



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 4, 2018 – 03:08 AM EST

PDB ID : 4V5B
Title : Structure of PDF binding helix in complex with the ribosome
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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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030736

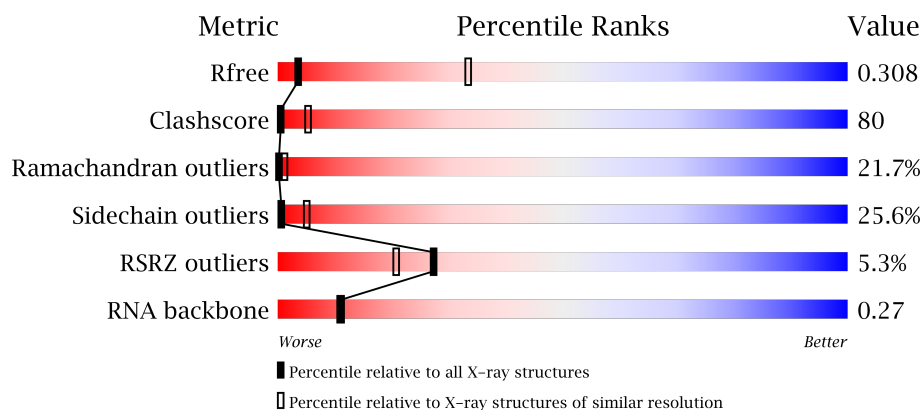
1 Overall quality at a glance

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}	100719	1291 (3.98-3.50)
Clashscore	112137	1437 (3.98-3.50)
Ramachandran outliers	110173	1382 (3.98-3.50)
Sidechain outliers	110143	1379 (3.98-3.50)
RSRZ outliers	101464	1320 (3.98-3.50)
RNA backbone	2435	1012 (4.52-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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>19%</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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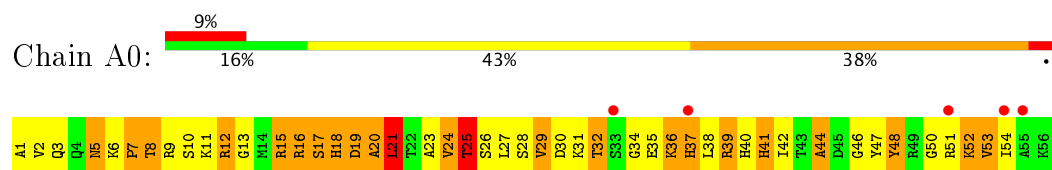
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	CQ	1	Total 1	O 1	0	0
55	CT	2	Total 2	O 2	0	0
55	CU	1	Total 1	O 1	0	0
55	DA	293	Total 293	O 293	0	0
55	DD	1	Total 1	O 1	0	0
55	DE	2	Total 2	O 2	0	0
55	DG	1	Total 1	O 1	0	0
55	DL	4	Total 4	O 4	0	0
55	DN	2	Total 2	O 2	0	0
55	DP	1	Total 1	O 1	0	0
55	DT	3	Total 3	O 3	0	0

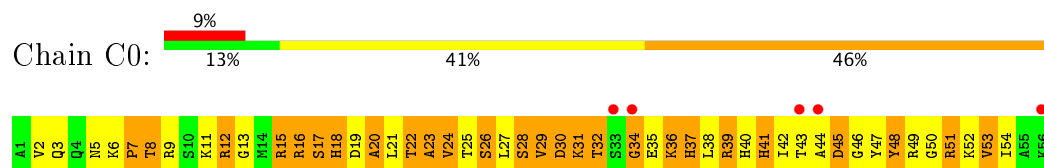
3 Residue-property plots [i](#)

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

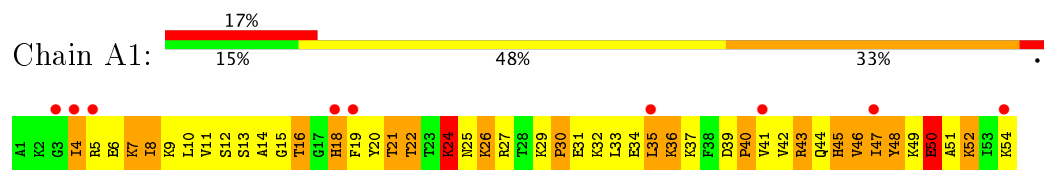
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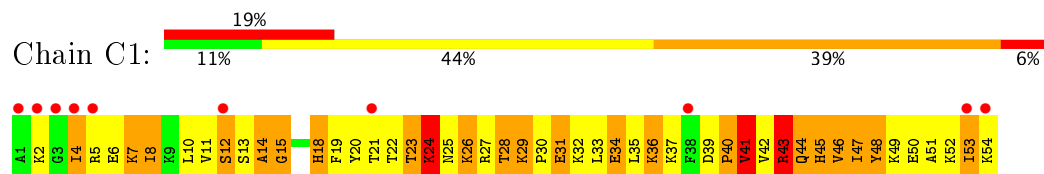
- Molecule 1: 50S RIBOSOMAL PROTEIN L32



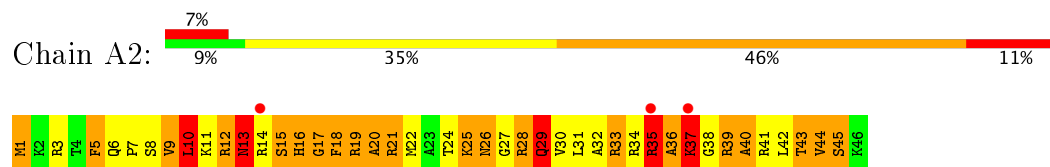
- Molecule 2: 50S RIBOSOMAL PROTEIN L33



- Molecule 2: 50S RIBOSOMAL PROTEIN L33



- Molecule 3: 50S RIBOSOMAL PROTEIN L34

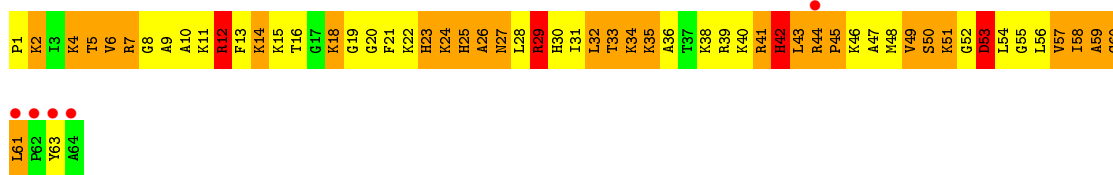


- Molecule 3: 50S RIBOSOMAL PROTEIN L34

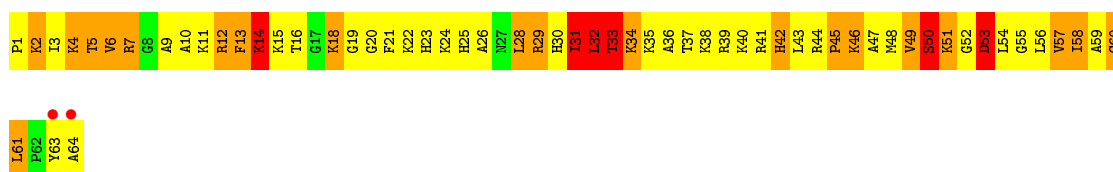




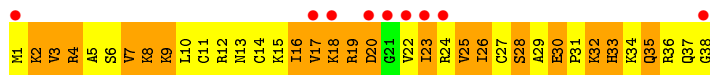
• Molecule 4: 50S RIBOSOMAL PROTEIN L35



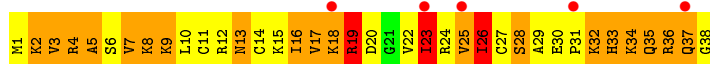
• Molecule 4: 50S RIBOSOMAL PROTEIN L35



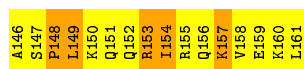
• Molecule 5: 50S RIBOSOMAL PROTEIN L36



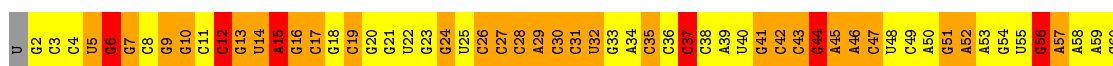
• Molecule 5: 50S RIBOSOMAL PROTEIN L36

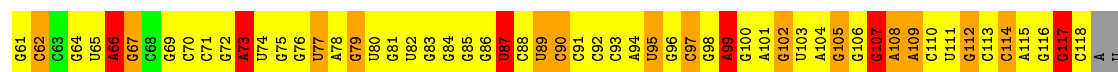


• Molecule 6: C-TERM HELIX PDF

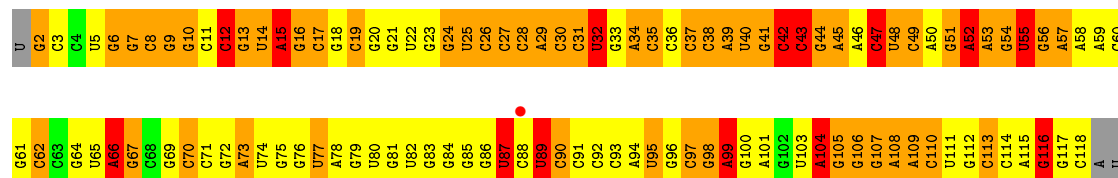


• Molecule 7: 5S RIBOSOMAL RNA

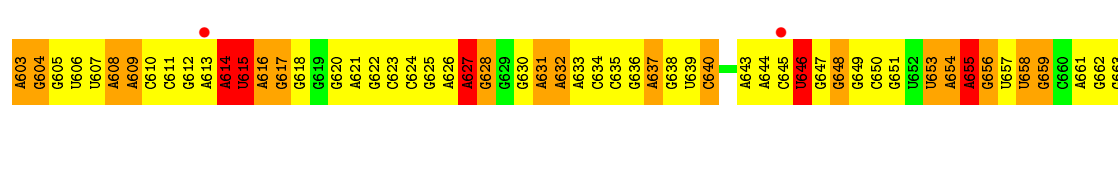
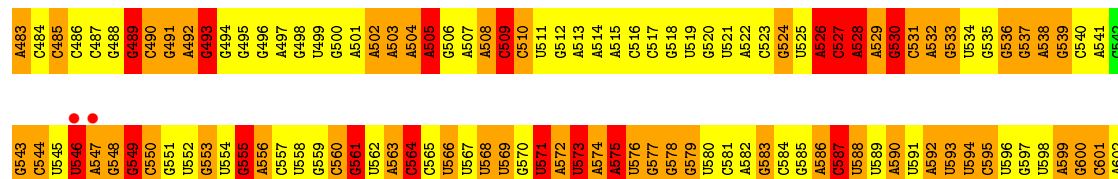
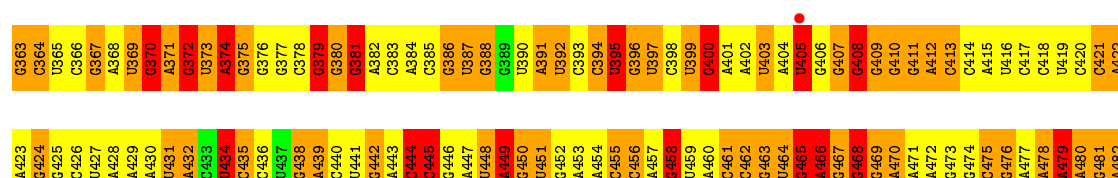
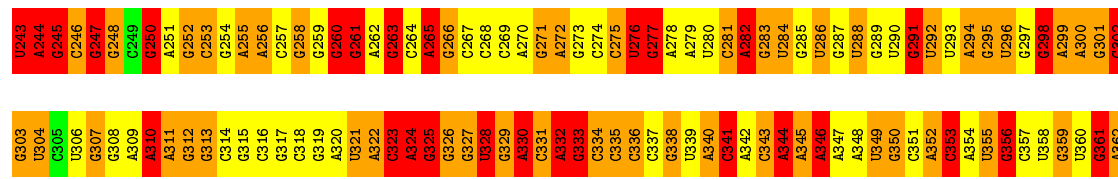
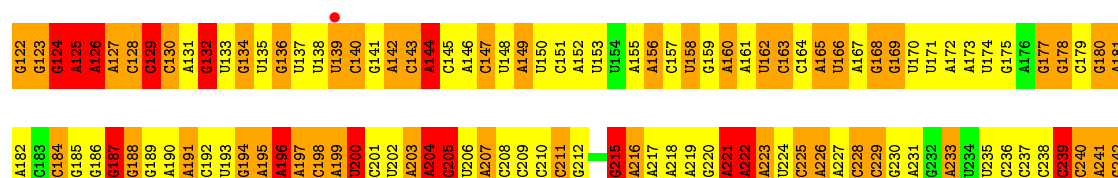
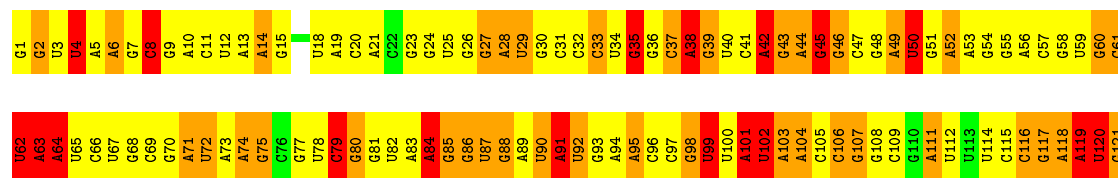




• Molecule 7: 5S RIBOSOMAL RNA

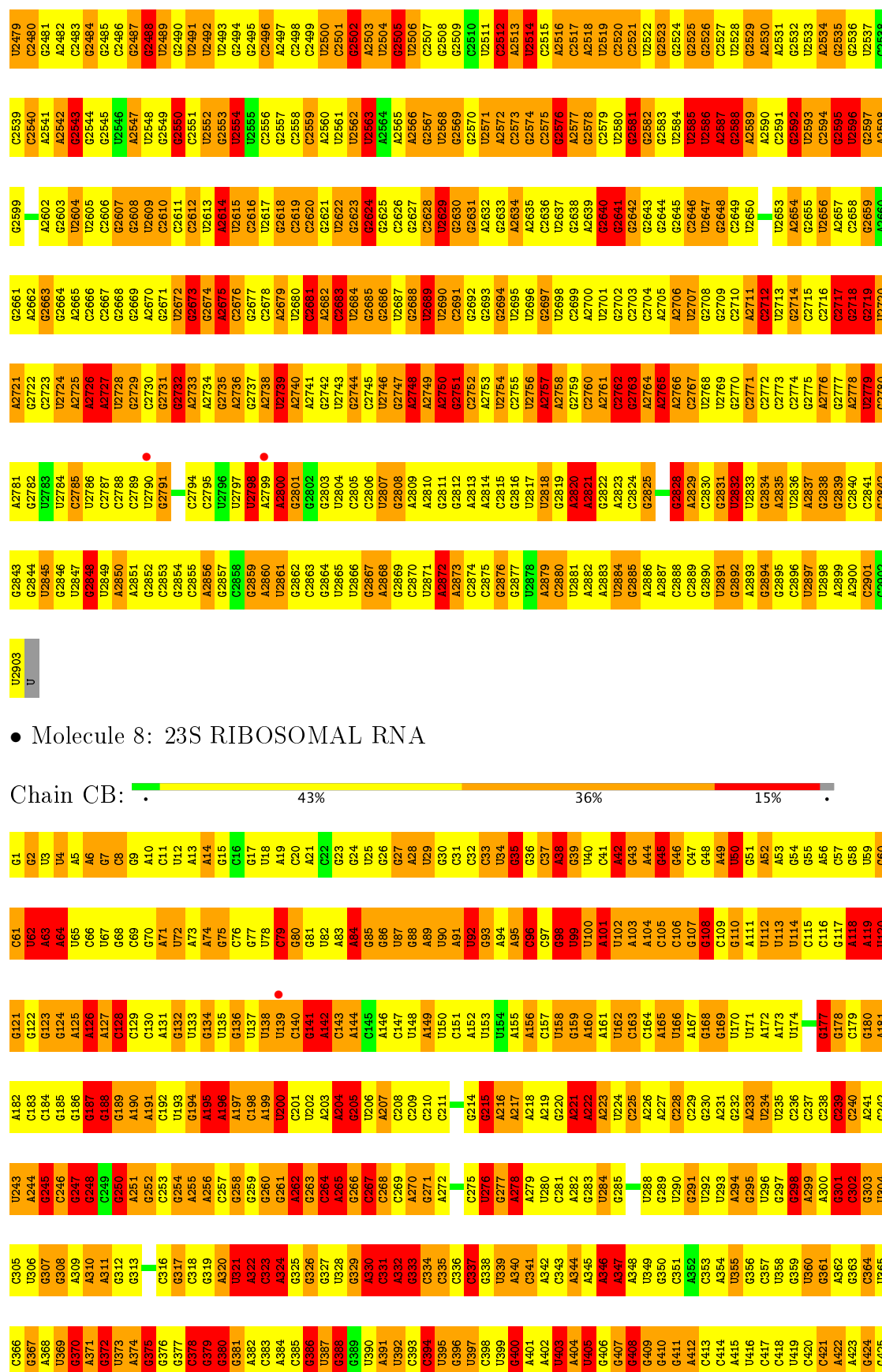


• Molecule 8: 23S RIBOSOMAL RNA



A1535	G1448	G1388	G1206	A1085	G1024	C964	G904	A844	G784	U724	G664
G1516	G1449	G1389	G1210	A1086	G1025	C965	A905	A845	G785	G725	G665
G1517	G1450	G1390	G1211	G1087	G1026	C966	G906	A846	G786	G726	G666
G1518	G1451	G1391	G1212	A1088	A1027	G967	G907	U847	G787	G727	G667
G1519	G1452	G1392	G1213	A1089	A1028	C968	C908	C848	A788	G728	G668
G1520	G1453	G1393	G1214	A1090	A1029	C969	A909	A849	A789	G729	G669
G1521	G1454	G1394	G1215	G1091	C1030	U970	A910	U850	U780	A730	A670
A1522	A1455	A1395	G1216	C1092	G1031	G971	A911	C851	C791	C731	A671
G1523	G1456	G1396	G1217	G1093	A1032	A972	C912	U852	A792	C732	G672
G1524	G1457	G1397	G1218	A1094	U1033	A973	G913	C853	A793	G733	G673
A1525	U1458	G1398	G1219	A1095	G1034	G974	U914	C854	A794	G734	G674
G1526	G1459	G1399	G1220	A1096	U1035	A975	C915	G855	G795	A735	A675
G1527	U1460	U1400	G1221	U1097	G1036	G976	G916	G856	C796	G736	A676
A1528	G1461	G1341	G1222	A1098	G1037	G977	A917	G857	G797	C737	A677
G1529	G1462	G1342	G1223	G1099	G1038	G978	U918	G858	G798	G738	G678
G1530	G1463	G1343	G1224	G1100	G1039	A979	U919	G859	G799	A739	C679
A1531	G1465	A1404	G1225	U1101	A1040	A980	A920	U860	A800	G740	C680
A1532	U1466	G1345	G1226	C1102	G1041	A981	C921	A861	G801	U741	G681
C1533	U1467	G1346	G1227	A1103	G1042	C982	C922	G862	A802	A742	G682
U1534	A1469	G1407	G1228	C1104	C1043	A983	G923	A863	U803	A743	G683
A1535	A1470	G1408	G1229	U1105	C1044	A984	G924	G864	A804	U744	G684
U1536	G1471	C1349	G1230	G1106	C1045	C985	A925	C865	A805	G745	A685
G1537	G1472	C1350	G1231	G1107	A1046	C986	G926	A866	C806	U746	G686
G1538	G1473	C1351	G1232	U1108	G1047	C987	A927	C867	U807	U747	G687
U1539	U1474	U1352	G1233	C1109	A1048	A988	A928	U868	G808	G748	G688
G1540	G1475	A1413	C1234	G1110	C1049	G989	U929	C889	A809	A749	G689
C1541	U1476	G1354	G1235	A1111	A1050	A990	G930	U870	U810	A750	G690
U1542	A1477	G1355	G1236	G1112	G1051	A991	C931	U871	U811	A751	C691
G1543	G1478	G1356	G1237	U1113	C1052	C992	U932	U872	C812	A752	C692
A1544	G1479	C1357	G1238	C1114	C1053	G993	A933	C873	U813	A753	A693
U1545	C1480	G1358	G1239	G1115	A1054	C994	U934	G874	C814	U754	G694
G1546	U1481	A1359	G1240	G1116	G1055	C995	C935	C875	C815	U755	G695
G1547	G1482	A1360	G1241	C1117	G1056	A996	A936	C876	C816	A756	G696
A1548	G1483	G1361	G1242	U1118	U1058	C997	G937	A877	C817	G757	G697
U1549	U1484	C1362	G1243	U1119	C1059	U999	G938	A878	C818	C758	C698
C1550	U1485	G1363	G1244	G1120	U1060	U999	G939	G	A819	G759	A699
A1551	U1486	G1364	G1245	C1121	U1061	A1000	G940	G	A820	G760	G700
U1552	U1487	A1365	G1246	G1122	U1062	A1001	A941	G	A821	A761	G701
A1553	C1488	A1366	A1247	C1123	G1063	G1002	G942	G	G822	U762	U702
C1554	C1489	A1367	G1248	G1124	G1063	G1003	A943	G	C823	G763	U703
G1555	A1490	G1368	G1249	G1125	C1064	U1004	C944	U	U824	A764	G704
C1556	G1491	G1369	U1249	A1126	U1065	C1005	A945	C	A825	C765	A705
U1557	G1492	G1370	G1250	U1127	U1066	C1006	C946	A	U826	U766	A706
C1558	C1493	G1371	G1251	G1128	A1067	C1007	A947	U	U827	U767	G707
U1559	A1494	U1372	G1252	A1129	G1068	A1008	C948	C	U828	G768	G708
G1560	A1495	A1373	A1253	U1130	A1069	A1009	G949	C	A829	U769	U709
C1561	U1496	G1374	A1254	G1131	A1070	A1010	G950	C	C830	G770	U710
U1562	U1497	U1375	U1255	U1132	G1071	G1011	C951	G	C831	G771	G711
U1563	C1498	G1376	G1256	A1133	C1072	U1012	G952	A	U832	C772	G712
C1564	C1499	G1377	C1257	G1134	C1073	C1013	G953	C	A833	U773	G713
C1565	U1498	U1378	U1258	C1135	C1075	A1014	G954	U	G834	G774	U714
A1566	A1499	C1379	G1259	G1136	C1076	U1015	G955	U	C835	G775	A715
G1567	A1500	G1380	A1260	U1137	A1077	G1016	U956	A	C836	G776	A716
U1568	A1501	G1381	C1261	G1138	U1078	G1017	C957	C	C837	G777	C717
A1569	U1506	G1382	A1262	G1139	C1079	U1018	U958	C898	C838	G778	A718
U1570	C1507	U1443	U1263	C1140	A1080	U1019	A959	A899	U839	U779	C719
A1571	A1508	A1384	A1264	U1141	U1081	A1020	A960	A900	C840	G780	U720
U1572	U1509	A1385	G1265	U1142	U1082	A1021	C961	C901	G841	A781	A721
G1573	G1510	C1386	G1266	A1143	U1083	G1022	G962	C902	U842	A782	A722
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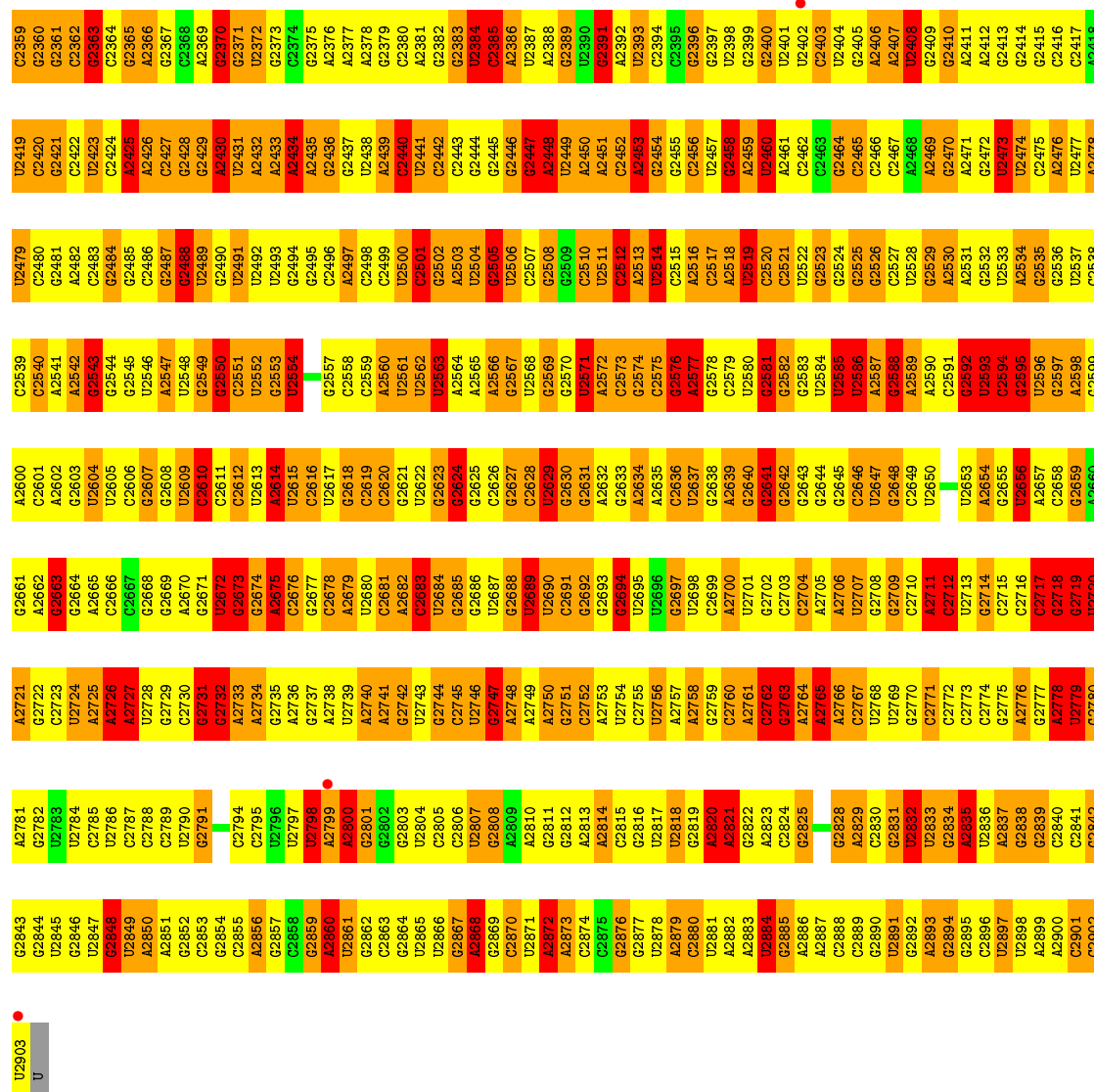




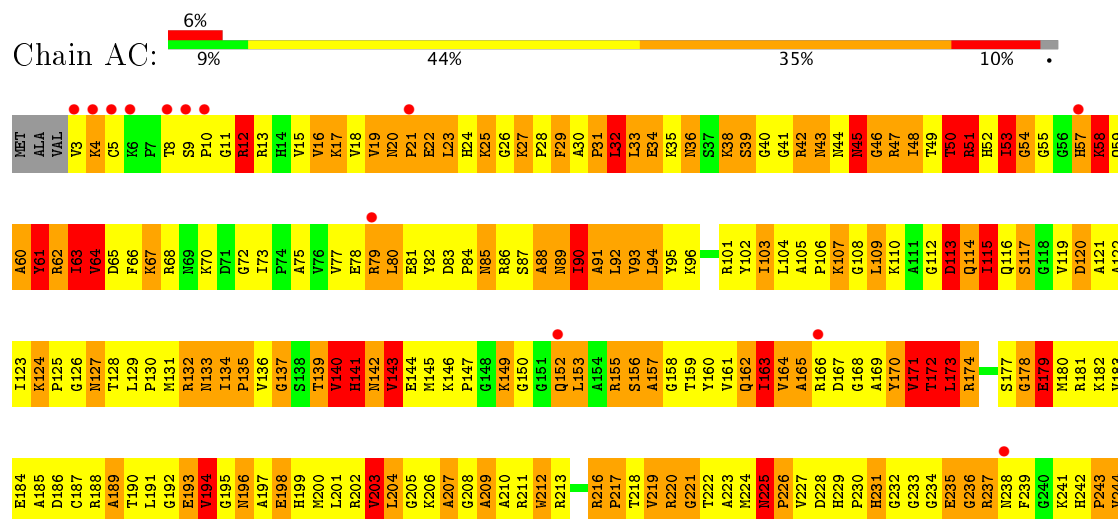
• Molecule 8: 23S RIBOSOMAL RNA

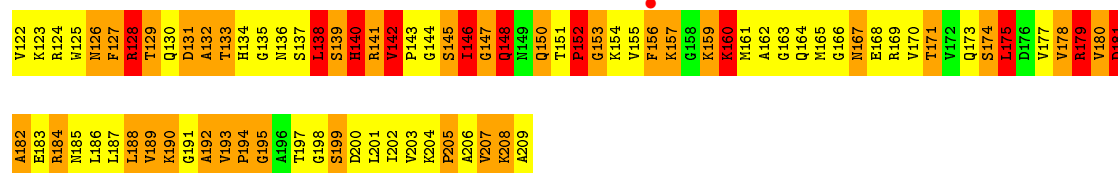
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U2301	G2241	U2181	G2061	C2001	C1879	U1813	A1757	G1697	A1636	U1576	A1516	G1452	U1392
G2302	G2242	A2062	G2062	G2002	U1880	U1814	U1758	A1698	A1637	C1577	G1517	A1453	A1393
G2303	C2243	C2063	C2063	A2003	C1881	A1819	A1759	A1699	C1639	U1578	C1518	C1454	U1394
G2304	A2184	G2064	G2064	G2004	U1882	U1820	C1760	A1700	C1638	A1579	G1519	G1455	A1395
U2305	U2185	C2065	C2065	A2005	U1883	A1821	C1761	A1701	A1640	A1580	U1520	G1456	U1396
C2306	G2246	C2066	C2066	C2006	G1884	C1822	A1762	G1702	A1641	U1581	G1521	U1457	U1397
G2307	U2187	U2067	U2067	U2007	A1885	G1823	G1763	G1703	G1642	C1582	A1522	U1458	C1398
G2308	U2188	G2068	G2068	C2008	C1886	C1824	C1764	C1704	G1643	U1583	U1523	G1459	C1399
A2309	C2248	C2069	C2069	A2009	U1887	U1825	U1765	A1705	C1644	U1584	G1524	U1460	U1400
G2310	G2250	U2070	U2070	G2010	G1888	A1826	G1766	G1706	G1645	C1585	A1525	C1461	G1401
A2311	C2071	A2071	C2071	U2011	A1889	U1827	G1767	G1707	C1646	U1586	C1526	C1462	U1402
U2312	C2072	U2072	C2072	G2012	A1890	G1828	C1768	C1708	U1647	G1587	G1527		A1403
G2313	C2073	C2073	C2073	A2013	A1891	A1829	U1769	U1709	U1648	G1588	A1528	G1465	C1404
A2314	U2074	A2014	A1953	A2014	C1892	C1830	G1770	G1710	G1649	U1589	G1529	U1466	U1405
G2315	U2075	U2075	G1954	A2015		G1831	C1771	A1711	A1650	A1590	G1530		U1406
G2316	A2135	U2076	U1955	U2016		C1832	A1772	U1712	G1651	A1591	G1531		G1407
A2317	C2077	U2077	U1956	U2017	G1896	C1833	A1773	A1713	A1652	A1592	A1532		U1408
G2318	C2078	G2078	C1957	G2018	G1897	U1834	C1774	U1714	G1653	A1593	C1533		U1409
A2319	U2079	A2080	G1958	A2019	U1898	G1835	U1775	G1715	A1654	U1594	U1534		G1471
C2320	A2080	C2080	G1959	A2020	A1899	C1836	G1776	U1716	A1655	C1595	A1535		U1411
G2201	U2081	C2021	A1960	C2021	A1900	C1837	U1777	A1717	C1656	A1596	C1536		U1412
U2202	U2076	U2022	C1961	U2022	A1901	C1838	U1778	G1718	U1657	A1597	G1537		G1475
C2263	G2083	C2083		C2023	C1902	G1839	U1779	G1719	C1658	A1598	G1538		C1413
G2204	C2084	C2084	G1964	G2024	G1903	G1840	A1780	U1720	G1659	U1599	U1539		U1415
A2205	U2085	U2085	C1965	C2025	G1904	U1841	U1781	G1721	G1660	C1600	G1540		G1478
C2206	U2086	C2026	A1966	U2026	C1905	C1842	U1782	G1661	G1661	C1601	G1541		C1417
C2207	G2087	C2027	C1967	G2027	G1906	C1843	A1783	G1723	U1662	U1602	U1542		U1418
G2208	A2088	U2028	G1968	U2028	A1907	C1844	A1784	G1724	G1663	A1603	G1543		A1419
C2209	C2089	G2039	A1969	C2039	C1908	G1845	A1785	U1725	A1664	C1604	A1544		A1420
U2210	A2090	A2030	A1970	A2030	C1909	G1846	A1786	C1726	A1665	C1605	A1545		G1421
A2211	C2091	U2091	U1971	C2031	G1910	U1847	A1787	C1727	G1666	C1606	G1546		G1422
G2212	U2092	C2032	G1972	G2032	U1911	C1848	C1788	C1728	G1667	C1607	C1547		G1423
C2213	G2093	A2033	G1973	A2033	A1912	G1849	A1789	U1729	A1668	A1608	U1548		G1424
G2214	A2094	U2034	C1974	U2034	A1913	G1850	C1790	C1730	A1669	A1549	A1549		G1425
C2215	A2095	G2035	G1975	G2035	C1914		A1791	G1731	C1670	A1610	C1550		G1426
G2216	C2096	C2036	U1976	C2036	U1915		G1792	C1732	U1671	C1611	A1551		A1427
A2217	A2097	A2037	A1977	A2037	A1916	A1853	C1793	G1733	A1672	C1612	A1552		G1428
U2218	U2098	G2038	U1978	G2038	U1917	A1854	A1794	G1734	G1673	G1613	A1553		C1429
G2219	C2099	U2039	U1979	U2039	A1918	U1856	C1795	A1735	G1674	A1614	U1554		G1430
U2220	G2100	G2040	G1980	G2040	A1919	C1857	U1796	U1736	C1675	C1615	G1555		A1431
C2221	A2101	U2041	A1981	U2041	C1920	A1858	G1797	U1737	A1676	A1616	C1556		G1432
G2222	C2102	A2042	U1982	A2042	G1921		U1798	G1738	A1677	C1617	C1557		A1433
C2223	C2103	C2043	G1983	C2043	G1922	G1861	G1799	A1739	A1678	A1618	C1558		A1434
G2224	C2104	C2044	G1984	C2044	U1923	G1862	C1800	G1740	A1679	G1619	U1559		G1435
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A2227	U2107	C2047	A1987	C2047	U1926	U1865	A1803	G1743	G1682	G1622	U1562		U1438
G2228	A2108	G2048	G1988	A2108	A1927	A1866	C1804	A1744	U1683	U1623	U1563		A1439
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G2230	A	C2050	C1990	C2050	G1929	C1868	C1806	A1746	C1685	C1625	C1565		A1504
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C2234	C	A2054	C1994	G1933	A1872	A1872	A1810	G1750		U1629	A1569		G1445
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U2236	G	G2056	C1996	U1935	C1874	C1874	U1812	C1752	U1692	G1631	A1571		G1447
G2237	A	G2057	C1997	A1936	A1875	A1875	U1813	G1753	U1693	A1632	A1572		G1448
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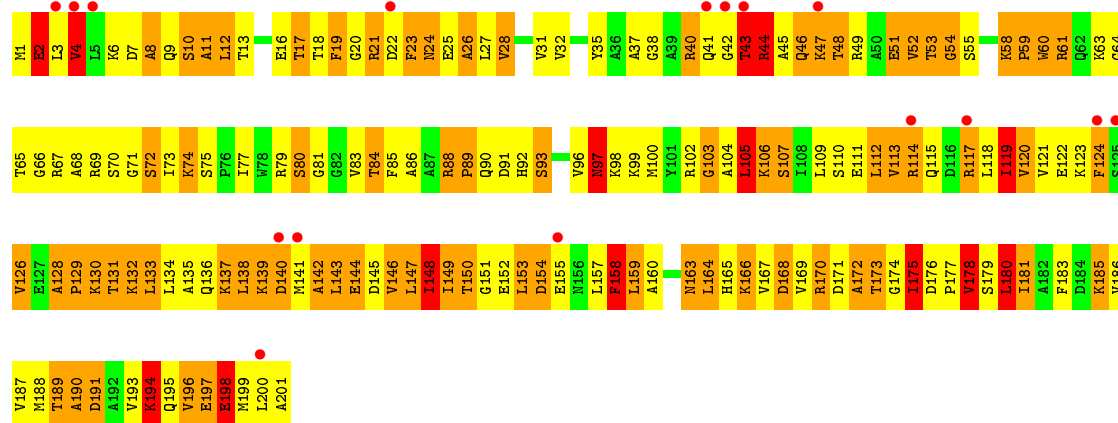
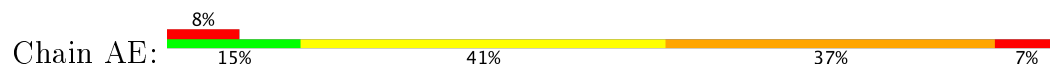


● Molecule 9: 50S RIBOSOMAL PROTEIN L2

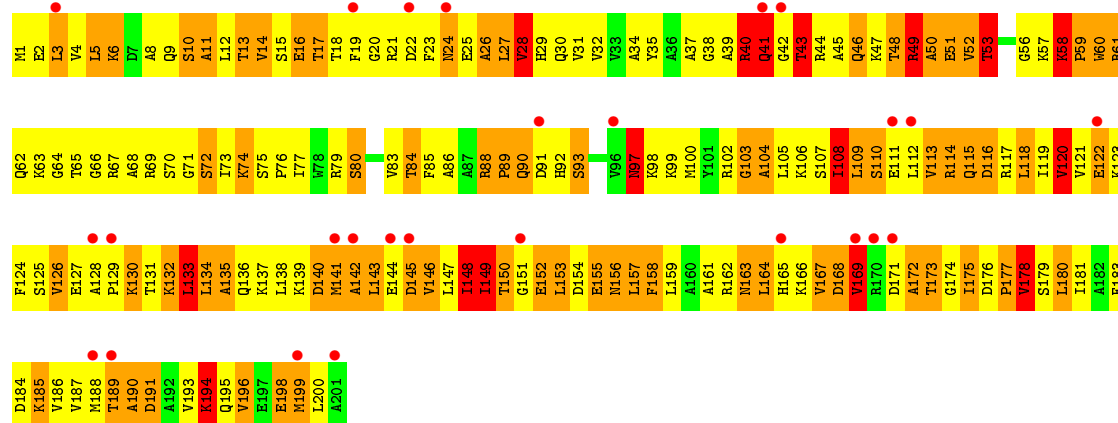




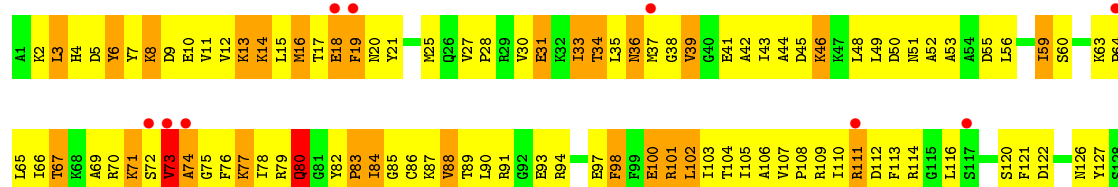
• Molecule 11: 50S RIBOSOMAL PROTEIN L4



• Molecule 11: 50S RIBOSOMAL PROTEIN L4

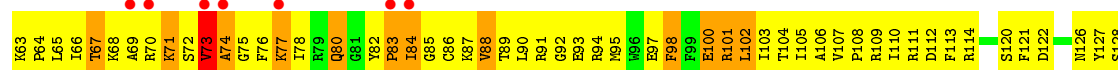


• Molecule 12: 50S RIBOSOMAL PROTEIN L5

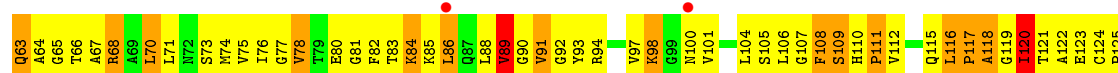
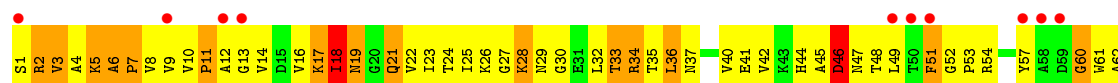




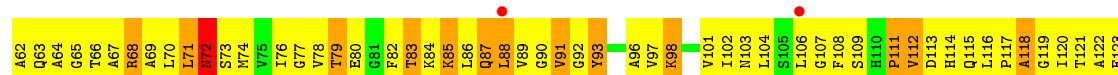
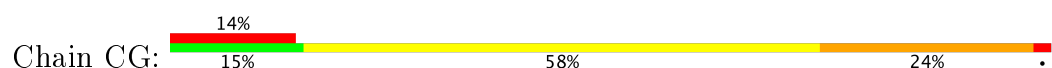
• Molecule 12: 50S RIBOSOMAL PROTEIN L5



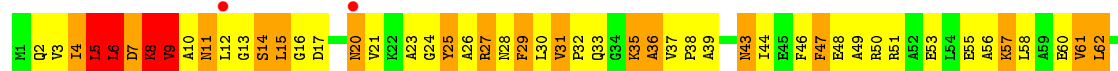
• Molecule 13: 50S RIBOSOMAL PROTEIN L6

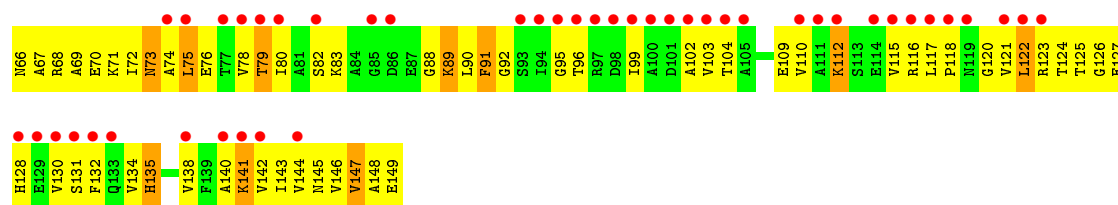


• Molecule 13: 50S RIBOSOMAL PROTEIN L6

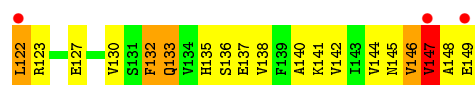
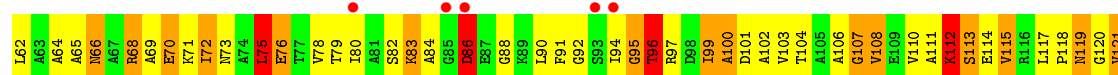
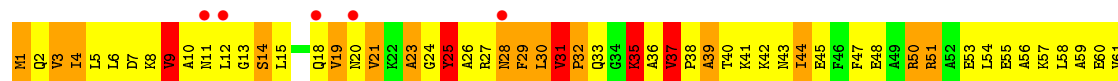
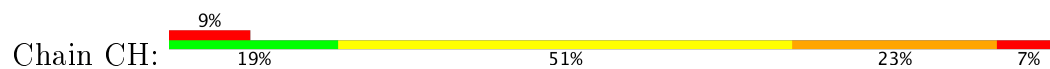


• Molecule 14: 50S RIBOSOMAL PROTEIN L9

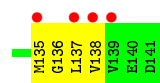
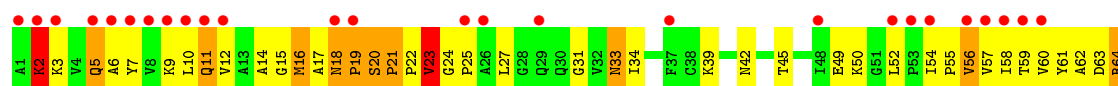




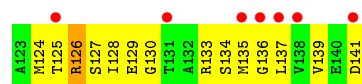
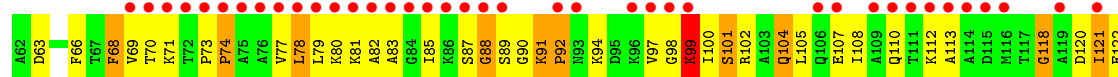
• Molecule 14: 50S RIBOSOMAL PROTEIN L9



• Molecule 15: 50S RIBOSOMAL PROTEIN L11

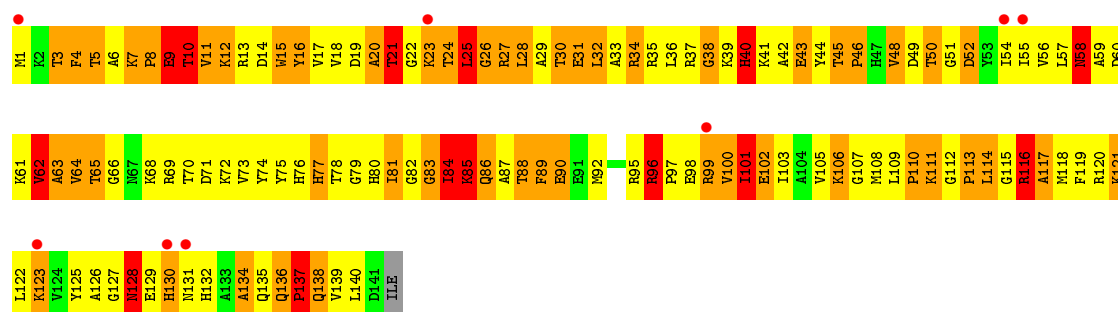


• Molecule 15: 50S RIBOSOMAL PROTEIN L11

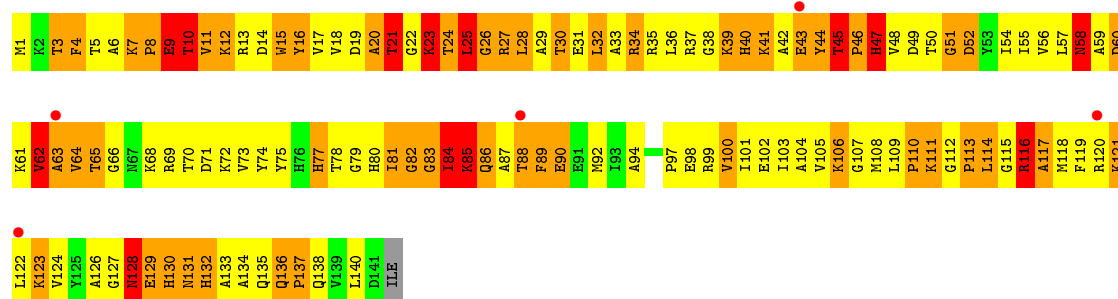


• Molecule 16: 50S RIBOSOMAL PROTEIN L13

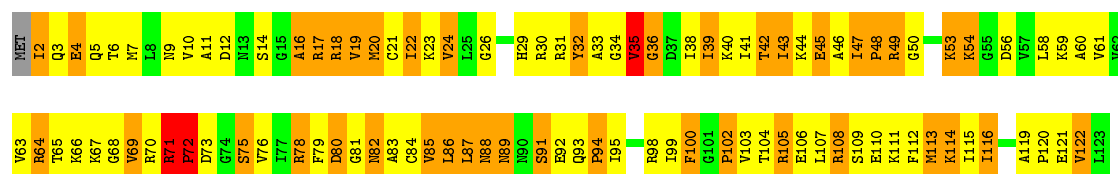
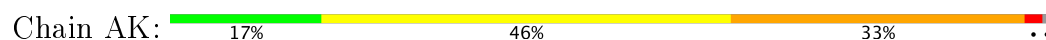




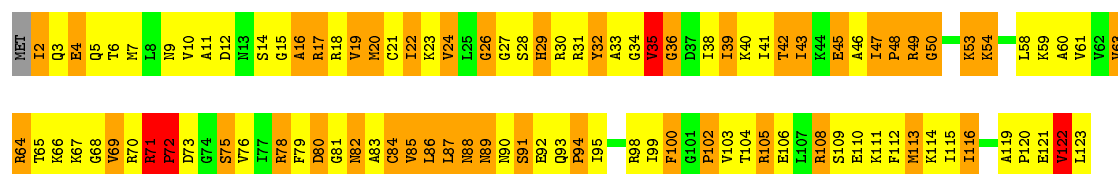
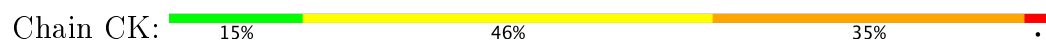
• Molecule 16: 50S RIBOSOMAL PROTEIN L13



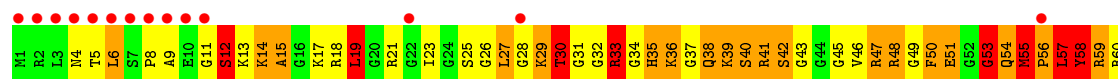
• Molecule 17: 50S RIBOSOMAL PROTEIN L14

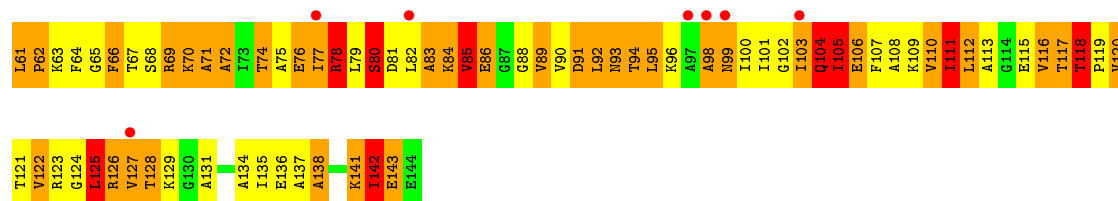


• Molecule 17: 50S RIBOSOMAL PROTEIN L14

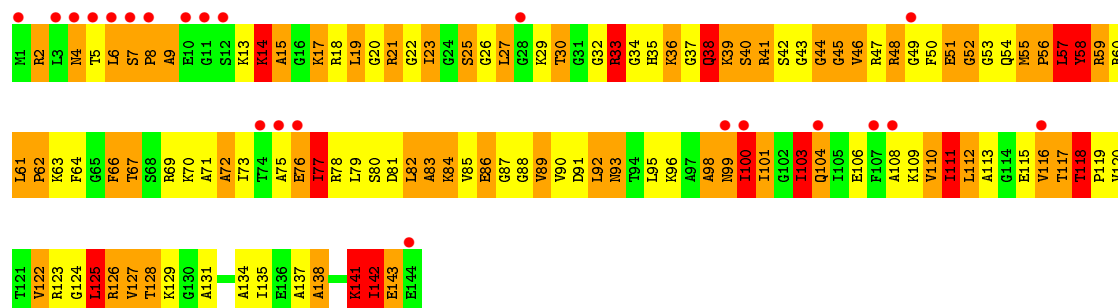
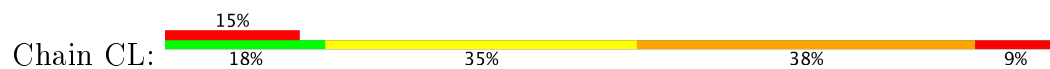


• Molecule 18: 50S RIBOSOMAL PROTEIN L15

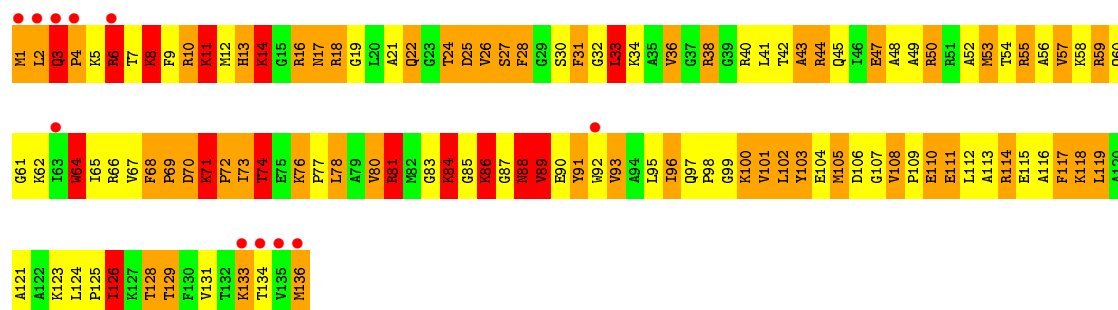




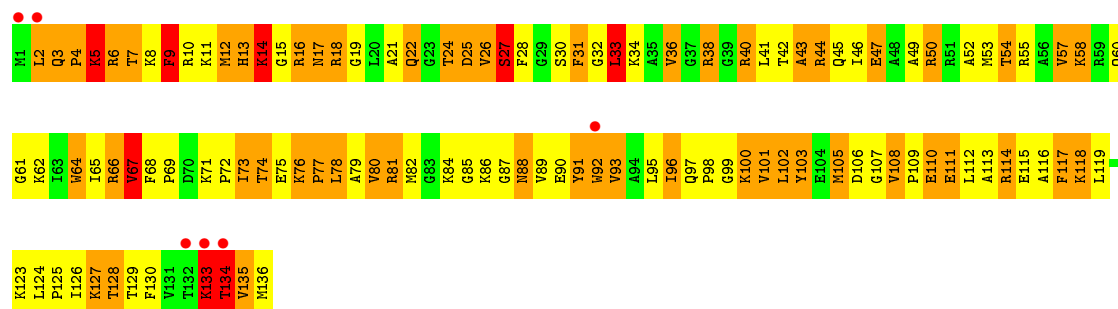
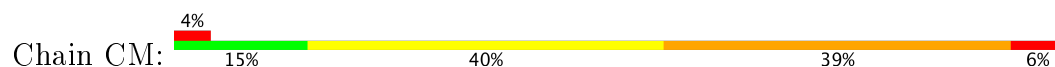
● Molecule 18: 50S RIBOSOMAL PROTEIN L15



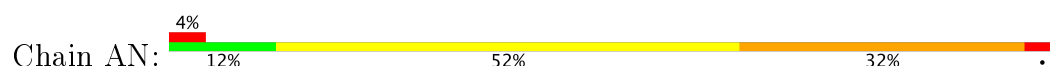
● Molecule 19: 50S RIBOSOMAL PROTEIN L16

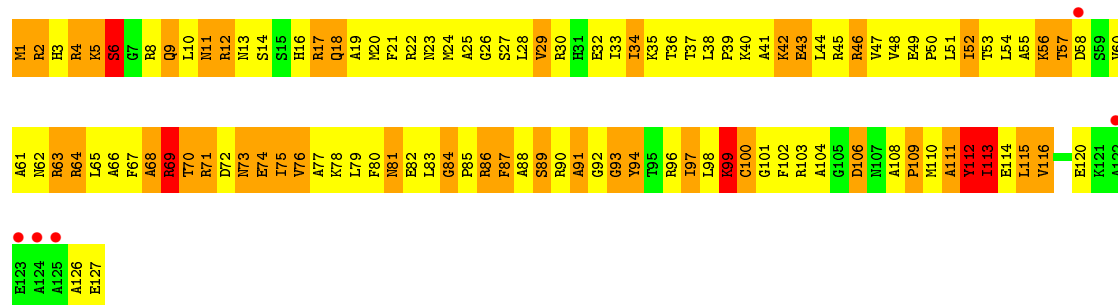


● Molecule 19: 50S RIBOSOMAL PROTEIN L16

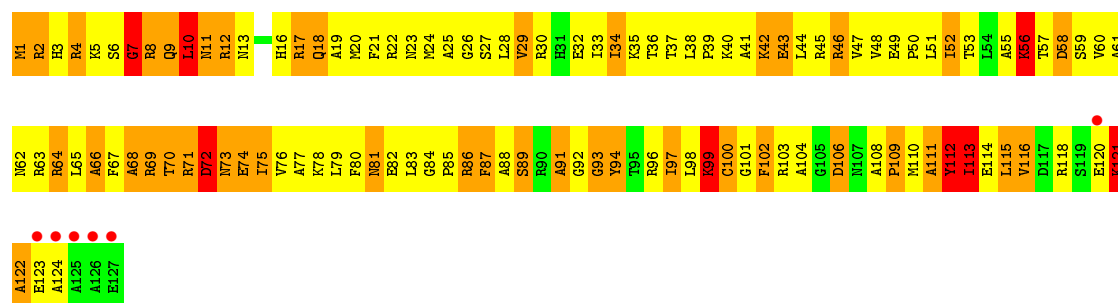
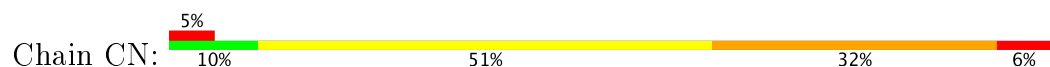


● Molecule 20: 50S RIBOSOMAL PROTEIN L17

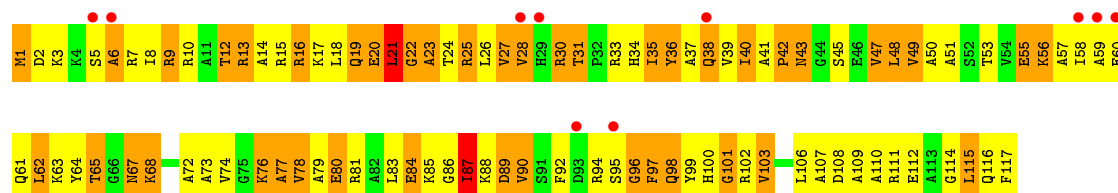
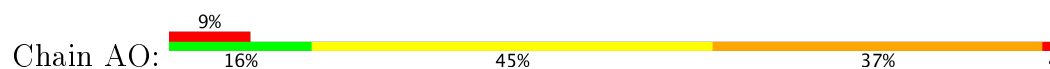




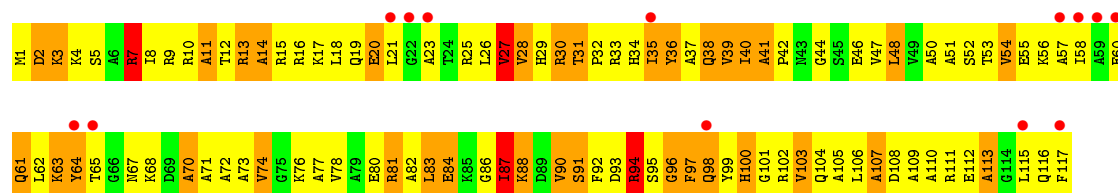
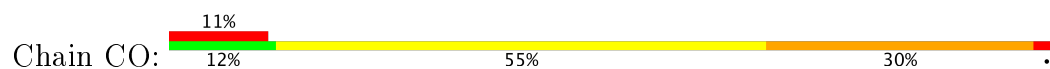
• Molecule 20: 50S RIBOSOMAL PROTEIN L17



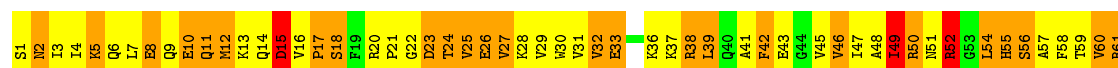
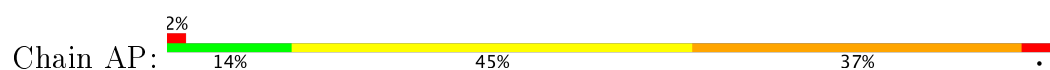
• Molecule 21: 50S RIBOSOMAL PROTEIN L18

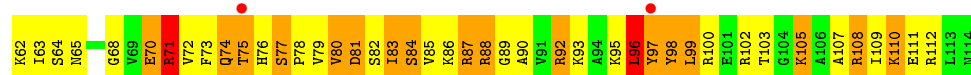


• Molecule 21: 50S RIBOSOMAL PROTEIN L18

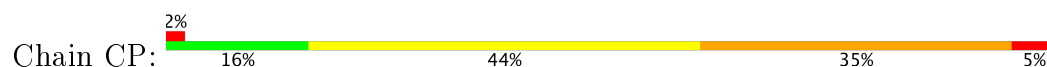


• Molecule 22: 50S RIBOSOMAL PROTEIN L19





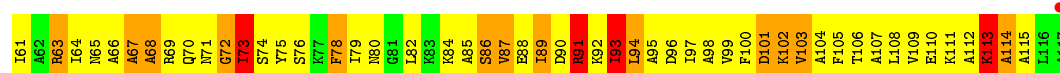
• Molecule 22: 50S RIBOSOMAL PROTEIN L19



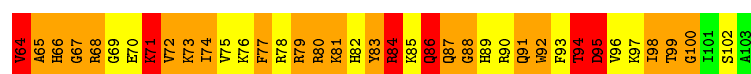
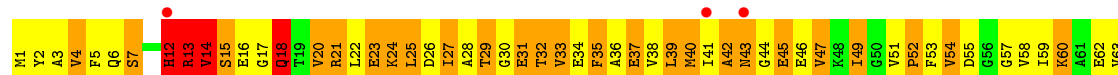
• Molecule 23: 50S RIBOSOMAL PROTEIN L20



• Molecule 23: 50S RIBOSOMAL PROTEIN L20



• Molecule 24: 50S RIBOSOMAL PROTEIN L21

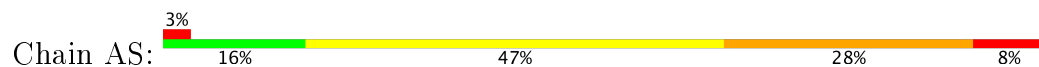


• Molecule 24: 50S RIBOSOMAL PROTEIN L21

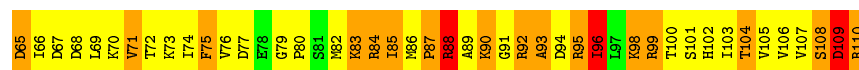
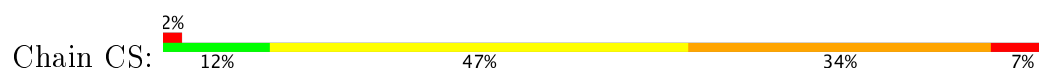




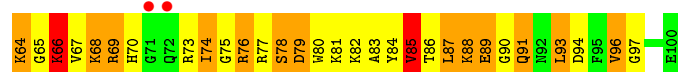
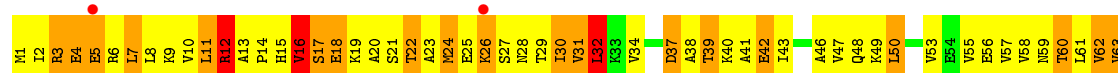
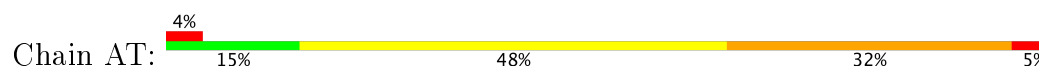
• Molecule 25: 50S RIBOSOMAL PROTEIN L22



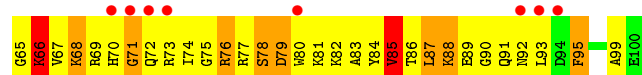
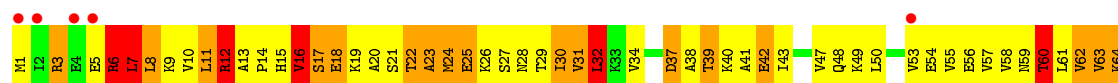
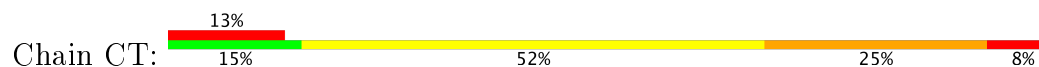
• Molecule 25: 50S RIBOSOMAL PROTEIN L22



• Molecule 26: 50S RIBOSOMAL PROTEIN L23

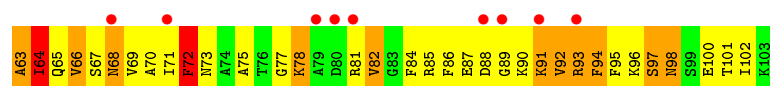


• Molecule 26: 50S RIBOSOMAL PROTEIN L23

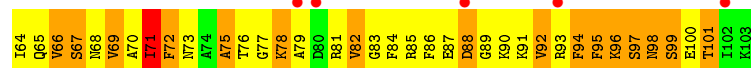
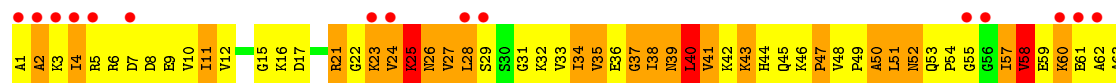
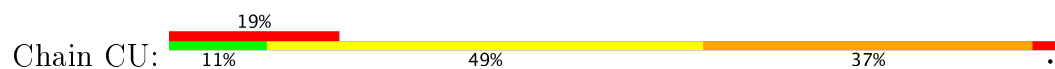


• Molecule 27: 50S RIBOSOMAL PROTEIN L24





• Molecule 27: 50S RIBOSOMAL PROTEIN L24



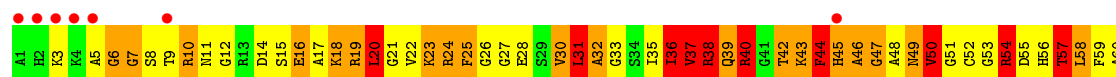
• Molecule 28: 50S RIBOSOMAL PROTEIN L25



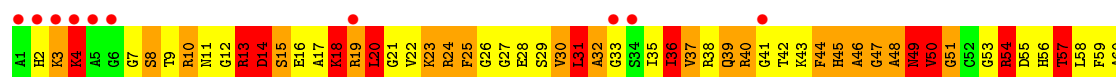
• Molecule 28: 50S RIBOSOMAL PROTEIN L25

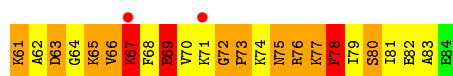


• Molecule 29: 50S RIBOSOMAL PROTEIN L27

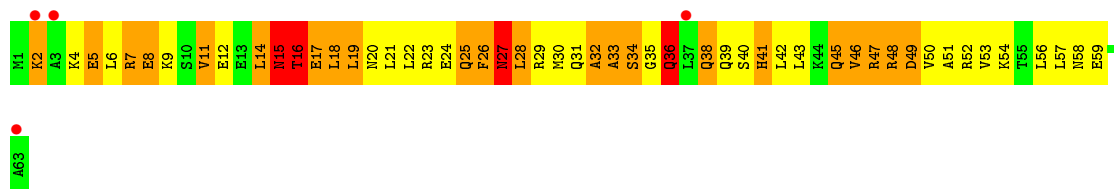
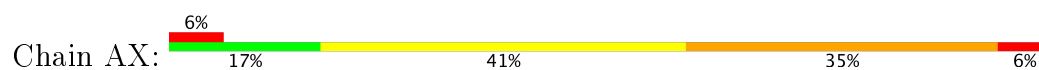


• Molecule 29: 50S RIBOSOMAL PROTEIN L27

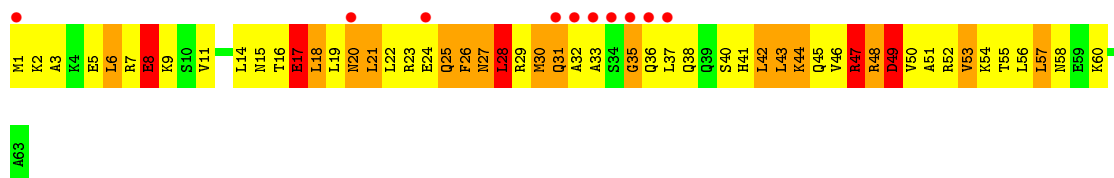
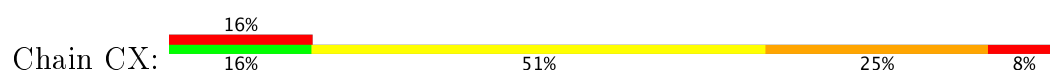




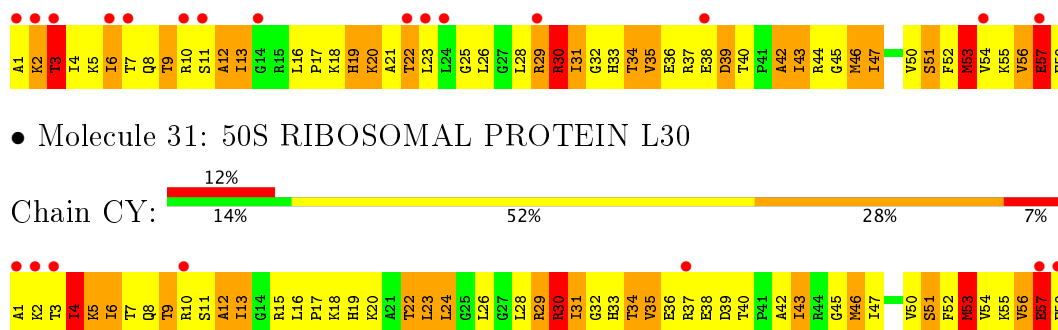
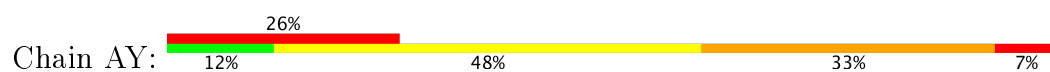
• Molecule 30: 50S RIBOSOMAL PROTEIN L29



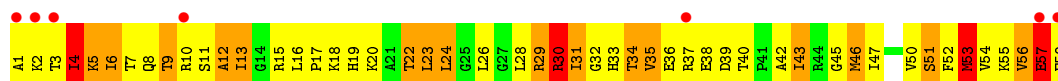
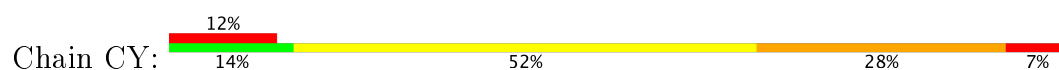
• Molecule 30: 50S RIBOSOMAL PROTEIN L29



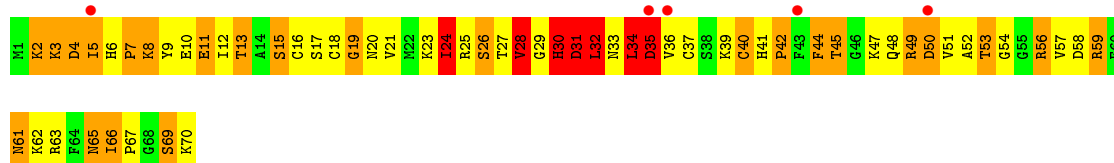
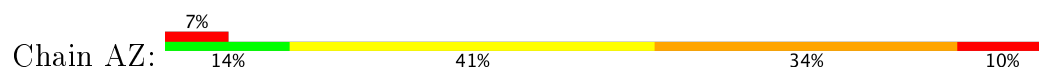
• Molecule 31: 50S RIBOSOMAL PROTEIN L30



• Molecule 31: 50S RIBOSOMAL PROTEIN L30



• Molecule 32: 50S RIBOSOMAL PROTEIN L31



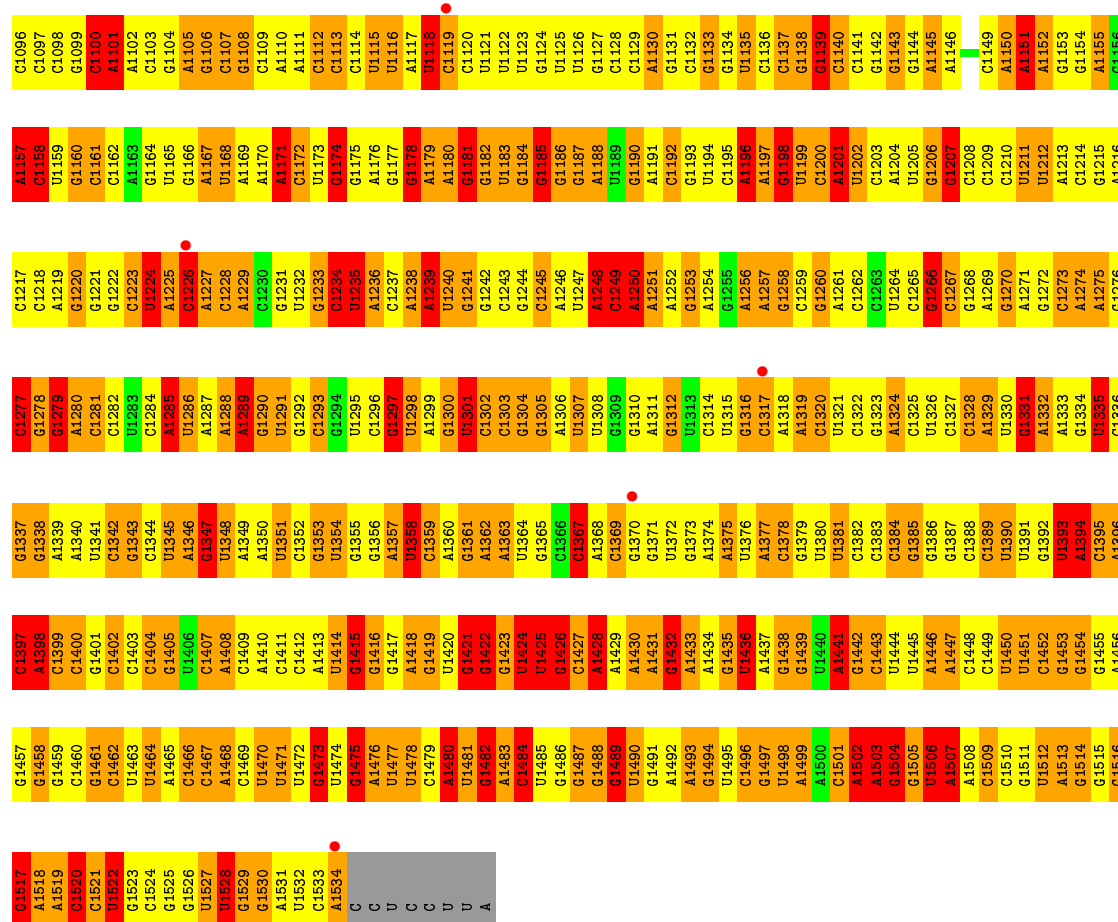
• Molecule 32: 50S RIBOSOMAL PROTEIN L31



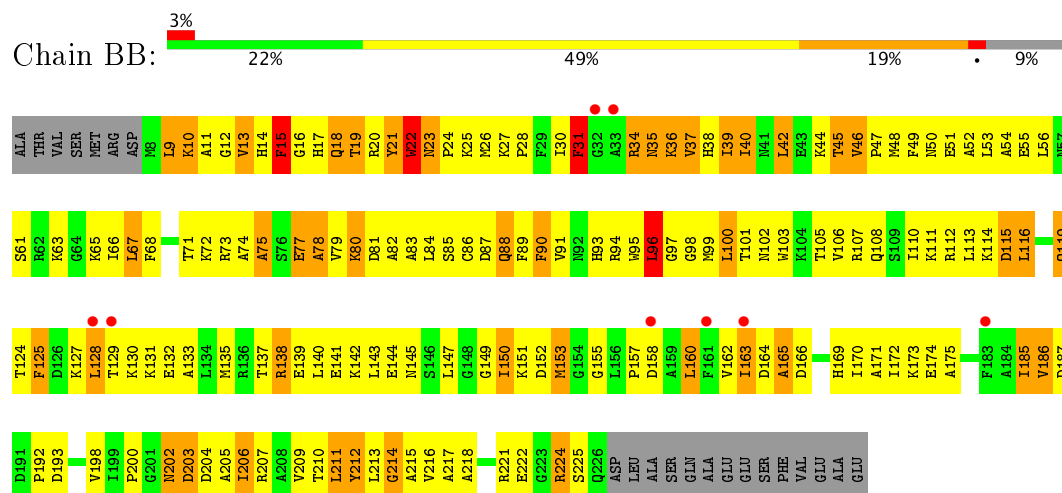
● Molecule 33: 16S RIBOSOMAL RNA

A	A	A	A	A	U	U5	G6	A7	A8	G9	A10	G11	G12	U13	G14	G15	A16	U17	C18	U19	G20	G21	G22	C23	U24	C25	G26	G27	A28	U29	U30	G31	G32	A33	G34	G35	C36	U37	G38	G39	A40	G41	G42	C43	A44	G45	G46	C47	C48	U49	A50	A51	G52	C53	A54	C55	A56	U56	G57	C58	A59	G60
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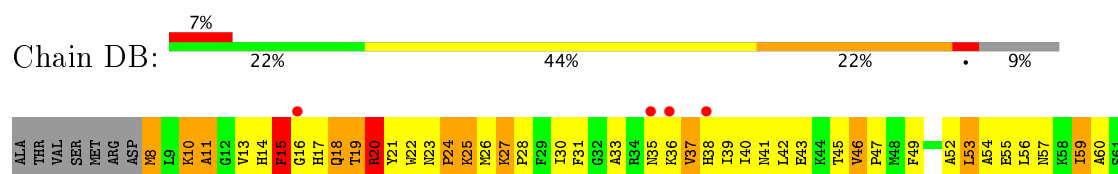
A1036	A974	U854	A794	G734	G674	C614	A554	G494	G433	A373	A313	U249	U185	U125	G61
C1037	A975	U855	C795	C735	A675	G615	U555	A495	U434	A374	C314	A250	C186	G126	U62
G1038	G976	C856	C796	C736	A676	G616	G556	A496	A435	G376	A315	G251	G187	G127	C63
C1039	G977	C857	C797	C737	A677	G617	G557	A497	G436	G377	C316	G252	C188	G128	G84
U1040	A978	C858	U798	C738	G678	C618	G558	A498	U437	G378	U317	A253	A189	A129	A65
G1041	G979	C859	G799	C739	G679	C619	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	A682	A622	U562	A502	A441	C381	A321	G257		U133	A71
C1045	A983	U863	G803	A743	G683	C623	A563	C503	G443	A383	U323	G258	A196	G134	A72
A1046	C984	A864	U804	C744	U684	C624	C564	C504	C444	A384	U324		A197	C135	C73
G1047	C985	A865	G805	G745	G685	C625	U565	G505	G445	G385	G325	U261	A198	C136	A74
G1048	U986	C866	C806	A746	U686	G626	G566	G506	G446	C386	A326	A262	G198	U137	A75
U1049	G987	G867	A807	A747	A687	G627	G567	C507	G447	C387	G327	A263	A199	G138	G76
G1050	G988	C868	C808	G748	G688	G628	G568	U508	G448	U388	A327	G264	G200	A139	A77
C1051	U989	G869	G809	A749	G689	A629	C569	A509	A449	C389	C328	G265	G201	U140	A78
U1052	C990	U870	C810	C750	G690	A630	U570	A510	G449	A390	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	A873	U813	A753	G693	G633	A573	C513	A452	C392	U332	C269		G144	C83
U1056	A994	C874	A814	C754	A694	C634	A574	C514	A453	A393	U333	A270	U209	G145	U84
G1057	C995	U875	A815	G755	A695	A635	G575	U515	G454	C394	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	C878	G818	C758	G698	U638	C578	C518	A457	C397	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	C402	C342	A279	U218	U154	U93
C1066	A1004	U884	G824	C764	A704	U644	G584	G524	U463	C403	U343	C280	U219	A155	G94
A1005	G945	C885	A825	G765	G705	G645	G585	C525	U464	C404	A344	C281	G220	C156	C95
G1068	U946	C886	C826	A766	A706	A646	C586	C526	A465	U405	G345	A282	C221	U157	U96
C1069	G947	C887	U827	A767	U707	C647	G587	C527	U466	C406	G346	G283	C222	G158	G97
U1070	U1008	C888	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	C890	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		A412	C352	G292	A228	G164	U103
U1076	A1014	C894	U834	G774	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	G416	A356	U296	G232	G168	G107
A1080	G1018	G898	G838	G778	A718	C658	U598	G538	A478	G417	G357	G297	C233	G169	G108
U1081	A1019	C899	C839	C779	C719	U659	C599	A539	U479	C418	U358	A298	C234	U170	A109
A1082	G1020	U900	C840	A780	C720	C660	A600	G540	U480	C419	G359	G299	C235	A171	C110
U1083	A1021	G901	C841	A781	G721	G661	G601	G541	G481	U420	G360	A300	A236	A172	G111
G1084	C1022	G902	U842	A782	G722	U662	A602	G542	A482	U421	G361	G301	G237	U173	G112
U1085	U1023	G903	U843	C783	U723	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	U1090	A908	C848	U788	A728	G668	A608	G548	C488	G427	U367	C307	U244	A179	A119
U1091	C1031	A909	G849	U789	A729	G669	A609	C549	C489	G428	U368	C308	U245	U180	A120
A1092	G1032	C970	U850	A790	G730	G670	U610	G550	C490	U429	G369	A309	U246	A181	U121
U1093	G1033	G911	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	G973	C853	U793	G733	A673	C613	A553	A493	A432	C372	C312	C248	G184	C124

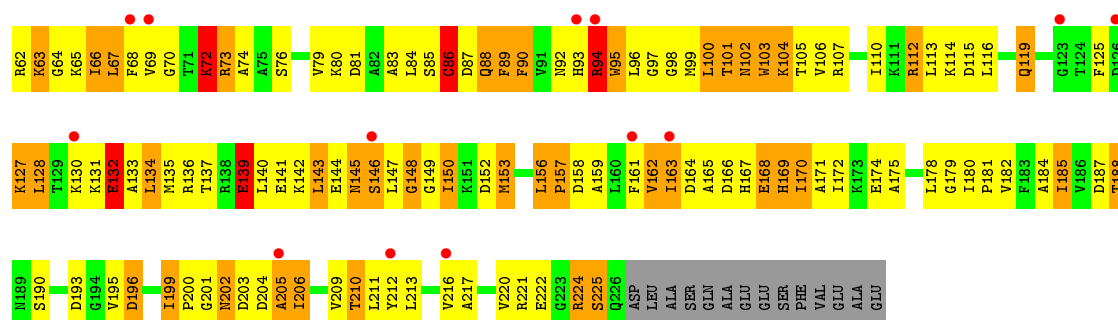


• Molecule 34: 30S RIBOSOMAL PROTEIN S2

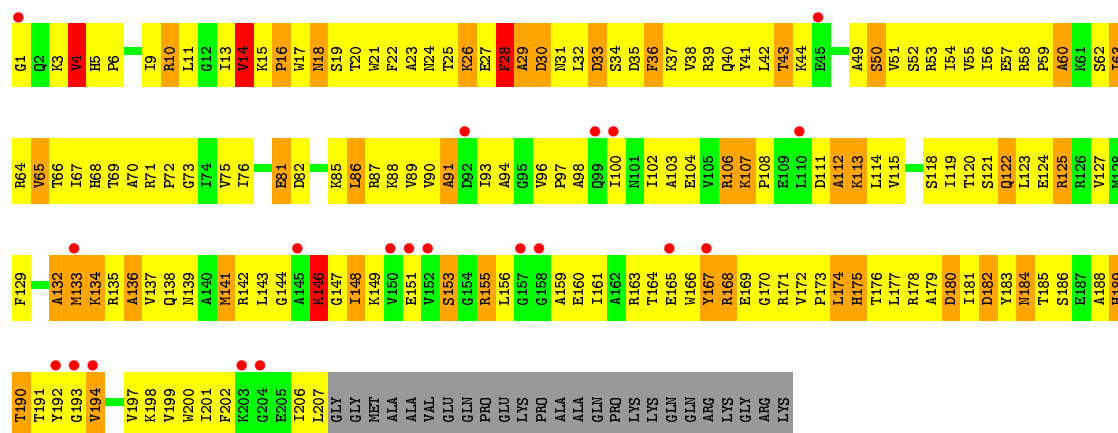
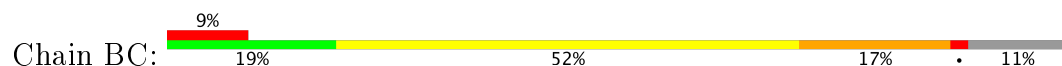


• Molecule 34: 30S RIBOSOMAL PROTEIN S2

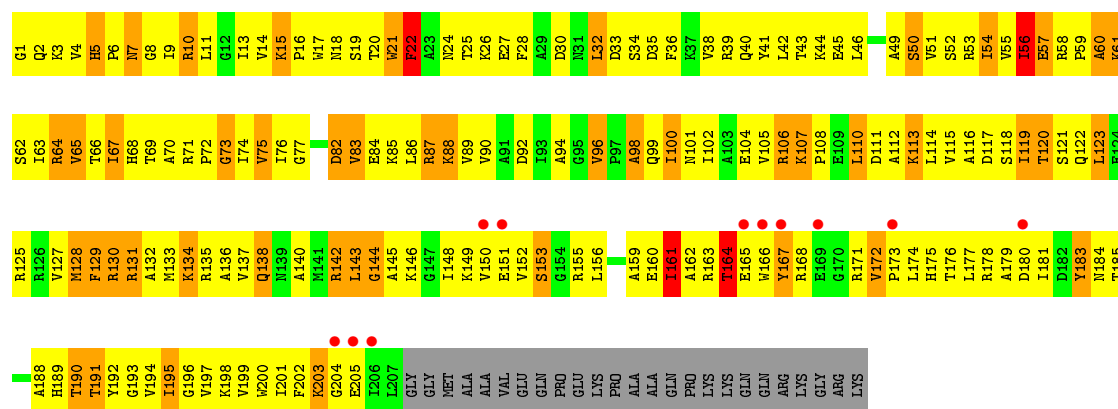
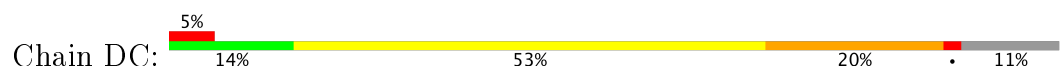




• Molecule 35: 30S RIBOSOMAL PROTEIN S3

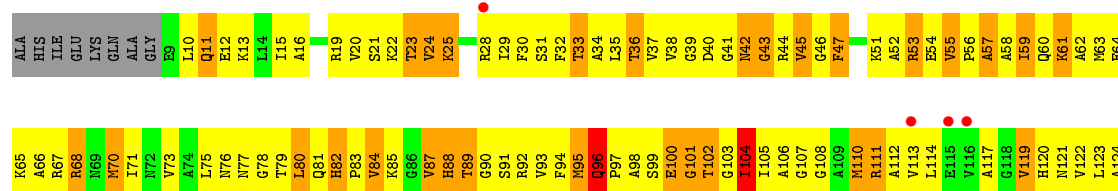


• Molecule 35: 30S RIBOSOMAL PROTEIN S3



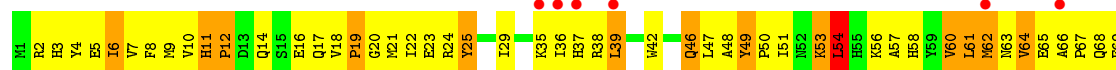
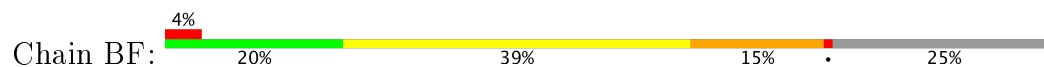
• Molecule 36: 30S RIBOSOMAL PROTEIN S4



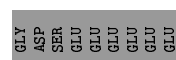
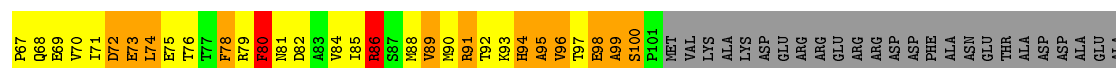




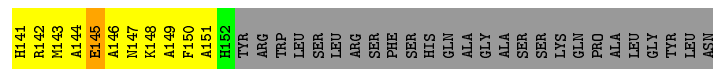
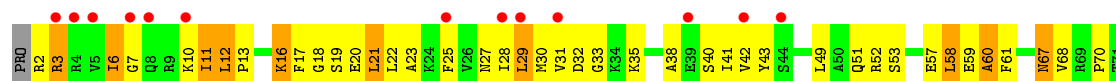
• Molecule 38: 30S RIBOSOMAL PROTEIN S6

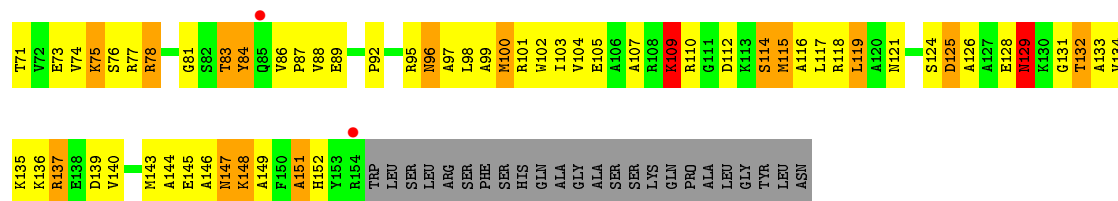


• Molecule 38: 30S RIBOSOMAL PROTEIN S6

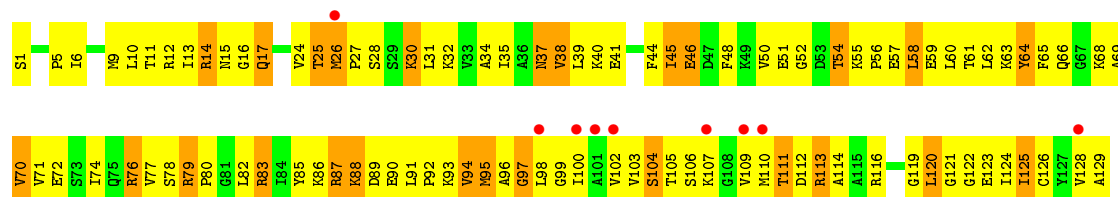


• Molecule 39: 30S RIBOSOMAL PROTEIN S7

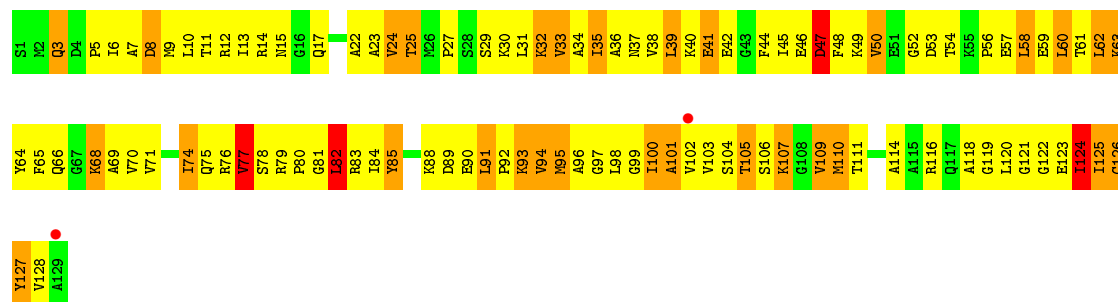




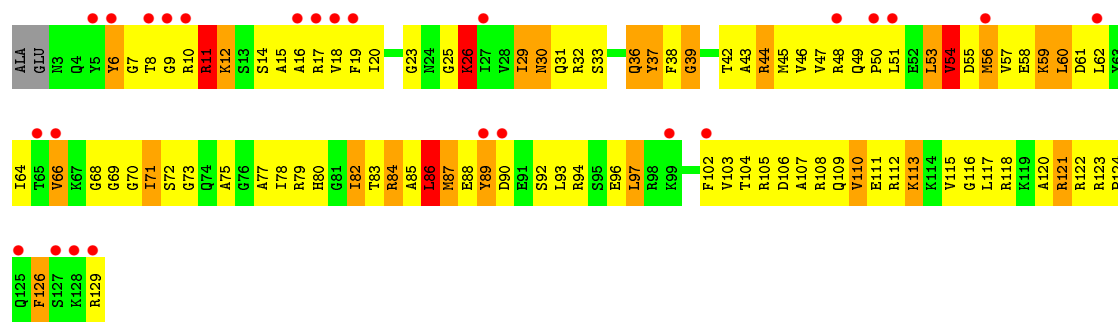
• Molecule 40: 30S RIBOSOMAL PROTEIN S8



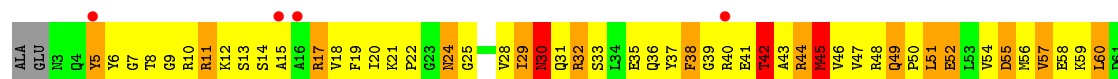
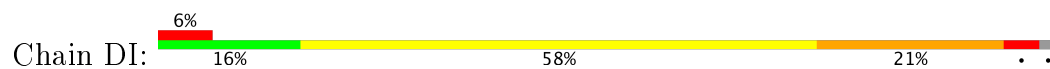
• Molecule 40: 30S RIBOSOMAL PROTEIN S8

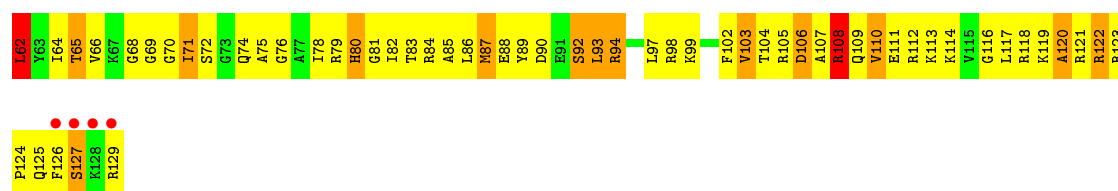


• Molecule 41: 30S RIBOSOMAL PROTEIN S9

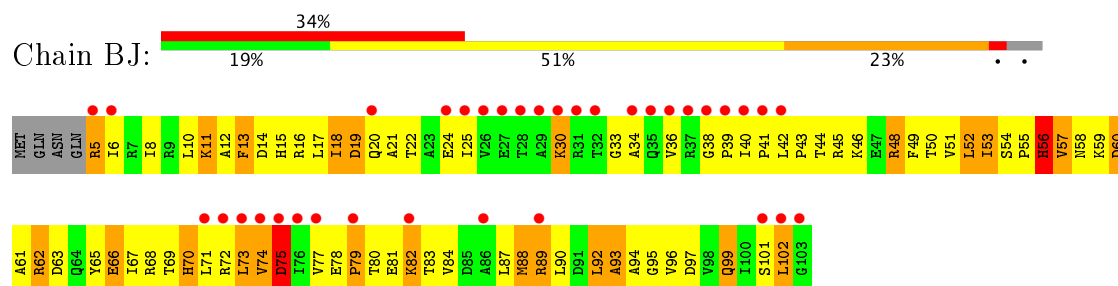


• Molecule 41: 30S RIBOSOMAL PROTEIN S9

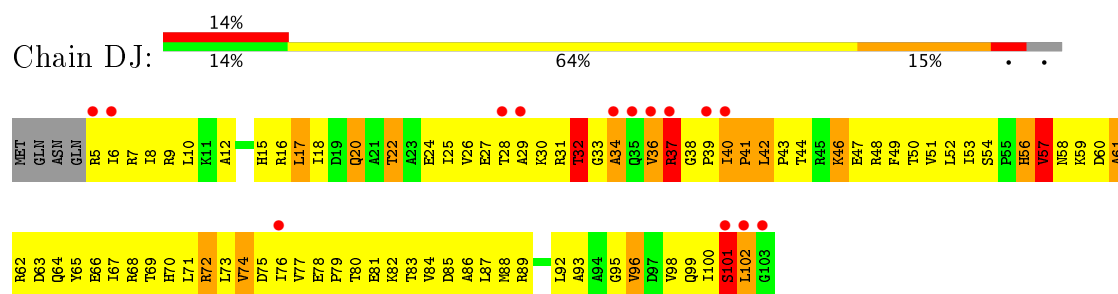




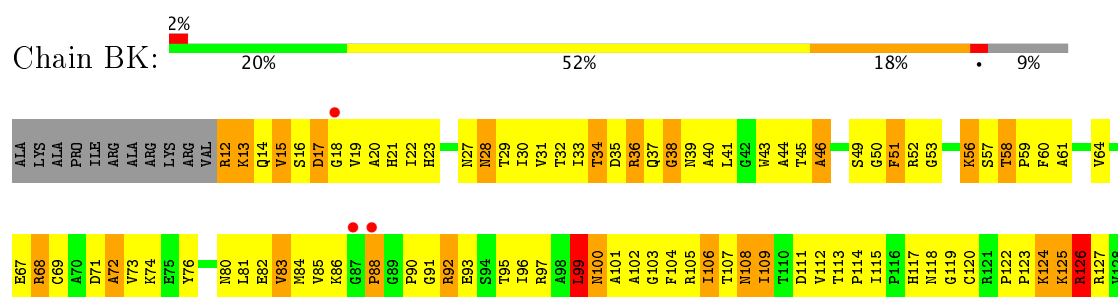
● Molecule 42: 30S RIBOSOMAL PROTEIN S10



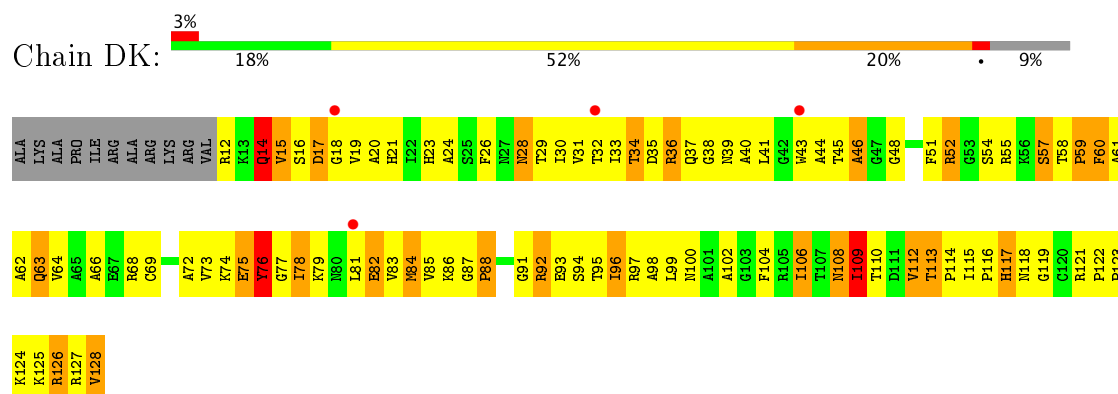
● Molecule 42: 30S RIBOSOMAL PROTEIN S10



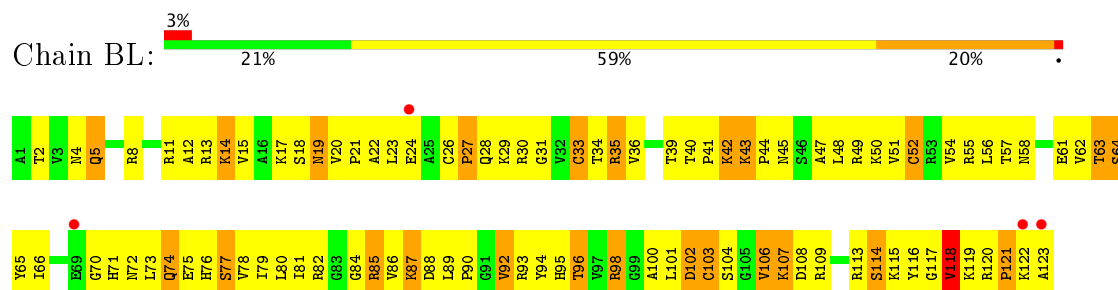
● Molecule 43: 30S RIBOSOMAL PROTEIN S11



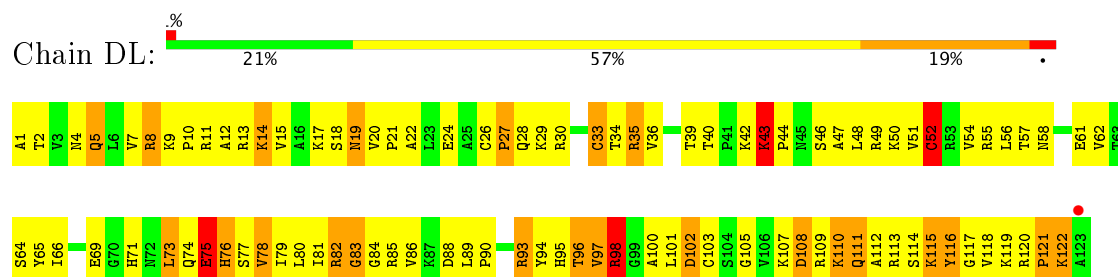
● Molecule 43: 30S RIBOSOMAL PROTEIN S11



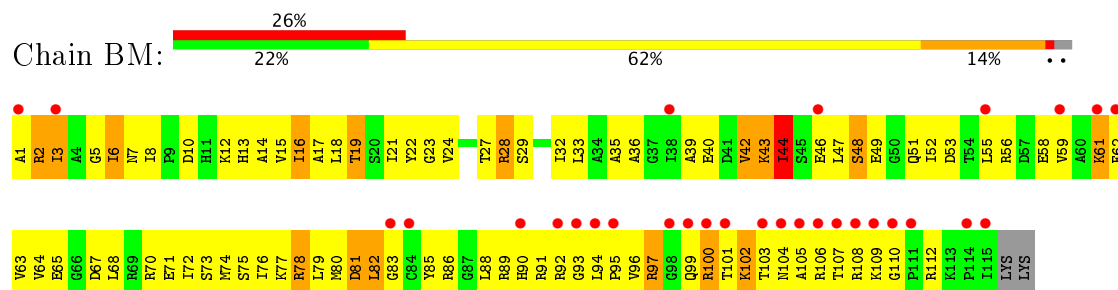
• Molecule 44: 30S RIBOSOMAL PROTEIN S12



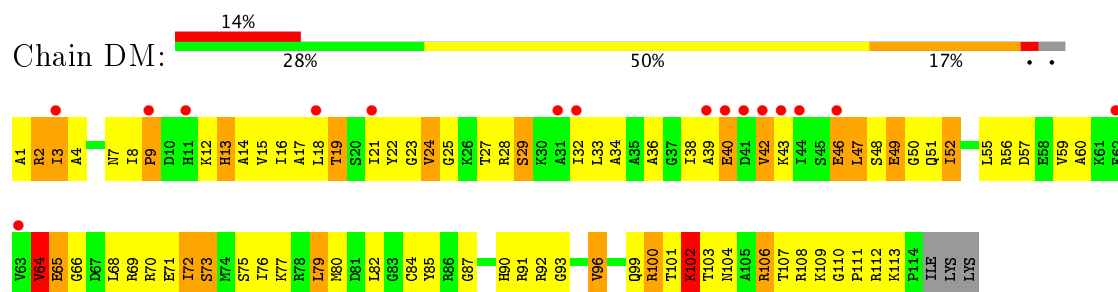
• Molecule 44: 30S RIBOSOMAL PROTEIN S12



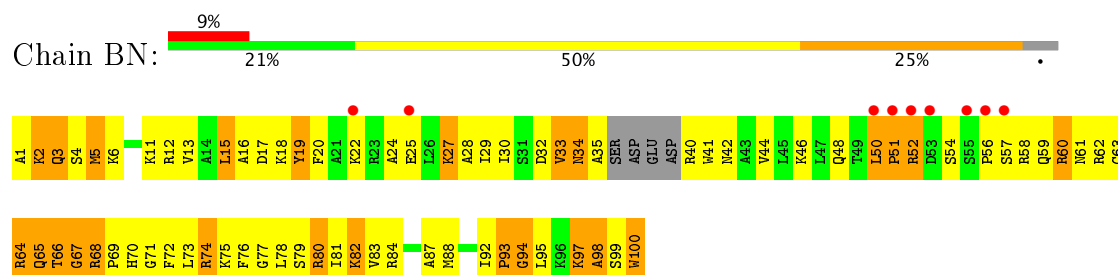
• Molecule 45: 30S RIBOSOMAL PROTEIN S13

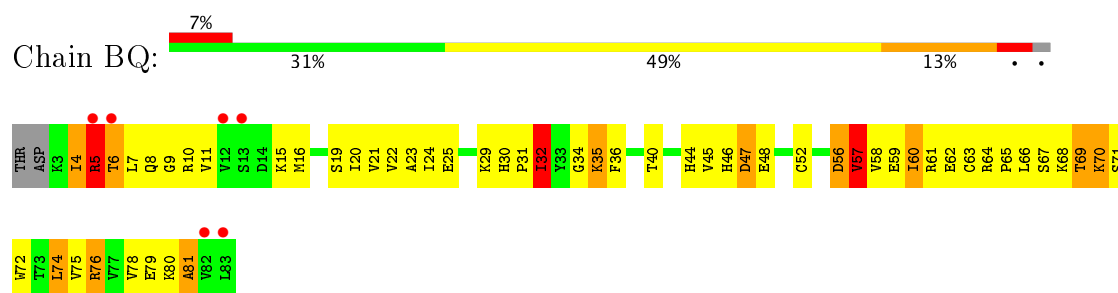


• Molecule 45: 30S RIBOSOMAL PROTEIN S13

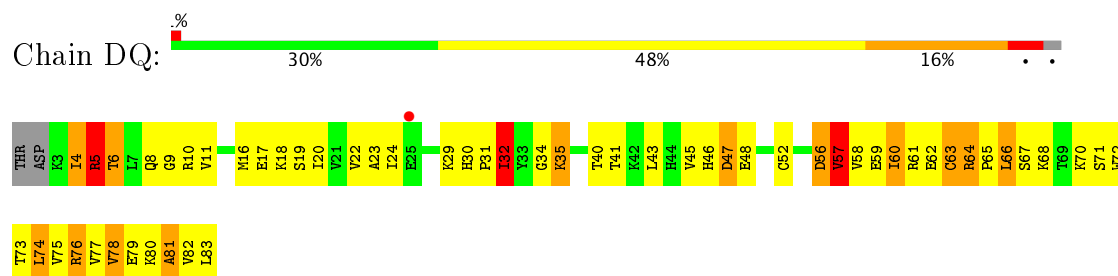


• Molecule 46: 30S RIBOSOMAL PROTEIN S14

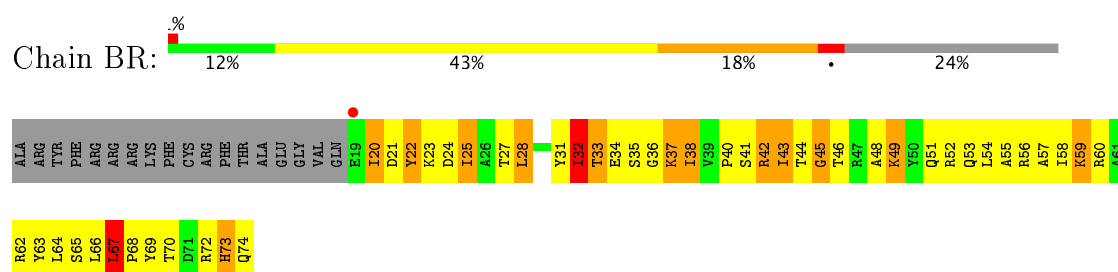




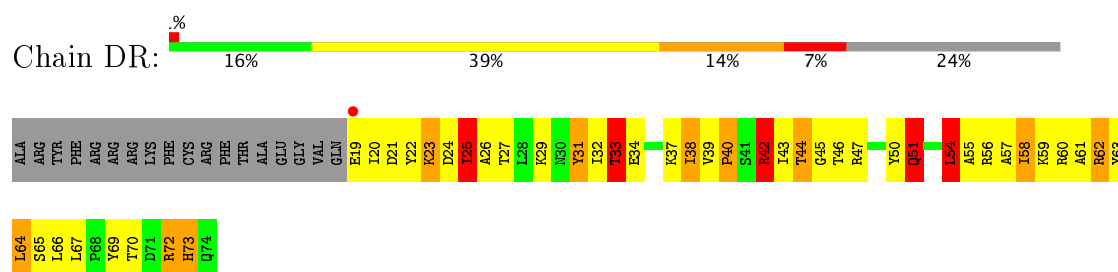
• Molecule 49: 30S RIBOSOMAL PROTEIN S17



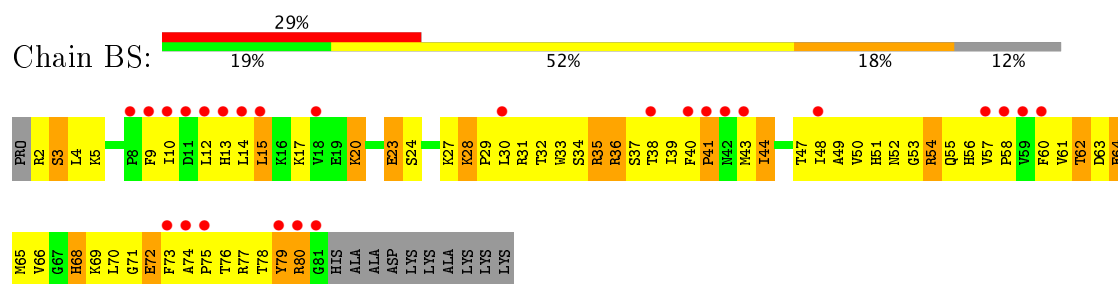
• Molecule 50: 30S RIBOSOMAL PROTEIN S18



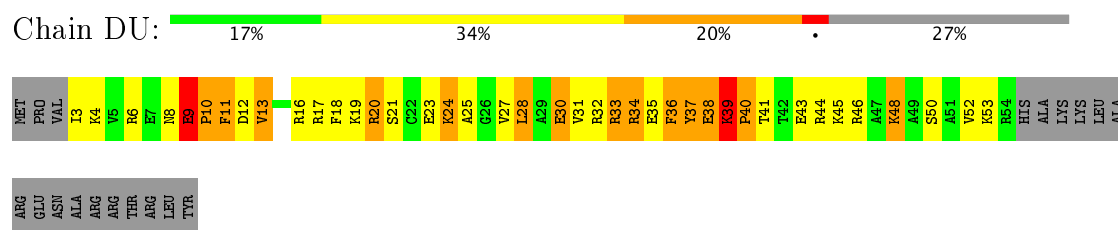
• Molecule 50: 30S RIBOSOMAL PROTEIN S18



• Molecule 51: 30S RIBOSOMAL PROTEIN S19



• Molecule 51: 30S RIBOSOMAL PROTEIN S19



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	90.4	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.10 , 15.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	284264	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	6966	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	3630	0
33	DA	32831	0	16521	4106	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	37666	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 37666 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	0
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	1
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	2
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	2
13	CG	174/176 (99%)	89 (51%)	52 (30%)	33 (19%)	0	2
14	AH	147/149 (99%)	94 (64%)	34 (23%)	19 (13%)	0	6
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	11
15	CI	137/141 (97%)	87 (64%)	32 (23%)	18 (13%)	0	6
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	2
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	0
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	0
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	0
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	0
25	CS	108/110 (98%)	52 (48%)	29 (27%)	27 (25%)	0	0

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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	0
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	5
28	CV	92/94 (98%)	57 (62%)	21 (23%)	14 (15%)	0	4
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	1
31	AY	56/58 (97%)	25 (45%)	17 (30%)	14 (25%)	0	0
31	CY	56/58 (97%)	26 (46%)	19 (34%)	11 (20%)	0	2
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	2
34	BB	217/240 (90%)	128 (59%)	65 (30%)	24 (11%)	0	9
34	DB	217/240 (90%)	124 (57%)	59 (27%)	34 (16%)	0	4
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	6
36	BD	203/205 (99%)	120 (59%)	57 (28%)	26 (13%)	0	6
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	4
38	BF	99/135 (73%)	62 (63%)	25 (25%)	12 (12%)	0	7
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	11
39	DG	151/178 (85%)	94 (62%)	43 (28%)	14 (9%)	1	13
40	BH	127/129 (98%)	73 (58%)	42 (33%)	12 (9%)	1	13
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	12
41	DI	125/129 (97%)	73 (58%)	32 (26%)	20 (16%)	0	4
42	BJ	97/103 (94%)	59 (61%)	23 (24%)	15 (16%)	0	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	DJ	97/103 (94%)	62 (64%)	24 (25%)	11 (11%)	0	8
43	BK	115/128 (90%)	69 (60%)	31 (27%)	15 (13%)	0	6
43	DK	115/128 (90%)	73 (64%)	30 (26%)	12 (10%)	0	10
44	BL	121/123 (98%)	67 (55%)	37 (31%)	17 (14%)	0	5
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	12
45	DM	112/117 (96%)	78 (70%)	20 (18%)	14 (12%)	0	7
46	BN	92/100 (92%)	58 (63%)	18 (20%)	16 (17%)	0	3
46	DN	92/100 (92%)	55 (60%)	18 (20%)	19 (21%)	0	2
47	BO	86/89 (97%)	51 (59%)	26 (30%)	9 (10%)	0	10
47	DO	86/89 (97%)	51 (59%)	26 (30%)	9 (10%)	0	10
48	BP	80/82 (98%)	43 (54%)	22 (28%)	15 (19%)	0	2
48	DP	79/82 (96%)	38 (48%)	24 (30%)	17 (22%)	0	1
49	BQ	79/83 (95%)	53 (67%)	15 (19%)	11 (14%)	0	5
49	DQ	79/83 (95%)	53 (67%)	16 (20%)	10 (13%)	0	6
50	BR	54/74 (73%)	25 (46%)	19 (35%)	10 (18%)	0	2
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	17
51	DS	79/91 (87%)	50 (63%)	20 (25%)	9 (11%)	0	8
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	5
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	17
2	A1	48/48 (100%)	40 (83%)	8 (17%)	2	18
2	C1	48/48 (100%)	36 (75%)	12 (25%)	1	5
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	10
9	AC	213/218 (98%)	150 (70%)	63 (30%)	0	3
9	CC	213/218 (98%)	147 (69%)	66 (31%)	0	3
10	AD	164/164 (100%)	112 (68%)	52 (32%)	0	2
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	3
12	AF	149/149 (100%)	129 (87%)	20 (13%)	4	28
12	CF	149/149 (100%)	131 (88%)	18 (12%)	6	32
13	AG	137/137 (100%)	103 (75%)	34 (25%)	1	5
13	CG	137/137 (100%)	106 (77%)	31 (23%)	1	7
14	AH	114/114 (100%)	87 (76%)	27 (24%)	1	6
14	CH	114/114 (100%)	85 (75%)	29 (25%)	0	5
15	AI	109/109 (100%)	93 (85%)	16 (15%)	3	24
15	CI	109/109 (100%)	98 (90%)	11 (10%)	9	40
16	AJ	114/116 (98%)	74 (65%)	40 (35%)	0	1

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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	3
20	CN	103/103 (100%)	69 (67%)	34 (33%)	0	2
21	AO	87/87 (100%)	64 (74%)	23 (26%)	0	4
21	CO	87/87 (100%)	69 (79%)	18 (21%)	1	9
22	AP	99/99 (100%)	79 (80%)	20 (20%)	1	10
22	CP	99/99 (100%)	81 (82%)	18 (18%)	2	13
23	AQ	89/89 (100%)	58 (65%)	31 (35%)	0	1
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	3
25	CS	93/93 (100%)	66 (71%)	27 (29%)	0	3
26	AT	83/84 (99%)	60 (72%)	23 (28%)	0	4
26	CT	83/84 (99%)	59 (71%)	24 (29%)	0	3
27	AU	83/84 (99%)	63 (76%)	20 (24%)	1	6
27	CU	83/84 (99%)	63 (76%)	20 (24%)	1	6
28	AV	78/78 (100%)	63 (81%)	15 (19%)	1	11
28	CV	78/78 (100%)	62 (80%)	16 (20%)	1	9
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	3
32	CZ	62/62 (100%)	43 (69%)	19 (31%)	0	3
34	BB	180/198 (91%)	143 (79%)	37 (21%)	1	9
34	DB	180/198 (91%)	140 (78%)	40 (22%)	1	7
35	BC	170/189 (90%)	142 (84%)	28 (16%)	2	18
35	DC	170/189 (90%)	130 (76%)	40 (24%)	1	6
36	BD	172/172 (100%)	137 (80%)	35 (20%)	1	10
36	DD	172/172 (100%)	126 (73%)	46 (27%)	0	4
37	BE	113/125 (90%)	86 (76%)	27 (24%)	1	6
37	DE	113/125 (90%)	82 (73%)	31 (27%)	0	4
38	BF	87/116 (75%)	71 (82%)	16 (18%)	2	13
38	DF	87/116 (75%)	67 (77%)	20 (23%)	1	7
39	BG	123/146 (84%)	105 (85%)	18 (15%)	3	25
39	DG	125/146 (86%)	95 (76%)	30 (24%)	1	6
40	BH	104/104 (100%)	78 (75%)	26 (25%)	1	5
40	DH	104/104 (100%)	78 (75%)	26 (25%)	1	5
41	BI	105/106 (99%)	81 (77%)	24 (23%)	1	7
41	DI	105/106 (99%)	82 (78%)	23 (22%)	1	7
42	BJ	86/90 (96%)	68 (79%)	18 (21%)	1	9
42	DJ	86/90 (96%)	71 (83%)	15 (17%)	2	16
43	BK	90/98 (92%)	68 (76%)	22 (24%)	1	6
43	DK	90/98 (92%)	61 (68%)	29 (32%)	0	2
44	BL	103/103 (100%)	82 (80%)	21 (20%)	1	9
44	DL	103/103 (100%)	79 (77%)	24 (23%)	1	6
45	BM	92/95 (97%)	76 (83%)	16 (17%)	2	16
45	DM	91/95 (96%)	74 (81%)	17 (19%)	2	12
46	BN	79/83 (95%)	66 (84%)	13 (16%)	2	18
46	DN	79/83 (95%)	64 (81%)	15 (19%)	2	12
47	BO	76/77 (99%)	63 (83%)	13 (17%)	2	17
47	DO	76/77 (99%)	60 (79%)	16 (21%)	1	9
48	BP	65/65 (100%)	54 (83%)	11 (17%)	2	17

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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	31
49	DQ	75/77 (97%)	63 (84%)	12 (16%)	3	20
50	BR	48/64 (75%)	39 (81%)	9 (19%)	2	12
50	DR	48/64 (75%)	35 (73%)	13 (27%)	0	4
51	BS	70/78 (90%)	59 (84%)	11 (16%)	3	22
51	DS	71/78 (91%)	53 (75%)	18 (25%)	0	5
52	BT	65/65 (100%)	55 (85%)	10 (15%)	3	22
52	DT	65/65 (100%)	57 (88%)	8 (12%)	5	31
53	BU	44/61 (72%)	39 (89%)	5 (11%)	7	35
53	DU	44/61 (72%)	31 (70%)	13 (30%)	0	3
All	All	9356/9707 (96%)	6965 (74%)	2391 (26%)	0	5

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, 95th 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 ²)	Q<0.9
1	A0	56/56 (100%)	0.29	5 (8%)	10 8	109, 149, 271, 317	0
1	C0	56/56 (100%)	0.30	5 (8%)	10 8	97, 120, 190, 244	0
2	A1	54/54 (100%)	0.83	9 (16%)	2 2	124, 143, 239, 296	0
2	C1	54/54 (100%)	1.11	10 (18%)	1 1	92, 113, 223, 254	0
3	A2	46/46 (100%)	0.53	3 (6%)	20 14	74, 92, 165, 271	0
3	C2	46/46 (100%)	0.05	3 (6%)	20 14	68, 103, 198, 264	0
4	A3	64/64 (100%)	0.13	5 (7%)	14 11	80, 106, 228, 309	0
4	C3	64/64 (100%)	-0.06	2 (3%)	49 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%)	0.74	5 (13%)	4 4	124, 144, 238, 298	0
6	A5	16/16 (100%)	-0.18	0	100 100	73, 108, 197, 216	0
7	AA	117/120 (97%)	-0.52	0	100 100	78, 127, 174, 316	0
7	CA	117/120 (97%)	-0.56	1 (0%)	84 75	71, 127, 170, 285	0
8	AB	2841/2904 (97%)	-0.43	33 (1%)	79 68	57, 105, 213, 373	0
8	CB	2841/2904 (97%)	-0.59	12 (0%)	92 88	41, 89, 202, 421	0
9	AC	268/273 (98%)	0.10	16 (5%)	23 16	71, 107, 196, 257	0
9	CC	268/273 (98%)	-0.06	12 (4%)	34 26	63, 91, 165, 248	0
10	AD	209/209 (100%)	0.22	8 (3%)	41 31	12, 127, 226, 325	0
10	CD	209/209 (100%)	-0.07	9 (4%)	36 27	11, 94, 186, 271	0
11	AE	201/201 (100%)	0.18	16 (7%)	13 10	92, 120, 206, 299	0
11	CE	201/201 (100%)	0.32	26 (12%)	4 4	88, 117, 224, 290	0
12	AF	178/178 (100%)	0.23	11 (6%)	21 15	121, 170, 253, 334	0
12	CF	178/178 (100%)	0.24	12 (6%)	19 13	92, 155, 224, 286	0
13	AG	176/176 (100%)	0.15	17 (9%)	8 7	100, 137, 207, 246	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	CG	176/176 (100%)	0.49	24 (13%) 3 4	88, 138, 222, 271	0
14	AH	149/149 (100%)	1.72	47 (31%) 0 1	71, 314, 427, 456	0
14	CH	149/149 (100%)	0.37	13 (8%) 11 9	107, 147, 233, 274	0
15	AI	141/141 (100%)	1.90	50 (35%) 0 1	155, 233, 307, 356	0
15	CI	141/141 (100%)	2.78	62 (43%) 0 1	219, 343, 422, 470	0
16	AJ	141/142 (99%)	0.05	8 (5%) 24 18	105, 130, 217, 267	0
16	CJ	141/142 (99%)	0.16	5 (3%) 44 34	104, 121, 207, 250	0
17	AK	122/123 (99%)	-0.22	0 100 100	81, 109, 162, 234	0
17	CK	122/123 (99%)	-0.48	0 100 100	80, 94, 127, 208	0
18	AL	144/144 (100%)	1.04	21 (14%) 3 3	94, 138, 281, 363	0
18	CL	144/144 (100%)	0.62	22 (15%) 2 2	83, 128, 275, 315	0
19	AM	136/136 (100%)	0.13	11 (8%) 13 10	105, 126, 222, 268	0
19	CM	136/136 (100%)	-0.03	6 (4%) 35 26	77, 108, 223, 279	0
20	AN	127/127 (100%)	0.04	5 (3%) 40 30	96, 114, 200, 251	0
20	CN	127/127 (100%)	-0.10	6 (4%) 32 24	58, 78, 155, 257	0
21	AO	117/117 (100%)	0.22	10 (8%) 11 10	107, 162, 236, 299	0
21	CO	117/117 (100%)	0.40	13 (11%) 6 6	52, 118, 211, 255	0
22	AP	114/114 (100%)	-0.10	2 (1%) 69 57	85, 123, 219, 281	0
22	CP	114/114 (100%)	-0.25	2 (1%) 69 57	77, 96, 196, 257	0
23	AQ	117/117 (100%)	-0.27	0 100 100	70, 106, 152, 203	0
23	CQ	117/117 (100%)	-0.29	1 (0%) 84 75	70, 93, 148, 225	0
24	AR	103/103 (100%)	0.20	3 (2%) 52 40	105, 145, 250, 346	0
24	CR	103/103 (100%)	0.28	8 (7%) 14 11	87, 132, 229, 286	0
25	AS	110/110 (100%)	0.11	3 (2%) 55 43	77, 106, 167, 279	0
25	CS	110/110 (100%)	-0.08	2 (1%) 69 57	49, 85, 152, 211	0
26	AT	100/100 (100%)	0.00	4 (4%) 39 29	94, 130, 222, 250	0
26	CT	100/100 (100%)	0.41	13 (13%) 4 4	85, 120, 248, 278	0
27	AU	103/103 (100%)	1.08	24 (23%) 1 1	90, 140, 235, 264	0
27	CU	103/103 (100%)	0.88	20 (19%) 1 1	118, 162, 256, 281	0
28	AV	94/94 (100%)	-0.23	3 (3%) 48 37	86, 136, 209, 234	0
28	CV	94/94 (100%)	-0.19	4 (4%) 36 27	87, 125, 194, 215	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
29	AW	84/84 (100%)	1.18	16 (19%) 1 1	116, 147, 244, 330	0
29	CW	84/84 (100%)	0.70	12 (14%) 3 3	111, 136, 238, 275	0
30	AX	63/63 (100%)	-0.05	4 (6%) 21 15	84, 130, 208, 247	0
30	CX	63/63 (100%)	0.42	10 (15%) 2 2	86, 150, 233, 320	0
31	AY	58/58 (100%)	1.52	15 (25%) 1 1	116, 143, 272, 279	0
31	CY	58/58 (100%)	0.96	7 (12%) 5 5	126, 138, 240, 249	0
32	AZ	70/70 (100%)	0.17	5 (7%) 17 12	66, 104, 170, 258	0
32	CZ	70/70 (100%)	-0.07	3 (4%) 36 27	70, 91, 169, 255	0
33	BA	1530/1542 (99%)	-0.32	18 (1%) 79 68	70, 137, 279, 497	0
33	DA	1530/1542 (99%)	-0.51	7 (0%) 90 85	45, 111, 224, 368	0
34	BB	219/240 (91%)	-0.02	8 (3%) 42 32	94, 175, 269, 316	0
34	DB	219/240 (91%)	0.20	17 (7%) 14 11	108, 159, 243, 292	0
35	BC	207/232 (89%)	0.18	20 (9%) 8 7	87, 169, 255, 315	0
35	DC	207/232 (89%)	-0.04	11 (5%) 27 21	113, 140, 207, 226	0
36	BD	205/205 (100%)	-0.19	2 (0%) 82 72	61, 139, 230, 325	0
36	DD	205/205 (100%)	-0.27	2 (0%) 82 72	71, 102, 169, 227	0
37	BE	151/166 (90%)	0.25	11 (7%) 16 12	75, 156, 254, 336	0
37	DE	151/166 (90%)	-0.00	6 (3%) 39 29	56, 99, 174, 250	0
38	BF	101/135 (74%)	-0.04	6 (5%) 23 17	57, 140, 224, 279	0
38	DF	101/135 (74%)	-0.11	0 100 100	110, 137, 200, 247	0
39	BG	151/178 (84%)	0.71	24 (15%) 2 2	94, 206, 288, 333	0
39	DG	153/178 (85%)	0.07	5 (3%) 47 36	44, 144, 206, 228	0
40	BH	129/129 (100%)	0.25	9 (6%) 17 13	76, 157, 231, 297	0
40	DH	129/129 (100%)	-0.23	2 (1%) 72 61	70, 98, 166, 216	0
41	BI	127/129 (98%)	0.89	25 (19%) 1 1	90, 194, 271, 307	0
41	DI	127/129 (98%)	0.31	8 (6%) 21 15	103, 165, 231, 281	0
42	BJ	99/103 (96%)	1.63	35 (35%) 0 1	131, 254, 373, 423	0
42	DJ	99/103 (96%)	0.58	14 (14%) 3 3	130, 173, 223, 237	0
43	BK	117/128 (91%)	-0.12	3 (2%) 56 45	54, 128, 245, 290	0
43	DK	117/128 (91%)	-0.06	4 (3%) 46 35	69, 100, 165, 222	0
44	BL	123/123 (100%)	0.01	4 (3%) 47 36	50, 138, 215, 332	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	DL	123/123 (100%)	-0.27	1 (0%) 86 77	64, 95, 150, 211	0
45	BM	115/117 (98%)	1.28	30 (26%) 1 1	144, 252, 315, 344	0
45	DM	114/117 (97%)	0.61	16 (14%) 3 3	113, 171, 221, 288	0
46	BN	96/100 (96%)	0.53	9 (9%) 9 7	85, 188, 308, 367	0
46	DN	96/100 (96%)	0.46	12 (12%) 4 5	105, 153, 250, 295	0
47	BO	88/89 (98%)	-0.13	1 (1%) 80 70	67, 133, 213, 255	0
47	DO	88/89 (98%)	-0.37	0 100 100	73, 105, 170, 201	0
48	BP	82/82 (100%)	1.01	18 (21%) 1 1	90, 168, 269, 347	0
48	DP	81/82 (98%)	0.41	7 (8%) 11 9	69, 93, 145, 202	0
49	BQ	81/83 (97%)	0.41	6 (7%) 15 11	101, 180, 266, 301	0
49	DQ	81/83 (97%)	-0.01	1 (1%) 79 68	65, 109, 172, 212	0
50	BR	56/74 (75%)	-0.22	1 (1%) 69 57	66, 117, 216, 283	0
50	DR	56/74 (75%)	0.38	1 (1%) 69 57	74, 103, 172, 253	0
51	BS	80/91 (87%)	1.65	26 (32%) 0 1	152, 267, 315, 366	0
51	DS	81/91 (89%)	0.76	14 (17%) 2 2	122, 182, 230, 249	0
52	BT	85/86 (98%)	-0.18	0 100 100	76, 155, 224, 256	0
52	DT	85/86 (98%)	0.13	3 (3%) 44 34	79, 97, 185, 219	0
53	BU	52/71 (73%)	0.04	3 (5%) 24 17	91, 171, 256, 300	0
53	DU	52/71 (73%)	-0.39	0 100 100	95, 140, 201, 249	0
All	All	20487/21050 (97%)	-0.05	1083 (5%) 27 21	11, 121, 254, 497	0

The worst 5 of 1083 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
15	CI	98	GLY	28.5
15	CI	83	ALA	21.9
18	AL	98	ALA	17.5
15	AI	70	THR	17.4
15	CI	137	LEU	16.6

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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 ²)	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(\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(\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(\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(\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(\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(\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(\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(\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.