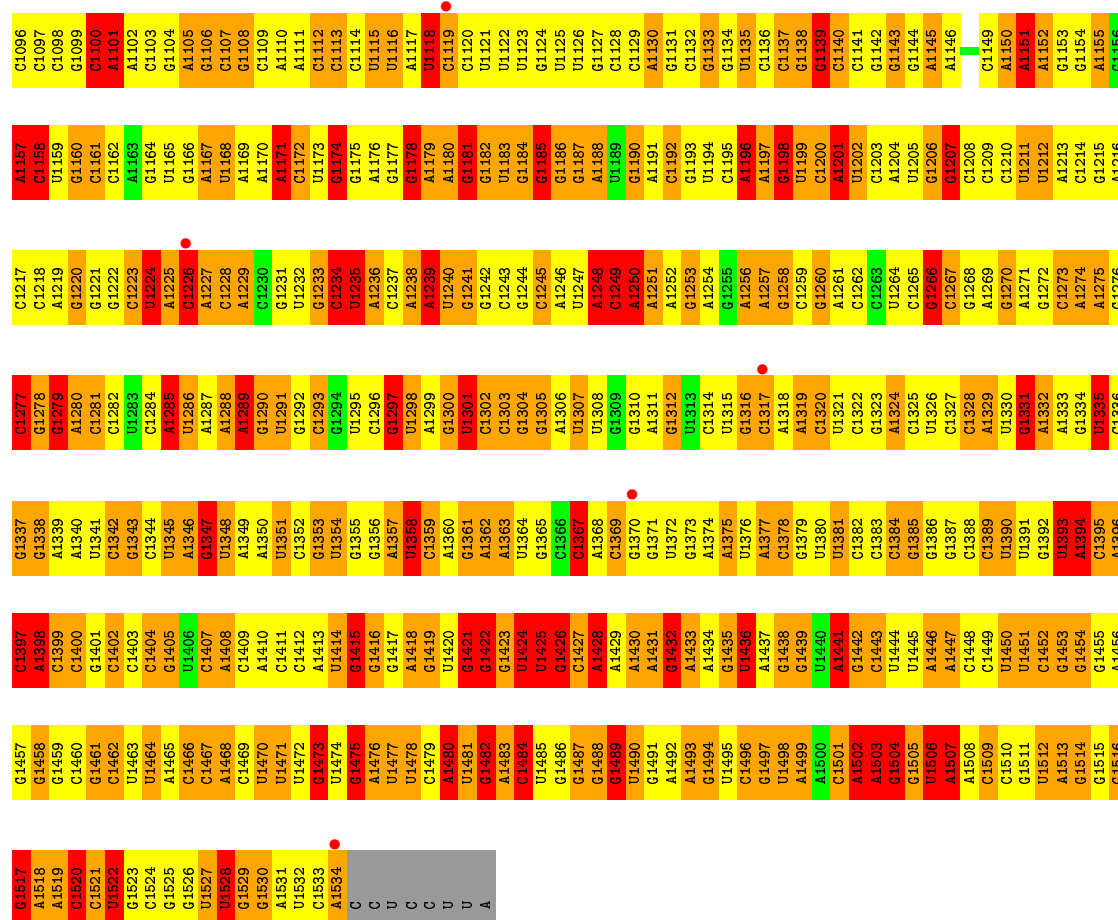


• Molecule 33: 16S RIBOSOMAL RNA

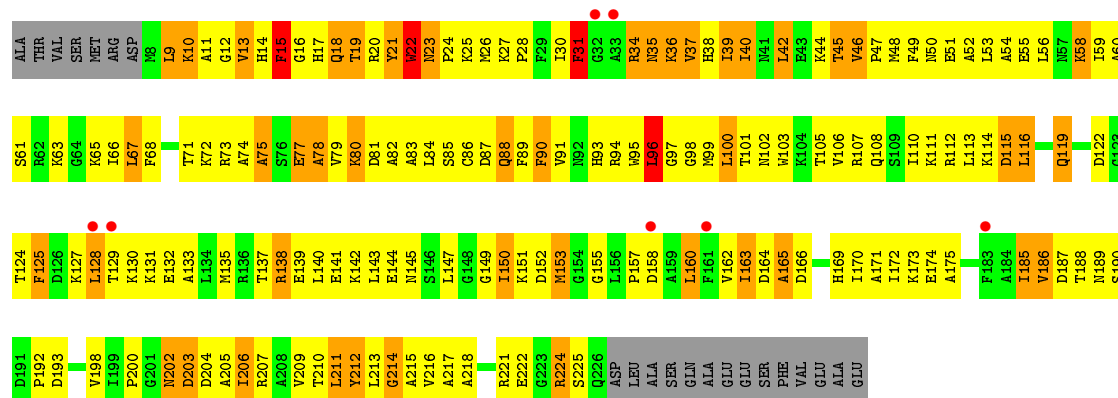


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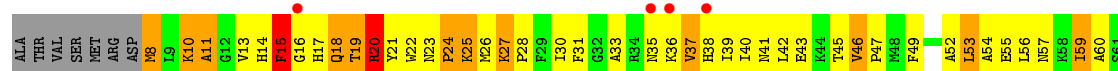
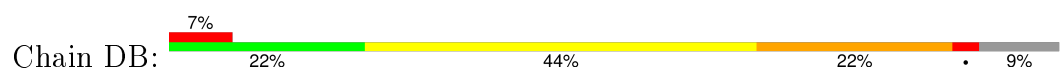
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C1037	A975	U855	C795	C735	A675	G615	U555	A495	U434	A374	C314	A250	C186	G126	U62
G1038	G976	C856	C796	C736	A676	G616	G556	A496	A435	G376	A315	G251	G187	G127	C63
C1039	G977	C857	C797	C737	A677	G617	G557	A497	A436	G377	C316	G252	C188	G128	G64
U1040	A978	C858	U798	C738	G678	C618	G558	A498	U437	G378	U317	A253	A189	A129	A65
G1041	G979	C859	G799	C739	G679	G619	A559	A499	U438	G379	G318	G254	A190	A130	A66
A1042	C980	A860	G800	U740	C680	C620	A560	G500	U439	C379	G319	G255	G191	A131	
G1043	U981	G861	A801	G741	A681	A621	U561	C501	U440	G380	A320	U256	A192	C132	U70
A1044	U982	G862	A802	G742	G682	A622	U562	A502	A441	C381	A321	G257		U133	A71
C1045	A983	U863	G803	A743	G683	C623	A563	C503	G442	A382	C322	G258	A196	G134	A72
A1046	C984	G864	U804	C744	U684	C624	C564	C504	C443	A383	U323		A197	C135	C73
G1047	C985	A865	G805	G745	G685	U625	U565	G505	G444	G384	G324	U261	A198	C136	A74
G1048	U986	C866	C806	A746	U686	G626	G566	G506	G445	G385	A325	A262	G198	U137	G75
U1049	G987	G867	A807	A747	A687	G627	G567	C507	G446	C386	G326	A263	A199	G138	G76
G1050	G988	C868	C808	G748	G688	G628	G568	U508	G447	U387	A327	G264	G200	A139	A77
C1051	U989	G869	G809	A749	G689	A629	C569	A509	A448	C388	C328	G265	G201	U140	A78
U1052	C990	U870	C810	C750	G690	A630	U570	A510	G449	A389	A329	G266	G202	G141	
G1053	U991	C871	C811	U751	G691	C631	G571	C511	G450	U390	C330	G267	G203	G142	A81
C1054	U992	A872	G812	G752	U692	U632	A572	U512	A451	C391	G331	U268	G204	A143	G82
A1055	G993	C873	U813	A753	G693	G633	A573	C513	A452	C392	G332	C269		G144	C83
U1056	A994	G874	A814	C754	A694	C634	A574	C514	A453	A393	U333	A270	U209	G145	U84
G1057	C995	U875	A815	G755	A695	A635	G575	G515	G454	G394	C334	C271	C210	G146	U85
A1058	A996	C876	A816	C756	A696	U636	C576	U516	G455	C395	C335	C272	G211	G147	G86
C1059	U997	A877	C817	U757	G697	G637	G577	C517	A456	C396	A336	U273	G212	G148	C87
U1060	G998	G878	G818	C758	G698	U638	C578	C518	G457	A397	G337	A274	G213	A149	U88
G1061	C999	C879	A819	A759	C699	G639	A579	C519	U458	U398	A338	C275	C214	U150	U89
U1062	A1000	C880	U820	G760	G700	A640	C580	A520	A459	G399	C339	G276	C215	A151	C90
C1063	C1001	G881	G821	G761	U701	U641	G581	C521	A460	C400	U340	C277	U216	A152	U91
G1064	G1002	C882	U822	U762	A702	A642	C582	C522	A461	C401	C341	G278	C217	C153	U92
U1065	C1003	C883	C823	G763	G703	G643	A583	A523	G462	A402	C342	A279	U218	U154	U93
C1066	A1004	U884	G824	C764	A704	U644	G584	G524	U463	C403	U343	C280	U219	A155	G94
A1067	G1005	C885	A825	G765	G705	G645	G585	C525	U464	C404	A344	C281	G220	C156	C95
G1068	U1006	G886	C826	A766	A706	A646	C586	C526	A465	U405	G345	A282	C221	U157	U96
C1069	U1007	G887	U827	A767	G707	C647	G587	C527	U466	C406	G346	G283	C222	G158	G97
U1070	U1008	A888	U828	A768	C708	A648	G588	C528	U467	U407	G347	C284	A223	G159	A98
C1071	U1009	A889	G829	G769	U709	A649	U589	G529	A468	A408	G348		U224	A160	C99
U1072	U1010	G890	G830	C770	G710	G650	U590	G530	C469	U409	A349	G289	C225	A161	G100
G1073	C1011	U891	A831	G771	G711	C651	U591	U531	C470	G410	G350	C290	G226	A162	A101
U1074	G1012	A892	G832	U772	A712	U652	G592	A532		A411	G351	U291	G227	G163	G102
G1075	C1013	C893	G833	G773	G713	U653	U593	A533	U473	A412	C352	G292	A228	G164	U103
U1076	A1014	G894	U834	C774	G714	G654	U594	U534	G474	G413	A353	G293	U229	G165	G104
G1077	G1015	C895	U835	G775	A715	A655	A595	A535	C475	A414	G354	U294	G230	U166	G105
U1078	A1016	C896	G836	G776	A716	G656	A596	C536	U476	A415	C355	C295	U231	A167	C106
G1079	U1017	C897	U837	A777	U717	U657	G597	C537	C477	C416	A356	U296	G232	G168	G107
A1080	G1018	G898	G838	G778	A718	C658	U598	G538	A478	C417	G357	G297	C233	G169	G108
U1081	A1019	C899	C839	C779	C719	U659	C599	A539	U479	C418	U358	A298	C234	U170	A109
A1082	G1020	A900	C840	A780	C720	C660	A600	G540	U480	C419	G359	G299	C235	A171	C110
U1083	A1021	U901	C841	A781	G721	G661	G601	G541	G481	U420	G360	A300	A236	A172	G111
G1084	A1022	G902	U842	A782	G722	U662	A602	G542	A482	U421	G361	G301	G237	U173	G112
U1085	U1023	G903	U843	C783	G723	A663	U603	U543	C483	C422	G362	G302	A238	A174	G113
G1086	U1024	U904	G844	A784	G724	G664	G604	G544	G484	C423	A363	A303	U239	C175	U114
U1087	G1025	U905	A845	G785	G725	A665	U605	C545	U485	G424	A364	U304	G240	C176	G115
G1088	G1026	A906	G846	G786	C726	G666	G606	A546	U486	G425	U365	G305	G241	G177	
U1089		C907	G847	A787	G727	G667	A607	A547	A487	U426	A366	A306	G242	C178	G116
G1090	U1030	A908	C848	U788	A728	G668	A608	G548	C488	G427	U367	C307	U244	A179	A119
U1091	C1031	A909	G849	U789	A729	G669	A609	C549	A489	G428	U368	C308	U245	U180	A120
A1092	G1032	C910	U850	G790	G730	G670	U610	G550	C490	U429	G369	A309	U246	A181	U121
U1093	G1033	U911	G851	G791	G731	G671	C611	U551	G491	A430	C370	G310	A247	A182	G122
G1094	C1034	C912	G852	A792	C732	U672	C612	U552	G492	A431	A371	C311	G248	C183	U123
U1095	A1035	G913	C853	U793	G733	A673	C613	A553	A493	A432	C372	C312	C248	G184	C124

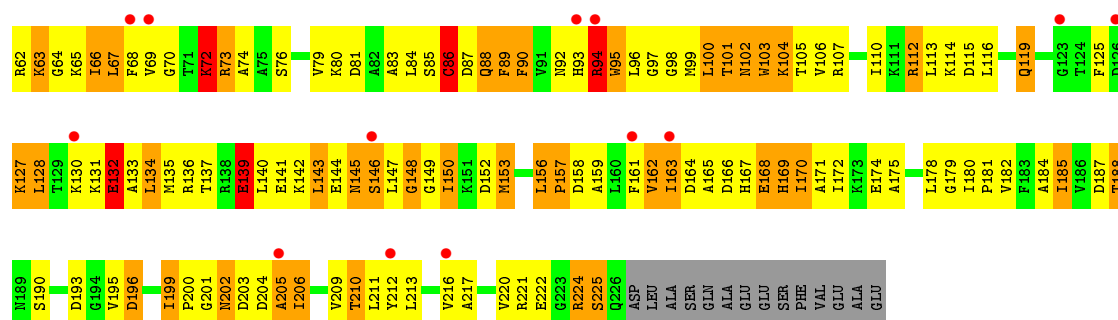


### • Molecule 34: 30S RIBOSOMAL PROTEIN S2

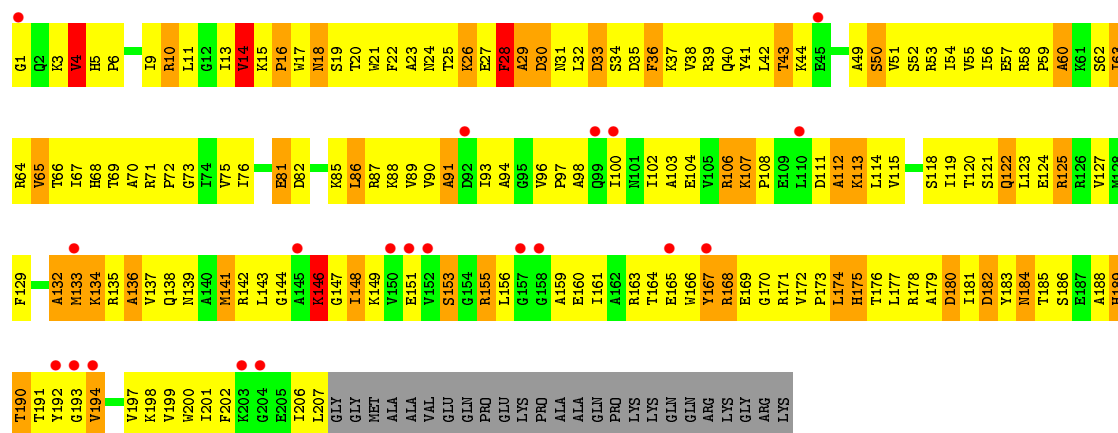
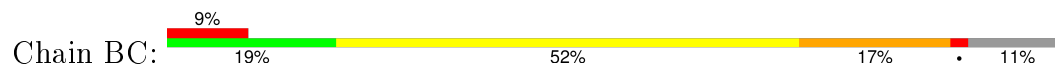


### • Molecule 34: 30S RIBOSOMAL PROTEIN S2

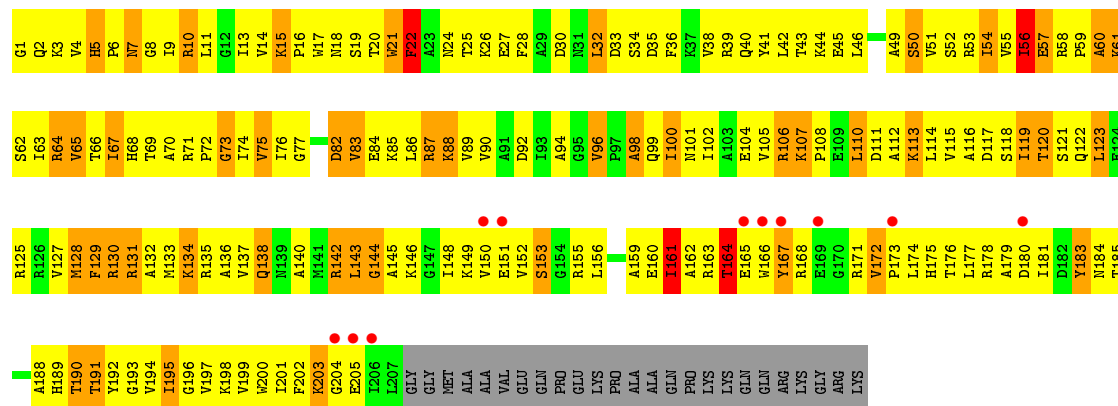
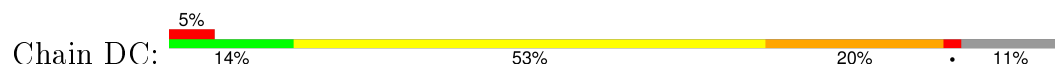




• Molecule 35: 30S RIBOSOMAL PROTEIN S3



• Molecule 35: 30S RIBOSOMAL PROTEIN S3



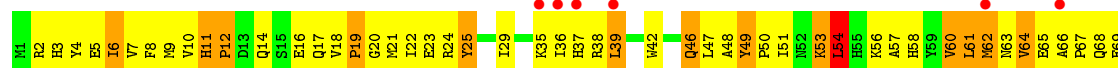
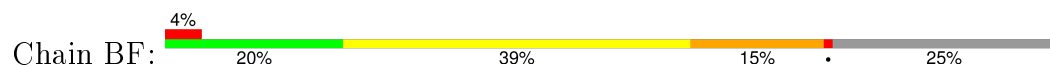
• Molecule 36: 30S RIBOSOMAL PROTEIN S4



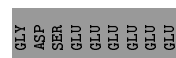
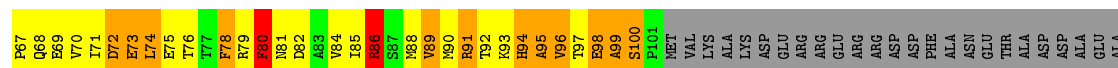




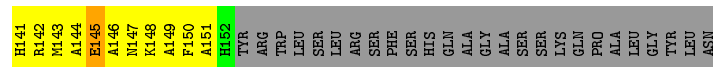
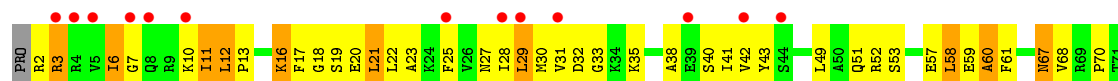
• Molecule 38: 30S RIBOSOMAL PROTEIN S6



• Molecule 38: 30S RIBOSOMAL PROTEIN S6

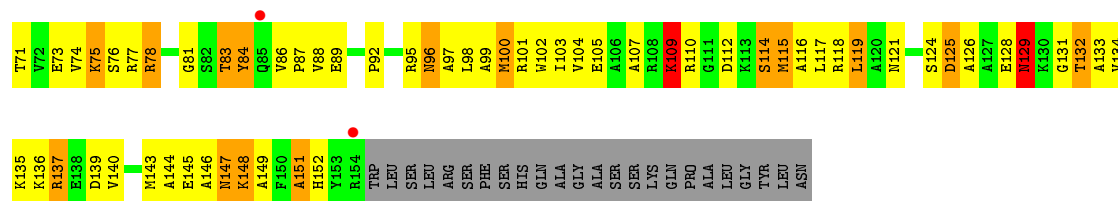


• Molecule 39: 30S RIBOSOMAL PROTEIN S7

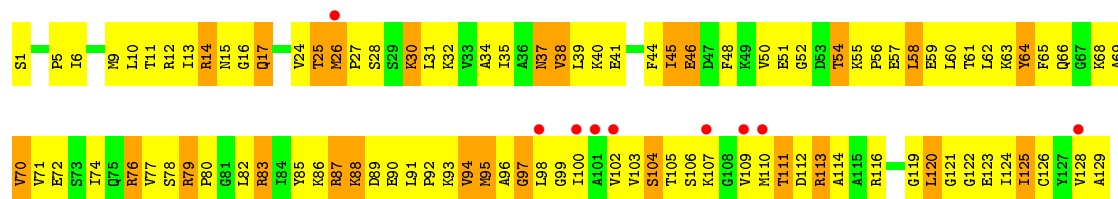


• Molecule 39: 30S RIBOSOMAL PROTEIN S7

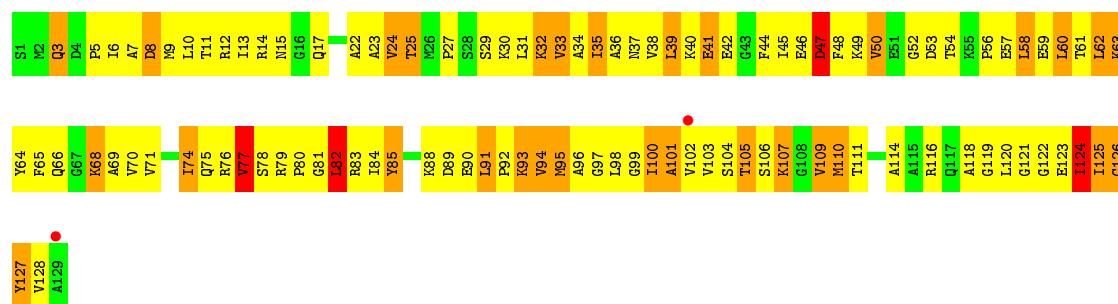




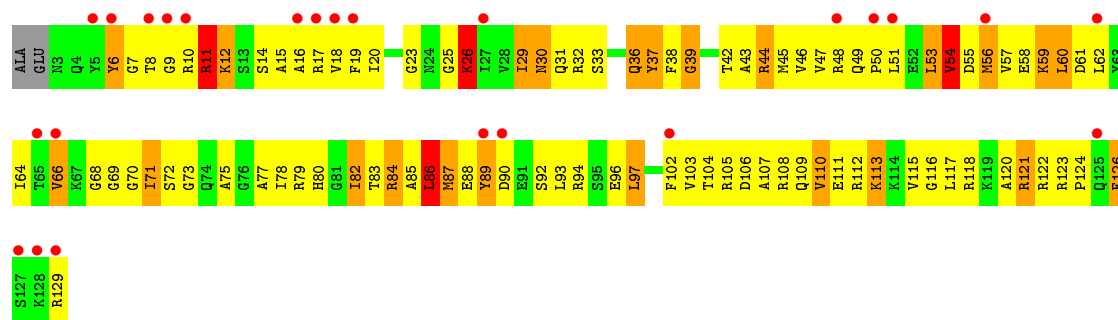
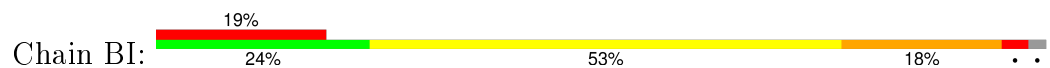
• Molecule 40: 30S RIBOSOMAL PROTEIN S8



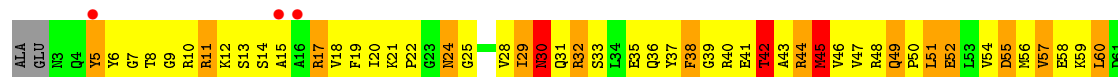
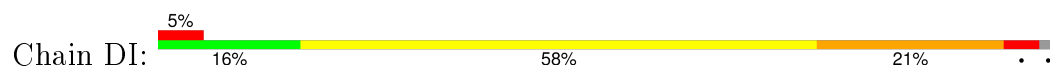
• Molecule 40: 30S RIBOSOMAL PROTEIN S8



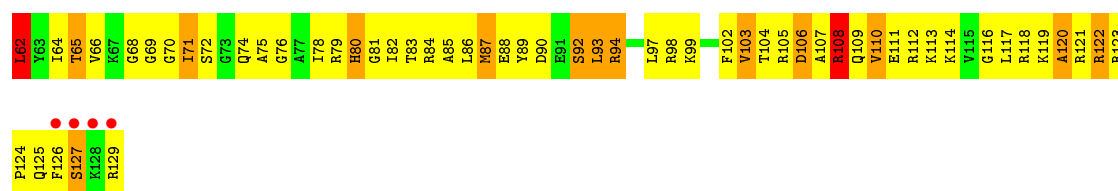
• Molecule 41: 30S RIBOSOMAL PROTEIN S9



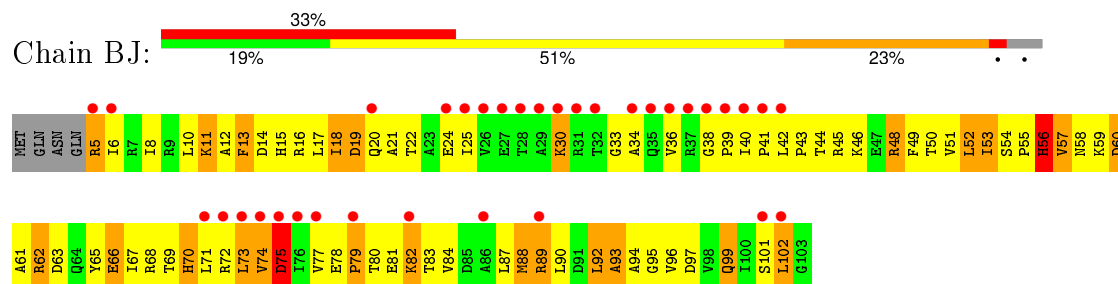
• Molecule 41: 30S RIBOSOMAL PROTEIN S9



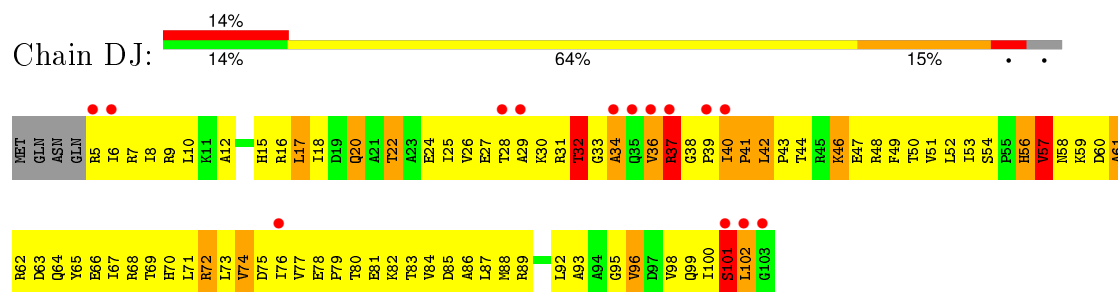




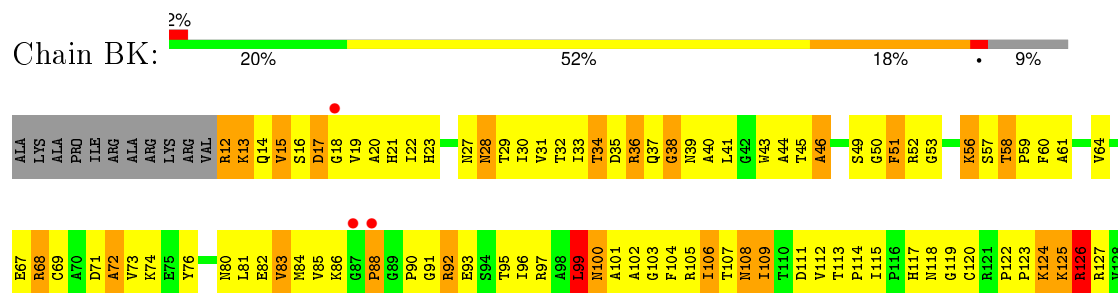
• Molecule 42: 30S RIBOSOMAL PROTEIN S10



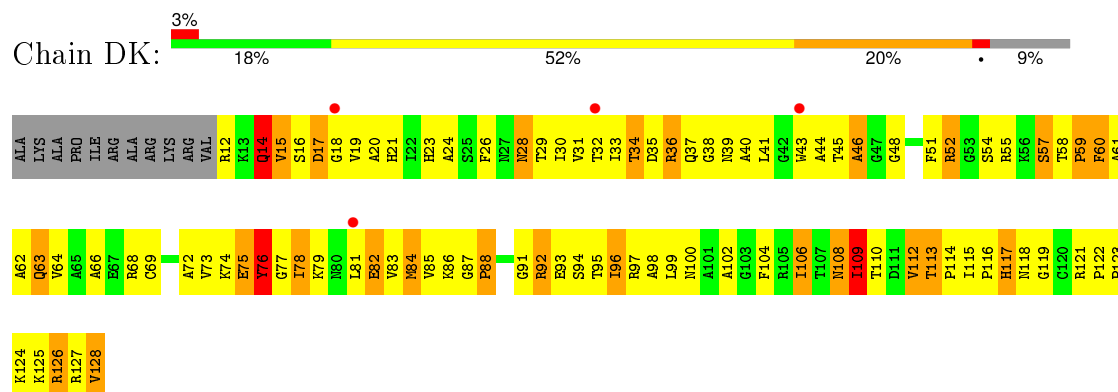
• Molecule 42: 30S RIBOSOMAL PROTEIN S10



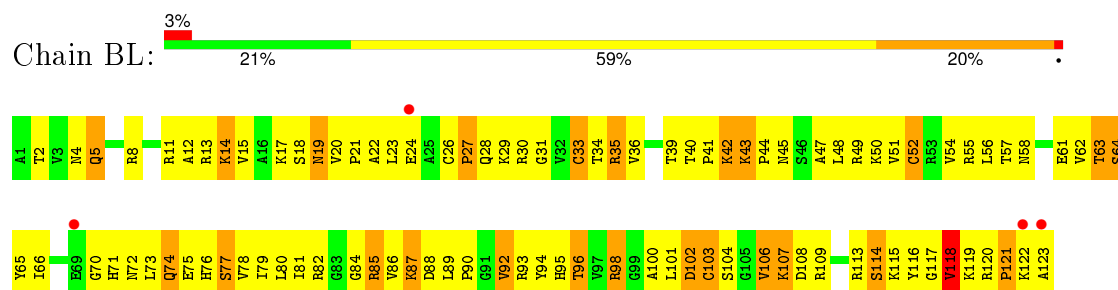
• Molecule 43: 30S RIBOSOMAL PROTEIN S11



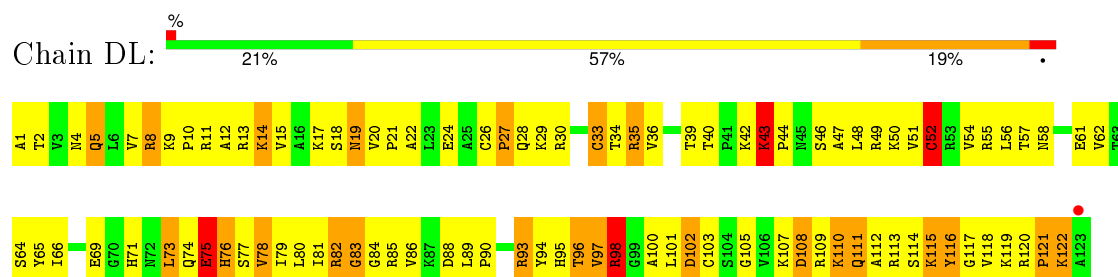
• Molecule 43: 30S RIBOSOMAL PROTEIN S11



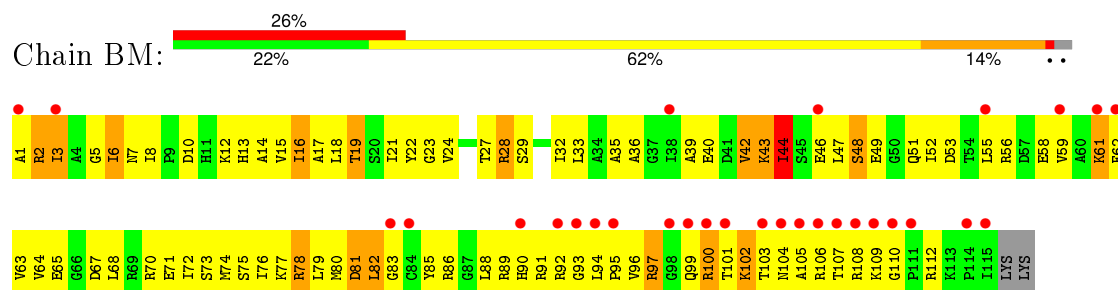
- Molecule 44: 30S RIBOSOMAL PROTEIN S12



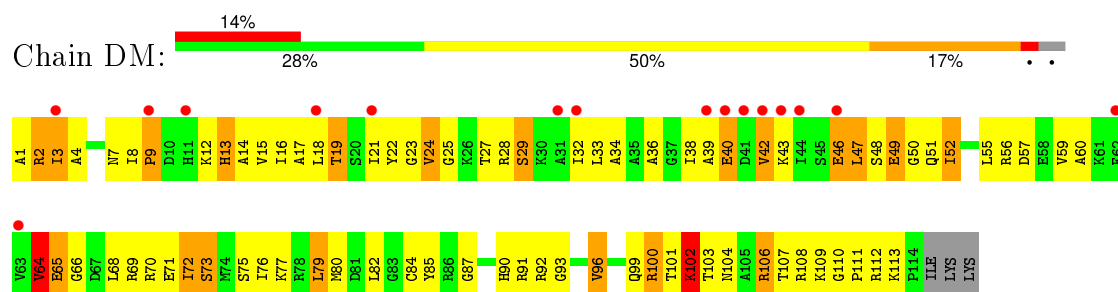
- Molecule 44: 30S RIBOSOMAL PROTEIN S12



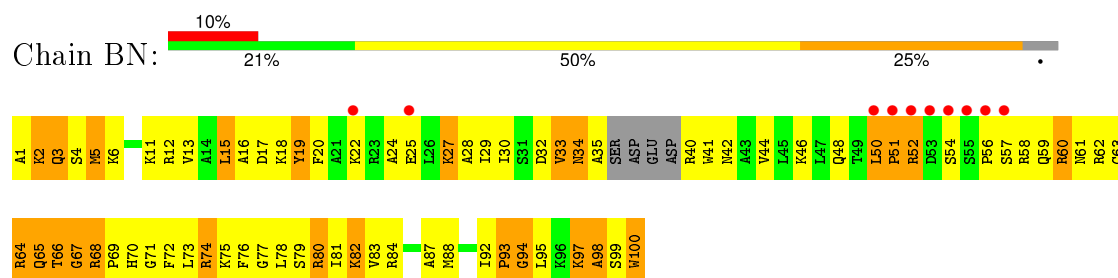
- Molecule 45: 30S RIBOSOMAL PROTEIN S13



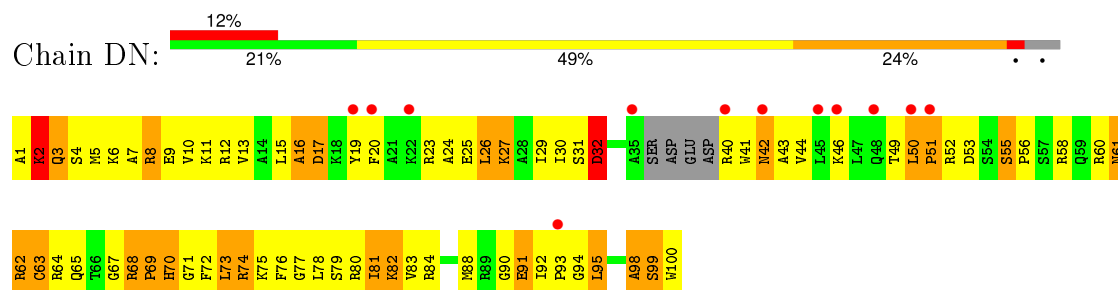
- Molecule 45: 30S RIBOSOMAL PROTEIN S13



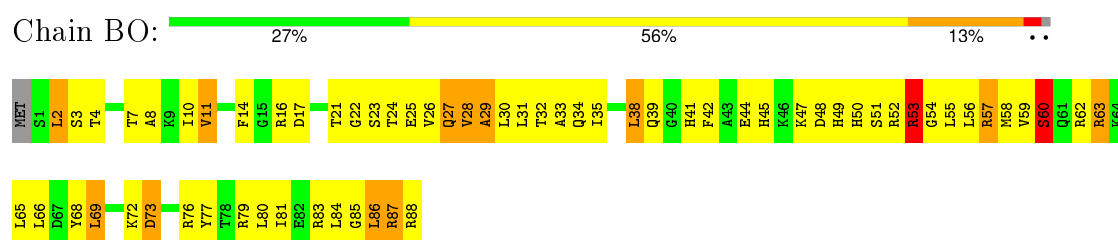
- Molecule 46: 30S RIBOSOMAL PROTEIN S14



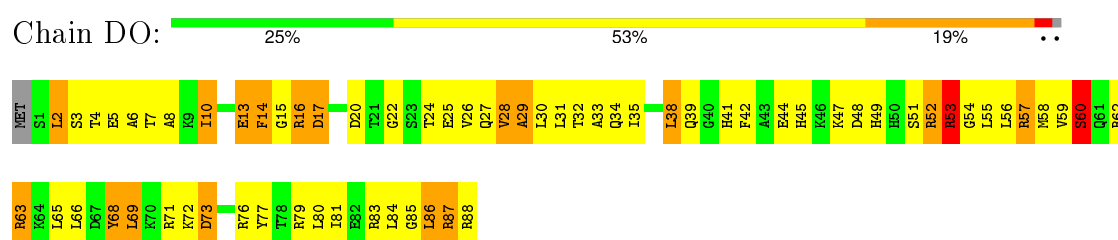
## • Molecule 46: 30S RIBOSOMAL PROTEIN S14



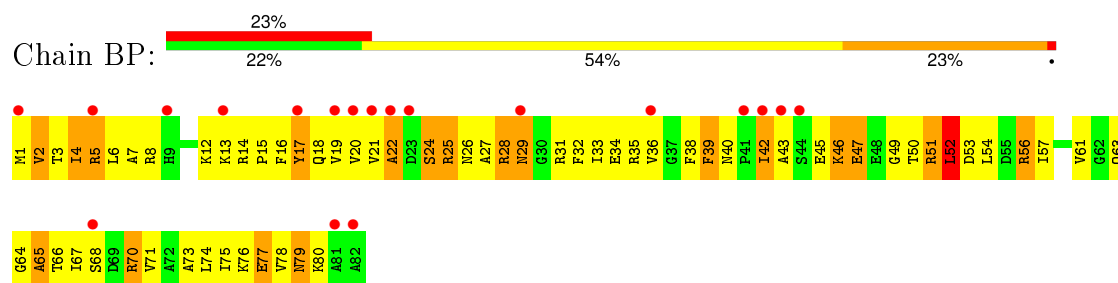
## • Molecule 47: 30S RIBOSOMAL PROTEIN S15



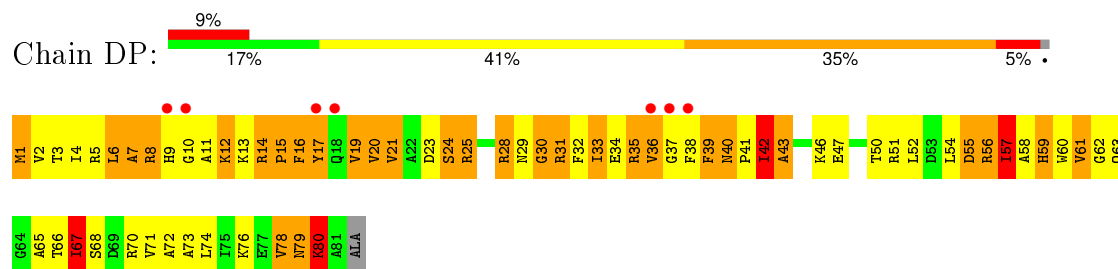
## • Molecule 47: 30S RIBOSOMAL PROTEIN S15



## • Molecule 48: 30S RIBOSOMAL PROTEIN S16

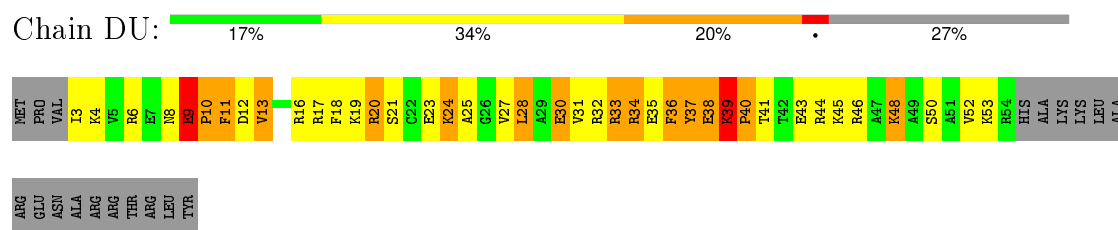


## • Molecule 48: 30S RIBOSOMAL PROTEIN S16



## • Molecule 49: 30S RIBOSOMAL PROTEIN S17





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	208.18Å 380.08Å 736.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.74 49.74 – 3.74	Depositor EDS
% Data completeness (in resolution range)	91.5 (50.00-3.74) 91.5 (49.74-3.74)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.52 (at 3.77Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.259 , 0.323 0.249 , 0.308	Depositor DCC
$R_{free}$ test set	5522 reflections (1.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	90.4	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.10 , 15.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.34$ , $\langle L^2 \rangle = 0.17$	Xtriage
Outliers	0 of 546832 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	284264	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.64% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	A0	0.41	0/450	0.71	0/599
1	C0	0.48	0/450	0.78	0/599
2	A1	0.42	0/448	0.69	0/594
2	C1	0.46	0/448	0.73	0/594
3	A2	0.46	0/380	0.76	0/498
3	C2	0.46	0/380	0.83	1/498 (0.2%)
4	A3	0.52	0/513	0.79	0/676
4	C3	0.54	0/513	0.91	0/676
5	A4	0.43	0/303	0.69	0/397
5	C4	0.46	0/303	0.78	0/397
6	A5	0.64	0/134	0.72	0/176
7	AA	0.76	3/2803 (0.1%)	1.48	39/4371 (0.9%)
7	CA	0.79	2/2803 (0.1%)	1.52	47/4371 (1.1%)
8	AB	0.82	7/68314 (0.0%)	1.58	975/106569 (0.9%)
8	CB	0.90	15/68314 (0.0%)	1.64	1204/106569 (1.1%)
9	AC	0.51	0/2093	0.81	2/2815 (0.1%)
9	CC	0.55	0/2093	0.82	1/2815 (0.0%)
10	AD	0.45	0/1586	0.72	0/2134
10	CD	0.51	0/1586	0.77	0/2134
11	AE	0.47	0/1571	0.77	0/2113
11	CE	0.50	0/1571	0.75	0/2113
12	AF	0.30	0/1444	0.53	0/1937
12	CF	0.32	0/1444	0.54	0/1937
13	AG	0.38	0/1343	0.62	0/1816
13	CG	0.37	0/1343	0.62	0/1816
14	AH	0.34	0/1122	0.60	0/1515
14	CH	0.37	0/1122	0.64	0/1515
15	AI	0.29	0/1046	0.52	0/1410
15	CI	0.26	0/1045	0.52	0/1406
16	AJ	0.43	0/1136	0.71	0/1531
16	CJ	0.50	0/1136	0.75	0/1531
17	AK	0.50	0/940	0.71	0/1260

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	CK	0.54	0/940	0.72	0/1260
18	AL	0.46	0/1062	0.84	1/1413 (0.1%)
18	CL	0.44	0/1062	0.81	0/1413
19	AM	0.46	0/1093	0.73	0/1460
19	CM	0.48	0/1093	0.77	0/1460
20	AN	0.41	0/1021	0.66	0/1364
20	CN	0.49	0/1021	0.73	0/1364
21	AO	0.38	0/910	0.69	0/1219
21	CO	0.45	0/910	0.77	0/1219
22	AP	0.44	0/929	0.77	1/1242 (0.1%)
22	CP	0.51	0/929	0.81	1/1242 (0.1%)
23	AQ	0.45	0/960	0.71	0/1278
23	CQ	0.53	0/960	0.81	1/1278 (0.1%)
24	AR	0.41	0/829	0.72	0/1107
24	CR	0.46	0/829	0.75	0/1107
25	AS	0.43	0/864	0.74	0/1156
25	CS	0.44	0/864	0.82	0/1156
26	AT	0.45	0/785	0.68	0/1050
26	CT	0.43	0/785	0.69	0/1050
27	AU	0.48	0/788	0.72	0/1053
27	CU	0.42	0/788	0.69	0/1053
28	AV	0.34	0/766	0.52	0/1025
28	CV	0.36	0/766	0.52	0/1025
29	AW	0.42	0/642	0.76	0/848
29	CW	0.45	0/642	0.78	0/848
30	AX	0.47	0/510	0.76	0/677
30	CX	0.40	0/510	0.69	0/677
31	AY	0.36	0/453	0.66	0/605
31	CY	0.34	0/453	0.67	0/605
32	AZ	0.56	0/559	0.94	2/745 (0.3%)
32	CZ	0.68	0/559	0.97	0/745
33	BA	0.70	4/36761 (0.0%)	1.42	407/57346 (0.7%)
33	DA	0.82	4/36762 (0.0%)	1.58	674/57350 (1.2%)
34	BB	0.32	0/1736	0.54	0/2340
34	DB	0.36	0/1736	0.61	0/2340
35	BC	0.33	0/1652	0.53	0/2227
35	DC	0.39	0/1652	0.61	0/2227
36	BD	0.36	0/1665	0.62	0/2227
36	DD	0.46	0/1665	0.68	0/2227
37	BE	0.37	0/1119	0.56	0/1506
37	DE	0.43	0/1119	0.67	0/1506
38	BF	0.40	1/836 (0.1%)	0.57	0/1130
38	DF	0.41	1/836 (0.1%)	0.63	1/1130 (0.1%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
39	BG	0.33	0/1188	0.52	0/1593
39	DG	0.38	0/1212	0.58	0/1626
40	BH	0.32	0/989	0.55	0/1326
40	DH	0.44	0/989	0.69	0/1326
41	BI	0.29	0/1034	0.51	0/1375
41	DI	0.33	0/1034	0.64	1/1375 (0.1%)
42	BJ	0.33	1/797 (0.1%)	0.53	0/1079
42	DJ	0.36	1/797 (0.1%)	0.57	0/1079
43	BK	0.35	0/893	0.61	0/1205
43	DK	0.43	0/893	0.70	0/1205
44	BL	0.33	0/969	0.58	0/1300
44	DL	0.42	0/969	0.67	0/1300
45	BM	0.29	0/893	0.50	0/1195
45	DM	0.37	1/885 (0.1%)	0.60	0/1183
46	BN	0.29	0/785	0.51	0/1043
46	DN	0.30	0/785	0.56	0/1043
47	BO	0.33	0/724	0.55	0/966
47	DO	0.38	0/724	0.63	0/966
48	BP	0.30	0/659	0.51	0/884
48	DP	0.49	0/649	0.69	0/872
49	BQ	0.37	0/658	0.59	0/883
49	DQ	0.39	0/666	0.65	0/892
50	BR	0.40	0/463	0.62	0/623
50	DR	0.49	0/463	0.70	0/623
51	BS	0.32	1/653 (0.2%)	0.50	0/879
51	DS	0.37	1/661 (0.2%)	0.62	0/890
52	BT	0.32	0/671	0.49	0/888
52	DT	0.39	0/671	0.58	0/888
53	BU	0.42	0/431	0.56	0/572
53	DU	0.55	0/431	0.73	0/572
All	All	0.73	42/306634 (0.0%)	1.39	3358/458333 (0.7%)

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	C0	0	2
4	C3	0	2
11	CE	0	3
13	AG	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
14	CH	0	1
16	AJ	0	1
16	CJ	0	1
18	AL	0	1
18	CL	0	1
19	AM	0	1
20	CN	0	2
22	AP	0	3
22	CP	0	4
24	CR	0	1
25	CS	0	2
26	CT	0	1
30	CX	0	1
32	AZ	0	1
32	CZ	0	1
All	All	0	30

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	DA	765	G	N9-C4	9.10	1.45	1.38
8	CB	301	G	C3'-O3'	7.66	1.52	1.42
7	CA	87	U	C1'-N1	7.10	1.59	1.48
7	AA	87	U	C1'-N1	6.70	1.58	1.48
33	DA	519	C	C1'-N1	6.38	1.58	1.48

The worst 5 of 3358 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	AB	2288	A	C2-N3-C4	-70.19	75.50	110.60
8	CB	2288	A	C2-N3-C4	-69.49	75.85	110.60
8	CB	2288	A	N1-C2-N3	59.84	159.22	129.30
8	AB	2288	A	C6-N1-C2	-58.83	83.30	118.60
8	AB	2288	A	N1-C2-N3	58.75	158.67	129.30

There are no chirality outliers.

5 of 30 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	AG	109	SER	Peptide
16	AJ	9	GLU	Peptide

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Mol	Chain	Res	Type	Group
18	AL	53	GLY	Peptide
19	AM	88	ASN	Peptide
22	AP	46	VAL	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A0	444	0	461	86	0
1	C0	444	0	461	112	0
2	A1	441	0	485	104	0
2	C1	441	0	485	89	0
3	A2	377	0	418	106	0
3	C2	377	0	418	104	0
4	A3	504	0	574	171	0
4	C3	504	0	574	137	0
5	A4	302	0	340	104	0
5	C4	302	0	340	99	0
6	A5	134	0	153	17	0
7	AA	2507	0	1270	277	0
7	CA	2507	0	1270	303	0
8	AB	60995	0	30679	6970	0
8	CB	60995	0	30678	7146	0
9	AC	2054	0	2122	607	0
9	CC	2054	0	2122	625	0
10	AD	1565	0	1616	443	0
10	CD	1565	0	1616	508	0
11	AE	1552	0	1619	432	0
11	CE	1552	0	1619	401	0
12	AF	1420	0	1460	177	0
12	CF	1420	0	1460	216	0
13	AG	1323	0	1374	196	0
13	CG	1323	0	1374	226	0
14	AH	1111	0	1148	160	0
14	CH	1111	0	1148	191	0
15	AI	1032	0	1088	100	0
15	CI	1032	0	1088	131	0
16	AJ	1113	0	1147	293	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	CJ	1113	0	1147	307	0
17	AK	931	0	1000	161	0
17	CK	931	0	1000	159	0
18	AL	1053	0	1129	403	0
18	CL	1053	0	1129	336	0
19	AM	1074	0	1157	276	0
19	CM	1074	0	1157	294	0
20	AN	1008	0	1045	219	0
20	CN	1008	0	1045	248	0
21	AO	900	0	935	206	0
21	CO	900	0	935	247	0
22	AP	917	0	965	248	0
22	CP	917	0	965	243	0
23	AQ	947	0	1022	269	0
23	CQ	947	0	1022	284	0
24	AR	816	0	839	236	0
24	CR	816	0	839	308	0
25	AS	857	0	922	172	0
25	CS	857	0	922	200	0
26	AT	778	0	840	178	0
26	CT	778	0	840	173	0
27	AU	780	0	834	183	0
27	CU	780	0	834	172	0
28	AV	753	0	780	100	0
28	CV	753	0	780	90	0
29	AW	634	0	656	205	0
29	CW	634	0	656	226	0
30	AX	509	0	543	111	0
30	CX	509	0	543	123	0
31	AY	449	0	491	66	0
31	CY	449	0	491	84	0
32	AZ	549	0	552	174	0
32	CZ	549	0	552	152	0
33	BA	32831	0	16522	3632	0
33	DA	32831	0	16521	4109	0
34	BB	1705	0	1732	245	0
34	DB	1705	0	1732	220	0
35	BC	1625	0	1699	214	0
35	DC	1625	0	1699	274	0
36	BD	1643	0	1710	284	0
36	DD	1643	0	1710	280	0
37	BE	1106	0	1148	176	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	DE	1106	0	1148	200	0
38	BF	818	0	808	114	0
38	DF	818	0	808	143	0
39	BG	1175	0	1230	116	0
39	DG	1197	0	1246	145	0
40	BH	979	0	1034	141	0
40	DH	979	0	1034	156	0
41	BI	1022	0	1070	141	0
41	DI	1022	0	1070	158	0
42	BJ	787	0	828	99	0
42	DJ	787	0	828	129	0
43	BK	877	0	887	127	0
43	DK	877	0	887	134	0
44	BL	955	0	1019	145	0
44	DL	955	0	1019	149	0
45	BM	884	0	944	125	0
45	DM	877	0	937	107	0
46	BN	774	0	827	138	0
46	DN	774	0	827	127	0
47	BO	716	0	742	96	0
47	DO	716	0	742	106	0
48	BP	649	0	666	109	0
48	DP	639	0	656	121	0
49	BQ	649	0	691	70	0
49	DQ	657	0	702	91	0
50	BR	456	0	478	75	0
50	DR	456	0	478	100	0
51	BS	638	0	665	112	0
51	DS	645	0	675	97	0
52	BT	665	0	714	85	0
52	DT	665	0	714	91	0
53	BU	426	0	449	81	0
53	DU	426	0	449	67	0
54	AB	109	0	0	0	0
54	AE	1	0	0	0	0
54	BA	58	0	0	0	0
54	BN	1	0	0	0	0
54	BT	1	0	0	0	0
54	CB	109	0	0	0	0
54	CC	1	0	0	0	0
54	CL	1	0	0	0	0
54	DA	61	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	DN	1	0	0	0	0
55	A2	2	0	0	2	0
55	AB	489	0	0	65	0
55	AC	3	0	0	1	0
55	AD	1	0	0	0	0
55	AE	3	0	0	2	0
55	AJ	2	0	0	2	0
55	AL	3	0	0	1	0
55	BA	284	0	0	26	0
55	BE	3	0	0	0	0
55	BI	2	0	0	0	0
55	BK	1	0	0	0	0
55	BL	2	0	0	0	0
55	BN	3	0	0	0	0
55	BP	1	0	0	0	0
55	BT	2	0	0	0	0
55	C0	1	0	0	0	0
55	C2	2	0	0	0	0
55	CB	485	0	0	65	0
55	CC	3	0	0	0	0
55	CD	1	0	0	0	0
55	CE	1	0	0	0	0
55	CJ	2	0	0	0	0
55	CK	1	0	0	0	0
55	CL	5	0	0	1	0
55	CN	3	0	0	2	0
55	CP	1	0	0	0	0
55	CQ	1	0	0	0	0
55	CT	2	0	0	0	0
55	CU	1	0	0	2	0
55	DA	293	0	0	18	0
55	DD	1	0	0	0	0
55	DE	2	0	0	0	0
55	DG	1	0	0	0	0
55	DL	4	0	0	0	0
55	DN	2	0	0	1	0
55	DP	1	0	0	0	0
55	DT	3	0	0	2	0
All	All	284264	0	190919	37675	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 80.

The worst 5 of 37675 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)
8:CB:2822:G:OP2	20:CN:2:ARG:HB3	1.29	1.26
33:DA:585:G:C8	33:DA:585:G:H5'	1.76	1.21
33:DA:235:C:H2'	33:DA:236:A:C8	1.77	1.19
1:C0:27:LEU:HG	8:CB:2886:A:C6	1.77	1.19
23:CQ:49:ARG:HG3	24:CR:77:PHE:CZ	1.79	1.18

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A0	54/56 (96%)	26 (48%)	13 (24%)	15 (28%)	0	0
1	C0	54/56 (96%)	24 (44%)	12 (22%)	18 (33%)	0	0
2	A1	52/54 (96%)	18 (35%)	15 (29%)	19 (36%)	0	0
2	C1	52/54 (96%)	18 (35%)	12 (23%)	22 (42%)	0	0
3	A2	44/46 (96%)	15 (34%)	16 (36%)	13 (30%)	0	0
3	C2	44/46 (96%)	16 (36%)	16 (36%)	12 (27%)	0	0
4	A3	62/64 (97%)	24 (39%)	17 (27%)	21 (34%)	0	0
4	C3	62/64 (97%)	29 (47%)	20 (32%)	13 (21%)	0	2
5	A4	36/38 (95%)	14 (39%)	13 (36%)	9 (25%)	0	1
5	C4	36/38 (95%)	9 (25%)	16 (44%)	11 (31%)	0	0
6	A5	14/16 (88%)	6 (43%)	5 (36%)	3 (21%)	0	2
9	AC	266/273 (97%)	101 (38%)	67 (25%)	98 (37%)	0	0
9	CC	266/273 (97%)	101 (38%)	70 (26%)	95 (36%)	0	0
10	AD	207/209 (99%)	80 (39%)	56 (27%)	71 (34%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	CD	207/209 (99%)	72 (35%)	65 (31%)	70 (34%)	0	0
11	AE	199/201 (99%)	76 (38%)	58 (29%)	65 (33%)	0	0
11	CE	199/201 (99%)	71 (36%)	63 (32%)	65 (33%)	0	0
12	AF	176/178 (99%)	95 (54%)	48 (27%)	33 (19%)	0	3
12	CF	176/178 (99%)	95 (54%)	45 (26%)	36 (20%)	0	2
13	AG	174/176 (99%)	98 (56%)	42 (24%)	34 (20%)	0	3
13	CG	174/176 (99%)	89 (51%)	52 (30%)	33 (19%)	0	3
14	AH	147/149 (99%)	94 (64%)	34 (23%)	19 (13%)	0	7
14	CH	147/149 (99%)	74 (50%)	39 (26%)	34 (23%)	0	1
15	AI	139/141 (99%)	92 (66%)	33 (24%)	14 (10%)	1	12
15	CI	137/141 (97%)	87 (64%)	32 (23%)	18 (13%)	0	7
16	AJ	139/142 (98%)	60 (43%)	34 (24%)	45 (32%)	0	0
16	CJ	139/142 (98%)	57 (41%)	37 (27%)	45 (32%)	0	0
17	AK	120/123 (98%)	67 (56%)	30 (25%)	23 (19%)	0	3
17	CK	120/123 (98%)	66 (55%)	29 (24%)	25 (21%)	0	2
18	AL	142/144 (99%)	53 (37%)	37 (26%)	52 (37%)	0	0
18	CL	142/144 (99%)	54 (38%)	39 (28%)	49 (34%)	0	0
19	AM	134/136 (98%)	51 (38%)	46 (34%)	37 (28%)	0	0
19	CM	134/136 (98%)	55 (41%)	45 (34%)	34 (25%)	0	1
20	AN	125/127 (98%)	55 (44%)	43 (34%)	27 (22%)	0	1
20	CN	125/127 (98%)	55 (44%)	44 (35%)	26 (21%)	0	2
21	AO	115/117 (98%)	49 (43%)	40 (35%)	26 (23%)	0	1
21	CO	115/117 (98%)	46 (40%)	41 (36%)	28 (24%)	0	1
22	AP	112/114 (98%)	48 (43%)	30 (27%)	34 (30%)	0	0
22	CP	112/114 (98%)	48 (43%)	31 (28%)	33 (30%)	0	0
23	AQ	115/117 (98%)	62 (54%)	26 (23%)	27 (24%)	0	1
23	CQ	115/117 (98%)	57 (50%)	30 (26%)	28 (24%)	0	1
24	AR	101/103 (98%)	31 (31%)	25 (25%)	45 (45%)	0	0
24	CR	101/103 (98%)	37 (37%)	23 (23%)	41 (41%)	0	0
25	AS	108/110 (98%)	58 (54%)	24 (22%)	26 (24%)	0	1
25	CS	108/110 (98%)	52 (48%)	29 (27%)	27 (25%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	AT	98/100 (98%)	42 (43%)	33 (34%)	23 (24%)	0	1
26	CT	98/100 (98%)	42 (43%)	33 (34%)	23 (24%)	0	1
27	AU	101/103 (98%)	40 (40%)	36 (36%)	25 (25%)	0	1
27	CU	101/103 (98%)	38 (38%)	31 (31%)	32 (32%)	0	0
28	AV	92/94 (98%)	58 (63%)	21 (23%)	13 (14%)	0	6
28	CV	92/94 (98%)	57 (62%)	21 (23%)	14 (15%)	0	5
29	AW	82/84 (98%)	20 (24%)	28 (34%)	34 (42%)	0	0
29	CW	82/84 (98%)	17 (21%)	29 (35%)	36 (44%)	0	0
30	AX	61/63 (97%)	17 (28%)	25 (41%)	19 (31%)	0	0
30	CX	61/63 (97%)	26 (43%)	22 (36%)	13 (21%)	0	2
31	AY	56/58 (97%)	25 (45%)	17 (30%)	14 (25%)	0	1
31	CY	56/58 (97%)	26 (46%)	19 (34%)	11 (20%)	0	3
32	AZ	68/70 (97%)	30 (44%)	19 (28%)	19 (28%)	0	0
32	CZ	68/70 (97%)	34 (50%)	21 (31%)	13 (19%)	0	3
34	BB	217/240 (90%)	128 (59%)	65 (30%)	24 (11%)	0	10
34	DB	217/240 (90%)	124 (57%)	59 (27%)	34 (16%)	0	5
35	BC	205/232 (88%)	116 (57%)	59 (29%)	30 (15%)	0	5
35	DC	205/232 (88%)	112 (55%)	67 (33%)	26 (13%)	0	7
36	BD	203/205 (99%)	120 (59%)	57 (28%)	26 (13%)	0	7
36	DD	203/205 (99%)	116 (57%)	50 (25%)	37 (18%)	0	3
37	BE	149/166 (90%)	94 (63%)	33 (22%)	22 (15%)	0	5
37	DE	149/166 (90%)	77 (52%)	49 (33%)	23 (15%)	0	5
38	BF	99/135 (73%)	62 (63%)	25 (25%)	12 (12%)	0	8
38	DF	99/135 (73%)	56 (57%)	22 (22%)	21 (21%)	0	2
39	BG	149/178 (84%)	100 (67%)	34 (23%)	15 (10%)	1	12
39	DG	151/178 (85%)	94 (62%)	43 (28%)	14 (9%)	1	15
40	BH	127/129 (98%)	73 (58%)	42 (33%)	12 (9%)	1	14
40	DH	127/129 (98%)	70 (55%)	34 (27%)	23 (18%)	0	3
41	BI	125/129 (97%)	78 (62%)	35 (28%)	12 (10%)	1	14
41	DI	125/129 (97%)	73 (58%)	32 (26%)	20 (16%)	0	5
42	BJ	97/103 (94%)	59 (61%)	23 (24%)	15 (16%)	0	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	DJ	97/103 (94%)	62 (64%)	24 (25%)	11 (11%)	0	9
43	BK	115/128 (90%)	69 (60%)	31 (27%)	15 (13%)	0	7
43	DK	115/128 (90%)	73 (64%)	30 (26%)	12 (10%)	1	11
44	BL	121/123 (98%)	67 (55%)	37 (31%)	17 (14%)	0	6
44	DL	121/123 (98%)	73 (60%)	32 (26%)	16 (13%)	0	6
45	BM	113/117 (97%)	70 (62%)	32 (28%)	11 (10%)	1	13
45	DM	112/117 (96%)	78 (70%)	20 (18%)	14 (12%)	0	8
46	BN	92/100 (92%)	58 (63%)	18 (20%)	16 (17%)	0	4
46	DN	92/100 (92%)	55 (60%)	18 (20%)	19 (21%)	0	2
47	BO	86/89 (97%)	51 (59%)	26 (30%)	9 (10%)	1	11
47	DO	86/89 (97%)	51 (59%)	26 (30%)	9 (10%)	1	11
48	BP	80/82 (98%)	43 (54%)	22 (28%)	15 (19%)	0	3
48	DP	79/82 (96%)	38 (48%)	24 (30%)	17 (22%)	0	2
49	BQ	79/83 (95%)	53 (67%)	15 (19%)	11 (14%)	0	6
49	DQ	79/83 (95%)	53 (67%)	16 (20%)	10 (13%)	0	7
50	BR	54/74 (73%)	25 (46%)	19 (35%)	10 (18%)	0	3
50	DR	54/74 (73%)	24 (44%)	19 (35%)	11 (20%)	0	2
51	BS	78/91 (86%)	52 (67%)	20 (26%)	6 (8%)	1	19
51	DS	79/91 (87%)	50 (63%)	20 (25%)	9 (11%)	0	9
52	BT	83/86 (96%)	51 (61%)	20 (24%)	12 (14%)	0	5
52	DT	83/86 (96%)	52 (63%)	20 (24%)	11 (13%)	0	6
53	BU	50/71 (70%)	26 (52%)	14 (28%)	10 (20%)	0	2
53	DU	50/71 (70%)	13 (26%)	27 (54%)	10 (20%)	0	2
All	All	11307/11918 (95%)	5696 (50%)	3156 (28%)	2455 (22%)	0	1

5 of 2455 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A0	19	ASP
1	A0	21	LEU
1	A0	25	THR
1	A0	29	VAL
1	A0	36	LYS

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A0	47/47 (100%)	34 (72%)	13 (28%)	0	4
1	C0	47/47 (100%)	39 (83%)	8 (17%)	2	19
2	A1	48/48 (100%)	40 (83%)	8 (17%)	3	20
2	C1	48/48 (100%)	36 (75%)	12 (25%)	1	6
3	A2	38/38 (100%)	18 (47%)	20 (53%)	0	0
3	C2	38/38 (100%)	20 (53%)	18 (47%)	0	0
4	A3	51/51 (100%)	34 (67%)	17 (33%)	0	2
4	C3	51/51 (100%)	30 (59%)	21 (41%)	0	1
5	A4	34/34 (100%)	21 (62%)	13 (38%)	0	1
5	C4	34/34 (100%)	19 (56%)	15 (44%)	0	0
6	A5	15/15 (100%)	12 (80%)	3 (20%)	1	11
9	AC	213/218 (98%)	150 (70%)	63 (30%)	0	4
9	CC	213/218 (98%)	147 (69%)	66 (31%)	0	3
10	AD	164/164 (100%)	112 (68%)	52 (32%)	0	3
10	CD	164/164 (100%)	111 (68%)	53 (32%)	0	2
11	AE	165/165 (100%)	120 (73%)	45 (27%)	0	4
11	CE	165/165 (100%)	118 (72%)	47 (28%)	0	4
12	AF	149/149 (100%)	129 (87%)	20 (13%)	5	31
12	CF	149/149 (100%)	131 (88%)	18 (12%)	6	34
13	AG	137/137 (100%)	103 (75%)	34 (25%)	1	6
13	CG	137/137 (100%)	106 (77%)	31 (23%)	1	8
14	AH	114/114 (100%)	87 (76%)	27 (24%)	1	7
14	CH	114/114 (100%)	85 (75%)	29 (25%)	1	6
15	AI	109/109 (100%)	93 (85%)	16 (15%)	4	27
15	CI	109/109 (100%)	98 (90%)	11 (10%)	9	44
16	AJ	114/116 (98%)	74 (65%)	40 (35%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	CJ	114/116 (98%)	76 (67%)	38 (33%)	0	2
17	AK	102/104 (98%)	68 (67%)	34 (33%)	0	2
17	CK	102/104 (98%)	65 (64%)	37 (36%)	0	1
18	AL	103/103 (100%)	61 (59%)	42 (41%)	0	1
18	CL	103/103 (100%)	63 (61%)	40 (39%)	0	1
19	AM	109/109 (100%)	59 (54%)	50 (46%)	0	0
19	CM	109/109 (100%)	66 (61%)	43 (39%)	0	1
20	AN	103/103 (100%)	74 (72%)	29 (28%)	0	4
20	CN	103/103 (100%)	69 (67%)	34 (33%)	0	2
21	AO	87/87 (100%)	64 (74%)	23 (26%)	0	5
21	CO	87/87 (100%)	69 (79%)	18 (21%)	1	10
22	AP	99/99 (100%)	79 (80%)	20 (20%)	1	11
22	CP	99/99 (100%)	81 (82%)	18 (18%)	2	15
23	AQ	89/89 (100%)	58 (65%)	31 (35%)	0	2
23	CQ	89/89 (100%)	55 (62%)	34 (38%)	0	1
24	AR	84/84 (100%)	59 (70%)	25 (30%)	0	3
24	CR	84/84 (100%)	52 (62%)	32 (38%)	0	1
25	AS	93/93 (100%)	66 (71%)	27 (29%)	0	4
25	CS	93/93 (100%)	66 (71%)	27 (29%)	0	4
26	AT	83/84 (99%)	60 (72%)	23 (28%)	0	4
26	CT	83/84 (99%)	59 (71%)	24 (29%)	0	4
27	AU	83/84 (99%)	63 (76%)	20 (24%)	1	7
27	CU	83/84 (99%)	63 (76%)	20 (24%)	1	7
28	AV	78/78 (100%)	63 (81%)	15 (19%)	2	13
28	CV	78/78 (100%)	62 (80%)	16 (20%)	1	11
29	AW	62/62 (100%)	42 (68%)	20 (32%)	0	2
29	CW	62/62 (100%)	39 (63%)	23 (37%)	0	1
30	AX	55/55 (100%)	40 (73%)	15 (27%)	0	4
30	CX	55/55 (100%)	38 (69%)	17 (31%)	0	3
31	AY	48/48 (100%)	33 (69%)	15 (31%)	0	3
31	CY	48/48 (100%)	32 (67%)	16 (33%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	AZ	62/62 (100%)	44 (71%)	18 (29%)	0	4
32	CZ	62/62 (100%)	43 (69%)	19 (31%)	0	3
34	BB	180/198 (91%)	143 (79%)	37 (21%)	1	10
34	DB	180/198 (91%)	140 (78%)	40 (22%)	1	8
35	BC	170/189 (90%)	142 (84%)	28 (16%)	3	20
35	DC	170/189 (90%)	130 (76%)	40 (24%)	1	7
36	BD	172/172 (100%)	137 (80%)	35 (20%)	1	11
36	DD	172/172 (100%)	126 (73%)	46 (27%)	0	5
37	BE	113/125 (90%)	86 (76%)	27 (24%)	1	7
37	DE	113/125 (90%)	82 (73%)	31 (27%)	0	4
38	BF	87/116 (75%)	71 (82%)	16 (18%)	2	14
38	DF	87/116 (75%)	67 (77%)	20 (23%)	1	8
39	BG	123/146 (84%)	105 (85%)	18 (15%)	4	27
39	DG	125/146 (86%)	95 (76%)	30 (24%)	1	7
40	BH	104/104 (100%)	78 (75%)	26 (25%)	1	6
40	DH	104/104 (100%)	78 (75%)	26 (25%)	1	6
41	BI	105/106 (99%)	81 (77%)	24 (23%)	1	8
41	DI	105/106 (99%)	82 (78%)	23 (22%)	1	9
42	BJ	86/90 (96%)	68 (79%)	18 (21%)	1	10
42	DJ	86/90 (96%)	71 (83%)	15 (17%)	2	17
43	BK	90/98 (92%)	68 (76%)	22 (24%)	1	7
43	DK	90/98 (92%)	61 (68%)	29 (32%)	0	2
44	BL	103/103 (100%)	82 (80%)	21 (20%)	1	11
44	DL	103/103 (100%)	79 (77%)	24 (23%)	1	7
45	BM	92/95 (97%)	76 (83%)	16 (17%)	2	17
45	DM	91/95 (96%)	74 (81%)	17 (19%)	2	14
46	BN	79/83 (95%)	66 (84%)	13 (16%)	3	20
46	DN	79/83 (95%)	64 (81%)	15 (19%)	2	13
47	BO	76/77 (99%)	63 (83%)	13 (17%)	2	18
47	DO	76/77 (99%)	60 (79%)	16 (21%)	1	10
48	BP	65/65 (100%)	54 (83%)	11 (17%)	2	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	DP	65/65 (100%)	42 (65%)	23 (35%)	0	1
49	BQ	74/77 (96%)	65 (88%)	9 (12%)	6	34
49	DQ	75/77 (97%)	63 (84%)	12 (16%)	3	22
50	BR	48/64 (75%)	39 (81%)	9 (19%)	2	14
50	DR	48/64 (75%)	35 (73%)	13 (27%)	0	4
51	BS	70/78 (90%)	59 (84%)	11 (16%)	3	24
51	DS	71/78 (91%)	53 (75%)	18 (25%)	1	6
52	BT	65/65 (100%)	55 (85%)	10 (15%)	3	24
52	DT	65/65 (100%)	57 (88%)	8 (12%)	6	34
53	BU	44/61 (72%)	39 (89%)	5 (11%)	7	37
53	DU	44/61 (72%)	31 (70%)	13 (30%)	0	4
All	All	9356/9707 (96%)	6965 (74%)	2391 (26%)	0	6

5 of 2391 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	BO	11	VAL
10	CD	188	LEU
43	DK	52	ARG
50	BR	22	TYR
5	C4	23	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 328 such sidechains are listed below:

Mol	Chain	Res	Type
45	BM	90	HIS
9	CC	196	ASN
44	DL	71	HIS
47	BO	39	GLN
52	BT	69	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
33	BA	1528/1542 (99%)	618 (40%)	204 (13%)
33	DA	1529/1542 (99%)	663 (43%)	211 (13%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
7	AA	116/120 (96%)	40 (34%)	12 (10%)
7	CA	117/120 (97%)	48 (41%)	15 (12%)
8	AB	2839/2904 (97%)	1140 (40%)	396 (13%)
8	CB	2838/2904 (97%)	1137 (40%)	386 (13%)
All	All	8967/9132 (98%)	3646 (40%)	1224 (13%)

5 of 3646 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	AA	6	G
7	AA	7	G
7	AA	9	G
7	AA	12	C
7	AA	13	G

5 of 1224 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
33	BA	1107	C
8	CB	396	G
33	DA	820	U
33	BA	1198	G
7	CA	44	G

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 343 ligands modelled in this entry, 343 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 [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
33	BA	1
15	CI	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BA	1045:C	O3'	1046:A	P	4.69
1	CI	72:THR	C	73:PRO	N	4.33



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A0	56/56 (100%)	0.31	5 (8%) 12 7	109, 149, 271, 317	0
1	C0	56/56 (100%)	0.32	5 (8%) 12 7	97, 120, 190, 244	0
2	A1	54/54 (100%)	0.85	9 (16%) 2 2	124, 143, 239, 296	0
2	C1	54/54 (100%)	1.12	11 (20%) 1 1	92, 113, 223, 254	0
3	A2	46/46 (100%)	0.54	3 (6%) 22 13	74, 92, 165, 271	0
3	C2	46/46 (100%)	0.07	3 (6%) 22 13	68, 103, 198, 264	0
4	A3	64/64 (100%)	0.15	5 (7%) 16 10	80, 106, 228, 309	0
4	C3	64/64 (100%)	-0.03	2 (3%) 52 38	69, 99, 174, 229	0
5	A4	38/38 (100%)	1.08	9 (23%) 1 1	115, 135, 250, 284	0
5	C4	38/38 (100%)	0.75	5 (13%) 4 4	124, 144, 238, 298	0
6	A5	16/16 (100%)	-0.16	0 100 100	73, 108, 197, 216	0
7	AA	117/120 (97%)	-0.47	0 100 100	78, 127, 174, 316	0
7	CA	117/120 (97%)	-0.50	1 (0%) 85 76	71, 127, 170, 285	0
8	AB	2841/2904 (97%)	-0.38	32 (1%) 82 71	57, 105, 213, 373	0
8	CB	2841/2904 (97%)	-0.53	12 (0%) 93 89	41, 89, 202, 421	0
9	AC	268/273 (98%)	0.13	14 (5%) 31 22	71, 107, 196, 257	0
9	CC	268/273 (98%)	-0.03	12 (4%) 37 26	63, 91, 165, 248	0
10	AD	209/209 (100%)	0.24	9 (4%) 39 27	12, 127, 226, 325	0
10	CD	209/209 (100%)	-0.04	9 (4%) 39 27	11, 94, 186, 271	0
11	AE	201/201 (100%)	0.21	17 (8%) 13 9	92, 120, 206, 299	0
11	CE	201/201 (100%)	0.34	26 (12%) 5 4	88, 117, 224, 290	0
12	AF	178/178 (100%)	0.26	13 (7%) 18 11	121, 170, 253, 334	0
12	CF	178/178 (100%)	0.26	12 (6%) 21 13	92, 155, 224, 286	0
13	AG	176/176 (100%)	0.17	17 (9%) 10 6	100, 137, 207, 246	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	CG	176/176 (100%)	0.51	24 (13%) 4 3	88, 138, 222, 271	0
14	AH	149/149 (100%)	1.74	48 (32%) 1 1	71, 314, 427, 456	0
14	CH	149/149 (100%)	0.40	13 (8%) 13 9	107, 147, 233, 274	0
15	AI	141/141 (100%)	1.91	51 (36%) 0 1	155, 233, 307, 356	0
15	CI	141/141 (100%)	2.79	62 (43%) 0 1	219, 343, 422, 470	0
16	AJ	141/142 (99%)	0.07	8 (5%) 27 18	105, 130, 217, 267	0
16	CJ	141/142 (99%)	0.18	5 (3%) 48 34	104, 121, 207, 250	0
17	AK	122/123 (99%)	-0.20	0 100 100	81, 109, 162, 234	0
17	CK	122/123 (99%)	-0.45	0 100 100	80, 94, 127, 208	0
18	AL	144/144 (100%)	1.06	21 (14%) 3 3	94, 138, 281, 363	0
18	CL	144/144 (100%)	0.64	22 (15%) 3 2	83, 128, 275, 315	0
19	AM	136/136 (100%)	0.15	12 (8%) 12 8	105, 126, 222, 268	0
19	CM	136/136 (100%)	-0.01	6 (4%) 38 26	77, 108, 223, 279	0
20	AN	127/127 (100%)	0.07	6 (4%) 35 24	96, 114, 200, 251	0
20	CN	127/127 (100%)	-0.07	6 (4%) 35 24	58, 78, 155, 257	0
21	AO	117/117 (100%)	0.24	10 (8%) 13 9	107, 162, 236, 299	0
21	CO	117/117 (100%)	0.42	13 (11%) 7 5	52, 118, 211, 255	0
22	AP	114/114 (100%)	-0.07	2 (1%) 71 58	85, 123, 219, 281	0
22	CP	114/114 (100%)	-0.22	2 (1%) 71 58	77, 96, 196, 257	0
23	AQ	117/117 (100%)	-0.24	0 100 100	70, 106, 152, 203	0
23	CQ	117/117 (100%)	-0.26	1 (0%) 85 76	70, 93, 148, 225	0
24	AR	103/103 (100%)	0.23	3 (2%) 55 40	105, 145, 250, 346	0
24	CR	103/103 (100%)	0.31	8 (7%) 16 10	87, 132, 229, 286	0
25	AS	110/110 (100%)	0.13	3 (2%) 58 43	77, 106, 167, 279	0
25	CS	110/110 (100%)	-0.06	2 (1%) 71 58	49, 85, 152, 211	0
26	AT	100/100 (100%)	0.03	4 (4%) 42 29	94, 130, 222, 250	0
26	CT	100/100 (100%)	0.43	13 (13%) 5 4	85, 120, 248, 278	0
27	AU	103/103 (100%)	1.10	24 (23%) 1 1	90, 140, 235, 264	0
27	CU	103/103 (100%)	0.90	21 (20%) 1 1	118, 162, 256, 281	0
28	AV	94/94 (100%)	-0.20	3 (3%) 51 37	86, 136, 209, 234	0
28	CV	94/94 (100%)	-0.16	4 (4%) 39 27	87, 125, 194, 215	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
29	AW	84/84 (100%)	1.19	16 (19%) 2 1	116, 147, 244, 330	0
29	CW	84/84 (100%)	0.71	12 (14%) 4 3	111, 136, 238, 275	0
30	AX	63/63 (100%)	-0.03	4 (6%) 23 14	84, 130, 208, 247	0
30	CX	63/63 (100%)	0.44	11 (17%) 2 1	86, 150, 233, 320	0
31	AY	58/58 (100%)	1.53	15 (25%) 1 1	116, 143, 272, 279	0
31	CY	58/58 (100%)	0.98	7 (12%) 6 5	126, 138, 240, 249	0
32	AZ	70/70 (100%)	0.20	5 (7%) 19 11	66, 104, 170, 258	0
32	CZ	70/70 (100%)	-0.04	3 (4%) 39 27	70, 91, 169, 255	0
33	BA	1530/1542 (99%)	-0.26	17 (1%) 82 71	70, 137, 279, 497	0
33	DA	1530/1542 (99%)	-0.45	7 (0%) 91 86	45, 111, 224, 368	0
34	BB	219/240 (91%)	0.00	7 (3%) 51 37	94, 175, 269, 316	0
34	DB	219/240 (91%)	0.23	17 (7%) 16 10	108, 159, 243, 292	0
35	BC	207/232 (89%)	0.20	20 (9%) 10 6	87, 169, 255, 315	0
35	DC	207/232 (89%)	-0.02	11 (5%) 30 21	113, 140, 207, 226	0
36	BD	205/205 (100%)	-0.16	2 (0%) 84 73	61, 139, 230, 325	0
36	DD	205/205 (100%)	-0.24	2 (0%) 84 73	71, 102, 169, 227	0
37	BE	151/166 (90%)	0.27	10 (6%) 22 13	75, 156, 254, 336	0
37	DE	151/166 (90%)	0.02	6 (3%) 42 29	56, 99, 174, 250	0
38	BF	101/135 (74%)	-0.02	6 (5%) 26 16	57, 140, 224, 279	0
38	DF	101/135 (74%)	-0.09	0 100 100	110, 137, 200, 247	0
39	BG	151/178 (84%)	0.73	26 (17%) 2 2	94, 206, 288, 333	0
39	DG	153/178 (85%)	0.09	5 (3%) 50 36	44, 144, 206, 228	0
40	BH	129/129 (100%)	0.27	9 (6%) 19 12	76, 157, 231, 297	0
40	DH	129/129 (100%)	-0.21	2 (1%) 74 61	70, 98, 166, 216	0
41	BI	127/129 (98%)	0.90	24 (18%) 2 1	90, 194, 271, 307	0
41	DI	127/129 (98%)	0.33	7 (5%) 29 19	103, 165, 231, 281	0
42	BJ	99/103 (96%)	1.63	34 (34%) 0 1	131, 254, 373, 423	0
42	DJ	99/103 (96%)	0.60	14 (14%) 4 3	130, 173, 223, 237	0
43	BK	117/128 (91%)	-0.09	3 (2%) 59 45	54, 128, 245, 290	0
43	DK	117/128 (91%)	-0.03	4 (3%) 49 35	69, 100, 165, 222	0
44	BL	123/123 (100%)	0.03	4 (3%) 50 36	50, 138, 215, 332	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	DL	123/123 (100%)	-0.25	1 (0%) 87 78	64, 95, 150, 211	0
45	BM	115/117 (98%)	1.29	30 (26%) 1 1	144, 252, 315, 344	0
45	DM	114/117 (97%)	0.63	16 (14%) 4 3	113, 171, 221, 288	0
46	BN	96/100 (96%)	0.56	10 (10%) 8 6	85, 188, 308, 367	0
46	DN	96/100 (96%)	0.48	12 (12%) 5 5	105, 153, 250, 295	0
47	BO	88/89 (98%)	-0.10	0 100 100	67, 133, 213, 255	0
47	DO	88/89 (98%)	-0.34	0 100 100	73, 105, 170, 201	0
48	BP	82/82 (100%)	1.03	19 (23%) 1 1	90, 168, 269, 347	0
48	DP	81/82 (98%)	0.43	7 (8%) 13 9	69, 93, 145, 202	0
49	BQ	81/83 (97%)	0.43	6 (7%) 17 11	101, 180, 266, 301	0
49	DQ	81/83 (97%)	0.01	1 (1%) 81 69	65, 109, 172, 212	0
50	BR	56/74 (75%)	-0.20	1 (1%) 71 58	66, 117, 216, 283	0
50	DR	56/74 (75%)	0.40	2 (3%) 46 33	74, 103, 172, 253	0
51	BS	80/91 (87%)	1.66	26 (32%) 1 1	152, 267, 315, 366	0
51	DS	81/91 (89%)	0.78	15 (18%) 2 1	122, 182, 230, 249	0
52	BT	85/86 (98%)	-0.15	0 100 100	76, 155, 224, 256	0
52	DT	85/86 (98%)	0.15	4 (4%) 35 24	79, 97, 185, 219	0
53	BU	52/71 (73%)	0.06	3 (5%) 26 17	91, 171, 256, 300	0
53	DU	52/71 (73%)	-0.36	0 100 100	95, 140, 201, 249	0
All	All	20487/21050 (97%)	-0.01	1091 (5%) 30 21	11, 121, 254, 497	0

The worst 5 of 1091 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
15	CI	98	GLY	28.1
15	CI	83	ALA	21.9
18	AL	98	ALA	17.6
15	AI	70	THR	17.3
15	CI	137	LEU	16.4

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	CB	3080	1/1	0.83	0.47	23.73	55,55,55,55	1
54	MG	AB	4091	1/1	0.94	0.44	14.38	34,34,34,34	0
54	MG	BA	4002	1/1	0.88	0.30	12.22	86,86,86,86	0
54	MG	CB	3028	1/1	0.99	0.31	8.56	46,46,46,46	0
54	MG	CB	3044	1/1	1.00	0.38	7.49	83,83,83,83	0
54	MG	CB	3041	1/1	0.96	0.19	6.86	19,19,19,19	0
54	MG	CB	3070	1/1	0.97	0.30	6.45	33,33,33,33	0
54	MG	DA	1644	1/1	0.94	0.30	4.85	53,53,53,53	0
54	MG	CB	3077	1/1	0.92	0.17	4.54	76,76,76,76	0
54	MG	BA	4027	1/1	0.94	0.30	4.53	68,68,68,68	0
54	MG	AB	4050	1/1	0.88	0.32	4.48	49,49,49,49	0
54	MG	AB	4057	1/1	0.96	0.29	4.10	49,49,49,49	0
54	MG	BA	4001	1/1	0.95	0.25	3.03	69,69,69,69	0
54	MG	AB	4082	1/1	0.99	0.27	2.80	50,50,50,50	0
54	MG	AB	4061	1/1	0.96	0.18	2.47	35,35,35,35	0
54	MG	AB	4085	1/1	0.97	0.24	2.28	53,53,53,53	0
54	MG	BA	4017	1/1	0.95	0.25	2.21	42,42,42,42	0
54	MG	CB	3029	1/1	0.92	0.18	1.96	39,39,39,39	0
54	MG	CB	3071	1/1	0.93	0.21	1.46	52,52,52,52	0
54	MG	CB	3040	1/1	0.95	0.23	1.31	46,46,46,46	0
54	MG	BA	4028	1/1	0.83	0.19	0.88	61,61,61,61	0
54	MG	AB	4065	1/1	0.98	0.17	0.85	20,20,20,20	0
54	MG	CB	3049	1/1	0.93	0.16	0.67	30,30,30,30	1
54	MG	AB	4101	1/1	0.96	0.17	0.60	25,25,25,25	0
54	MG	AB	4013	1/1	0.87	0.18	0.53	46,46,46,46	0
54	MG	BA	4033	1/1	0.95	0.21	0.52	90,90,90,90	0
54	MG	DA	1611	1/1	0.91	0.16	0.36	51,51,51,51	0
54	MG	AB	4029	1/1	0.98	0.16	0.32	55,55,55,55	0
54	MG	AB	4011	1/1	0.98	0.18	0.16	45,45,45,45	0
54	MG	DA	1616	1/1	0.97	0.15	0.14	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	1638	1/1	0.99	0.13	-0.18	12,12,12,12	0
54	MG	CB	3081	1/1	0.96	0.13	-0.20	10,10,10,10	0
54	MG	CB	3095	1/1	0.96	0.16	-0.27	22,22,22,22	0
54	MG	CB	3073	1/1	0.99	0.14	-0.31	14,14,14,14	0
54	MG	CB	3048	1/1	0.99	0.19	-0.48	4,4,4,4	0
54	MG	AB	4038	1/1	0.96	0.12	-0.56	30,30,30,30	0
54	MG	DA	1646	1/1	0.99	0.18	-0.56	50,50,50,50	0
54	MG	DA	1615	1/1	0.98	0.12	-0.62	95,95,95,95	0
54	MG	CB	3037	1/1	0.95	0.13	-0.63	10,10,10,10	0
54	MG	AB	4097	1/1	0.95	0.15	-0.65	17,17,17,17	0
54	MG	AB	4109	1/1	0.91	0.14	-0.76	34,34,34,34	0
54	MG	CL	201	1/1	0.95	0.07	-0.97	43,43,43,43	0
54	MG	AB	4005	1/1	0.98	0.14	-1.03	11,11,11,11	0
54	MG	BA	4008	1/1	0.94	0.12	-1.06	21,21,21,21	0
54	MG	AB	4051	1/1	0.99	0.12	-1.15	7,7,7,7	0
54	MG	CB	3059	1/1	0.95	0.12	-1.18	12,12,12,12	0
54	MG	CB	3056	1/1	0.97	0.15	-1.19	8,8,8,8	0
54	MG	BA	4038	1/1	0.96	0.10	-1.41	50,50,50,50	0
54	MG	BA	4006	1/1	0.97	0.12	-1.50	42,42,42,42	0
54	MG	CB	3043	1/1	0.92	0.07	-1.50	69,69,69,69	0
54	MG	CB	3024	1/1	0.99	0.11	-1.53	21,21,21,21	0
54	MG	AB	4081	1/1	0.98	0.11	-1.56	60,60,60,60	0
54	MG	CC	301	1/1	0.99	0.07	-1.59	89,89,89,89	0
54	MG	BA	4014	1/1	0.88	0.12	-1.59	44,44,44,44	0
54	MG	AB	4055	1/1	0.97	0.07	-1.70	68,68,68,68	0
54	MG	DA	1604	1/1	0.98	0.13	-1.73	35,35,35,35	0
54	MG	AE	301	1/1	0.98	0.13	-1.76	10,10,10,10	0
54	MG	CB	3033	1/1	0.96	0.11	-1.79	33,33,33,33	0
54	MG	DN	201	1/1	0.96	0.09	-1.80	48,48,48,48	0
54	MG	CB	3019	1/1	0.97	0.12	-1.81	11,11,11,11	0
54	MG	AB	4084	1/1	0.94	0.09	-1.85	21,21,21,21	0
54	MG	DA	1641	1/1	0.94	0.09	-1.90	63,63,63,63	0
54	MG	CB	3084	1/1	0.97	0.10	-1.93	24,24,24,24	0
54	MG	DA	1635	1/1	0.97	0.15	-1.99	41,41,41,41	0
54	MG	CB	3098	1/1	0.97	0.08	-2.01	7,7,7,7	0
54	MG	AB	4093	1/1	0.94	0.09	-2.21	4,4,4,4	0
54	MG	CB	3074	1/1	0.93	0.11	-2.31	33,33,33,33	0
54	MG	CB	3008	1/1	0.98	0.11	-2.49	16,16,16,16	0
54	MG	AB	4001	1/1	0.96	0.06	-2.52	5,5,5,5	0
54	MG	CB	3025	1/1	0.97	0.09	-2.54	27,27,27,27	0
54	MG	AB	4019	1/1	0.99	0.11	-2.56	29,29,29,29	0
54	MG	DA	1631	1/1	0.99	0.05	-2.62	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	AB	4036	1/1	0.88	0.09	-2.67	12,12,12,12	0
54	MG	CB	3057	1/1	0.97	0.11	-2.68	7,7,7,7	0
54	MG	CB	3069	1/1	0.99	0.10	-2.80	10,10,10,10	0
54	MG	CB	3018	1/1	0.98	0.10	-2.92	25,25,25,25	0
54	MG	CB	3088	1/1	0.99	0.05	-3.00	52,52,52,52	0
54	MG	CB	3062	1/1	0.98	0.08	-3.20	7,7,7,7	0
54	MG	AB	4086	1/1	0.99	0.10	-3.50	39,39,39,39	0
54	MG	AB	4068	1/1	0.98	0.08	-3.53	21,21,21,21	0
54	MG	DA	1654	1/1	0.98	0.07	-3.55	13,13,13,13	0
54	MG	CB	3002	1/1	0.99	0.08	-3.61	54,54,54,54	0
54	MG	BA	4036	1/1	0.93	0.08	-3.81	5,5,5,5	0
54	MG	CB	3047	1/1	0.99	0.06	-4.00	10,10,10,10	0
54	MG	CB	3001	1/1	0.99	0.04	-4.53	9,9,9,9	0
54	MG	DA	1639	1/1	0.98	0.09	-4.73	79,79,79,79	0
54	MG	CB	3003	1/1	0.99	0.05	-5.14	8,8,8,8	0
54	MG	AB	4083	1/1	0.94	0.12	-5.18	29,29,29,29	0
54	MG	BA	4040	1/1	0.99	0.07	-8.09	49,49,49,49	0
54	MG	CB	3105	1/1	0.99	0.05	-11.66	20,20,20,20	0
54	MG	AB	4106	1/1	0.98	0.06	-	9,9,9,9	0
54	MG	DA	1637	1/1	0.96	0.20	-	109,109,109,109	0
54	MG	BA	4043	1/1	0.89	0.69	-	25,25,25,25	0
54	MG	AB	4022	1/1	0.95	0.33	-	11,11,11,11	0
54	MG	DA	1610	1/1	0.83	0.22	-	48,48,48,48	0
54	MG	AB	4042	1/1	0.94	0.14	-	90,90,90,90	0
54	MG	AB	4074	1/1	0.97	0.12	-	50,50,50,50	0
54	MG	CB	3083	1/1	0.99	0.12	-	9,9,9,9	0
54	MG	CB	3005	1/1	0.97	0.17	-	26,26,26,26	0
54	MG	BA	4025	1/1	0.90	0.17	-	37,37,37,37	0
54	MG	CB	3075	1/1	0.97	0.14	-	61,61,61,61	0
54	MG	AB	4066	1/1	0.98	0.13	-	33,33,33,33	0
54	MG	DA	1622	1/1	0.99	0.37	-	27,27,27,27	0
54	MG	CB	3092	1/1	0.94	0.11	-	7,7,7,7	0
54	MG	AB	4041	1/1	0.97	0.09	-	11,11,11,11	0
54	MG	CB	3053	1/1	0.96	0.12	-	5,5,5,5	0
54	MG	BA	4054	1/1	0.81	1.04	-	90,90,90,90	0
54	MG	CB	3066	1/1	0.97	0.18	-	45,45,45,45	0
54	MG	BA	4053	1/1	0.77	0.55	-	109,109,109,109	0
54	MG	CB	3055	1/1	0.99	0.06	-	5,5,5,5	0
54	MG	DA	1617	1/1	0.98	0.10	-	10,10,10,10	0
54	MG	CB	3030	1/1	0.97	0.18	-	17,17,17,17	0
54	MG	CB	3091	1/1	0.97	0.11	-	42,42,42,42	0
54	MG	AB	4025	1/1	0.94	0.22	-	129,129,129,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	CB	3104	1/1	0.97	0.46	-	6,6,6,6	0
54	MG	BA	4045	1/1	0.99	0.10	-	59,59,59,59	0
54	MG	AB	4015	1/1	0.98	0.09	-	3,3,3,3	0
54	MG	BA	4034	1/1	0.93	0.18	-	48,48,48,48	0
54	MG	AB	4032	1/1	0.98	0.17	-	35,35,35,35	0
54	MG	CB	3063	1/1	0.95	0.20	-	11,11,11,11	0
54	MG	CB	3106	1/1	0.95	0.24	-	20,20,20,20	0
54	MG	DA	1647	1/1	0.96	0.30	-	30,30,30,30	0
54	MG	AB	4072	1/1	0.96	0.14	-	44,44,44,44	0
54	MG	CB	3051	1/1	0.98	0.25	-	12,12,12,12	0
54	MG	AB	4008	1/1	0.96	0.09	-	38,38,38,38	0
54	MG	AB	4040	1/1	0.99	0.12	-	77,77,77,77	0
54	MG	AB	4023	1/1	0.93	0.19	-	66,66,66,66	0
54	MG	AB	4006	1/1	0.98	0.08	-	12,12,12,12	0
54	MG	DA	1620	1/1	0.97	0.09	-	19,19,19,19	0
54	MG	BA	4015	1/1	0.95	0.11	-	59,59,59,59	0
54	MG	DA	1649	1/1	0.95	0.14	-	45,45,45,45	0
54	MG	BA	4039	1/1	0.94	0.24	-	31,31,31,31	0
54	MG	BA	4005	1/1	0.99	0.21	-	59,59,59,59	0
54	MG	DA	1629	1/1	0.98	0.24	-	52,52,52,52	0
54	MG	AB	4090	1/1	0.93	0.27	-	37,37,37,37	0
54	MG	CB	3038	1/1	0.74	0.18	-	58,58,58,58	0
54	MG	AB	4079	1/1	0.99	0.20	-	43,43,43,43	0
54	MG	AB	4037	1/1	0.97	0.13	-	25,25,25,25	0
54	MG	AB	4052	1/1	0.99	0.09	-	25,25,25,25	0
54	MG	CB	3097	1/1	0.98	0.10	-	9,9,9,9	0
54	MG	BA	4020	1/1	0.95	0.39	-	77,77,77,77	0
54	MG	DA	1655	1/1	0.98	0.07	-	12,12,12,12	0
54	MG	AB	4010	1/1	0.98	0.10	-	32,32,32,32	0
54	MG	CB	3032	1/1	0.95	0.27	-	52,52,52,52	0
54	MG	AB	4058	1/1	0.98	0.09	-	20,20,20,20	0
54	MG	CB	3021	1/1	0.97	0.05	-	22,22,22,22	0
54	MG	CB	3076	1/1	0.91	0.29	-	15,15,15,15	0
54	MG	CB	3015	1/1	0.97	0.15	-	9,9,9,9	0
54	MG	AB	4089	1/1	0.99	0.06	-	31,31,31,31	0
54	MG	BA	4052	1/1	0.94	0.13	-	33,33,33,33	0
54	MG	CB	3016	1/1	0.99	0.07	-	18,18,18,18	0
54	MG	AB	4003	1/1	0.96	0.15	-	26,26,26,26	0
54	MG	CB	3007	1/1	0.99	0.15	-	25,25,25,25	0
54	MG	DA	1606	1/1	0.96	0.09	-	18,18,18,18	0
54	MG	AB	4100	1/1	0.99	0.17	-	25,25,25,25	0
54	MG	AB	4088	1/1	0.93	0.14	-	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	1613	1/1	0.95	0.19	-	62,62,62,62	0
54	MG	AB	4095	1/1	0.93	0.14	-	47,47,47,47	0
54	MG	AB	4047	1/1	0.90	0.29	-	48,48,48,48	0
54	MG	AB	4004	1/1	0.98	0.15	-	41,41,41,41	0
54	MG	DA	1658	1/1	0.98	0.45	-	47,47,47,47	0
54	MG	AB	4053	1/1	0.95	0.12	-	14,14,14,14	0
54	MG	CB	3086	1/1	0.99	0.10	-	17,17,17,17	0
54	MG	BA	4051	1/1	0.98	0.13	-	79,79,79,79	0
54	MG	CB	3078	1/1	0.95	0.12	-	57,57,57,57	0
54	MG	BA	4047	1/1	0.98	0.09	-	29,29,29,29	0
54	MG	CB	3042	1/1	0.98	0.08	-	18,18,18,18	0
54	MG	CB	3109	1/1	0.99	0.09	-	16,16,16,16	0
54	MG	CB	3010	1/1	0.93	0.15	-	30,30,30,30	0
54	MG	CB	3014	1/1	0.94	0.25	-	33,33,33,33	0
54	MG	DA	1627	1/1	0.96	0.14	-	51,51,51,51	0
54	MG	CB	3058	1/1	0.98	0.07	-	31,31,31,31	0
54	MG	AB	4080	1/1	0.97	0.13	-	17,17,17,17	0
54	MG	AB	4069	1/1	0.92	0.17	-	51,51,51,51	0
54	MG	CB	3061	1/1	0.95	0.12	-	31,31,31,31	0
54	MG	CB	3006	1/1	0.96	0.08	-	19,19,19,19	0
54	MG	AB	4056	1/1	0.98	0.36	-	9,9,9,9	0
54	MG	AB	4098	1/1	0.92	0.38	-	37,37,37,37	0
54	MG	BA	4003	1/1	0.98	0.20	-	29,29,29,29	0
54	MG	CB	3054	1/1	0.99	0.23	-	13,13,13,13	0
54	MG	DA	1632	1/1	0.85	0.39	-	90,90,90,90	0
54	MG	DA	1630	1/1	0.94	0.07	-	29,29,29,29	0
54	MG	DA	1628	1/1	0.94	0.32	-	33,33,33,33	1
54	MG	AB	4105	1/1	0.98	0.09	-	33,33,33,33	0
54	MG	AB	4070	1/1	0.99	0.16	-	20,20,20,20	0
54	MG	CB	3035	1/1	0.97	0.09	-	20,20,20,20	0
54	MG	AB	4045	1/1	0.93	0.09	-	51,51,51,51	0
54	MG	DA	1624	1/1	0.94	0.30	-	57,57,57,57	0
54	MG	DA	1614	1/1	0.98	0.19	-	25,25,25,25	0
54	MG	BA	4048	1/1	0.96	0.12	-	73,73,73,73	0
54	MG	AB	4002	1/1	0.97	0.18	-	27,27,27,27	0
54	MG	BA	4056	1/1	0.65	0.32	-	81,81,81,81	0
54	MG	BA	4016	1/1	0.98	0.06	-	47,47,47,47	0
54	MG	CB	3064	1/1	0.97	0.15	-	63,63,63,63	0
54	MG	BA	4012	1/1	0.94	0.20	-	54,54,54,54	0
54	MG	AB	4103	1/1	0.95	0.20	-	13,13,13,13	0
54	MG	AB	4034	1/1	0.94	0.19	-	51,51,51,51	0
54	MG	DA	1643	1/1	0.98	0.09	-	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	1650	1/1	0.98	0.13	-	48,48,48,48	0
54	MG	DA	1602	1/1	0.97	0.08	-	13,13,13,13	0
54	MG	BA	4029	1/1	0.89	0.11	-	44,44,44,44	0
54	MG	DA	1601	1/1	0.97	0.09	-	28,28,28,28	0
54	MG	CB	3072	1/1	0.96	0.19	-	42,42,42,42	0
54	MG	BA	4032	1/1	0.99	0.20	-	27,27,27,27	0
54	MG	CB	3082	1/1	0.96	0.14	-	17,17,17,17	0
54	MG	AB	4033	1/1	0.97	0.31	-	52,52,52,52	0
54	MG	CB	3009	1/1	0.93	0.12	-	13,13,13,13	0
54	MG	AB	4039	1/1	0.99	0.06	-	25,25,25,25	0
54	MG	DA	1640	1/1	0.92	0.16	-	17,17,17,17	0
54	MG	CB	3034	1/1	0.96	0.16	-	7,7,7,7	0
54	MG	DA	1608	1/1	0.79	0.32	-	41,41,41,41	0
54	MG	DA	1636	1/1	0.89	0.07	-	43,43,43,43	0
54	MG	BA	4042	1/1	0.94	0.27	-	69,69,69,69	0
54	MG	AB	4030	1/1	0.98	0.07	-	34,34,34,34	0
54	MG	BA	4035	1/1	0.97	0.55	-	30,30,30,30	0
54	MG	AB	4046	1/1	0.95	0.10	-	26,26,26,26	0
54	MG	BA	4023	1/1	0.77	0.16	-	63,63,63,63	1
54	MG	CB	3087	1/1	0.93	0.27	-	25,25,25,25	0
54	MG	DA	1645	1/1	0.98	0.08	-	56,56,56,56	0
54	MG	BA	4030	1/1	0.98	0.49	-	34,34,34,34	0
54	MG	CB	3022	1/1	0.97	0.08	-	21,21,21,21	0
54	MG	AB	4014	1/1	0.99	0.22	-	18,18,18,18	0
54	MG	CB	3090	1/1	0.97	0.12	-	67,67,67,67	0
54	MG	DA	1621	1/1	0.98	0.16	-	18,18,18,18	0
54	MG	CB	3079	1/1	0.94	0.16	-	54,54,54,54	0
54	MG	CB	3050	1/1	0.91	0.10	-	45,45,45,45	0
54	MG	DA	1648	1/1	0.98	0.11	-	43,43,43,43	0
54	MG	BA	4011	1/1	0.90	0.08	-	56,56,56,56	0
54	MG	AB	4017	1/1	0.99	0.39	-	10,10,10,10	0
54	MG	AB	4009	1/1	0.94	0.13	-	58,58,58,58	0
54	MG	AB	4054	1/1	0.99	0.10	-	10,10,10,10	0
54	MG	AB	4043	1/1	0.99	0.47	-	16,16,16,16	0
54	MG	CB	3089	1/1	0.96	0.14	-	38,38,38,38	0
54	MG	CB	3100	1/1	0.93	0.15	-	43,43,43,43	0
54	MG	CB	3004	1/1	0.97	0.14	-	9,9,9,9	0
54	MG	BA	4018	1/1	0.95	0.12	-	64,64,64,64	0
54	MG	BA	4044	1/1	0.94	0.21	-	86,86,86,86	0
54	MG	BA	4058	1/1	0.98	0.06	-	78,78,78,78	0
54	MG	AB	4007	1/1	0.94	0.15	-	37,37,37,37	0
54	MG	DA	1653	1/1	0.95	0.13	-	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	CB	3103	1/1	0.97	0.36	-	10,10,10,10	0
54	MG	CB	3099	1/1	0.91	0.40	-	43,43,43,43	0
54	MG	BA	4021	1/1	0.88	0.32	-	28,28,28,28	1
54	MG	BA	4009	1/1	0.98	0.10	-	34,34,34,34	0
54	MG	AB	4059	1/1	0.97	0.12	-	55,55,55,55	0
54	MG	DA	1651	1/1	0.91	0.17	-	56,56,56,56	0
54	MG	DA	1607	1/1	0.91	0.20	-	54,54,54,54	0
54	MG	DA	1626	1/1	0.85	0.26	-	11,11,11,11	1
54	MG	BA	4050	1/1	0.96	0.16	-	51,51,51,51	0
54	MG	BA	4055	1/1	0.99	0.11	-	27,27,27,27	0
54	MG	AB	4044	1/1	0.97	0.05	-	17,17,17,17	0
54	MG	AB	4092	1/1	0.94	0.48	-	27,27,27,27	1
54	MG	DA	1609	1/1	0.93	0.21	-	56,56,56,56	0
54	MG	CB	3107	1/1	0.90	0.16	-	22,22,22,22	0
54	MG	DA	1623	1/1	0.99	0.32	-	20,20,20,20	0
54	MG	BA	4037	1/1	0.88	0.11	-	58,58,58,58	0
54	MG	AB	4096	1/1	0.90	0.35	-	46,46,46,46	0
54	MG	AB	4102	1/1	0.99	0.09	-	63,63,63,63	0
54	MG	CB	3065	1/1	0.96	0.10	-	26,26,26,26	0
54	MG	CB	3060	1/1	0.94	0.20	-	78,78,78,78	0
54	MG	AB	4077	1/1	0.97	0.28	-	28,28,28,28	0
54	MG	CB	3045	1/1	0.98	0.33	-	67,67,67,67	0
54	MG	AB	4087	1/1	0.98	0.12	-	38,38,38,38	0
54	MG	BA	4013	1/1	0.88	0.32	-	73,73,73,73	0
54	MG	CB	3093	1/1	0.95	0.26	-	3,3,3,3	0
54	MG	DA	1603	1/1	0.99	0.10	-	22,22,22,22	0
54	MG	BT	101	1/1	0.90	0.22	-	27,27,27,27	0
54	MG	AB	4024	1/1	0.96	0.14	-	54,54,54,54	0
54	MG	AB	4018	1/1	0.98	0.05	-	32,32,32,32	0
54	MG	AB	4094	1/1	0.98	0.05	-	15,15,15,15	0
54	MG	BA	4019	1/1	0.98	0.28	-	11,11,11,11	0
54	MG	AB	4020	1/1	0.98	0.46	-	67,67,67,67	0
54	MG	CB	3046	1/1	0.99	0.09	-	29,29,29,29	0
54	MG	AB	4060	1/1	0.98	0.10	-	36,36,36,36	0
54	MG	CB	3052	1/1	0.96	0.20	-	43,43,43,43	0
54	MG	AB	4027	1/1	0.98	0.20	-	22,22,22,22	0
54	MG	DA	1612	1/1	0.69	0.45	-	81,81,81,81	0
54	MG	DA	1656	1/1	0.98	0.07	-	15,15,15,15	0
54	MG	DA	1619	1/1	0.88	0.62	-	64,64,64,64	0
54	MG	CB	3096	1/1	0.97	0.21	-	38,38,38,38	0
54	MG	AB	4048	1/1	0.94	0.24	-	22,22,22,22	0
54	MG	CB	3020	1/1	0.97	0.20	-	8,8,8,8	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	AB	4078	1/1	0.95	0.15	-	35,35,35,35	0
54	MG	AB	4076	1/1	0.98	0.35	-	23,23,23,23	0
54	MG	BA	4046	1/1	0.93	0.32	-	62,62,62,62	0
54	MG	AB	4021	1/1	0.97	0.11	-	33,33,33,33	0
54	MG	CB	3101	1/1	0.99	0.33	-	8,8,8,8	0
54	MG	DA	1642	1/1	0.99	0.06	-	31,31,31,31	0
54	MG	DA	1605	1/1	0.96	0.14	-	76,76,76,76	0
54	MG	CB	3108	1/1	0.86	0.59	-	53,53,53,53	1
54	MG	BA	4049	1/1	0.96	0.15	-	100,100,100,100	0
54	MG	CB	3023	1/1	0.96	0.09	-	7,7,7,7	0
54	MG	AB	4099	1/1	0.96	0.41	-	12,12,12,12	1
54	MG	AB	4012	1/1	0.96	0.08	-	44,44,44,44	0
54	MG	CB	3039	1/1	0.99	0.08	-	27,27,27,27	0
54	MG	AB	4049	1/1	0.99	0.28	-	21,21,21,21	0
54	MG	CB	3026	1/1	0.94	0.11	-	10,10,10,10	0
54	MG	BA	4026	1/1	0.93	0.17	-	75,75,75,75	0
54	MG	CB	3036	1/1	0.98	0.31	-	19,19,19,19	0
54	MG	CB	3102	1/1	0.98	0.18	-	17,17,17,17	0
54	MG	CB	3068	1/1	0.97	0.11	-	59,59,59,59	0
54	MG	BA	4007	1/1	0.94	0.72	-	81,81,81,81	0
54	MG	DA	1661	1/1	0.95	0.11	-	13,13,13,13	0
54	MG	DA	1625	1/1	0.94	0.19	-	37,37,37,37	1
54	MG	AB	4073	1/1	0.97	0.18	-	21,21,21,21	0
54	MG	DA	1652	1/1	0.99	0.03	-	21,21,21,21	0
54	MG	DA	1657	1/1	0.98	0.71	-	63,63,63,63	0
54	MG	BA	4010	1/1	0.99	0.09	-	17,17,17,17	0
54	MG	BA	4057	1/1	0.91	0.11	-	29,29,29,29	0
54	MG	CB	3031	1/1	0.98	0.12	-	55,55,55,55	0
54	MG	AB	4026	1/1	0.96	0.14	-	78,78,78,78	0
54	MG	BA	4031	1/1	0.97	0.11	-	40,40,40,40	0
54	MG	CB	3085	1/1	0.98	0.18	-	16,16,16,16	0
54	MG	BA	4004	1/1	0.97	0.12	-	34,34,34,34	0
54	MG	AB	4062	1/1	0.84	0.16	-	30,30,30,30	0
54	MG	CB	3012	1/1	0.97	0.07	-	10,10,10,10	0
54	MG	AB	4035	1/1	0.99	0.07	-	39,39,39,39	0
54	MG	AB	4071	1/1	0.98	0.26	-	29,29,29,29	0
54	MG	AB	4107	1/1	0.94	0.12	-	6,6,6,6	0
54	MG	BN	201	1/1	0.97	0.18	-	61,61,61,61	0
54	MG	DA	1660	1/1	0.96	0.24	-	14,14,14,14	0
54	MG	DA	1618	1/1	0.96	0.07	-	30,30,30,30	0
54	MG	CB	3067	1/1	0.98	0.14	-	9,9,9,9	0
54	MG	DA	1659	1/1	0.93	0.23	-	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	1634	1/1	0.90	0.36	-	110,110,110,110	0
54	MG	AB	4031	1/1	0.94	0.17	-	56,56,56,56	0
54	MG	AB	4104	1/1	0.99	0.11	-	26,26,26,26	0
54	MG	BA	4022	1/1	0.99	0.23	-	14,14,14,14	0
54	MG	CB	3027	1/1	0.98	0.10	-	40,40,40,40	0
54	MG	CB	3013	1/1	0.99	0.06	-	14,14,14,14	0
54	MG	BA	4041	1/1	0.97	0.11	-	54,54,54,54	0
54	MG	AB	4108	1/1	0.95	0.19	-	9,9,9,9	0
54	MG	DA	1633	1/1	0.98	0.06	-	3,3,3,3	0
54	MG	AB	4075	1/1	0.96	0.12	-	41,41,41,41	0
54	MG	AB	4064	1/1	0.94	0.12	-	43,43,43,43	0
54	MG	CB	3094	1/1	0.85	0.15	-	16,16,16,16	0
54	MG	AB	4016	1/1	0.99	0.20	-	68,68,68,68	0
54	MG	AB	4063	1/1	0.99	0.29	-	16,16,16,16	0
54	MG	CB	3017	1/1	0.97	0.11	-	13,13,13,13	0
54	MG	AB	4067	1/1	0.96	0.12	-	31,31,31,31	0
54	MG	CB	3011	1/1	0.98	0.10	-	33,33,33,33	0
54	MG	AB	4028	1/1	0.98	0.12	-	16,16,16,16	0
54	MG	BA	4024	1/1	0.90	0.35	-	32,32,32,32	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.