



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:04 PM GMT

PDB ID : 4V9D
Title : Structures of the bacterial ribosome in classical and hybrid states of tRNA binding
Authors : Dunkle, J.A.; Wang, L.; Feldman, M.B.; Pulk, A.; Chen, V.B.; Kapral, G.J.; Noeske, J.; Richardson, J.S.; Blanchard, S.C.; Cate, J.H.D.
Deposited on : 2012-07-31
Resolution : 3.00 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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

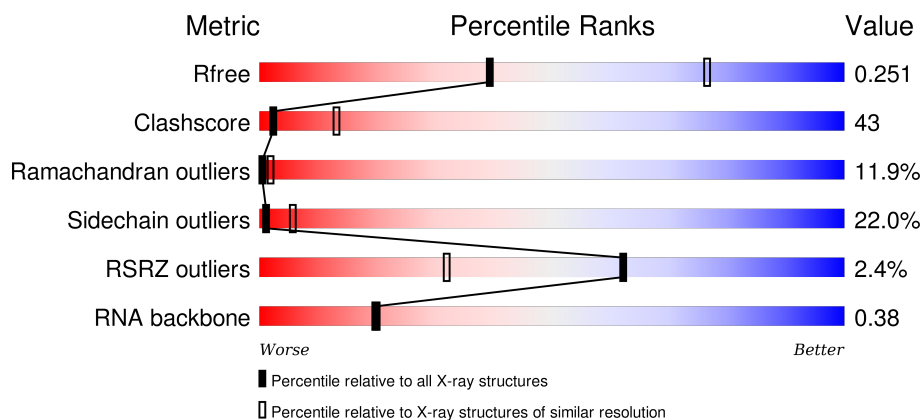
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



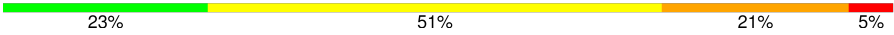


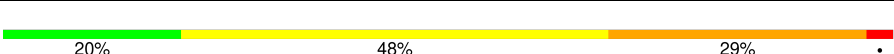
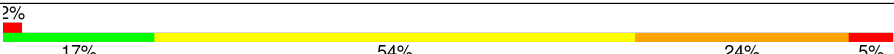
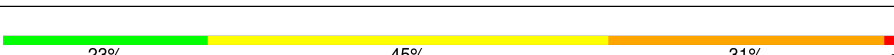
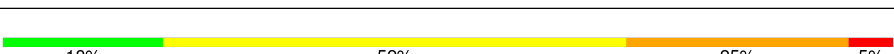
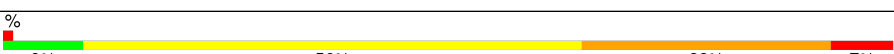
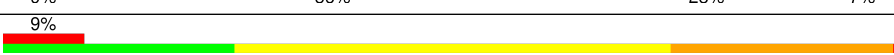
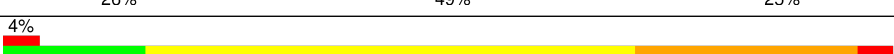
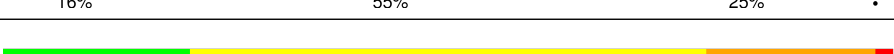
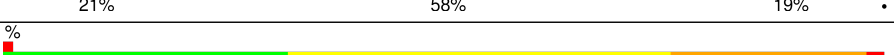
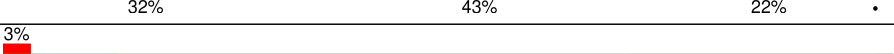
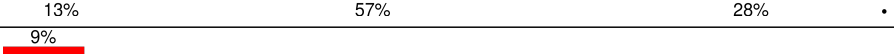


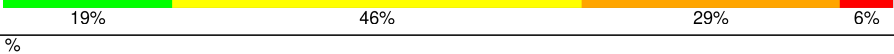
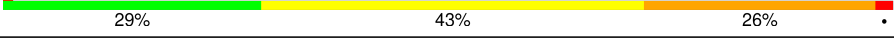
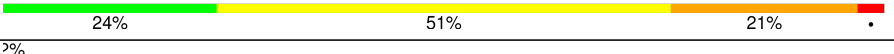
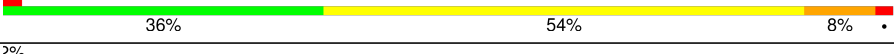
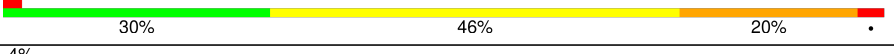
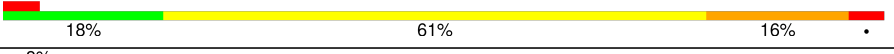
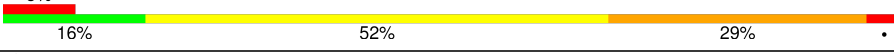


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)
RNA backbone	2183	1036 (3.40-2.60)

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	AA	1539	<div> <div>14%</div> <div>54%</div> <div>28%</div> <div>•</div> </div>
1	BA	1539	<div> <div>13%</div> <div>55%</div> <div>28%</div> <div>•</div> </div>
2	AB	218	<div> <div>7%</div> <div>10%</div> <div>45%</div> <div>36%</div> <div>9%</div> </div>
2	BB	218	<div> <div>6%</div> <div>15%</div> <div>51%</div> <div>26%</div> <div>8%</div> </div>

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Mol	Chain	Length	Quality of chain
3	AC	206	
3	BC	206	
4	AD	205	
4	BD	205	
5	AE	150	
5	BE	150	
6	AF	100	
6	BF	100	
7	AG	151	
7	BG	151	
8	AH	129	
8	BH	129	
9	AI	127	
9	BI	127	
10	AJ	98	
10	BJ	98	
11	AK	117	
11	BK	117	
12	AL	123	
12	BL	123	
13	AM	114	
13	BM	114	
14	AN	100	
14	BN	100	
15	AO	88	

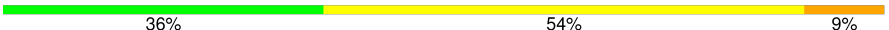

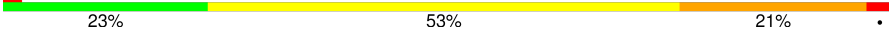
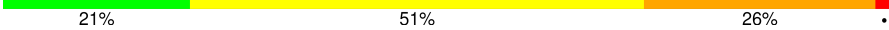


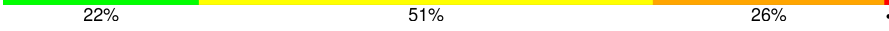
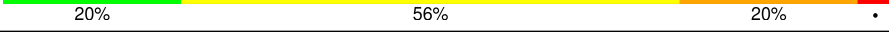



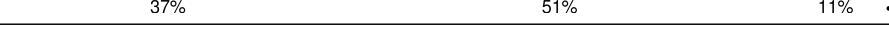







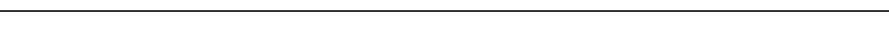

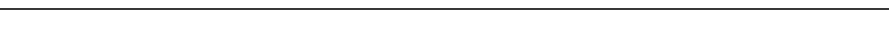
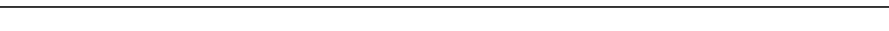


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Mol	Chain	Length	Quality of chain
15	BO	88	
16	AP	82	
16	BP	82	
17	AQ	80	
17	BQ	80	
18	AR	55	
18	BR	55	
19	AS	79	
19	BS	79	
20	AT	85	
20	BT	85	
21	AU	51	
21	BU	51	
22	AV	76	
22	BV	76	
23	AX	16	
23	BX	16	
24	AY	183	
25	CA	2903	
25	DA	2903	
26	CB	119	
27	CC	271	
27	DC	271	
28	CD	209	
28	DD	209	

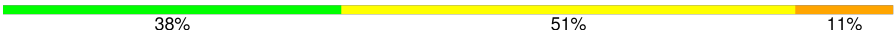

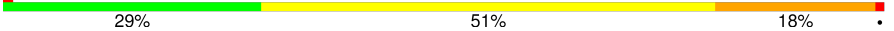





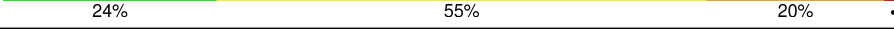


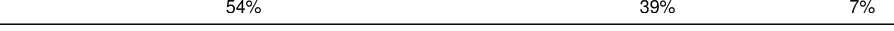


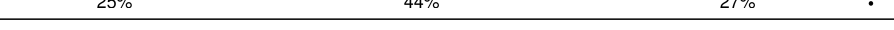




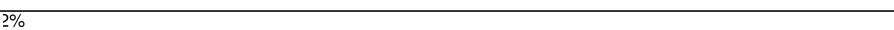

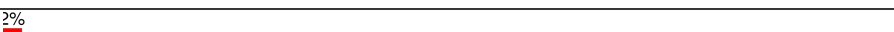
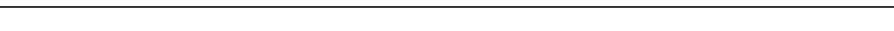


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Mol	Chain	Length	Quality of chain
29	CE	201	
29	DE	201	
30	CF	177	
30	DF	177	
31	CG	176	
31	DG	176	
32	CH	149	
32	DH	149	
33	CI	141	
33	DI	141	
34	CJ	142	
34	DJ	142	
35	CK	122	
35	DK	122	
36	CL	143	
36	DL	143	
37	CM	136	
37	DM	136	
38	CN	120	
38	DN	120	
39	CO	116	
39	DO	116	
40	CP	114	
40	DP	114	
41	CQ	117	

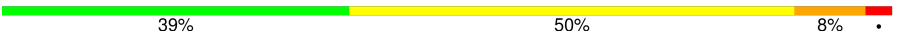


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Mol	Chain	Length	Quality of chain
41	DQ	117	
42	CR	103	
42	DR	103	
43	CS	110	
43	DS	110	
44	CT	93	
44	DT	93	
45	CU	102	
45	DU	102	
46	CV	94	
46	DV	94	
47	CW	76	
48	CX	77	
48	DX	77	
49	CY	63	
49	DY	63	
50	CZ	58	
50	DZ	58	
51	C0	56	
51	D0	56	
52	C1	50	
52	D1	50	
53	C2	46	
53	D2	46	
54	C3	64	

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Mol	Chain	Length	Quality of chain
54	D3	64	
55	C4	38	
55	D4	38	
56	DB	118	
57	DW	75	

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
58	MG	AA	1604	-	-	-	X
58	MG	AA	1622	-	-	-	X
58	MG	CA	3066	-	-	-	X
58	MG	CA	3121	-	-	-	X
58	MG	CA	3132	-	-	-	X
58	MG	CA	3147	-	-	-	X
58	MG	CA	3153	-	-	-	X
58	MG	CA	3155	-	-	-	X
58	MG	CA	3159	-	-	-	X
58	MG	CA	3163	-	-	-	X
58	MG	CA	3165	-	-	-	X
58	MG	CA	3175	-	-	-	X
58	MG	CA	3186	-	-	-	X
58	MG	CA	3188	-	-	-	X
58	MG	DA	3108	-	-	-	X
58	MG	DA	3116	-	-	-	X
58	MG	DA	3131	-	-	-	X
58	MG	DA	3139	-	-	-	X
58	MG	DA	3142	-	-	-	X
58	MG	DA	3152	-	-	-	X
58	MG	DA	3154	-	-	-	X
58	MG	DA	3157	-	-	-	X

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 292354 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1538	Total	C	N	O	P	0	0	0
			32995	14716	6050	10691	1538			
1	BA	1539	Total	C	N	O	P	0	0	0
			33015	14725	6052	10699	1539			

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	218	Total	C	N	O	S	0	0	0
			1705	1081	305	312	7			
2	BB	218	Total	C	N	O	S	0	0	0
			1705	1081	305	312	7			

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0	0
			1625	1028	305	289	3			
3	BC	206	Total	C	N	O	S	0	0	0
			1625	1028	305	289	3			

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	150	Total	C	N	O	S	0	0	0
			1106	687	211	202	6			
5	BE	150	Total	C	N	O	S	0	0	0
			1106	687	211	202	6			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	100	Total	C	N	O	S	0	0	0
			818	515	148	149	6			
6	BF	100	Total	C	N	O	S	0	0	0
			818	515	148	149	6			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	151	Total	C	N	O	S	0	0	0
			1182	735	227	216	4			
7	BG	151	Total	C	N	O	S	0	0	0
			1182	735	227	216	4			

- Molecule 8 is a protein called 30S ribosomal protein S8.

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

- Molecule 9 is a protein called 30S ribosomal protein S9.

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

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	98	Total	C	N	O	S	0	0	0
			787	493	150	143	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	BJ	98	Total	C	N	O	S	0	0	0
			787	493	150	143	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

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

- Molecule 12 is a protein called 30S ribosomal protein S12.

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

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	114	Total	C	N	O	S	0	0	0
			884	546	178	157	3			
13	BM	114	Total	C	N	O	S	0	0	0
			884	546	178	157	3			

- Molecule 14 is a protein called 30S ribosomal protein S14.

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

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			
15	BO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			
16	BP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	80	Total	C	N	O	S	0	0	0
			649	411	121	114	3			
17	BQ	80	Total	C	N	O	S	0	0	0
			649	411	121	114	3			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	55	Total	C	N	O	0	0	0
			456	288	86	82			
18	BR	55	Total	C	N	O	0	0	0
			456	288	86	82			

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	79	Total	C	N	O	S	0	0	0
			638	408	120	108	2			
19	BS	79	Total	C	N	O	S	0	0	0
			638	408	120	108	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

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

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AU	51	Total	C	N	O	S	0	0	0
			426	265	86	74	1			
21	BU	51	Total	C	N	O	S	0	0	0
			426	265	86	74	1			

- Molecule 22 is a RNA chain called phenylalanine specific transfer RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	76	Total	C	N	O	P	0	0	0
			1623	723	290	534	76			
22	BV	76	Total	C	N	O	P	0	0	0
			1623	723	290	534	76			

- Molecule 23 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AX	15	Total	C	N	O	P	0	0	0
			324	145	61	103	15			
23	BX	16	Total	C	N	O	P	0	0	0
			346	155	66	109	16			

- Molecule 24 is a protein called ribosome recycling factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AY	183	Total	C	N	O	S	0	0	0
			1419	871	260	283	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AY	2	GLY	-	EXPRESSION TAG	UNP P0A805

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	CA	2897	Total	C	N	O	P	0	0	0
			62195	27745	11446	20107	2897			
25	DA	2896	Total	C	N	O	P	0	0	0
			62173	27735	11441	20101	2896			

- Molecule 26 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	CB	119	Total	C	N	O	P	0	0	0
			2548	1135	466	829	118			

- Molecule 27 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	CC	271	Total	C	N	O	S	0	0	0
			2083	1288	423	365	7			
27	DC	271	Total	C	N	O	S	0	0	0
			2083	1288	423	365	7			

- Molecule 28 is a protein called 50S ribosomal protein L3.

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

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

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

- Molecule 30 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	CF	177	Total	C	N	O	S	0	0	0
			1411	899	249	257	6			
30	DF	177	Total	C	N	O	S	0	0	0
			1411	899	249	257	6			

- Molecule 31 is a protein called 50S ribosomal protein L6.

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

- Molecule 32 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	CH	149	Total	C	N	O	S	0	0	0
			1110	699	197	213	1			
32	DH	149	Total	C	N	O	S	0	0	0
			1110	699	197	213	1			

- Molecule 33 is a protein called 50S ribosomal protein L11.

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

- Molecule 34 is a protein called 50S ribosomal protein L13.

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

- Molecule 35 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	CK	122	Total	C	N	O	S	0	0	0
			939	587	180	166	6			
35	DK	122	Total	C	N	O	S	0	0	0
			939	587	180	166	6			

- Molecule 36 is a protein called 50S ribosomal protein L15.

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

- Molecule 37 is a protein called 50S ribosomal protein L16.

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

- Molecule 38 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	CN	120	Total	C	N	O	S	0	0	0
			961	593	196	167	5			
38	DN	120	Total	C	N	O	S	0	0	0
			961	593	196	167	5			

- Molecule 39 is a protein called 50S ribosomal protein L18.

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

- Molecule 40 is a protein called 50S ribosomal protein L19.

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

- Molecule 41 is a protein called 50S ribosomal protein L20.

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

- Molecule 42 is a protein called 50S ribosomal protein L21.

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

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

- Molecule 43 is a protein called 50S ribosomal protein L22.

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

- Molecule 44 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	CT	93	Total	C	N	O	S	0	0	0
			739	466	139	132	2			
44	DT	93	Total	C	N	O	S	0	0	0
			739	466	139	132	2			

- Molecule 45 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	CU	102	Total	C	N	O	S	0	0	0
			780	492	146	142				
45	DU	102	Total	C	N	O	S	0	0	0
			780	492	146	142				

- Molecule 46 is a protein called 50S ribosomal protein L25.

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

- Molecule 47 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	CW	76	Total	C	N	O	S	0	0	0
			575	356	117	101	1			

- Molecule 48 is a protein called 50S ribosomal protein L28.

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

- Molecule 49 is a protein called 50S ribosomal protein L29.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	C0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			
51	D0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
52	C1	50	Total	C	N	O	0	0	0
			410	263	75	72			
52	D1	50	Total	C	N	O	0	0	0
			410	263	75	72			

- Molecule 53 is a protein called 50S ribosomal protein L34.

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

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

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	C3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			
54	D3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

- Molecule 55 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	C4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			
55	D4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

- Molecule 56 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	DB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			

- Molecule 57 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	DW	75	Total	C	N	O	S	0	0	0
			564	350	113	100	1			

- Molecule 58 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	BA	56	Total	Mg	0	0
			56	56		
58	CA	194	Total	Mg	0	0
			194	194		
58	DQ	1	Total	Mg	0	0
			1	1		
58	CB	4	Total	Mg	0	0
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	DL	1	Total 1	Mg 1	0	0
58	AA	72	Total 72	Mg 72	0	0
58	CQ	1	Total 1	Mg 1	0	0
58	DA	166	Total 166	Mg 166	0	0
58	DB	3	Total 3	Mg 3	0	0

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	D4	1	Total 1	Zn 1	0	0
59	C4	1	Total 1	Zn 1	0	0

- Molecule 60 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AA	197	Total 197	O 197	0	0
60	AN	4	Total 4	O 4	0	0
60	AT	1	Total 1	O 1	0	0
60	AU	1	Total 1	O 1	0	0
60	BA	190	Total 190	O 190	0	0
60	BL	1	Total 1	O 1	0	0
60	BN	5	Total 5	O 5	0	0
60	BT	1	Total 1	O 1	0	0
60	BU	1	Total 1	O 1	0	0
60	CA	625	Total 625	O 625	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	CB	13	Total 13	O 13	0	0
60	CC	8	Total 8	O 8	0	0
60	CD	2	Total 2	O 2	0	0
60	CE	2	Total 2	O 2	0	0
60	CF	1	Total 1	O 1	0	0
60	CJ	1	Total 1	O 1	0	0
60	CL	6	Total 6	O 6	0	0
60	CN	4	Total 4	O 4	0	0
60	CS	1	Total 1	O 1	0	0
60	CV	1	Total 1	O 1	0	0
60	C2	1	Total 1	O 1	0	0
60	C3	1	Total 1	O 1	0	0
60	C4	2	Total 2	O 2	0	0
60	DA	622	Total 622	O 622	0	0
60	DB	14	Total 14	O 14	0	0
60	DC	4	Total 4	O 4	0	0
60	DD	5	Total 5	O 5	0	0
60	DE	2	Total 2	O 2	0	0
60	DJ	1	Total 1	O 1	0	0
60	DL	4	Total 4	O 4	0	0
60	DN	1	Total 1	O 1	0	0

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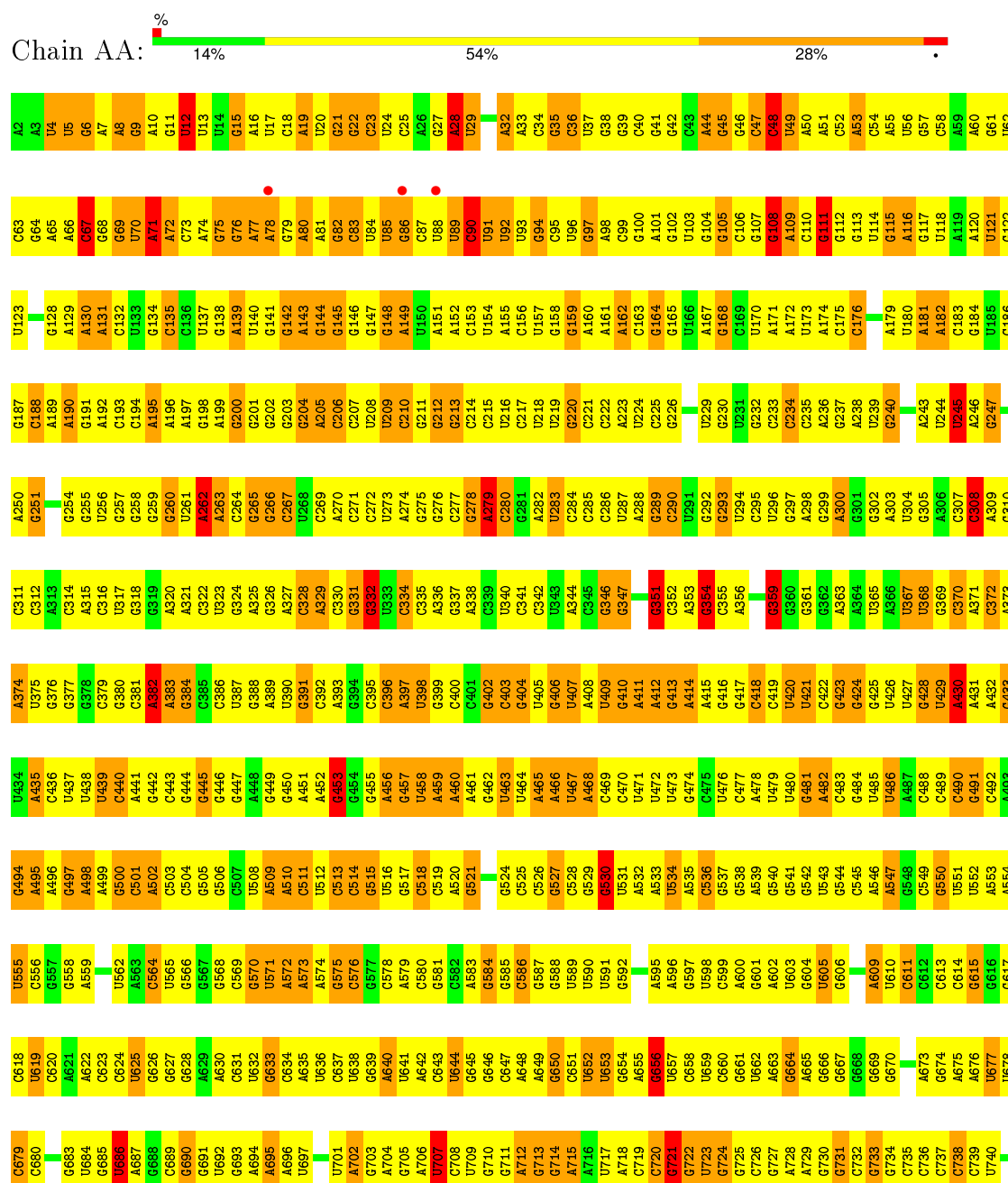
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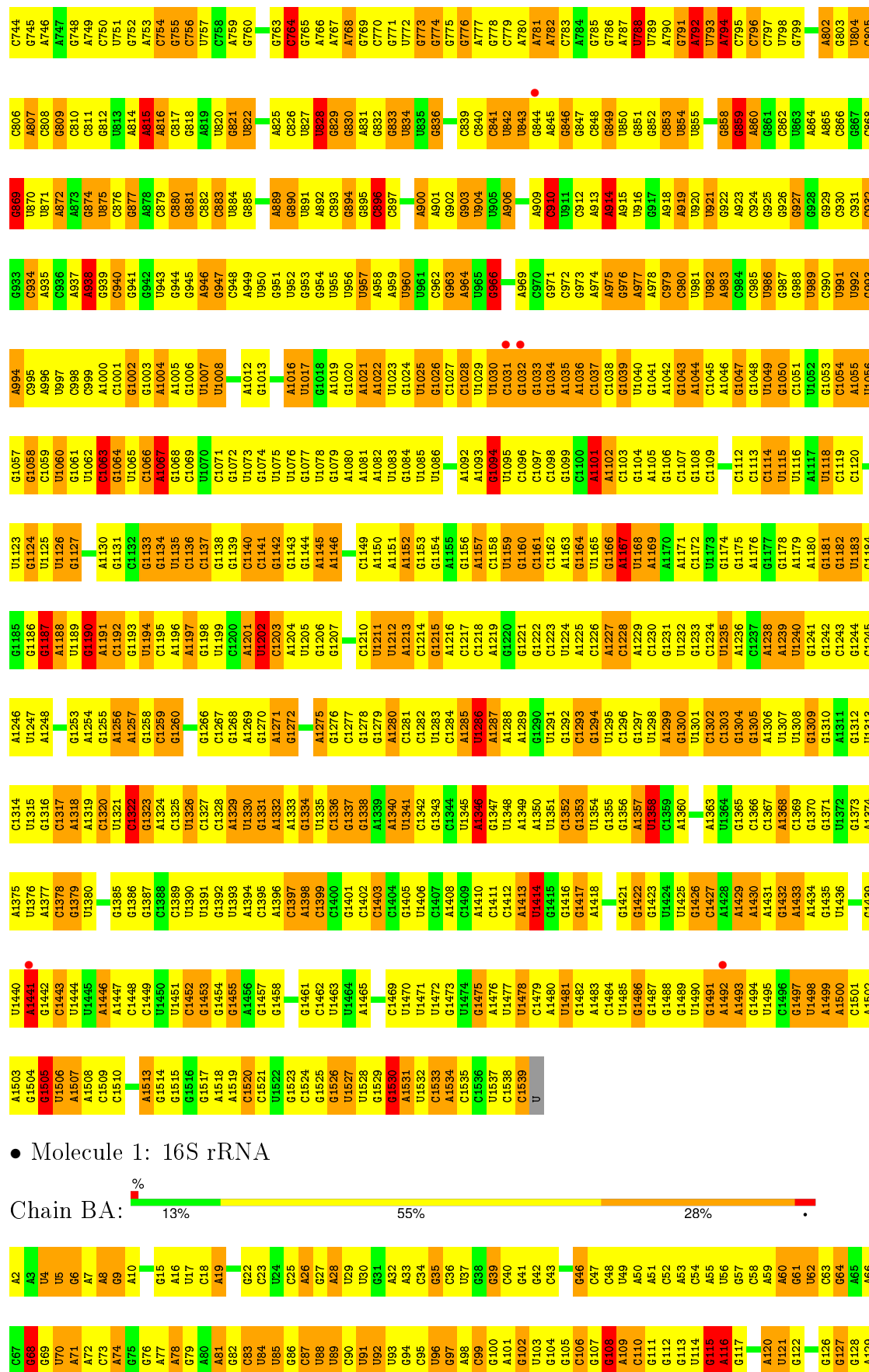
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	DR	1	Total 1	O 1	0	0
60	D2	1	Total 1	O 1	0	0
60	D3	2	Total 2	O 2	0	0
60	D4	1	Total 1	O 1	0	0

3 Residue-property plots


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

• Molecule 1: 16S rRNA

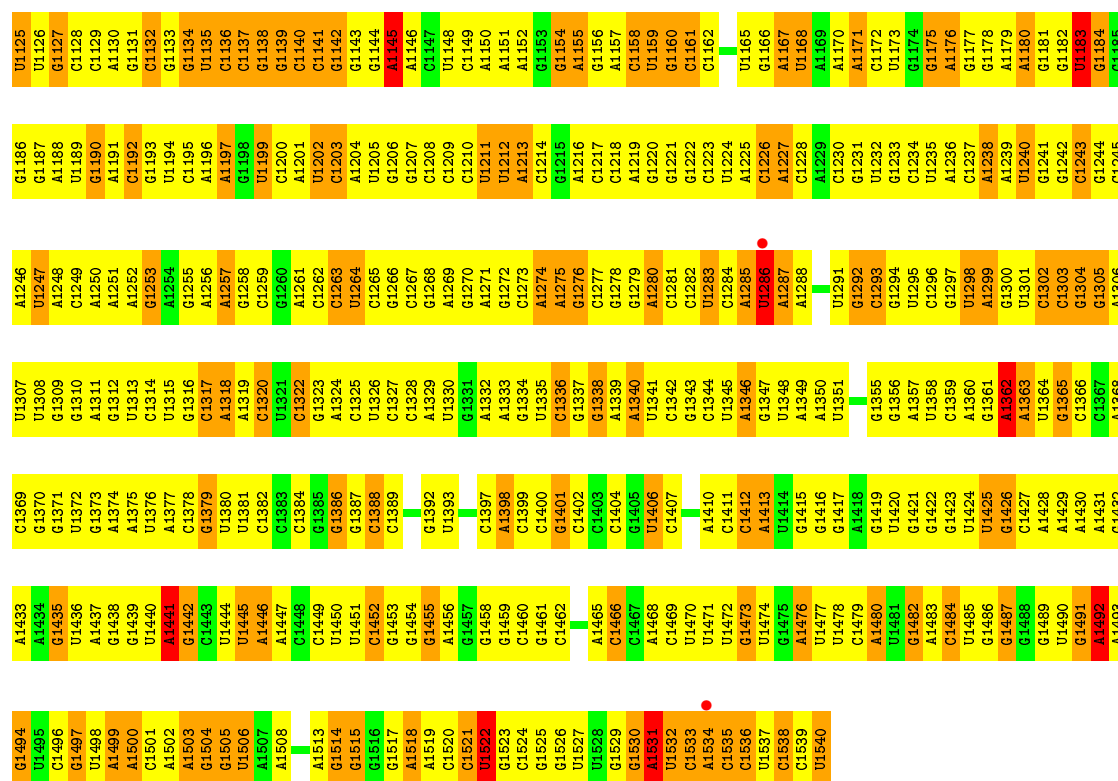




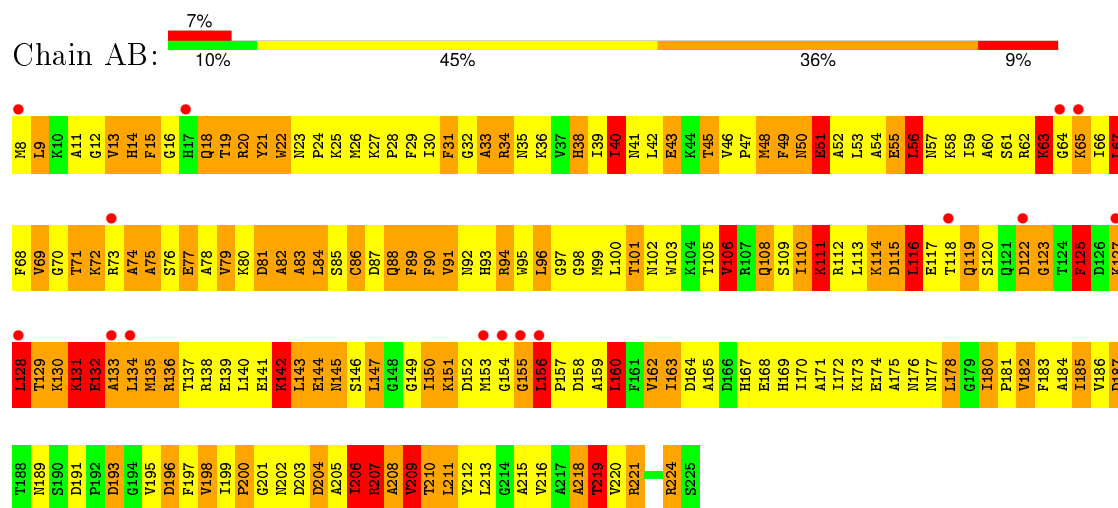
- Molecule 1: 16S rRNA

Chain BA:  13% 55% 28%

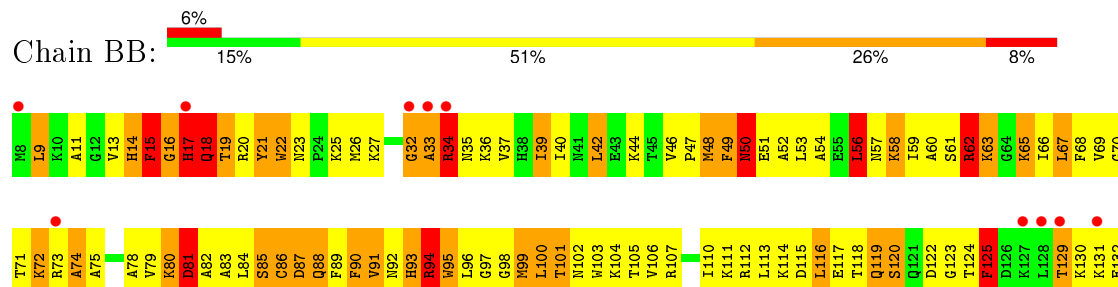
U1065	C1066	A1005	G939	G877	A815	G689	G628	A502	C381	G319	G255	G191	A130
C1066	A1067	G1007	G940	A878	A816	G690	A629	C503	A382	A320	U256	A192	A131
A1068	G879	G818	G941	G879	C817	G691	A630	C504	A383	A321	G257	C193	C132
C1069	G818	G818	G942	C880	C818	U692	A631	C505	A384	C322	G258	C194	U133
U1070	G881	A819	U943	G881	A819	G693	U632	G506	C385	G325	G259	A195	G134
C1071	G882	U820	G944	G882	U820	A694	G633	C507	C386	A325	G260	A196	C135
G1072	C883	G821		U757	G821	A695	C634	A572	U387	G326	U261	A197	C136
U1073	U884	U822		C758	U822		A635	A573	G388	A327		A198	U137
C1074	G885	G823		A759	G823	C699	U636	A574	C389	C328	C264	A199	G138
G1075	A889	G824			G824	G700	A636	C511	U390	A329		G200	
U1076	G890	A825		U701	A825	U701	U638	C513	U391	G330	G266	G201	
C1077	G891	C826		A702	C826	G702	G639		C392	G331	C267	G202	
G1078	U892	U827		G763	U827	G703	A640	U516	A393	G332	U268	G203	A143
U1078	A892	U828		G765	U828	A704	U841	G517	G394	U333	C269	G204	G144
G1079	C893	G829		A766	G829	G705	A642	C518	C395	U334	A270	A205	G145
A1080	G894	G830		A767	G830	A706	C643	C519	C396	C335	C271	C206	G146
U1081	G895	A831		A768	A831	U707	U644	U458	A397	A336	C272	C207	G147
A1082	G896	G832		G769	G832	C708	G645	A583	U398	G337	U273	U208	G148
U1083	C897	G833		C770	G833	U709	G646	C522	A398	A338	A274	U209	A149
G1084	G898	U834		G771	U834	G710	C647	G524	C400	C339	G275	C210	U150
U1085	C899	U835			U835	G711	A648	C525	C401	U340	G276	G211	A151
A1086	A900	G836		G775	G836	A712	A649	C526	G402	C341	C277	G212	A152
G1087	A901	U837		A777	U837	G713	G650	G527	C403	C342	G278	G213	G153
U1088	G902			G778		G714	C651	G530	G404	U343	A279	C214	U154
C1089	G903	C840		C779	C840	A715	U652	U581	U405	A344	C280	C215	A155
U1090	U904	C841		A780	U904	A716	U653	U582	G406	C345	G281	U216	C156
A1091	U905	U842		A781	U842	U717	A654	A532	U407	G346	A282	U219	U157
C1092	A906	U843		A782	U843	A718	G655	A533	A408	C347	G293	U220	G158
A1093	G844	G844		A783	G844	C719	U656	U534	U409	C348	C282	G221	G159
G1094	C972	A845		C783	A845	C720	U657	A535	G410	A349	C285	C221	A160
U1095	G846	A909		A784	A909	G721	G658	C536	A411	G350	C286	C222	A161
C1096	A974	C847		G785	C847	G722	U659	G537	A412	G351		A223	A162
U1097	A975	C848		G786	C848	U723	G660	G538	G413	C352	G289	G226	C163
G1098	G976	A913		A787	A913	G724	U661	A539	A414	A353	C290	G226	G164
U1099	A977	G913		U788	G913	G725	U662	G540	A415	G354	U291	G165	G165
C1100	A978	G914		A789	G914	C726	A663	G541	G416	G477	G292	U229	U166
A1101	G979	C853		A790	C853	G727	G664	G542	G417	G357	G293	U230	A167
U1102	C980	U954		G791	U954	A728	A665	U543	C418	U358	U294	U231	G168
C1103	U951	U955		A792	U955	U729	U666	G544	C419	G359	G295	G232	C169
G1104	A952	C856		U793	C856	G730	A667	C545	U421	G361	U296	C233	U170
C1105	A953	C857		A794	C857	G731	U668	A546	C422	G362	G297	C234	A171
U1106	G984	U920		C795	U920	G732	G669	A547	G423	A363	G299	A236	U173
G1107	C985	G858		U798	G858	G733	G671	G548	G424	A364	A300	C237	U174
C1108	U986	A860		G799	A860	G734	U672	C549	G425	U365		C237	C175
U1109	G987	G861		U799	G861	G735	A673	G550	U426	A366	A303	G240	C176
A1110	C988	C862		G800	C862	C736	A674	U551	U427	U367	U304	G241	G177
C1111	U989	U863		U801	U863	A675	G675	U552	G428	U368	G242	G242	C178
G1112	C990	A864		A802	A864	C738	A676	A553	U429	G369	A306	A243	A179
C1113	U991	G926		G803	G926	C739	U677	A554	C430	C370	A307	U244	U180
U1114	G992	C866		U804	C866	U740	U678	U555	A430	A371	C308	U245	A181
C1115	U993	G867		C805	G867	G741	C679	C556	A431	C372	A309	A246	A182
U1116	A994	C868		C806	C868	G742	U679	G557	A432	C373	A310	G247	C183
A1117	C995	G869		A807	G869	A743	A681	G558	G433	A374	G310	C248	G184
U1118	G1057	U870		C808	U870	C744	G682	A559	U434	A374	G311	G249	G185
C1119	C933	U871		G809	U871	G745	A683	A560	A435	U375	G312	U250	C186
U1120	G934	A872		C810	A872	G746	U684	U561	C436	G376	A313	G251	G187
C1121	A935	A873		C811	A873	A747	G685	U562	U437	G377		U252	C188
U1122	C936	G874		G812	G874	G748	U686	A563	U438	G378	C316	G253	G189
G1124	U1003	U875		U813	U875	A749	G687	G564	U439	C379	U317	G254	A190
	A1004	C876		A814	C876	C750	G688	U565	C440	G380	G318		

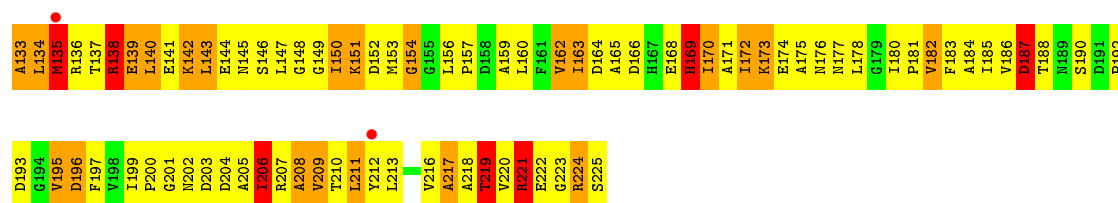


• Molecule 2: 30S ribosomal protein S2

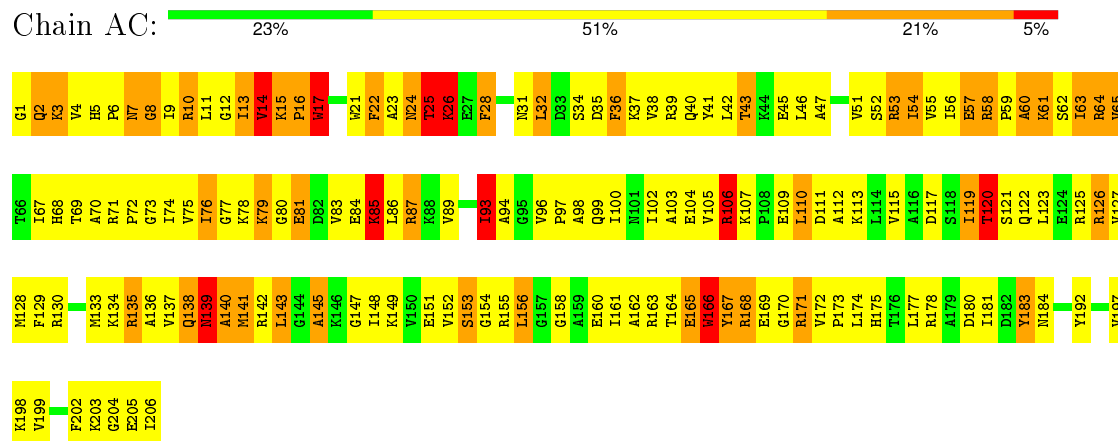


• Molecule 2: 30S ribosomal protein S2

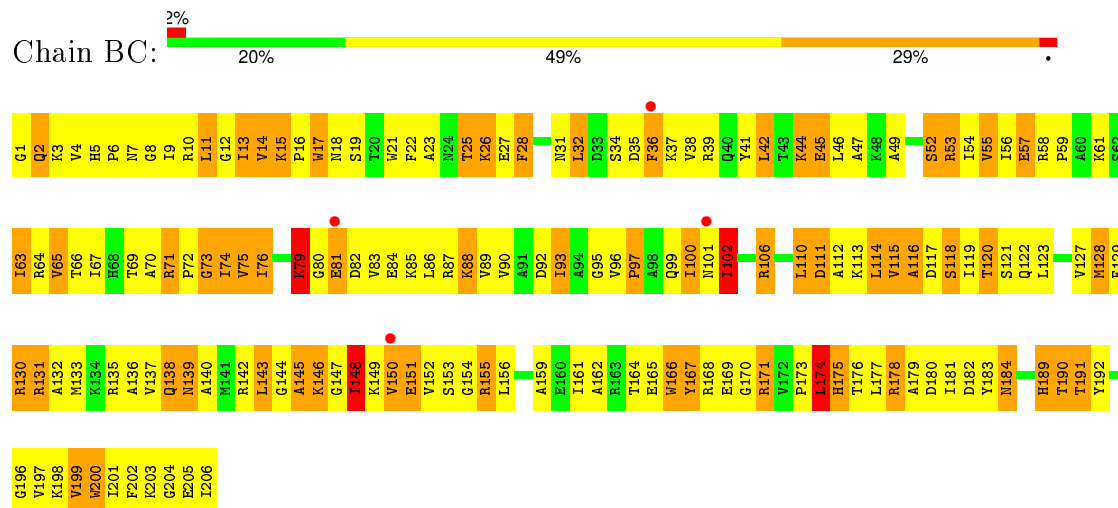




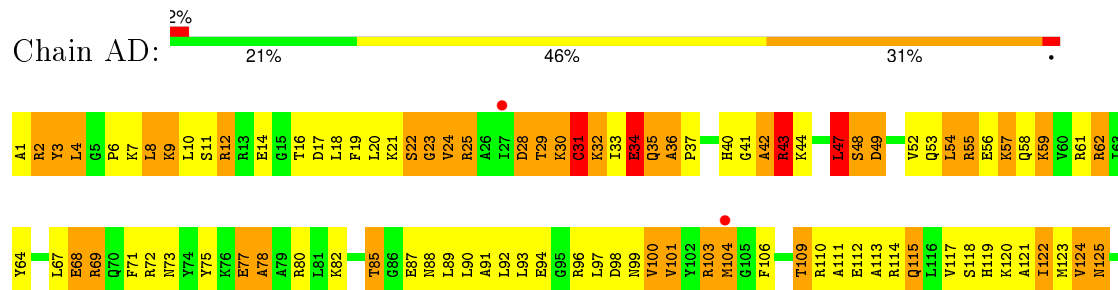
• Molecule 3: 30S ribosomal protein S3

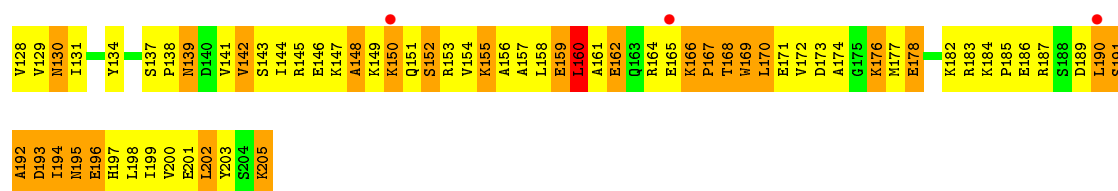


• Molecule 3: 30S ribosomal protein S3



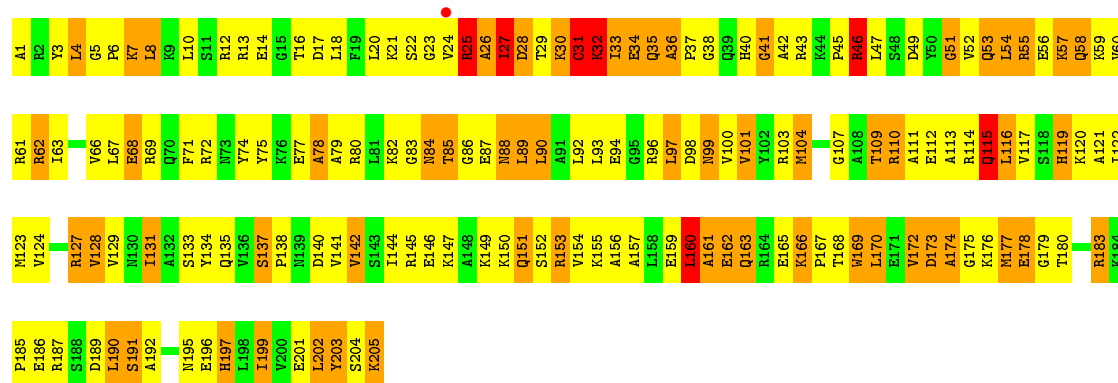
• Molecule 4: 30S ribosomal protein S4





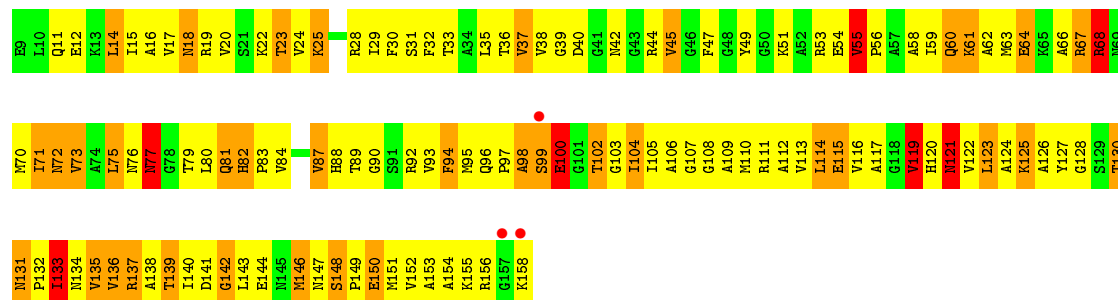
• Molecule 4: 30S ribosomal protein S4

Chain BD: 20% 48% 29%



• Molecule 5: 30S ribosomal protein S5

Chain AE: 2% 17% 54% 24% 5%

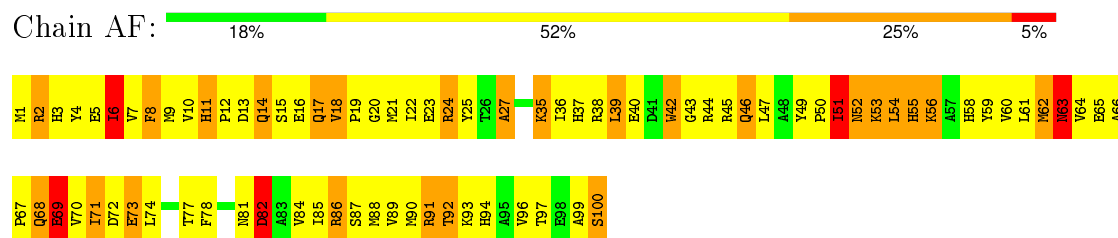


• Molecule 5: 30S ribosomal protein S5

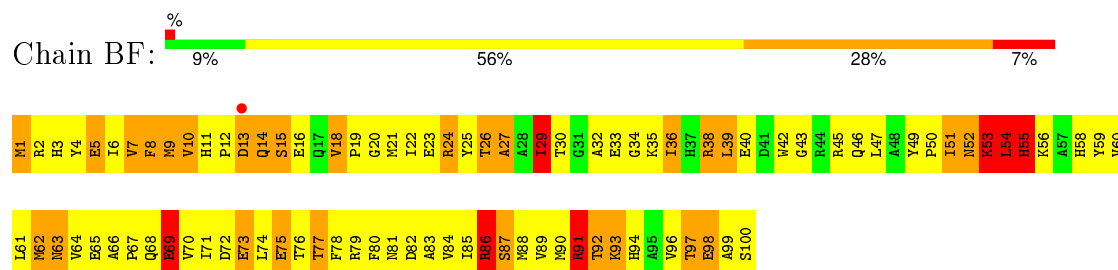
Chain BE: 23% 45% 31%



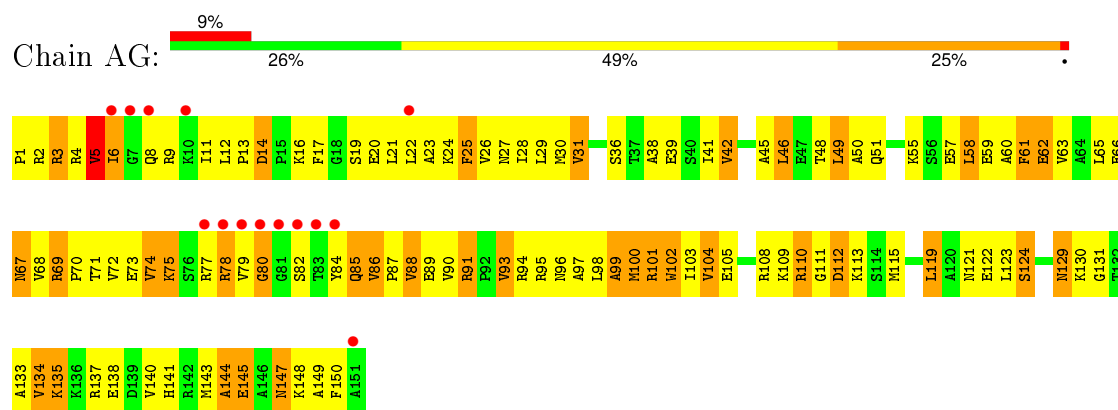
• Molecule 6: 30S ribosomal protein S6



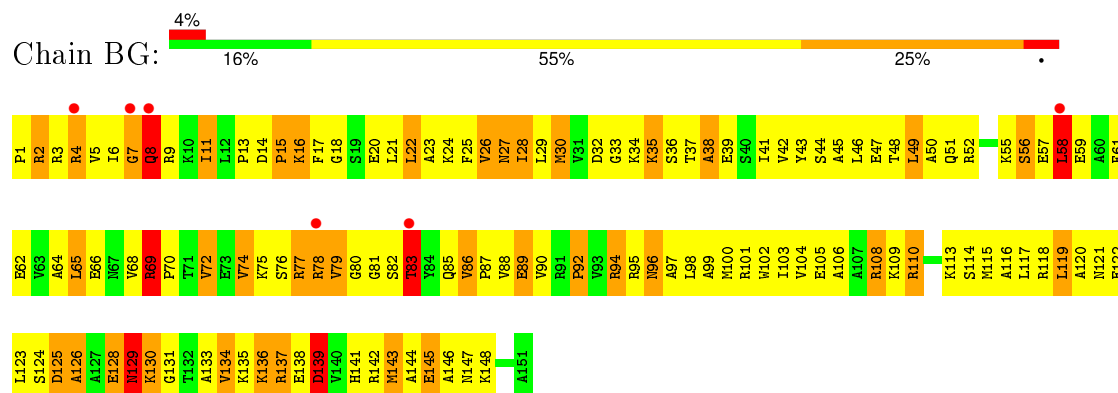
• Molecule 6: 30S ribosomal protein S6



• Molecule 7: 30S ribosomal protein S7



• Molecule 7: 30S ribosomal protein S7

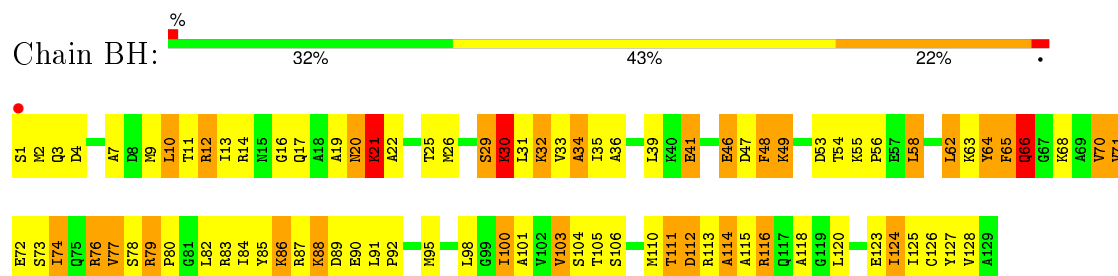


• Molecule 8: 30S ribosomal protein S8

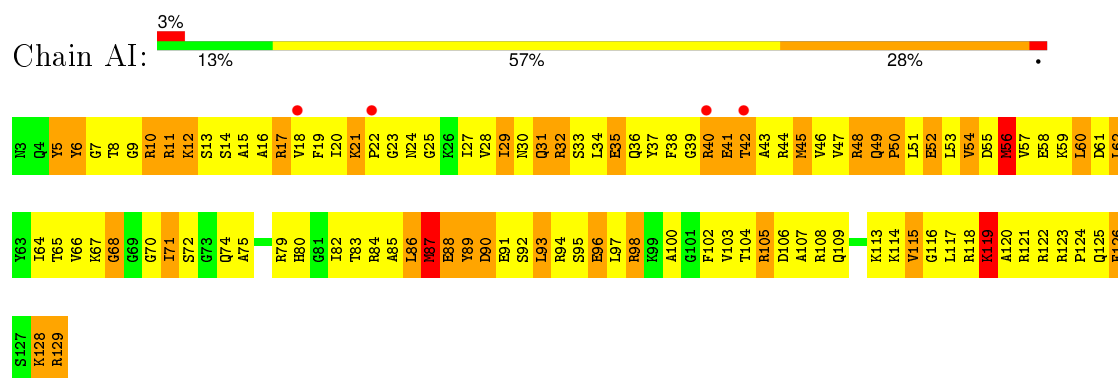




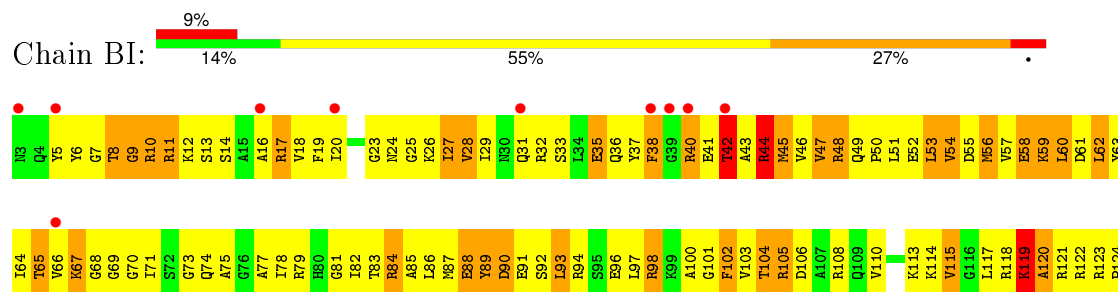
• Molecule 8: 30S ribosomal protein S8



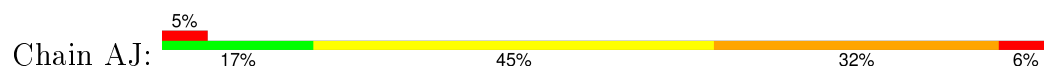
• Molecule 9: 30S ribosomal protein S9

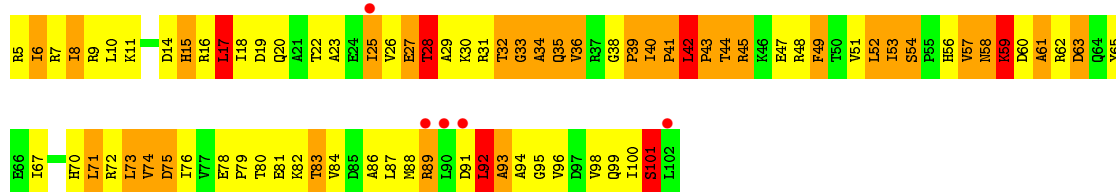


• Molecule 9: 30S ribosomal protein S9

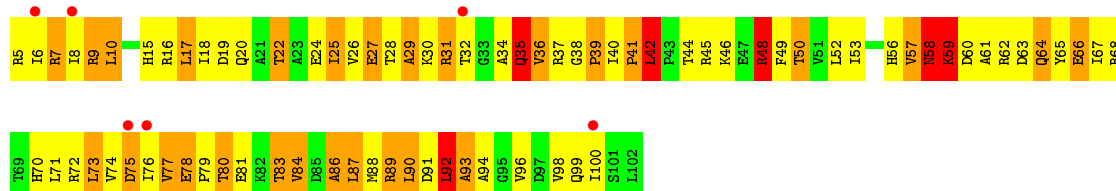
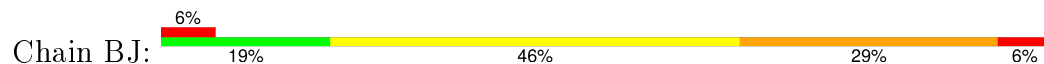


• Molecule 10: 30S ribosomal protein S10

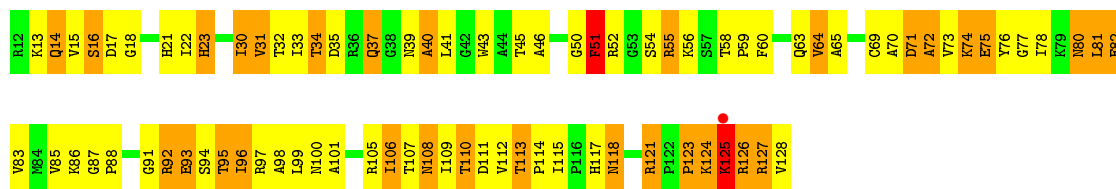




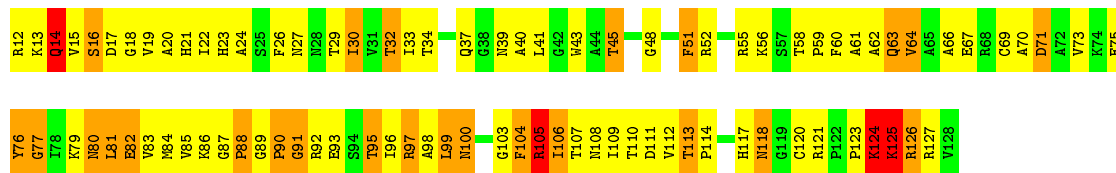
• Molecule 10: 30S ribosomal protein S10



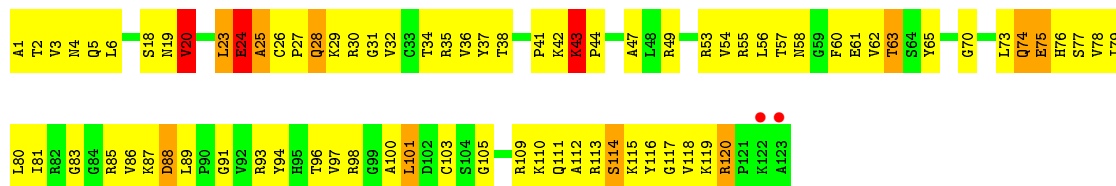
• Molecule 11: 30S ribosomal protein S11



• Molecule 11: 30S ribosomal protein S11

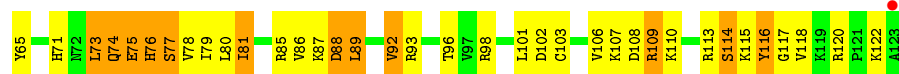
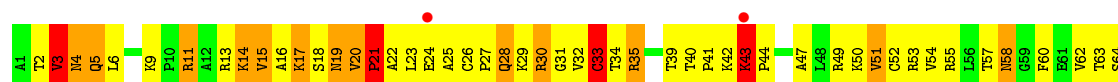


• Molecule 12: 30S ribosomal protein S12

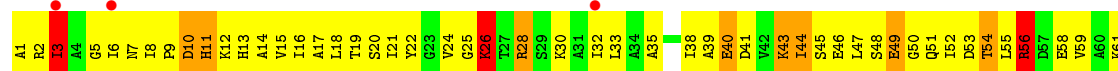


• Molecule 12: 30S ribosomal protein S12

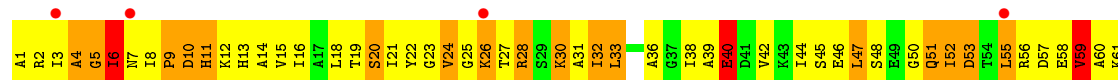
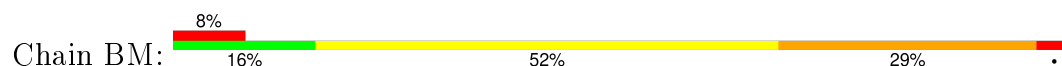


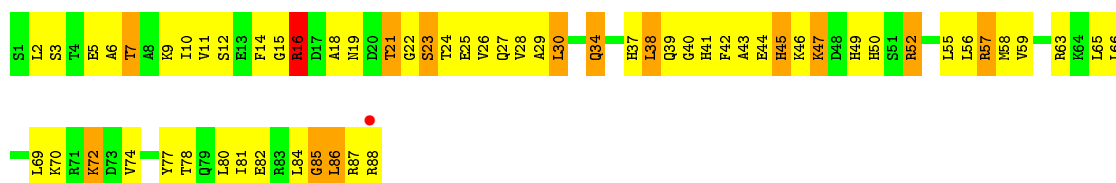


• Molecule 13: 30S ribosomal protein S13

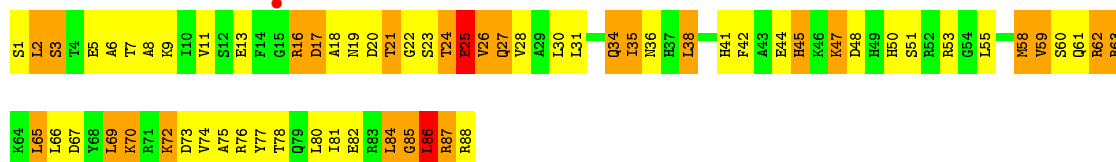


• Molecule 13: 30S ribosomal protein S13

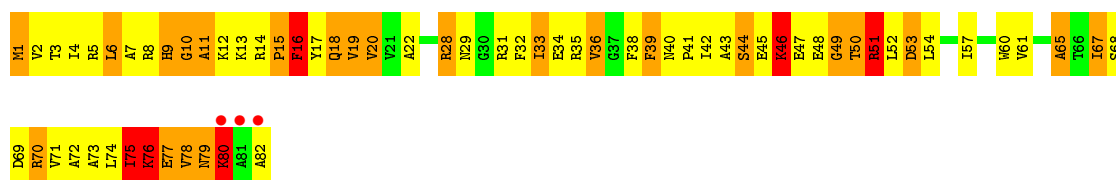
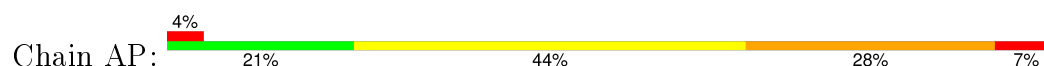




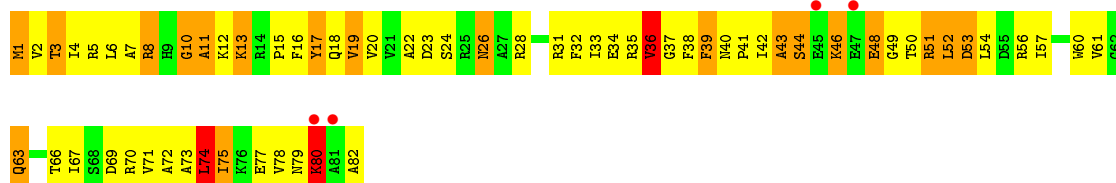
• Molecule 15: 30S ribosomal protein S15



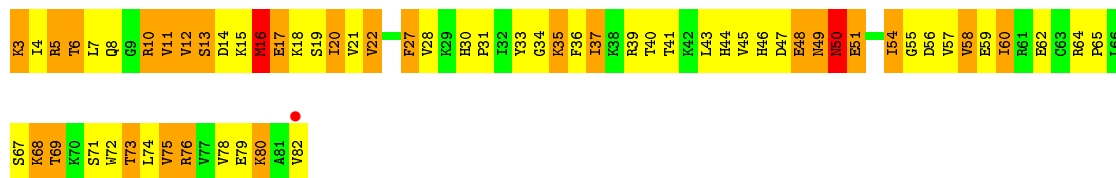
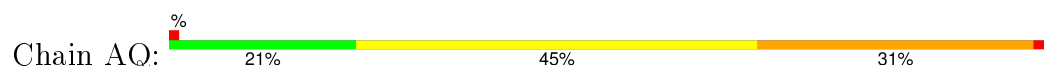
• Molecule 16: 30S ribosomal protein S16



• Molecule 16: 30S ribosomal protein S16

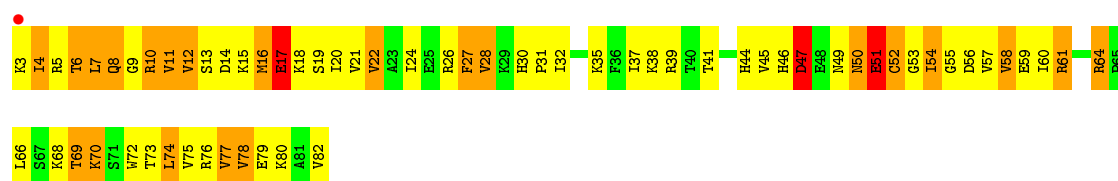


• Molecule 17: 30S ribosomal protein S17

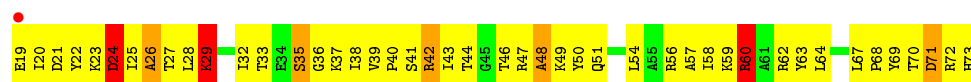


• Molecule 17: 30S ribosomal protein S17

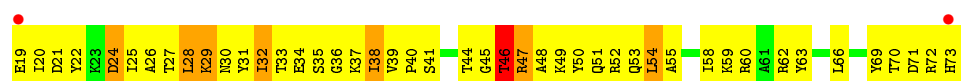




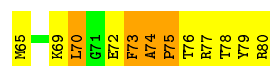
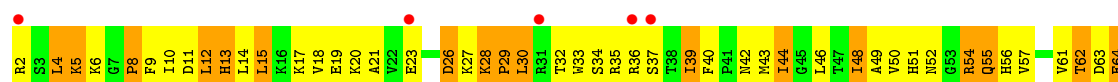
• Molecule 18: 30S ribosomal protein S18



• Molecule 18: 30S ribosomal protein S18



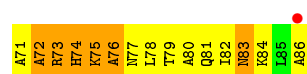
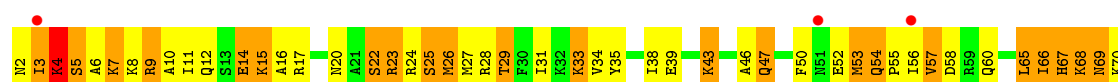
• Molecule 19: 30S ribosomal protein S19



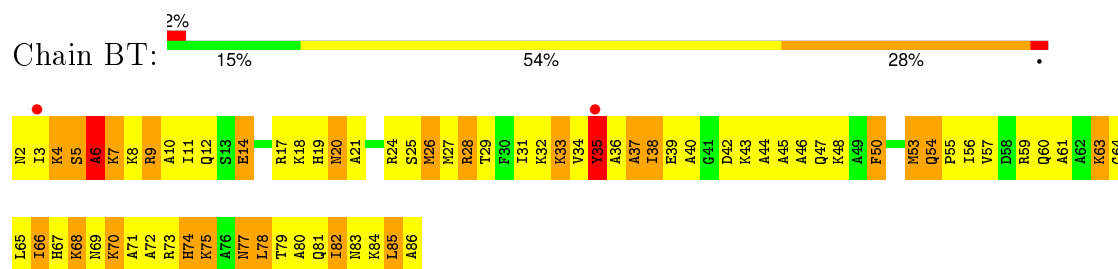
• Molecule 19: 30S ribosomal protein S19



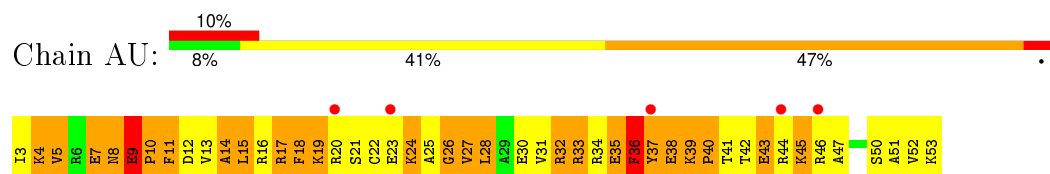
• Molecule 20: 30S ribosomal protein S20



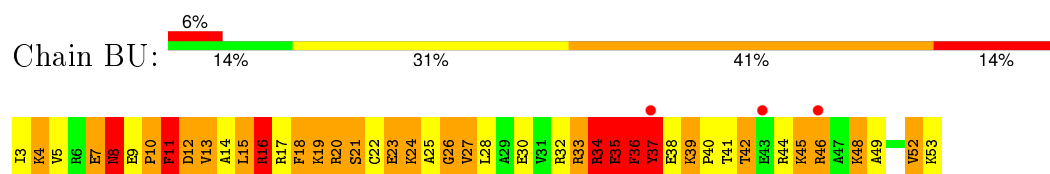
- Molecule 20: 30S ribosomal protein S20



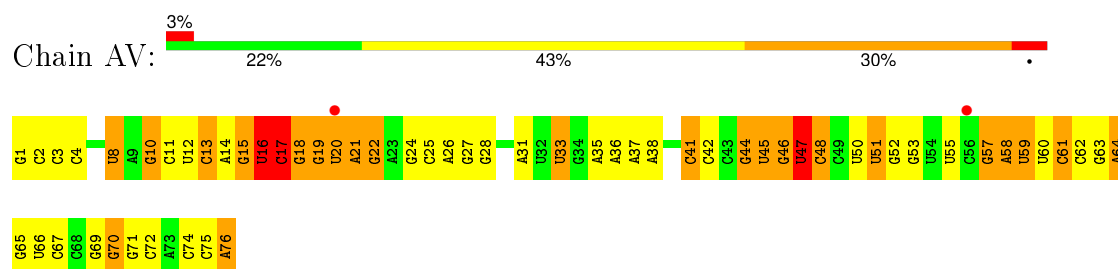
- Molecule 21: 30S ribosomal protein S21



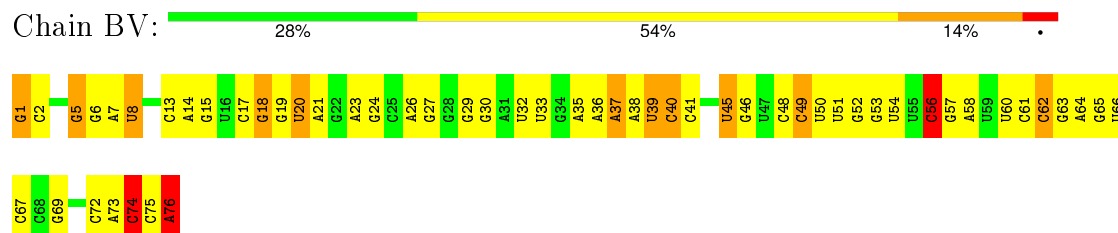
- Molecule 21: 30S ribosomal protein S21



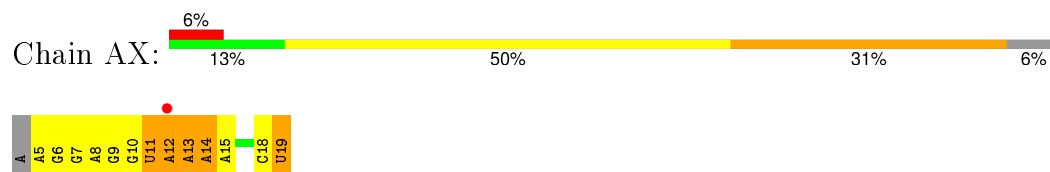
- Molecule 22: phenylalanine specific transfer RNA



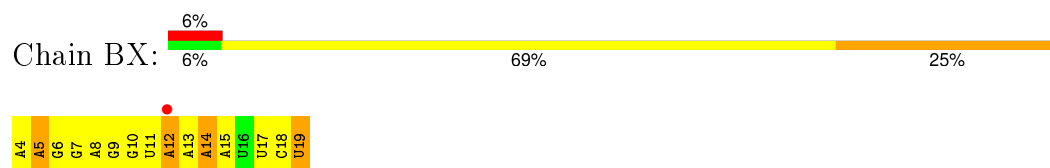
- Molecule 22: phenylalanine specific transfer RNA



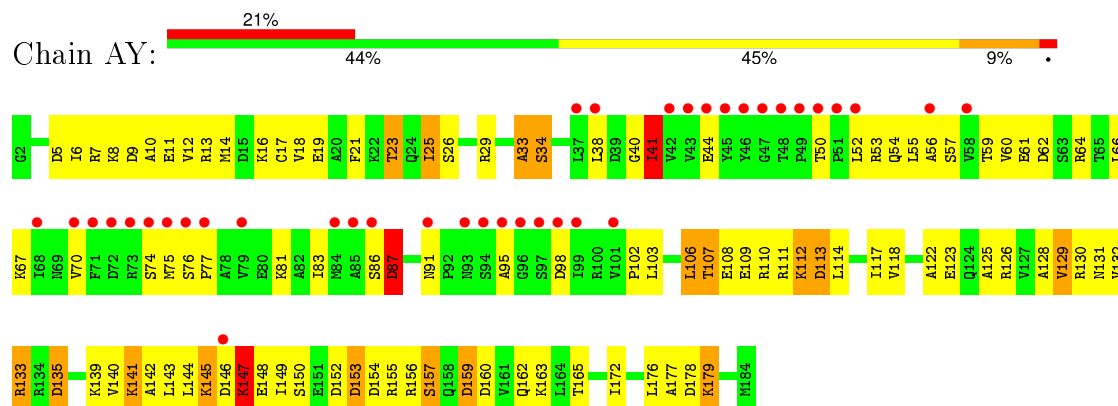
- Molecule 23: messenger RNA



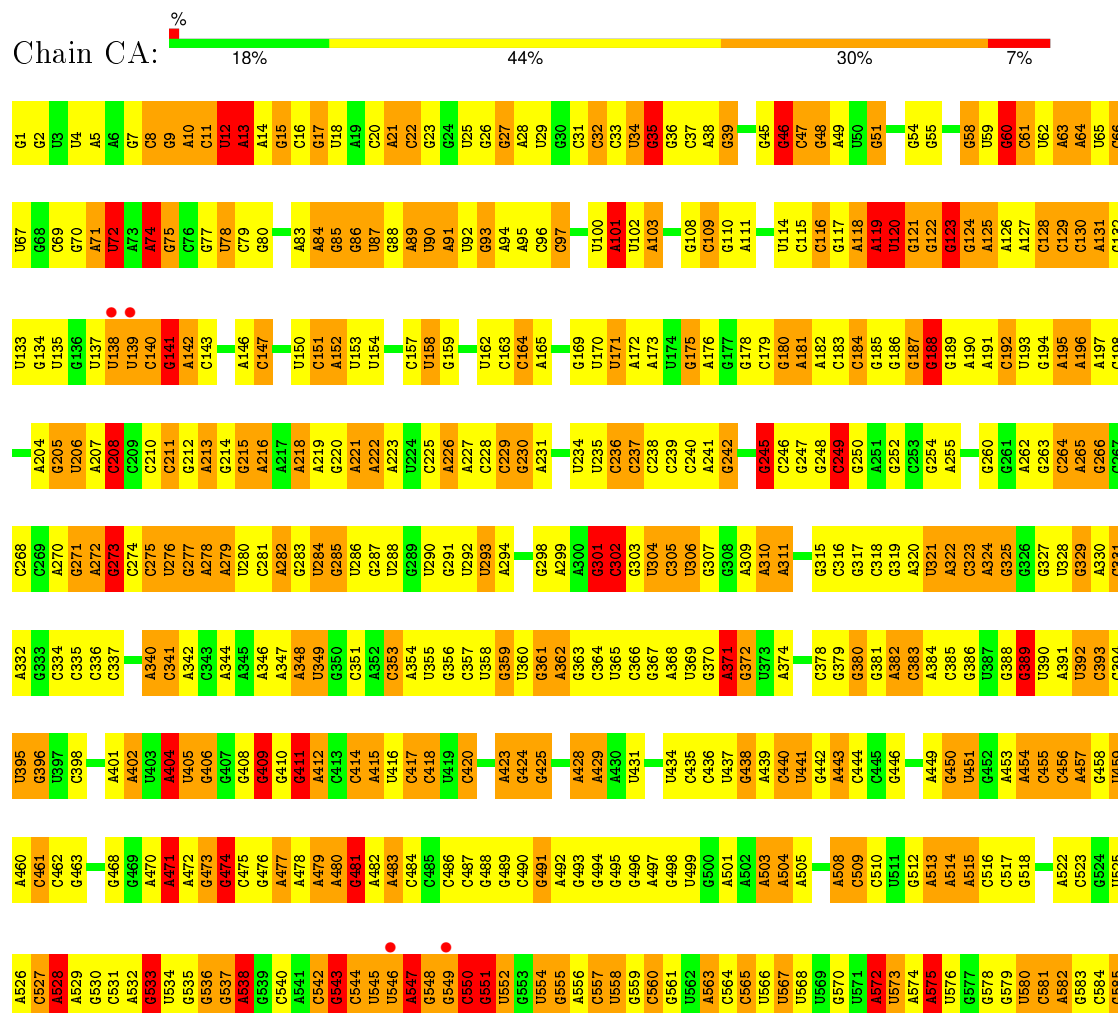
- Molecule 23: messenger RNA



- Molecule 24: ribosome recycling factor

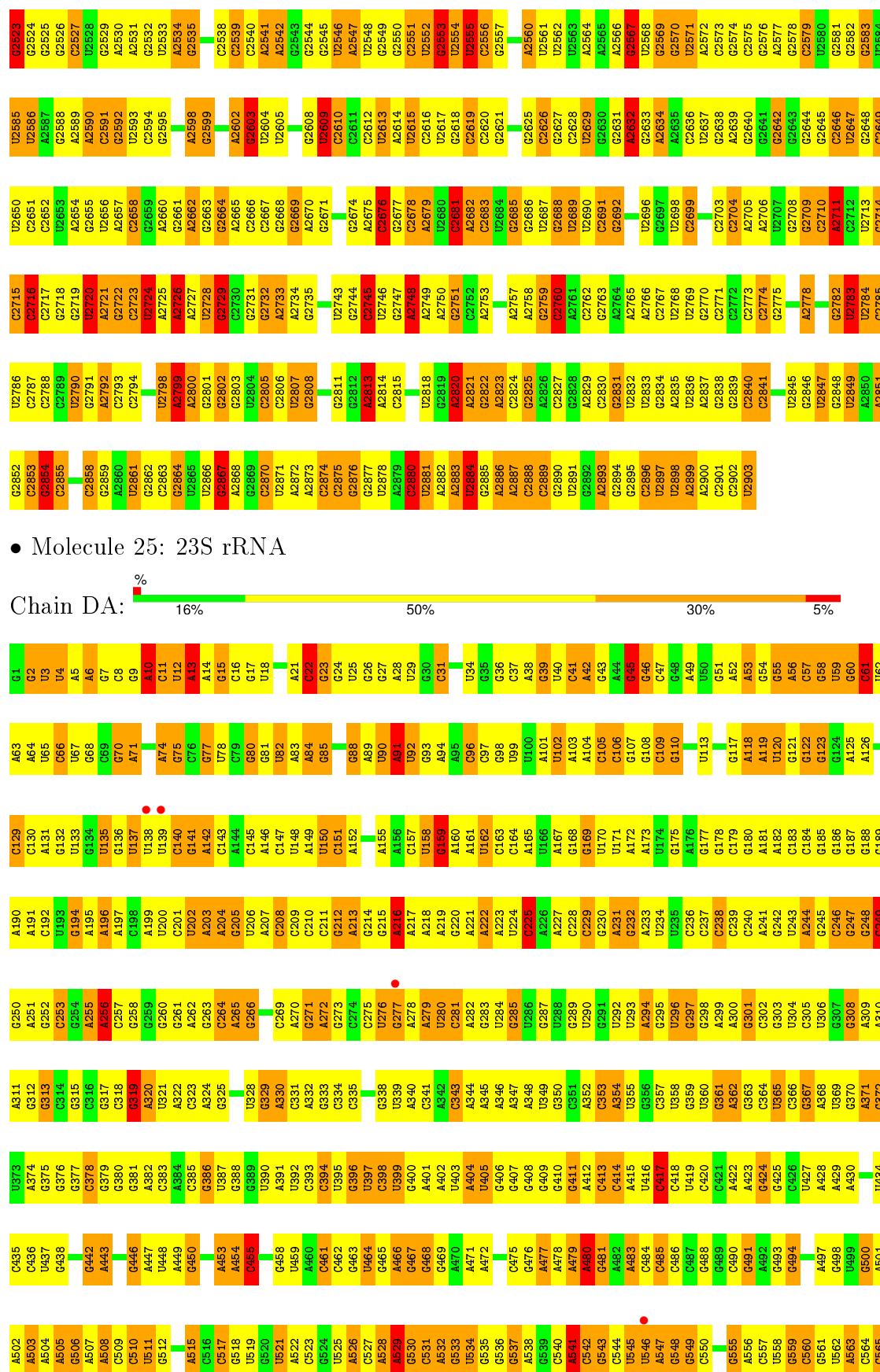


- Molecule 25: 23S rRNA



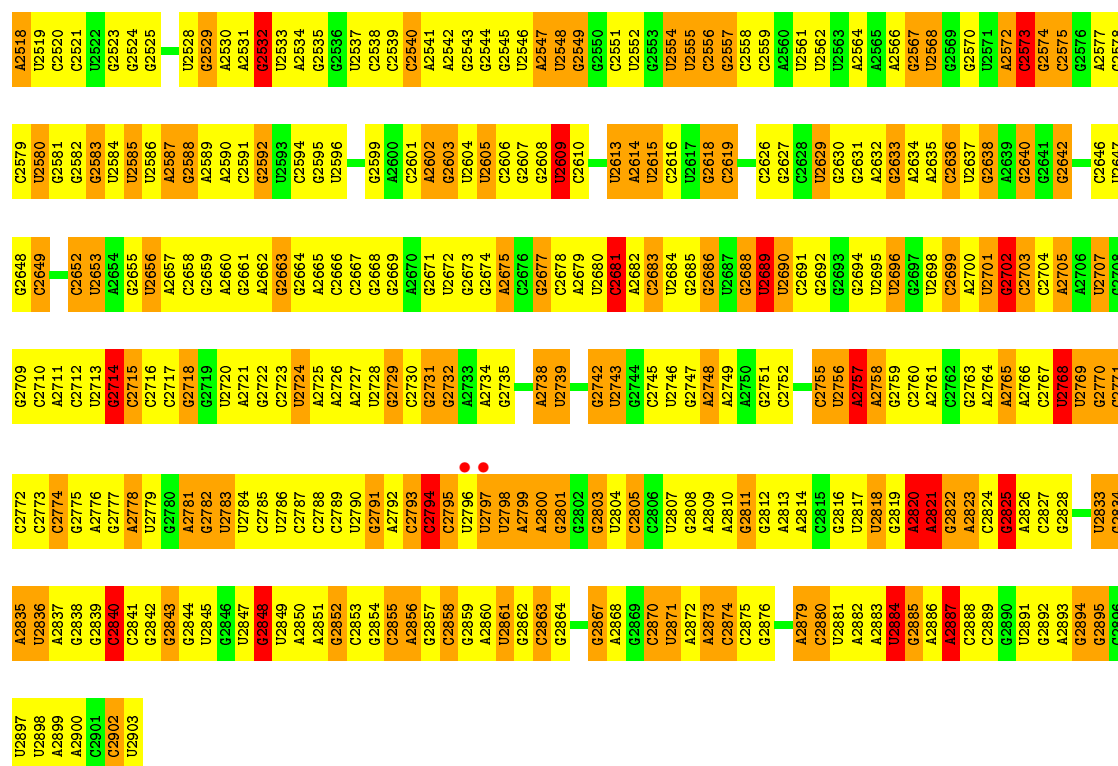
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U1523	U1460	U1273	A1143	A1272	A1144	U1083	U1023	C961	C897	C835	G775	U714	U654	U588
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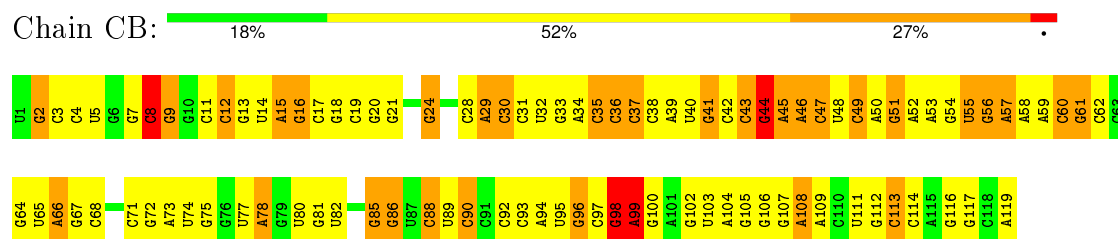


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C1562	U1501	G1441	A1381	A1321	G1252	U1190	G1128	A1069	C1007	G942	A878	A753	U689	A627	
U1563	A1502	U1442	G1382	A1322	A1253	G1191	A1129	A1070	A1008	A943	G879	A754	A699	A628	
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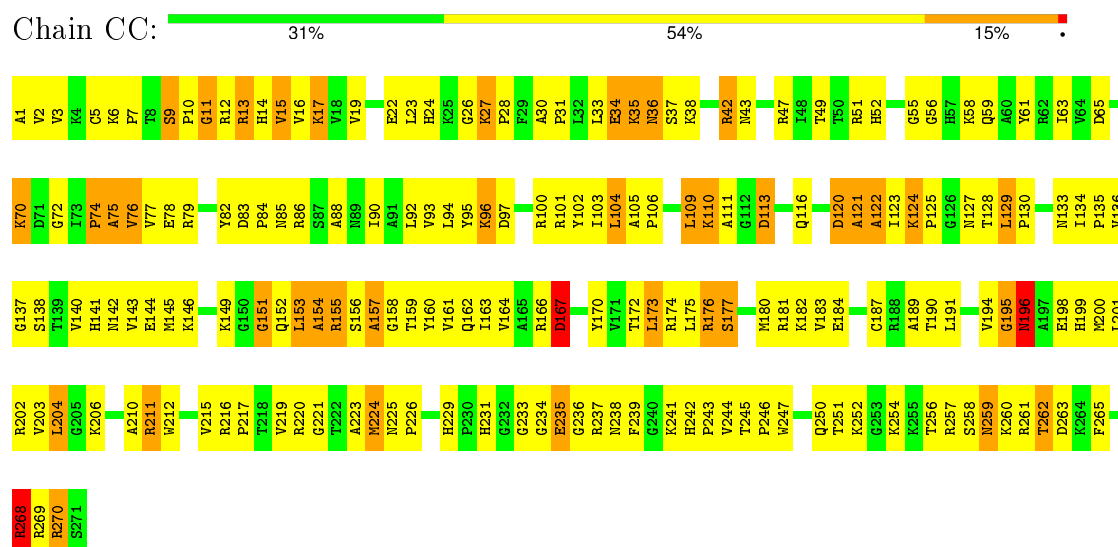
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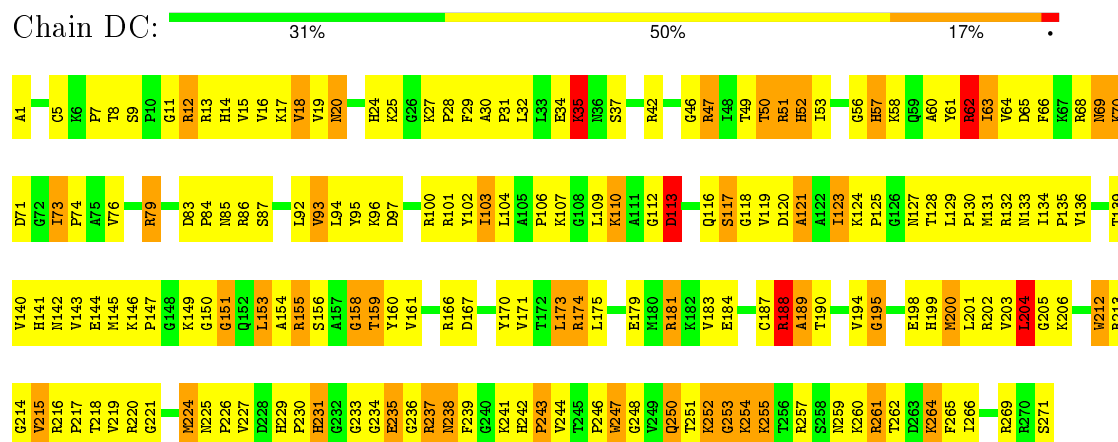
• Molecule 26: 5S rRNA



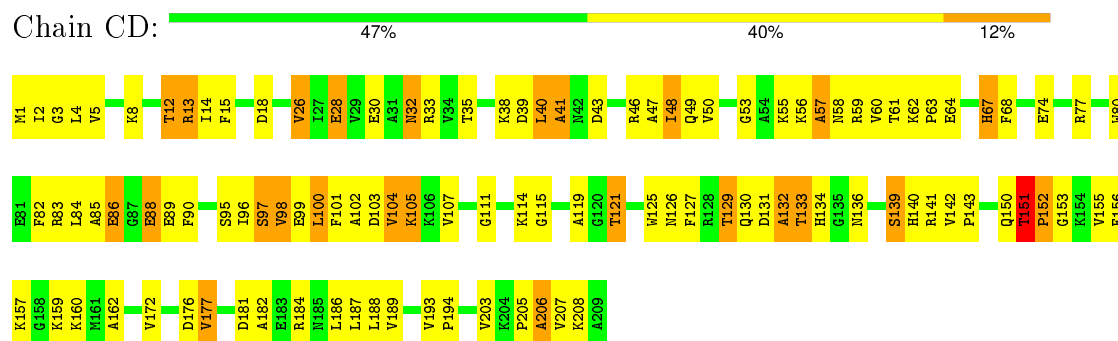
• Molecule 27: 50S ribosomal protein L2



- Molecule 27: 50S ribosomal protein L2



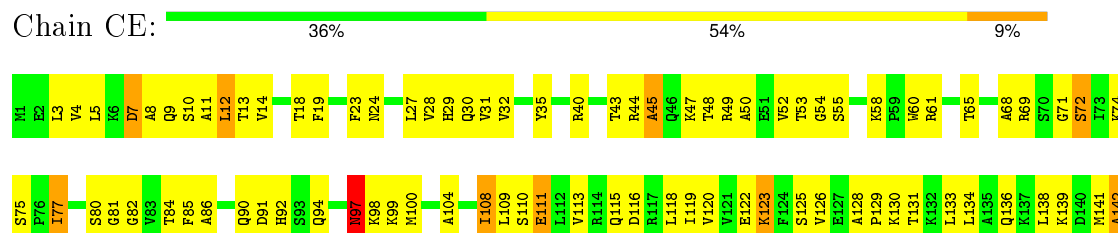
- Molecule 28: 50S ribosomal protein L3



- Molecule 28: 50S ribosomal protein L3



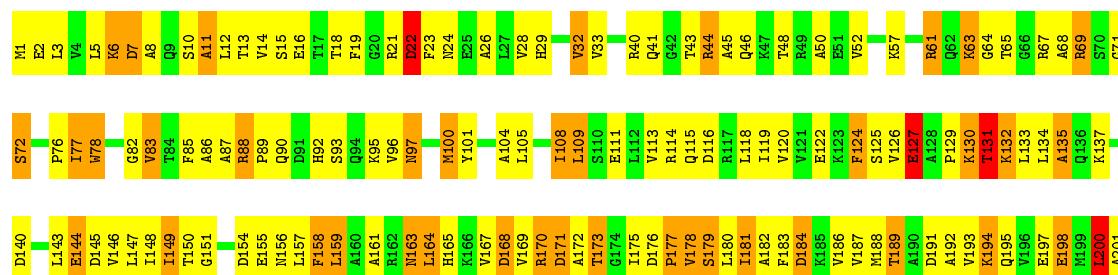
- Molecule 29: 50S ribosomal protein L4





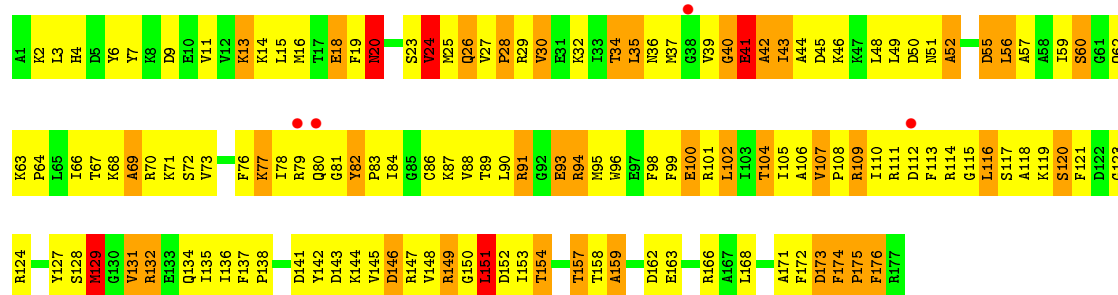
• Molecule 29: 50S ribosomal protein L4

Chain DE: 32% 47% 19%



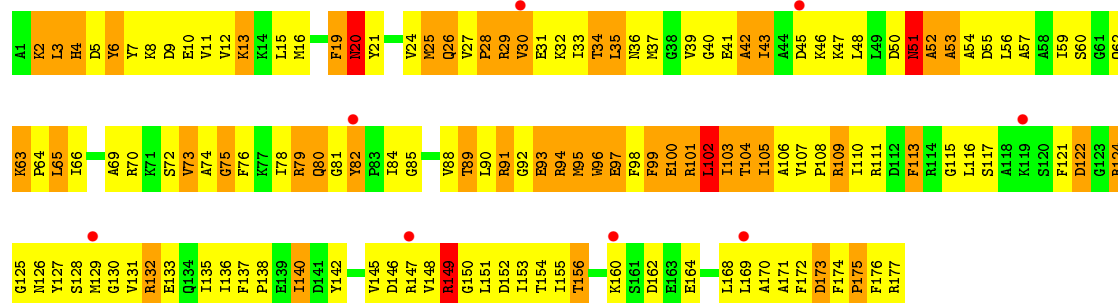
• Molecule 30: 50S ribosomal protein L5

Chain CF: 2% 23% 53% 21%



• Molecule 30: 50S ribosomal protein L5

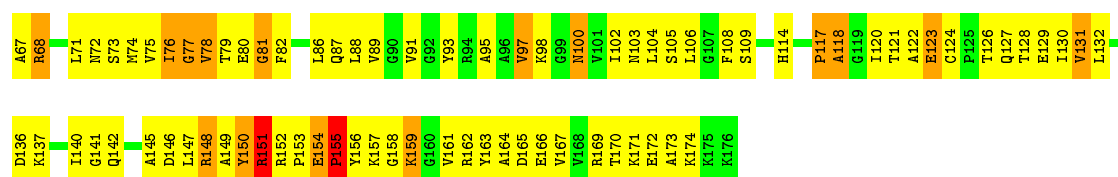
Chain DF: 5% 21% 51% 26%



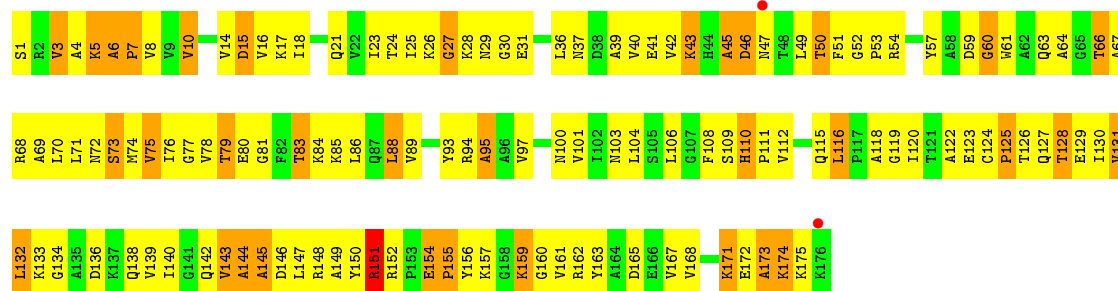
• Molecule 31: 50S ribosomal protein L6

Chain CG: 31% 53% 15%

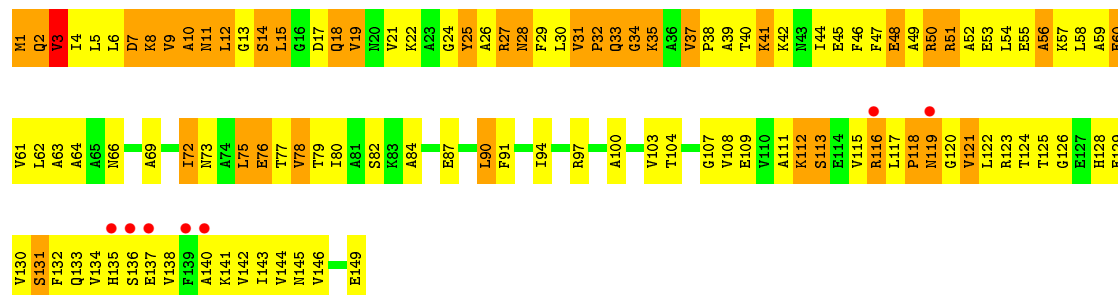




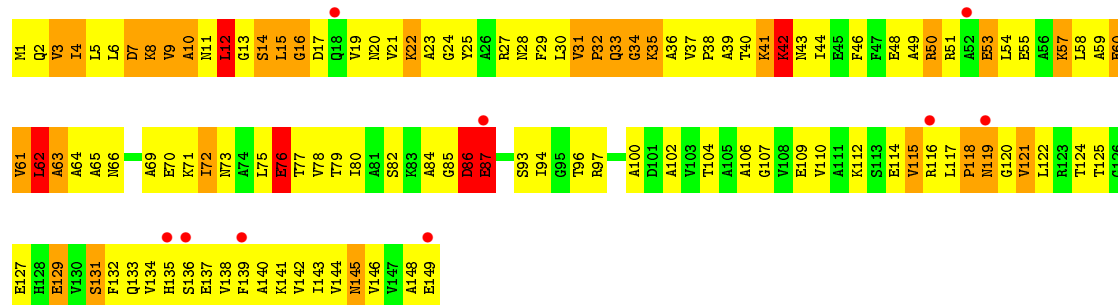
• Molecule 31: 50S ribosomal protein L6



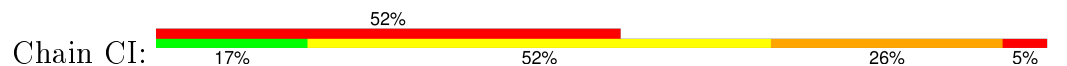
• Molecule 32: 50S ribosomal protein L9

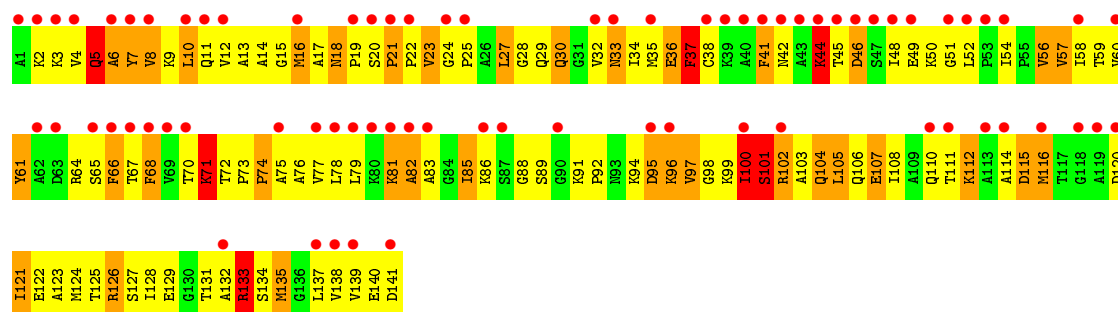


• Molecule 32: 50S ribosomal protein L9

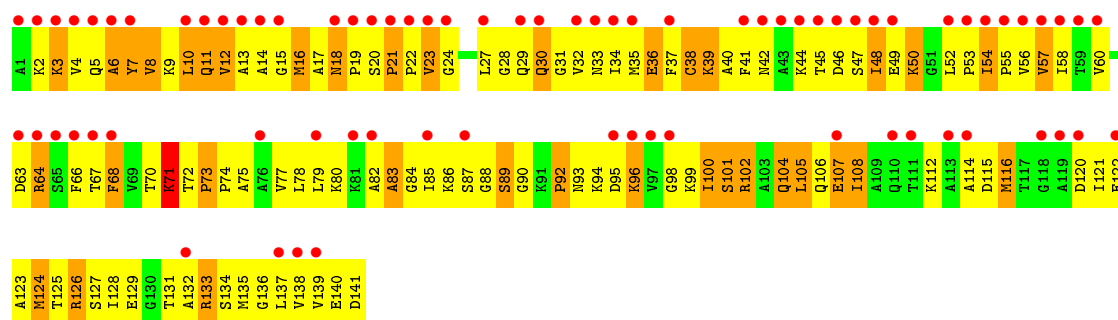
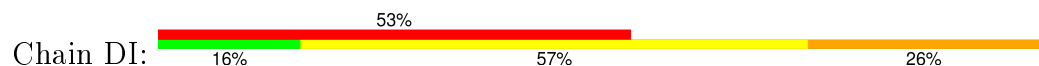


• Molecule 33: 50S ribosomal protein L11

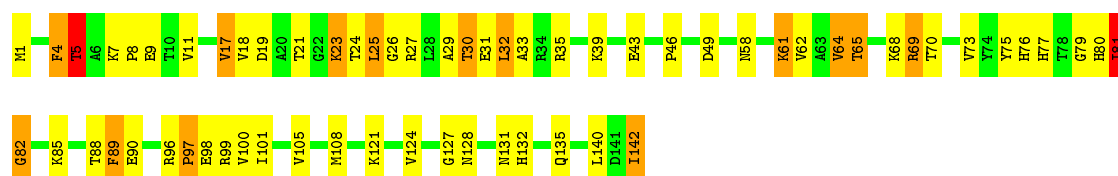




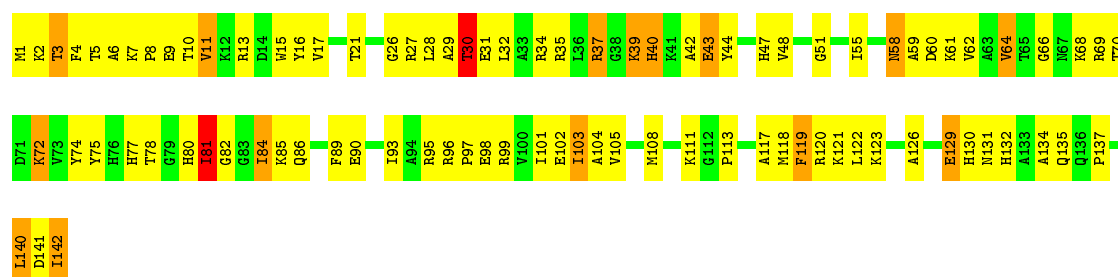
• Molecule 33: 50S ribosomal protein L11



• Molecule 34: 50S ribosomal protein L13

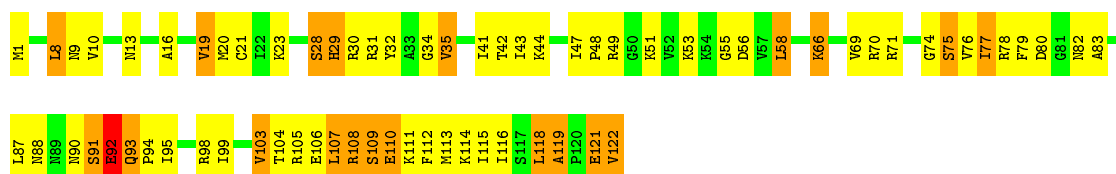


• Molecule 34: 50S ribosomal protein L13



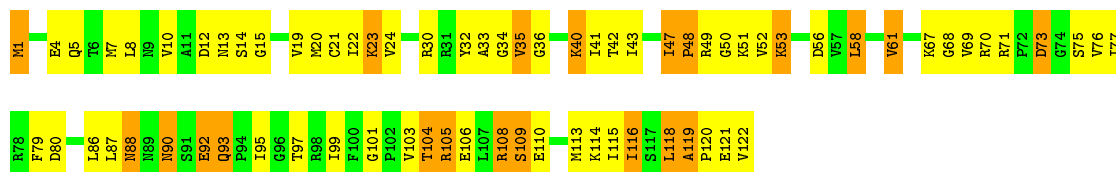
• Molecule 35: 50S ribosomal protein L14





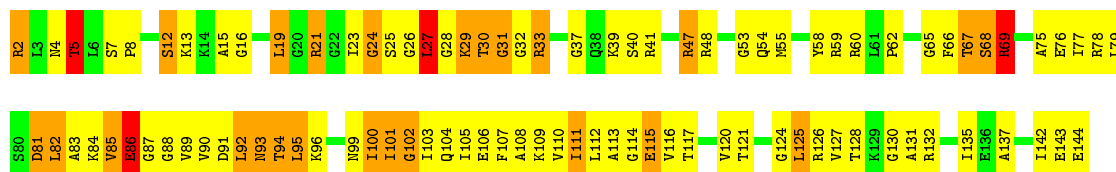
• Molecule 35: 50S ribosomal protein L14

Chain DK: 40% 43% 17%



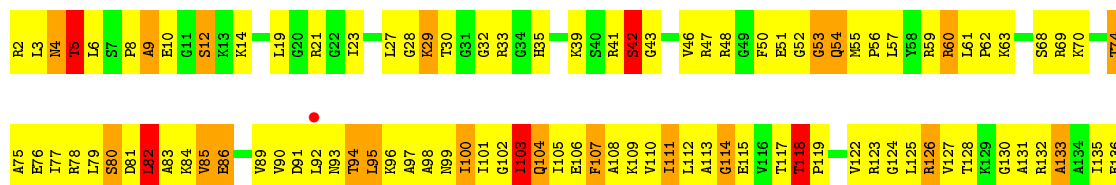
• Molecule 36: 50S ribosomal protein L15

Chain CL: 34% 46% 17%



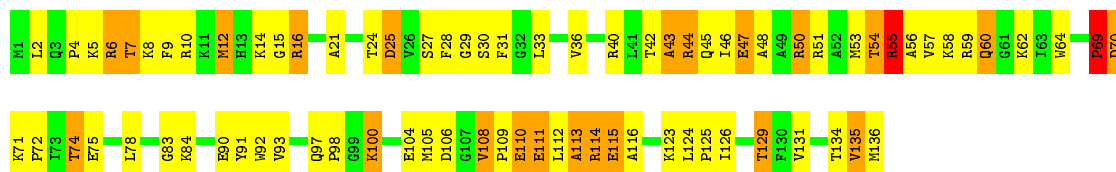
• Molecule 36: 50S ribosomal protein L15

Chain DL: 2% 27% 55% 14%

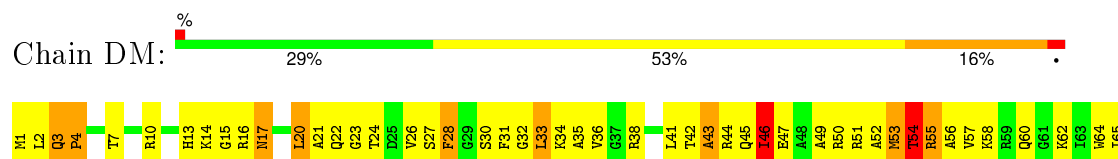


• Molecule 37: 50S ribosomal protein L16

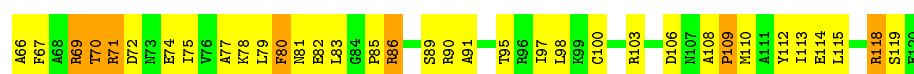
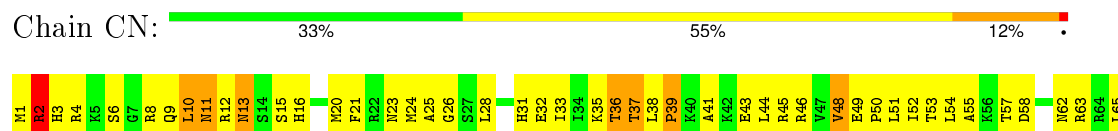
Chain CM: 42% 40% 16%



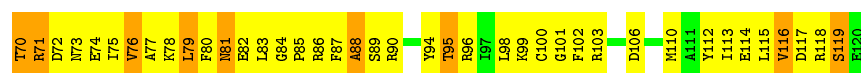
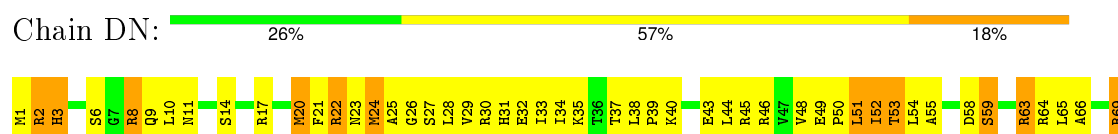
• Molecule 37: 50S ribosomal protein L16



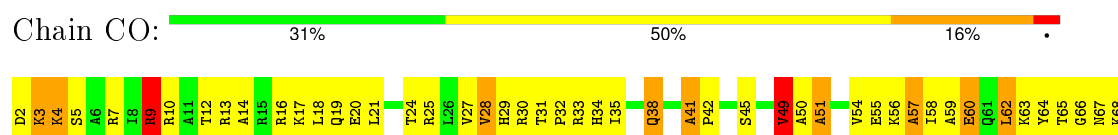
- Molecule 38: 50S ribosomal protein L17



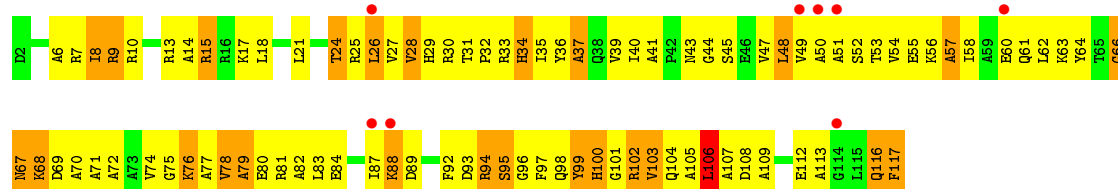
- Molecule 38: 50S ribosomal protein L17



- Molecule 39: 50S ribosomal protein L18

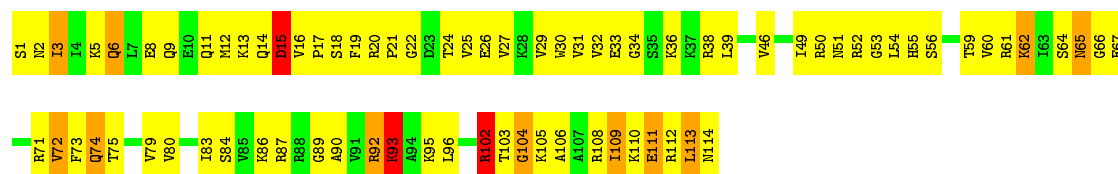


- Molecule 39: 50S ribosomal protein L18



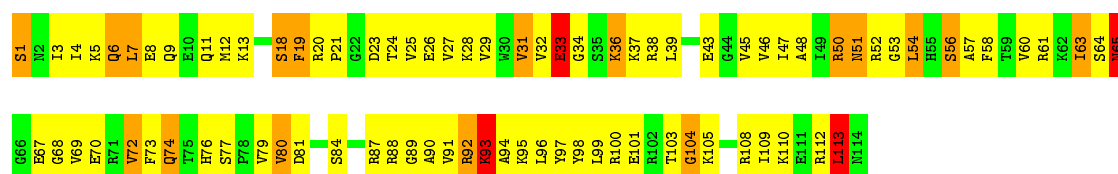
- Molecule 40: 50S ribosomal protein L19

Chain CP: 



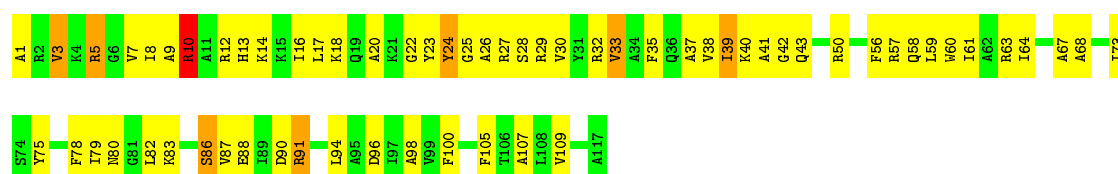
- Molecule 40: 50S ribosomal protein L19

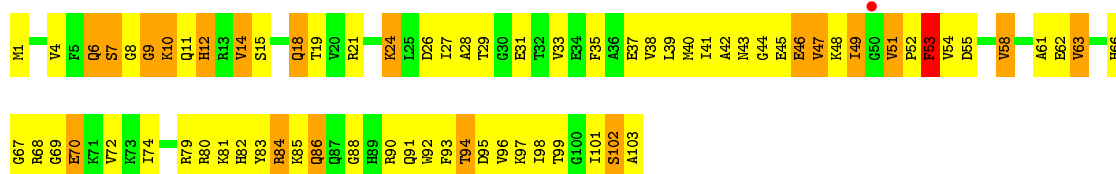
Chain DP: 



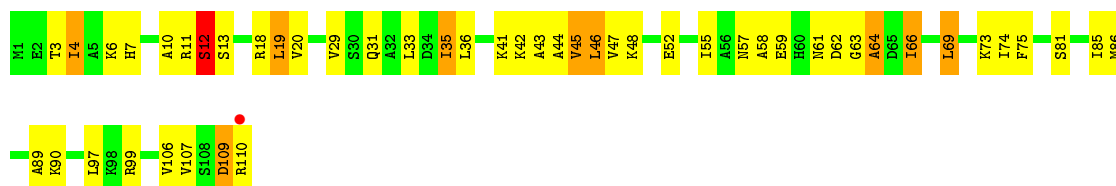
- Molecule 41: 50S ribosomal protein L20

Chain CQ: 

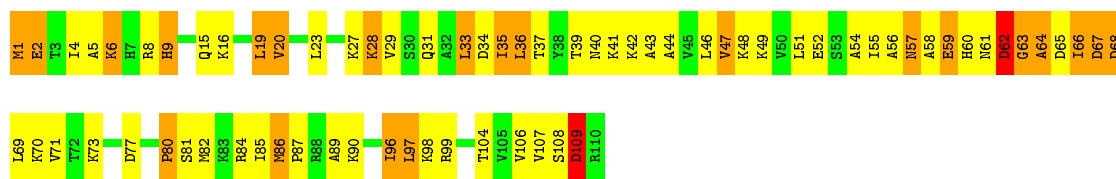




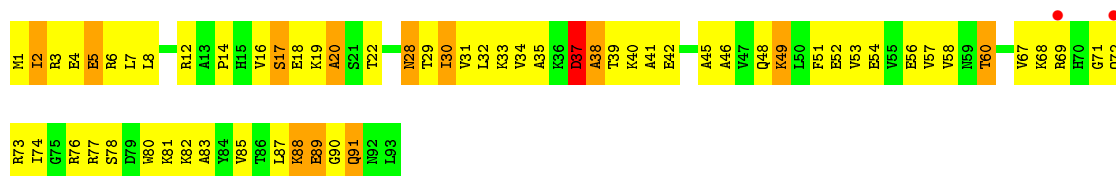
• Molecule 43: 50S ribosomal protein L22



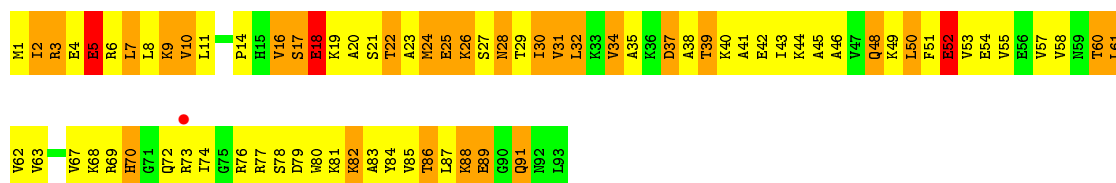
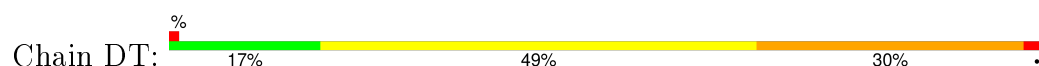
• Molecule 43: 50S ribosomal protein L22



• Molecule 44: 50S ribosomal protein L23

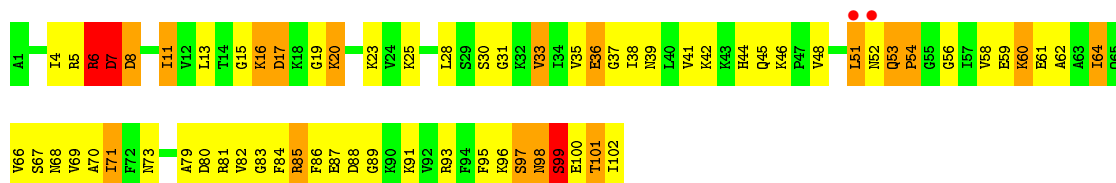


• Molecule 44: 50S ribosomal protein L23

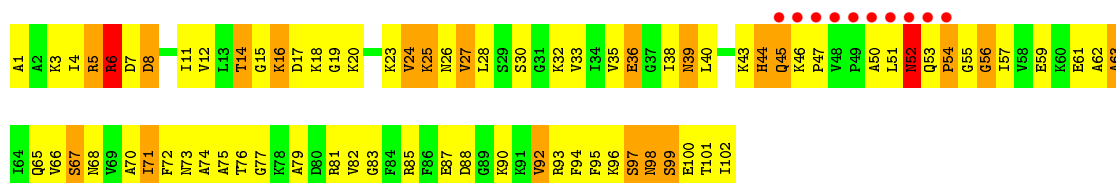


• Molecule 45: 50S ribosomal protein L24

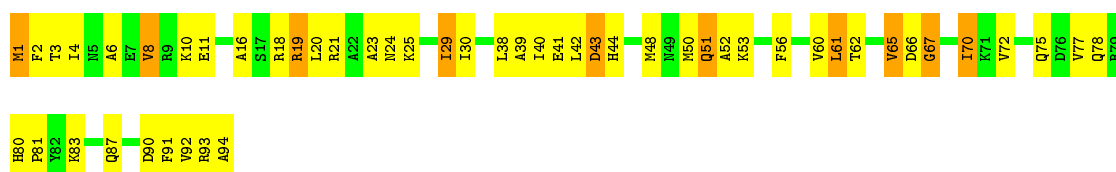




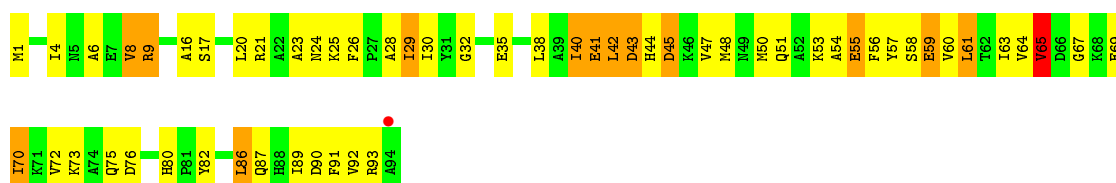
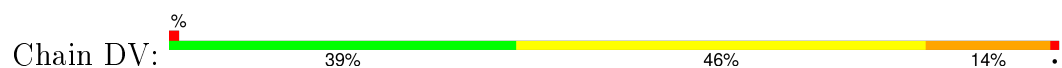
• Molecule 45: 50S ribosomal protein L24



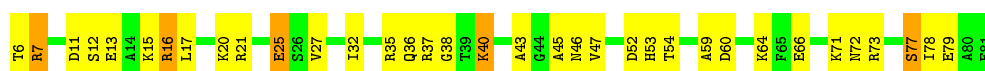
• Molecule 46: 50S ribosomal protein L25



• Molecule 46: 50S ribosomal protein L25



• Molecule 47: 50S ribosomal protein L27



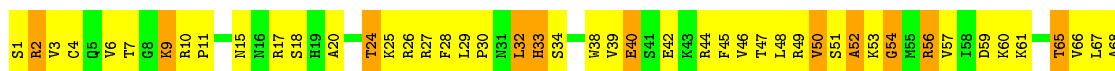
• Molecule 48: 50S ribosomal protein L28





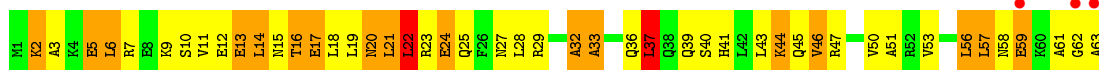
- Molecule 48: 50S ribosomal protein L28

Chain DX: 32% 51% 17%



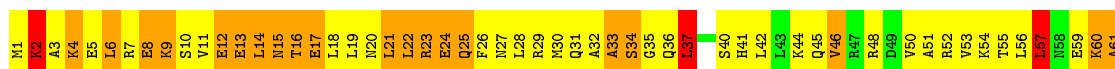
- Molecule 49: 50S ribosomal protein L29

Chain CY: 5% 25% 44% 27%



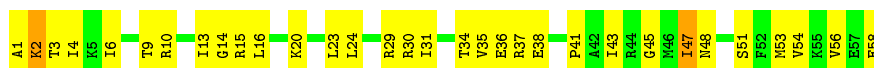
- Molecule 49: 50S ribosomal protein L29

Chain DY: 13% 51% 32% 5%



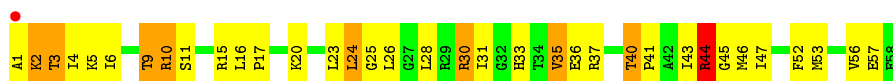
- Molecule 50: 50S ribosomal protein L30

Chain CZ: 45% 52%



- Molecule 50: 50S ribosomal protein L30

Chain DZ: 2% 40% 45% 14%

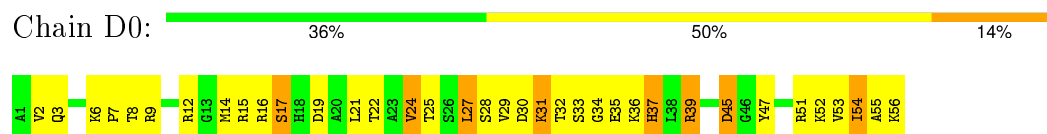


- Molecule 51: 50S ribosomal protein L32

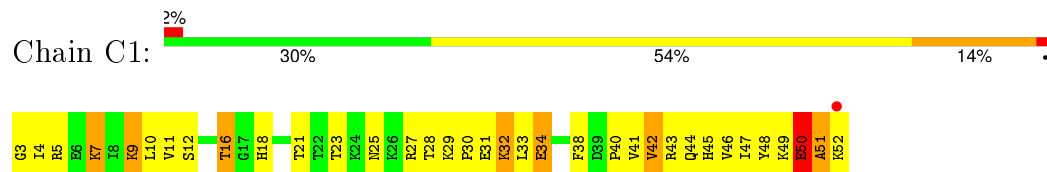
Chain C0: 48% 38% 14%



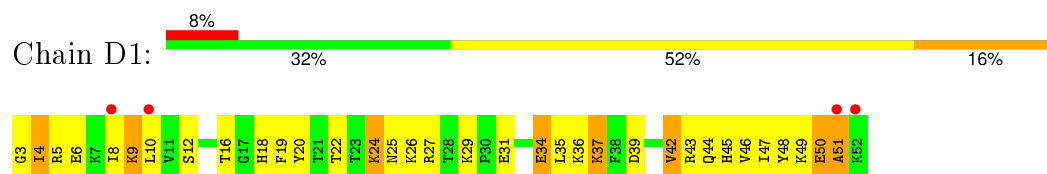
- Molecule 51: 50S ribosomal protein L32



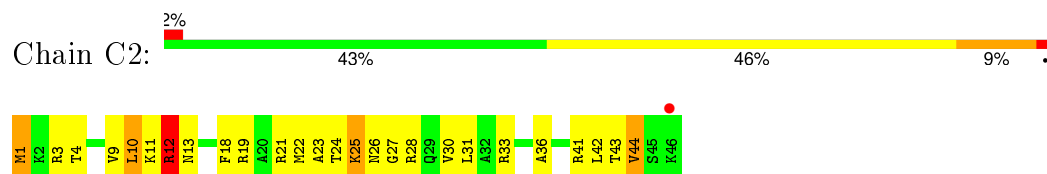
- Molecule 52: 50S ribosomal protein L33



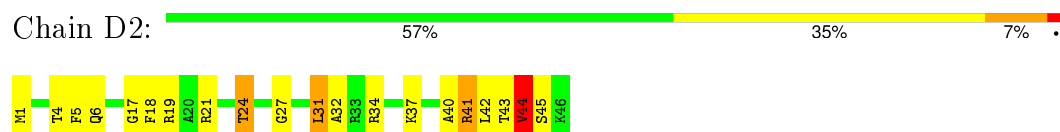
- Molecule 52: 50S ribosomal protein L33



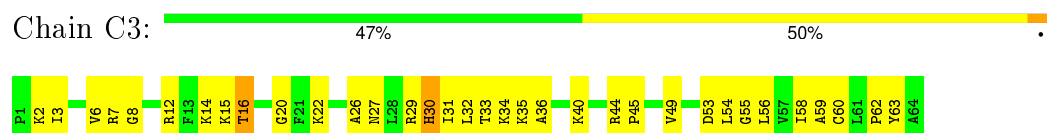
- Molecule 53: 50S ribosomal protein L34



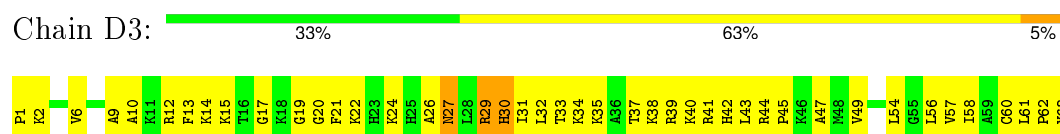
- Molecule 53: 50S ribosomal protein L34



- Molecule 54: 50S ribosomal protein L35



- Molecule 54: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L36

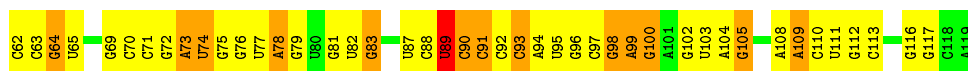
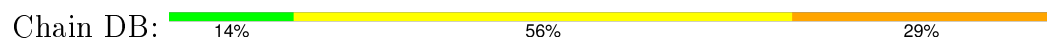




- Molecule 55: 50S ribosomal protein L36



- Molecule 56: 5S rRNA



- Molecule 57: 50S ribosomal protein L27



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.67Å 438.07Å 613.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.00 69.21 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.00) 83.5 (69.21-3.00)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 3.01Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.202 , 0.260 0.195 , 0.251	Depositor DCC
R_{free} test set	19047 reflections (2.03%)	DCC
Wilson B-factor (Å ²)	44.7	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 22.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 938380 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	292354	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.44% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AA	0.87	8/36944 (0.0%)	1.28	318/57632 (0.6%)
1	BA	0.86	8/36966 (0.0%)	1.30	335/57666 (0.6%)
2	AB	0.60	0/1736	0.79	0/2338
2	BB	0.54	0/1736	0.72	0/2338
3	AC	0.56	0/1652	0.72	0/2225
3	BC	0.51	0/1652	0.72	1/2225 (0.0%)
4	AD	0.59	0/1665	0.74	1/2227 (0.0%)
4	BD	0.65	0/1665	0.80	1/2227 (0.0%)
5	AE	0.62	0/1119	0.85	0/1504
5	BE	0.62	0/1119	0.85	0/1504
6	AF	0.65	0/836	0.82	1/1128 (0.1%)
6	BF	0.55	0/836	0.80	1/1128 (0.1%)
7	AG	0.50	0/1196	0.67	0/1602
7	BG	0.48	0/1196	0.67	0/1602
8	AH	0.60	0/989	0.77	0/1326
8	BH	0.58	0/989	0.74	0/1326
9	AI	0.48	0/1034	0.71	0/1375
9	BI	0.53	0/1034	0.75	0/1375
10	AJ	0.57	0/797	0.74	0/1077
10	BJ	0.52	0/797	0.76	1/1077 (0.1%)
11	AK	0.67	0/893	0.82	0/1205
11	BK	0.59	0/893	0.75	0/1205
12	AL	0.61	0/969	0.81	0/1300
12	BL	0.72	0/969	0.92	0/1300
13	AM	0.52	0/893	0.74	0/1193
13	BM	0.50	0/893	0.71	0/1193
14	AN	0.55	0/785	0.76	0/1043
14	BN	0.51	0/785	0.65	0/1043
15	AO	0.55	0/722	0.73	0/964
15	BO	0.53	0/722	0.73	0/964
16	AP	0.54	0/659	0.82	1/884 (0.1%)
16	BP	0.61	0/659	0.79	1/884 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.57	0/658	0.74	0/881
17	BQ	0.62	0/658	0.76	0/881
18	AR	0.61	0/463	0.69	0/621
18	BR	0.54	0/463	0.68	0/621
19	AS	0.48	0/653	0.73	0/877
19	BS	0.55	0/653	0.67	0/877
20	AT	0.54	0/671	0.69	0/888
20	BT	0.57	0/671	0.73	0/888
21	AU	0.93	0/431	0.96	0/570
21	BU	0.78	0/431	0.85	0/570
22	AV	0.76	1/1813 (0.1%)	1.22	14/2823 (0.5%)
22	BV	0.74	1/1813 (0.1%)	1.22	10/2823 (0.4%)
23	AX	0.86	0/363	1.11	0/564
23	BX	0.73	0/388	1.09	0/603
24	AY	0.65	0/1430	0.74	0/1924
25	CA	1.60	600/69659 (0.9%)	1.67	2062/108672 (1.9%)
25	DA	1.07	82/69633 (0.1%)	1.48	1284/108629 (1.2%)
26	CB	1.33	5/2847 (0.2%)	1.58	77/4440 (1.7%)
27	CC	0.80	0/2122	0.90	1/2852 (0.0%)
27	DC	0.68	1/2122 (0.0%)	0.86	1/2852 (0.0%)
28	CD	0.96	0/1586	0.92	1/2134 (0.0%)
28	DD	0.70	0/1586	0.87	2/2134 (0.1%)
29	CE	0.91	0/1571	0.89	1/2113 (0.0%)
29	DE	0.67	0/1571	0.81	0/2113
30	CF	0.64	0/1435	0.74	0/1926
30	DF	0.51	0/1435	0.67	0/1926
31	CG	0.75	0/1343	0.85	1/1816 (0.1%)
31	DG	0.51	0/1343	0.69	0/1816
32	CH	0.68	1/1121 (0.1%)	0.77	0/1515
32	DH	0.66	1/1121 (0.1%)	0.80	1/1515 (0.1%)
33	CI	0.72	0/1046	0.74	0/1410
33	DI	0.67	0/1046	0.72	0/1410
34	CJ	1.01	0/1152	0.84	1/1551 (0.1%)
34	DJ	0.77	0/1152	0.82	0/1551
35	CK	0.91	3/948 (0.3%)	0.94	1/1268 (0.1%)
35	DK	0.68	0/948	0.84	0/1268
36	CL	0.94	0/1054	1.01	0/1403
36	DL	0.65	0/1054	0.85	0/1403
37	CM	0.94	0/1093	0.96	0/1460
37	DM	0.64	0/1093	0.80	0/1460
38	CN	0.91	0/974	0.96	1/1301 (0.1%)
38	DN	0.67	0/974	0.82	0/1301
39	CO	0.76	0/902	0.87	1/1209 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	DO	0.50	0/902	0.66	0/1209
40	CP	0.89	0/929	0.88	1/1242 (0.1%)
40	DP	0.71	0/929	0.82	0/1242
41	CQ	1.14	0/960	0.96	1/1278 (0.1%)
41	DQ	0.80	0/960	0.79	0/1278
42	CR	1.01	1/829 (0.1%)	0.98	0/1107
42	DR	0.79	0/829	0.90	1/1107 (0.1%)
43	CS	1.08	1/864 (0.1%)	0.97	1/1156 (0.1%)
43	DS	0.71	0/864	0.89	1/1156 (0.1%)
44	CT	0.82	0/745	0.86	0/994
44	DT	0.59	0/745	0.74	0/994
45	CU	0.91	0/788	0.90	0/1051
45	DU	0.66	0/788	0.76	0/1051
46	CV	0.79	0/766	0.81	0/1025
46	DV	0.53	0/766	0.69	0/1025
47	CW	1.02	0/582	0.97	0/769
48	CX	0.78	0/635	0.84	0/848
48	DX	0.61	0/635	0.77	0/848
49	CY	0.76	0/510	0.96	1/677 (0.1%)
49	DY	0.56	0/510	0.77	0/677
50	CZ	1.04	0/453	0.94	0/605
50	DZ	0.58	0/453	0.78	0/605
51	C0	0.95	0/450	0.98	2/599 (0.3%)
51	D0	0.71	0/450	0.89	1/599 (0.2%)
52	C1	0.74	0/417	0.76	0/554
52	D1	0.50	0/417	0.66	0/554
53	C2	1.03	0/380	0.99	2/498 (0.4%)
53	D2	0.70	0/380	0.84	0/498
54	C3	0.94	0/513	0.85	0/676
54	D3	0.60	0/513	0.78	1/676 (0.1%)
55	C4	0.92	0/303	0.99	0/397
55	D4	0.68	0/303	0.76	0/397
56	DB	0.75	0/2828	1.23	18/4410 (0.4%)
57	DW	0.60	0/571	0.72	0/755
All	All	1.08	713/315257 (0.2%)	1.34	4150/471496 (0.9%)

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
4	AD	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	BD	0	1
5	AE	0	1
5	BE	0	2
6	BF	0	1
9	AI	0	1
11	AK	0	1
11	BK	0	2
12	BL	0	2
13	AM	0	1
14	AN	0	1
20	BT	0	1
21	AU	0	2
21	BU	0	1
27	CC	0	1
27	DC	0	1
28	CD	0	2
28	DD	0	1
32	DH	0	2
33	CI	0	1
34	DJ	0	1
39	DO	0	1
42	CR	0	1
45	CU	0	1
50	CZ	0	1
All	All	0	31

The worst 5 of 713 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	CA	1142	A	N9-C4	-18.22	1.26	1.37
25	CA	984	A	N9-C4	-13.29	1.29	1.37
25	DA	984	A	N9-C4	-10.51	1.31	1.37
25	CA	984	A	C5-C6	-10.44	1.31	1.41
25	CA	528	A	N7-C5	-10.29	1.33	1.39

The worst 5 of 4150 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	CA	984	A	C2-N3-C4	-18.86	101.17	110.60
25	CA	2250	G	N3-C4-C5	17.23	137.22	128.60
25	CA	1638	C	N1-C2-O2	-16.64	108.92	118.90
25	CA	1142	A	C2-N3-C4	-16.61	102.29	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	CA	1142	A	N3-C4-C5	16.11	138.07	126.80

There are no chirality outliers.

5 of 31 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	AD	47	LEU	Peptide
5	AE	100	GLU	Peptide
9	AI	5	TYR	Peptide
11	AK	125	LYS	Peptide
13	AM	111	PRO	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	AA	32995	0	16607	2052	0
1	BA	33015	0	16617	2194	0
2	AB	1705	0	1732	374	0
2	BB	1705	0	1732	298	0
3	AC	1625	0	1699	235	0
3	BC	1625	0	1699	237	0
4	AD	1643	0	1710	291	0
4	BD	1643	0	1710	228	0
5	AE	1106	0	1148	214	0
5	BE	1106	0	1148	211	0
6	AF	818	0	808	116	0
6	BF	818	0	808	156	0
7	AG	1182	0	1240	116	0
7	BG	1182	0	1240	166	0
8	AH	979	0	1034	161	0
8	BH	979	0	1034	119	0
9	AI	1022	0	1070	189	0
9	BI	1022	0	1070	186	0
10	AJ	787	0	828	178	0
10	BJ	787	0	828	142	0
11	AK	877	0	887	160	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	BK	877	0	887	136	0
12	AL	955	0	1019	94	0
12	BL	955	0	1019	118	0
13	AM	884	0	944	163	0
13	BM	884	0	944	144	0
14	AN	774	0	827	130	0
14	BN	774	0	827	131	0
15	AO	714	0	737	61	0
15	BO	714	0	737	87	0
16	AP	649	0	666	106	0
16	BP	649	0	666	87	0
17	AQ	649	0	691	118	0
17	BQ	649	0	691	103	0
18	AR	456	0	478	46	0
18	BR	456	0	478	57	0
19	AS	638	0	665	88	0
19	BS	638	0	665	96	0
20	AT	665	0	714	84	0
20	BT	665	0	714	129	0
21	AU	426	0	449	139	0
21	BU	426	0	449	119	0
22	AV	1623	0	821	88	0
22	BV	1623	0	821	47	0
23	AX	324	0	162	19	0
23	BX	346	0	173	24	0
24	AY	1419	0	1467	97	0
25	CA	62195	0	31271	2445	0
25	DA	62173	0	31270	3398	0
26	CB	2548	0	1292	98	0
27	CC	2083	0	2157	227	0
27	DC	2083	0	2157	213	0
28	CD	1565	0	1616	129	0
28	DD	1565	0	1616	114	0
29	CE	1552	0	1619	143	0
29	DE	1552	0	1619	163	0
30	CF	1411	0	1447	202	0
30	DF	1411	0	1447	197	0
31	CG	1323	0	1374	146	0
31	DG	1323	0	1374	177	0
32	CH	1110	0	1148	145	0
32	DH	1110	0	1148	210	0
33	CI	1032	0	1088	246	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	DI	1032	0	1088	180	0
34	CJ	1129	0	1162	57	0
34	DJ	1129	0	1162	96	0
35	CK	939	0	1012	75	0
35	DK	939	0	1012	79	0
36	CL	1045	0	1117	130	0
36	DL	1045	0	1117	168	0
37	CM	1074	0	1157	96	0
37	DM	1074	0	1157	127	0
38	CN	961	0	1000	94	0
38	DN	961	0	1000	124	0
39	CO	892	0	923	84	0
39	DO	892	0	923	141	0
40	CP	917	0	965	93	0
40	DP	917	0	965	107	0
41	CQ	947	0	1022	63	0
41	DQ	947	0	1022	83	0
42	CR	816	0	839	84	0
42	DR	816	0	839	99	0
43	CS	857	0	922	42	0
43	DS	857	0	922	82	0
44	CT	739	0	807	71	0
44	DT	739	0	807	114	0
45	CU	780	0	834	66	0
45	DU	780	0	834	111	0
46	CV	753	0	780	59	0
46	DV	753	0	780	71	0
47	CW	575	0	589	27	0
48	CX	625	0	655	41	0
48	DX	625	0	655	58	0
49	CY	509	0	543	88	0
49	DY	509	0	543	109	0
50	CZ	449	0	491	26	0
50	DZ	449	0	491	47	0
51	C0	444	0	461	35	0
51	D0	444	0	461	41	0
52	C1	410	0	440	37	0
52	D1	410	0	440	45	0
53	C2	377	0	418	26	0
53	D2	377	0	418	18	0
54	C3	504	0	574	40	0
54	D3	504	0	574	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	C4	302	0	340	23	0
55	D4	302	0	340	34	0
56	DB	2529	0	1281	163	0
57	DW	564	0	576	36	0
58	AA	72	0	0	0	0
58	BA	56	0	0	0	0
58	CA	194	0	0	0	0
58	CB	4	0	0	0	0
58	CQ	1	0	0	0	0
58	DA	166	0	0	0	0
58	DB	3	0	0	0	0
58	DL	1	0	0	0	0
58	DQ	1	0	0	0	0
59	C4	1	0	0	0	0
59	D4	1	0	0	0	0
60	AA	197	0	0	11	0
60	AN	4	0	0	0	0
60	AT	1	0	0	0	0
60	AU	1	0	0	0	0
60	BA	190	0	0	12	0
60	BL	1	0	0	0	0
60	BN	5	0	0	1	0
60	BT	1	0	0	0	0
60	BU	1	0	0	0	0
60	C2	1	0	0	0	0
60	C3	1	0	0	0	0
60	C4	2	0	0	0	0
60	CA	625	0	0	62	0
60	CB	13	0	0	0	0
60	CC	8	0	0	0	0
60	CD	2	0	0	0	0
60	CE	2	0	0	0	0
60	CF	1	0	0	0	0
60	CJ	1	0	0	0	0
60	CL	6	0	0	2	0
60	CN	4	0	0	0	0
60	CS	1	0	0	0	0
60	CV	1	0	0	0	0
60	D2	1	0	0	0	0
60	D3	2	0	0	0	0
60	D4	1	0	0	0	0
60	DA	622	0	0	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	DB	14	0	0	0	0
60	DC	4	0	0	0	0
60	DD	5	0	0	2	0
60	DE	2	0	0	0	0
60	DJ	1	0	0	0	0
60	DL	4	0	0	1	0
60	DN	1	0	0	0	0
60	DR	1	0	0	0	0
All	All	292354	0	195461	20868	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 43.

The worst 5 of 20868 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)
32:DH:93:SER:OG	32:DH:121:VAL:HG12	1.46	1.15
1:BA:1053:G:H4'	1:BA:1054:C:H5'	1.29	1.11
32:DH:93:SER:OG	32:DH:121:VAL:CG1	2.03	1.06
25:DA:1153:C:OP2	60:DA:3363:HOH:O	1.78	1.01
12:BL:33:CYS:HA	12:BL:54:VAL:HA	1.44	0.99

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	216/218 (99%)	109 (50%)	49 (23%)	58 (27%)	0	0
2	BB	216/218 (99%)	112 (52%)	49 (23%)	55 (26%)	0	0
3	AC	204/206 (99%)	125 (61%)	49 (24%)	30 (15%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	BC	204/206 (99%)	126 (62%)	47 (23%)	31 (15%)	0	1
4	AD	203/205 (99%)	123 (61%)	41 (20%)	39 (19%)	0	0
4	BD	203/205 (99%)	136 (67%)	36 (18%)	31 (15%)	0	1
5	AE	148/150 (99%)	87 (59%)	38 (26%)	23 (16%)	0	1
5	BE	148/150 (99%)	90 (61%)	31 (21%)	27 (18%)	0	0
6	AF	98/100 (98%)	62 (63%)	21 (21%)	15 (15%)	0	1
6	BF	98/100 (98%)	54 (55%)	23 (24%)	21 (21%)	0	0
7	AG	149/151 (99%)	86 (58%)	41 (28%)	22 (15%)	0	1
7	BG	149/151 (99%)	79 (53%)	46 (31%)	24 (16%)	0	1
8	AH	127/129 (98%)	79 (62%)	37 (29%)	11 (9%)	1	4
8	BH	127/129 (98%)	82 (65%)	32 (25%)	13 (10%)	1	3
9	AI	125/127 (98%)	76 (61%)	34 (27%)	15 (12%)	0	2
9	BI	125/127 (98%)	77 (62%)	33 (26%)	15 (12%)	0	2
10	AJ	96/98 (98%)	60 (62%)	14 (15%)	22 (23%)	0	0
10	BJ	96/98 (98%)	64 (67%)	14 (15%)	18 (19%)	0	0
11	AK	115/117 (98%)	84 (73%)	17 (15%)	14 (12%)	0	2
11	BK	115/117 (98%)	81 (70%)	19 (16%)	15 (13%)	0	1
12	AL	121/123 (98%)	85 (70%)	29 (24%)	7 (6%)	2	12
12	BL	121/123 (98%)	91 (75%)	16 (13%)	14 (12%)	0	2
13	AM	112/114 (98%)	78 (70%)	22 (20%)	12 (11%)	0	2
13	BM	112/114 (98%)	65 (58%)	24 (21%)	23 (20%)	0	0
14	AN	92/100 (92%)	47 (51%)	27 (29%)	18 (20%)	0	0
14	BN	92/100 (92%)	39 (42%)	30 (33%)	23 (25%)	0	0
15	AO	86/88 (98%)	57 (66%)	22 (26%)	7 (8%)	1	5
15	BO	86/88 (98%)	52 (60%)	17 (20%)	17 (20%)	0	0
16	AP	80/82 (98%)	48 (60%)	11 (14%)	21 (26%)	0	0
16	BP	80/82 (98%)	47 (59%)	22 (28%)	11 (14%)	0	1
17	AQ	78/80 (98%)	47 (60%)	18 (23%)	13 (17%)	0	1
17	BQ	78/80 (98%)	48 (62%)	18 (23%)	12 (15%)	0	1
18	AR	53/55 (96%)	34 (64%)	13 (24%)	6 (11%)	0	2
18	BR	53/55 (96%)	31 (58%)	19 (36%)	3 (6%)	2	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	AS	77/79 (98%)	36 (47%)	29 (38%)	12 (16%)	0	1
19	BS	77/79 (98%)	56 (73%)	14 (18%)	7 (9%)	1	4
20	AT	83/85 (98%)	37 (45%)	31 (37%)	15 (18%)	0	0
20	BT	83/85 (98%)	46 (55%)	23 (28%)	14 (17%)	0	1
21	AU	49/51 (96%)	20 (41%)	15 (31%)	14 (29%)	0	0
21	BU	49/51 (96%)	22 (45%)	10 (20%)	17 (35%)	0	0
24	AY	181/183 (99%)	135 (75%)	35 (19%)	11 (6%)	2	11
27	CC	269/271 (99%)	216 (80%)	32 (12%)	21 (8%)	1	6
27	DC	269/271 (99%)	198 (74%)	43 (16%)	28 (10%)	1	3
28	CD	207/209 (99%)	166 (80%)	30 (14%)	11 (5%)	2	14
28	DD	207/209 (99%)	162 (78%)	35 (17%)	10 (5%)	3	17
29	CE	199/201 (99%)	158 (79%)	32 (16%)	9 (4%)	3	18
29	DE	199/201 (99%)	142 (71%)	38 (19%)	19 (10%)	1	3
30	CF	175/177 (99%)	118 (67%)	38 (22%)	19 (11%)	0	2
30	DF	175/177 (99%)	113 (65%)	34 (19%)	28 (16%)	0	1
31	CG	174/176 (99%)	129 (74%)	30 (17%)	15 (9%)	1	4
31	DG	174/176 (99%)	106 (61%)	43 (25%)	25 (14%)	0	1
32	CH	147/149 (99%)	95 (65%)	29 (20%)	23 (16%)	0	1
32	DH	147/149 (99%)	95 (65%)	27 (18%)	25 (17%)	0	1
33	CI	139/141 (99%)	65 (47%)	47 (34%)	27 (19%)	0	0
33	DI	139/141 (99%)	71 (51%)	46 (33%)	22 (16%)	0	1
34	CJ	140/142 (99%)	123 (88%)	11 (8%)	6 (4%)	3	19
34	DJ	140/142 (99%)	112 (80%)	24 (17%)	4 (3%)	6	29
35	CK	120/122 (98%)	88 (73%)	24 (20%)	8 (7%)	1	8
35	DK	120/122 (98%)	87 (72%)	21 (18%)	12 (10%)	1	3
36	CL	141/143 (99%)	99 (70%)	21 (15%)	21 (15%)	0	1
36	DL	141/143 (99%)	88 (62%)	36 (26%)	17 (12%)	0	2
37	CM	134/136 (98%)	110 (82%)	15 (11%)	9 (7%)	1	8
37	DM	134/136 (98%)	97 (72%)	23 (17%)	14 (10%)	1	3
38	CN	118/120 (98%)	91 (77%)	21 (18%)	6 (5%)	2	15
38	DN	118/120 (98%)	82 (70%)	28 (24%)	8 (7%)	1	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	CO	114/116 (98%)	83 (73%)	17 (15%)	14 (12%)	0	2
39	DO	114/116 (98%)	77 (68%)	25 (22%)	12 (10%)	1	3
40	CP	112/114 (98%)	96 (86%)	12 (11%)	4 (4%)	4	24
40	DP	112/114 (98%)	86 (77%)	19 (17%)	7 (6%)	2	9
41	CQ	115/117 (98%)	100 (87%)	13 (11%)	2 (2%)	11	46
41	DQ	115/117 (98%)	95 (83%)	18 (16%)	2 (2%)	11	46
42	CR	101/103 (98%)	84 (83%)	9 (9%)	8 (8%)	1	5
42	DR	101/103 (98%)	78 (77%)	14 (14%)	9 (9%)	1	4
43	CS	108/110 (98%)	90 (83%)	12 (11%)	6 (6%)	2	13
43	DS	108/110 (98%)	78 (72%)	19 (18%)	11 (10%)	1	3
44	CT	91/93 (98%)	67 (74%)	13 (14%)	11 (12%)	0	2
44	DT	91/93 (98%)	59 (65%)	20 (22%)	12 (13%)	0	1
45	CU	100/102 (98%)	74 (74%)	14 (14%)	12 (12%)	0	2
45	DU	100/102 (98%)	73 (73%)	14 (14%)	13 (13%)	0	1
46	CV	92/94 (98%)	78 (85%)	12 (13%)	2 (2%)	8	38
46	DV	92/94 (98%)	71 (77%)	15 (16%)	6 (6%)	1	8
47	CW	74/76 (97%)	68 (92%)	4 (5%)	2 (3%)	6	32
48	CX	75/77 (97%)	64 (85%)	9 (12%)	2 (3%)	6	32
48	DX	75/77 (97%)	54 (72%)	15 (20%)	6 (8%)	1	5
49	CY	61/63 (97%)	34 (56%)	13 (21%)	14 (23%)	0	0
49	DY	61/63 (97%)	28 (46%)	16 (26%)	17 (28%)	0	0
50	CZ	56/58 (97%)	50 (89%)	6 (11%)	0	100	100
50	DZ	56/58 (97%)	50 (89%)	4 (7%)	2 (4%)	4	24
51	C0	54/56 (96%)	44 (82%)	8 (15%)	2 (4%)	4	23
51	D0	54/56 (96%)	39 (72%)	10 (18%)	5 (9%)	1	4
52	C1	48/50 (96%)	32 (67%)	12 (25%)	4 (8%)	1	5
52	D1	48/50 (96%)	36 (75%)	10 (21%)	2 (4%)	3	20
53	C2	44/46 (96%)	37 (84%)	6 (14%)	1 (2%)	8	36
53	D2	44/46 (96%)	31 (70%)	8 (18%)	5 (11%)	0	2
54	C3	62/64 (97%)	56 (90%)	6 (10%)	0	100	100
54	D3	62/64 (97%)	49 (79%)	11 (18%)	2 (3%)	5	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	C4	36/38 (95%)	31 (86%)	4 (11%)	1 (3%)	6	30
55	D4	36/38 (95%)	31 (86%)	4 (11%)	1 (3%)	6	30
57	DW	73/75 (97%)	57 (78%)	12 (16%)	4 (6%)	2	13
All	All	11416/11626 (98%)	7804 (68%)	2248 (20%)	1364 (12%)	0	2

5 of 1364 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	15	PHE
2	AB	21	TYR
2	AB	33	ALA
2	AB	63	LYS
2	AB	67	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	180/180 (100%)	114 (63%)	66 (37%)	0	1
2	BB	180/180 (100%)	131 (73%)	49 (27%)	0	2
3	AC	170/170 (100%)	127 (75%)	43 (25%)	1	3
3	BC	170/170 (100%)	123 (72%)	47 (28%)	0	2
4	AD	172/172 (100%)	132 (77%)	40 (23%)	1	4
4	BD	172/172 (100%)	123 (72%)	49 (28%)	0	2
5	AE	113/113 (100%)	80 (71%)	33 (29%)	0	2
5	BE	113/113 (100%)	87 (77%)	26 (23%)	1	5
6	AF	87/87 (100%)	60 (69%)	27 (31%)	0	2
6	BF	87/87 (100%)	61 (70%)	26 (30%)	0	2
7	AG	124/124 (100%)	90 (73%)	34 (27%)	0	2
7	BG	124/124 (100%)	85 (68%)	39 (32%)	0	2
8	AH	104/104 (100%)	78 (75%)	26 (25%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	BH	104/104 (100%)	78 (75%)	26 (25%)	1	3
9	AI	105/105 (100%)	74 (70%)	31 (30%)	0	2
9	BI	105/105 (100%)	67 (64%)	38 (36%)	0	1
10	AJ	86/86 (100%)	63 (73%)	23 (27%)	0	3
10	BJ	86/86 (100%)	61 (71%)	25 (29%)	0	2
11	AK	90/90 (100%)	66 (73%)	24 (27%)	0	3
11	BK	90/90 (100%)	67 (74%)	23 (26%)	0	3
12	AL	103/103 (100%)	86 (84%)	17 (16%)	3	13
12	BL	103/103 (100%)	75 (73%)	28 (27%)	0	2
13	AM	92/92 (100%)	73 (79%)	19 (21%)	1	7
13	BM	92/92 (100%)	71 (77%)	21 (23%)	1	5
14	AN	79/83 (95%)	56 (71%)	23 (29%)	0	2
14	BN	79/83 (95%)	60 (76%)	19 (24%)	1	4
15	AO	76/76 (100%)	61 (80%)	15 (20%)	1	9
15	BO	76/76 (100%)	60 (79%)	16 (21%)	1	6
16	AP	65/65 (100%)	45 (69%)	20 (31%)	0	2
16	BP	65/65 (100%)	48 (74%)	17 (26%)	0	3
17	AQ	74/74 (100%)	54 (73%)	20 (27%)	0	3
17	BQ	74/74 (100%)	47 (64%)	27 (36%)	0	1
18	AR	48/48 (100%)	40 (83%)	8 (17%)	3	13
18	BR	48/48 (100%)	40 (83%)	8 (17%)	3	13
19	AS	70/70 (100%)	56 (80%)	14 (20%)	1	8
19	BS	70/70 (100%)	53 (76%)	17 (24%)	1	4
20	AT	65/65 (100%)	45 (69%)	20 (31%)	0	2
20	BT	65/65 (100%)	47 (72%)	18 (28%)	0	2
21	AU	44/44 (100%)	23 (52%)	21 (48%)	0	0
21	BU	44/44 (100%)	26 (59%)	18 (41%)	0	0
24	AY	157/157 (100%)	139 (88%)	18 (12%)	7	28
27	CC	216/216 (100%)	182 (84%)	34 (16%)	3	15
27	DC	216/216 (100%)	173 (80%)	43 (20%)	1	8
28	CD	164/164 (100%)	143 (87%)	21 (13%)	5	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	DD	164/164 (100%)	135 (82%)	29 (18%)	2	11
29	CE	165/165 (100%)	143 (87%)	22 (13%)	5	21
29	DE	165/165 (100%)	126 (76%)	39 (24%)	1	4
30	CF	148/148 (100%)	112 (76%)	36 (24%)	1	4
30	DF	148/148 (100%)	114 (77%)	34 (23%)	1	5
31	CG	137/137 (100%)	114 (83%)	23 (17%)	2	13
31	DG	137/137 (100%)	119 (87%)	18 (13%)	5	22
32	CH	114/114 (100%)	89 (78%)	25 (22%)	1	6
32	DH	114/114 (100%)	92 (81%)	22 (19%)	2	9
33	CI	109/109 (100%)	78 (72%)	31 (28%)	0	2
33	DI	109/109 (100%)	83 (76%)	26 (24%)	1	4
34	CJ	116/116 (100%)	97 (84%)	19 (16%)	3	14
34	DJ	116/116 (100%)	95 (82%)	21 (18%)	2	11
35	CK	103/103 (100%)	85 (82%)	18 (18%)	2	12
35	DK	103/103 (100%)	85 (82%)	18 (18%)	2	12
36	CL	102/102 (100%)	81 (79%)	21 (21%)	1	7
36	DL	102/102 (100%)	81 (79%)	21 (21%)	1	7
37	CM	109/109 (100%)	87 (80%)	22 (20%)	1	8
37	DM	109/109 (100%)	87 (80%)	22 (20%)	1	8
38	CN	100/100 (100%)	83 (83%)	17 (17%)	2	13
38	DN	100/100 (100%)	80 (80%)	20 (20%)	1	8
39	CO	86/86 (100%)	68 (79%)	18 (21%)	1	7
39	DO	86/86 (100%)	66 (77%)	20 (23%)	1	4
40	CP	99/99 (100%)	78 (79%)	21 (21%)	1	6
40	DP	99/99 (100%)	76 (77%)	23 (23%)	1	5
41	CQ	89/89 (100%)	76 (85%)	13 (15%)	4	18
41	DQ	89/89 (100%)	74 (83%)	15 (17%)	2	13
42	CR	84/84 (100%)	70 (83%)	14 (17%)	3	13
42	DR	84/84 (100%)	66 (79%)	18 (21%)	1	6
43	CS	93/93 (100%)	83 (89%)	10 (11%)	8	30
43	DS	93/93 (100%)	71 (76%)	22 (24%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	CT	80/80 (100%)	69 (86%)	11 (14%)	4	20
44	DT	80/80 (100%)	57 (71%)	23 (29%)	0	2
45	CU	83/83 (100%)	64 (77%)	19 (23%)	1	5
45	DU	83/83 (100%)	63 (76%)	20 (24%)	1	4
46	CV	78/78 (100%)	63 (81%)	15 (19%)	2	10
46	DV	78/78 (100%)	63 (81%)	15 (19%)	2	10
47	CW	56/58 (97%)	50 (89%)	6 (11%)	8	31
48	CX	67/67 (100%)	56 (84%)	11 (16%)	3	14
48	DX	67/67 (100%)	56 (84%)	11 (16%)	3	14
49	CY	55/55 (100%)	46 (84%)	9 (16%)	3	14
49	DY	55/55 (100%)	43 (78%)	12 (22%)	1	6
50	CZ	48/48 (100%)	40 (83%)	8 (17%)	3	13
50	DZ	48/48 (100%)	38 (79%)	10 (21%)	1	7
51	C0	47/47 (100%)	41 (87%)	6 (13%)	5	23
51	D0	47/47 (100%)	41 (87%)	6 (13%)	5	23
52	C1	45/45 (100%)	38 (84%)	7 (16%)	3	16
52	D1	45/45 (100%)	37 (82%)	8 (18%)	2	11
53	C2	38/38 (100%)	32 (84%)	6 (16%)	3	15
53	D2	38/38 (100%)	33 (87%)	5 (13%)	5	22
54	C3	51/51 (100%)	48 (94%)	3 (6%)	24	63
54	D3	51/51 (100%)	48 (94%)	3 (6%)	24	63
55	C4	34/34 (100%)	28 (82%)	6 (18%)	2	12
55	D4	34/34 (100%)	27 (79%)	7 (21%)	1	7
57	DW	55/57 (96%)	47 (86%)	8 (14%)	4	18
All	All	9482/9494 (100%)	7392 (78%)	2090 (22%)	1	6

5 of 2090 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	BN	25	GLU
30	CF	55	ASP
42	DR	48	LYS
15	BO	87	ARG
21	BU	4	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 211 such sidechains are listed below:

Mol	Chain	Res	Type
27	CC	116	GLN
34	CJ	58	ASN
45	DU	26	ASN
28	CD	67	HIS
30	CF	62	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1537/1539 (99%)	441 (28%)	28 (1%)
1	BA	1538/1539 (99%)	445 (28%)	20 (1%)
22	AV	75/76 (98%)	29 (38%)	1 (1%)
22	BV	75/76 (98%)	15 (20%)	1 (1%)
23	AX	14/16 (87%)	5 (35%)	0
23	BX	15/16 (93%)	4 (26%)	0
25	CA	2895/2903 (99%)	747 (25%)	53 (1%)
25	DA	2893/2903 (99%)	764 (26%)	48 (1%)
26	CB	118/119 (99%)	24 (20%)	1 (0%)
56	DB	117/118 (99%)	34 (29%)	3 (2%)
All	All	9277/9305 (99%)	2508 (27%)	155 (1%)

5 of 2508 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	6	G
1	AA	7	A
1	AA	9	G
1	AA	12	U

5 of 155 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	CA	1046	A
25	CA	1800	C
25	DA	2311	A
25	CA	1133	A
25	CA	1301	A

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 500 ligands modelled in this entry, 500 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	AA	1538/1539 (99%)	-0.64	8 (0%) 91 76	0, 31, 105, 170	0
1	BA	1539/1539 (100%)	-0.58	10 (0%) 90 73	0, 33, 101, 147	0
2	AB	218/218 (100%)	0.62	15 (6%) 20 7	12, 52, 84, 115	0
2	BB	218/218 (100%)	0.44	12 (5%) 29 11	19, 59, 88, 113	0
3	AC	206/206 (100%)	-0.30	0 100 100	0, 35, 69, 93	0
3	BC	206/206 (100%)	0.26	4 (1%) 70 41	9, 46, 75, 92	0
4	AD	205/205 (100%)	0.11	5 (2%) 62 32	14, 42, 73, 98	0
4	BD	205/205 (100%)	-0.24	1 (0%) 91 76	0, 24, 64, 82	0
5	AE	150/150 (100%)	-0.13	3 (2%) 68 39	0, 32, 68, 105	0
5	BE	150/150 (100%)	-0.36	0 100 100	0, 31, 68, 98	0
6	AF	100/100 (100%)	-0.35	0 100 100	0, 33, 68, 86	0
6	BF	100/100 (100%)	0.02	1 (1%) 84 60	17, 54, 80, 93	0
7	AG	151/151 (100%)	0.53	14 (9%) 11 4	12, 56, 86, 111	0
7	BG	151/151 (100%)	0.04	6 (3%) 42 17	20, 54, 81, 94	0
8	AH	129/129 (100%)	-0.47	0 100 100	0, 32, 60, 71	0
8	BH	129/129 (100%)	-0.23	1 (0%) 87 67	4, 34, 58, 82	0
9	AI	127/127 (100%)	0.20	4 (3%) 52 24	6, 54, 79, 108	0
9	BI	127/127 (100%)	0.40	11 (8%) 13 4	20, 55, 85, 117	0
10	AJ	98/98 (100%)	0.45	5 (5%) 32 12	8, 55, 89, 104	0
10	BJ	98/98 (100%)	0.42	6 (6%) 25 9	25, 58, 82, 113	0
11	AK	117/117 (100%)	-0.36	1 (0%) 85 64	0, 19, 50, 87	0
11	BK	117/117 (100%)	-0.22	0 100 100	0, 32, 66, 79	0
12	AL	123/123 (100%)	-0.30	2 (1%) 74 47	0, 22, 67, 93	0
12	BL	123/123 (100%)	-0.26	3 (2%) 62 32	0, 17, 58, 93	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	114/114 (100%)	0.11	5 (4%) 38 16	9, 53, 87, 100	0
13	BM	114/114 (100%)	0.77	9 (7%) 15 5	26, 63, 87, 97	0
14	AN	96/100 (96%)	-0.01	1 (1%) 84 60	12, 45, 84, 107	0
14	BN	96/100 (96%)	0.29	4 (4%) 40 16	10, 56, 84, 98	0
15	AO	88/88 (100%)	-0.38	1 (1%) 82 58	0, 28, 55, 93	0
15	BO	88/88 (100%)	-0.05	1 (1%) 82 58	1, 33, 66, 89	0
16	AP	82/82 (100%)	0.15	3 (3%) 45 19	5, 30, 73, 86	0
16	BP	82/82 (100%)	-0.10	4 (4%) 33 13	0, 24, 67, 91	0
17	AQ	80/80 (100%)	0.05	1 (1%) 79 53	8, 42, 75, 96	0
17	BQ	80/80 (100%)	-0.08	1 (1%) 79 53	7, 44, 79, 94	0
18	AR	55/55 (100%)	-0.36	1 (1%) 71 43	0, 25, 59, 93	0
18	BR	55/55 (100%)	-0.09	2 (3%) 46 20	5, 38, 80, 101	0
19	AS	79/79 (100%)	0.55	5 (6%) 23 9	21, 52, 83, 98	0
19	BS	79/79 (100%)	0.82	9 (11%) 7 2	37, 65, 83, 95	0
20	AT	85/85 (100%)	0.22	4 (4%) 35 14	7, 37, 67, 80	0
20	BT	85/85 (100%)	0.23	2 (2%) 62 32	8, 38, 69, 96	0
21	AU	51/51 (100%)	0.23	5 (9%) 10 4	7, 39, 74, 77	0
21	BU	51/51 (100%)	0.30	3 (5%) 26 10	8, 47, 74, 80	0
22	AV	76/76 (100%)	-0.21	2 (2%) 59 29	0, 70, 127, 154	0
22	BV	76/76 (100%)	-0.31	0 100 100	22, 43, 72, 119	0
23	AX	15/16 (93%)	0.44	1 (6%) 21 7	6, 76, 115, 133	0
23	BX	16/16 (100%)	0.22	1 (6%) 23 9	16, 77, 102, 124	0
24	AY	183/183 (100%)	0.75	38 (20%) 1 1	0, 50, 96, 117	0
25	CA	2897/2903 (99%)	-0.51	35 (1%) 81 55	0, 0, 103, 162	0
25	DA	2896/2903 (99%)	-0.59	27 (0%) 85 64	0, 15, 109, 162	0
26	CB	119/119 (100%)	-0.84	0 100 100	0, 7, 32, 85	0
27	CC	271/271 (100%)	-0.61	0 100 100	0, 1, 29, 56	0
27	DC	271/271 (100%)	-0.52	0 100 100	0, 19, 47, 77	0
28	CD	209/209 (100%)	-0.62	0 100 100	0, 0, 19, 61	0
28	DD	209/209 (100%)	-0.54	1 (0%) 91 76	0, 10, 52, 66	0
29	CE	201/201 (100%)	-0.52	0 100 100	0, 0, 39, 84	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
29	DE	201/201 (100%)	-0.37	0 100 100	0, 21, 60, 89	0
30	CF	177/177 (100%)	0.09	4 (2%) 64 33	0, 35, 82, 91	0
30	DF	177/177 (100%)	0.44	8 (4%) 37 15	12, 58, 84, 95	0
31	CG	176/176 (100%)	-0.35	0 100 100	0, 15, 48, 88	0
31	DG	176/176 (100%)	0.22	2 (1%) 82 58	15, 48, 73, 93	0
32	CH	149/149 (100%)	0.12	7 (4%) 35 14	0, 52, 87, 100	0
32	DH	149/149 (100%)	0.64	9 (6%) 25 9	8, 58, 92, 107	0
33	CI	141/141 (100%)	2.40	74 (52%) 0 0	44, 79, 102, 124	0
33	DI	141/141 (100%)	2.52	75 (53%) 0 0	54, 82, 104, 118	0
34	CJ	142/142 (100%)	-0.60	0 100 100	0, 0, 21, 56	0
34	DJ	142/142 (100%)	-0.43	0 100 100	0, 8, 37, 65	0
35	CK	122/122 (100%)	-0.63	0 100 100	0, 0, 27, 73	0
35	DK	122/122 (100%)	-0.44	0 100 100	0, 15, 50, 71	0
36	CL	143/143 (100%)	-0.53	0 100 100	0, 0, 27, 68	0
36	DL	143/143 (100%)	-0.28	3 (2%) 67 36	0, 18, 56, 82	0
37	CM	136/136 (100%)	-0.60	0 100 100	0, 0, 21, 83	0
37	DM	136/136 (100%)	-0.15	1 (0%) 89 70	0, 21, 55, 88	0
38	CN	120/120 (100%)	-0.56	0 100 100	0, 0, 14, 68	0
38	DN	120/120 (100%)	-0.49	0 100 100	0, 12, 44, 78	0
39	CO	116/116 (100%)	-0.54	0 100 100	0, 11, 39, 49	0
39	DO	116/116 (100%)	0.36	8 (6%) 20 7	5, 49, 78, 98	0
40	CP	114/114 (100%)	-0.60	0 100 100	0, 0, 47, 70	0
40	DP	114/114 (100%)	-0.44	0 100 100	0, 21, 51, 81	0
41	CQ	117/117 (100%)	-0.59	0 100 100	0, 0, 7, 63	0
41	DQ	117/117 (100%)	-0.69	0 100 100	0, 2, 27, 45	0
42	CR	103/103 (100%)	-0.56	0 100 100	0, 0, 35, 57	0
42	DR	103/103 (100%)	-0.59	1 (0%) 84 60	0, 10, 46, 78	0
43	CS	110/110 (100%)	-0.45	1 (0%) 85 64	0, 0, 22, 98	0
43	DS	110/110 (100%)	-0.62	0 100 100	0, 8, 40, 77	0
44	CT	93/93 (100%)	-0.25	2 (2%) 65 35	0, 6, 68, 78	0
44	DT	93/93 (100%)	0.15	1 (1%) 82 58	0, 35, 71, 96	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
45	CU	102/102 (100%)	-0.48	2 (1%) 68 39	0, 5, 42, 79	0
45	DU	102/102 (100%)	0.38	10 (9%) 10 4	0, 34, 74, 100	0
46	CV	94/94 (100%)	-0.54	0 100 100	0, 6, 42, 62	0
46	DV	94/94 (100%)	-0.08	1 (1%) 82 58	11, 43, 68, 82	0
47	CW	76/76 (100%)	-0.53	0 100 100	0, 1, 31, 69	0
48	CX	77/77 (100%)	-0.46	0 100 100	0, 1, 47, 74	0
48	DX	77/77 (100%)	-0.40	0 100 100	0, 23, 55, 67	0
49	CY	63/63 (100%)	-0.30	3 (4%) 34 14	0, 14, 56, 97	0
49	DY	63/63 (100%)	-0.16	0 100 100	8, 43, 70, 111	0
50	CZ	58/58 (100%)	-0.52	0 100 100	0, 0, 13, 50	0
50	DZ	58/58 (100%)	-0.37	1 (1%) 73 45	0, 20, 52, 72	0
51	C0	56/56 (100%)	-0.58	0 100 100	0, 0, 25, 69	0
51	D0	56/56 (100%)	-0.53	0 100 100	0, 10, 53, 94	0
52	C1	50/50 (100%)	-0.01	1 (2%) 68 39	0, 8, 51, 93	0
52	D1	50/50 (100%)	0.51	4 (8%) 15 5	21, 38, 70, 88	0
53	C2	46/46 (100%)	-0.49	1 (2%) 65 35	0, 0, 15, 101	0
53	D2	46/46 (100%)	-0.63	0 100 100	0, 10, 26, 94	0
54	C3	64/64 (100%)	-0.60	0 100 100	0, 0, 11, 38	0
54	D3	64/64 (100%)	-0.41	0 100 100	0, 15, 35, 52	0
55	C4	38/38 (100%)	-0.36	0 100 100	0, 1, 32, 72	0
55	D4	38/38 (100%)	-0.10	0 100 100	3, 26, 59, 65	0
56	DB	118/118 (100%)	-0.70	0 100 100	6, 58, 86, 106	0
57	DW	75/75 (100%)	-0.14	1 (1%) 79 53	0, 27, 54, 94	0
All	All	20908/20931 (99%)	-0.30	498 (2%) 62 32	0, 23, 86, 170	0

The worst 5 of 498 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
33	CI	52	LEU	11.0
33	DI	2	LYS	9.7
33	DI	59	THR	9.2
33	DI	4	VAL	9.1
33	CI	48	ILE	8.8

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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
58	MG	DA	3131	1/1	0.90	0.58	37.92	55,55,55,55	0
58	MG	CA	3132	1/1	0.93	0.40	20.75	24,24,24,24	0
58	MG	DA	3139	1/1	0.96	0.28	13.50	0,0,0,0	0
58	MG	CA	3147	1/1	0.98	0.26	12.45	0,0,0,0	0
58	MG	CA	3159	1/1	0.98	0.26	10.09	0,0,0,0	0
58	MG	CA	3186	1/1	0.98	0.27	8.84	0,0,0,0	0
58	MG	AA	1604	1/1	0.91	0.18	8.53	22,22,22,22	0
58	MG	DA	3154	1/1	0.96	0.17	8.45	0,0,0,0	0
58	MG	DA	3157	1/1	0.97	0.22	6.86	0,0,0,0	0
58	MG	CA	3121	1/1	0.95	0.19	4.89	0,0,0,0	0
58	MG	CA	3175	1/1	0.95	0.17	4.51	0,0,0,0	0
58	MG	CA	3153	1/1	0.95	0.29	4.32	0,0,0,0	0
58	MG	CA	3066	1/1	0.98	0.22	4.32	0,0,0,0	0
58	MG	CA	3155	1/1	0.96	0.37	4.23	0,0,0,0	0
58	MG	CA	3188	1/1	0.96	0.15	4.06	2,2,2,2	0
58	MG	CA	3165	1/1	0.96	0.19	3.90	0,0,0,0	0
58	MG	CA	3163	1/1	0.97	0.20	3.49	0,0,0,0	0
58	MG	DA	3152	1/1	0.92	0.17	3.47	6,6,6,6	0
58	MG	DA	3142	1/1	0.98	0.16	2.97	0,0,0,0	0
58	MG	AA	1622	1/1	0.96	0.17	2.47	0,0,0,0	0
58	MG	DA	3116	1/1	0.85	0.14	2.18	13,13,13,13	0
58	MG	DA	3108	1/1	0.99	0.17	2.09	0,0,0,0	0
58	MG	CA	3161	1/1	0.98	0.19	1.90	0,0,0,0	0
58	MG	BA	1640	1/1	0.98	0.14	1.47	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	CA	3110	1/1	0.97	0.17	1.17	0,0,0,0	0
58	MG	CA	3064	1/1	0.98	0.18	0.72	0,0,0,0	0
58	MG	CA	3025	1/1	0.93	0.17	0.64	0,0,0,0	0
58	MG	CA	3152	1/1	0.98	0.18	0.57	0,0,0,0	0
58	MG	CA	3012	1/1	0.98	0.18	0.52	0,0,0,0	0
58	MG	AA	1656	1/1	0.96	0.13	0.52	14,14,14,14	0
58	MG	DA	3063	1/1	0.92	0.15	0.52	0,0,0,0	0
58	MG	CA	3106	1/1	0.84	0.18	0.42	0,0,0,0	0
58	MG	CA	3084	1/1	0.78	0.11	0.39	22,22,22,22	0
58	MG	BA	1646	1/1	0.95	0.14	0.15	10,10,10,10	0
58	MG	CA	3050	1/1	1.00	0.16	0.13	0,0,0,0	0
58	MG	DA	3040	1/1	0.96	0.14	0.10	5,5,5,5	0
58	MG	CA	3130	1/1	0.98	0.18	0.09	0,0,0,0	0
58	MG	DA	3145	1/1	0.95	0.11	-0.02	0,0,0,0	0
58	MG	DA	3057	1/1	0.89	0.14	-0.06	14,14,14,14	0
58	MG	DA	3151	1/1	0.99	0.15	-0.08	11,11,11,11	0
58	MG	DA	3013	1/1	0.96	0.14	-0.12	0,0,0,0	0
58	MG	DA	3109	1/1	0.94	0.13	-0.21	2,2,2,2	0
58	MG	CA	3131	1/1	0.98	0.15	-0.23	0,0,0,0	0
58	MG	CA	3017	1/1	0.98	0.16	-0.44	0,0,0,0	0
58	MG	CA	3105	1/1	0.84	0.16	-0.58	0,0,0,0	0
58	MG	CA	3145	1/1	0.97	0.13	-0.73	0,0,0,0	0
58	MG	DA	3017	1/1	0.98	0.13	-0.78	0,0,0,0	0
58	MG	AA	1636	1/1	0.92	0.08	-0.79	0,0,0,0	0
58	MG	DA	3136	1/1	0.85	0.11	-0.81	28,28,28,28	0
58	MG	CA	3041	1/1	0.95	0.16	-0.89	0,0,0,0	0
58	MG	CA	3109	1/1	0.95	0.15	-0.92	0,0,0,0	0
58	MG	AA	1607	1/1	0.94	0.08	-0.95	10,10,10,10	0
58	MG	DA	3101	1/1	0.87	0.12	-1.01	0,0,0,0	0
58	MG	BA	1631	1/1	0.78	0.13	-1.03	35,35,35,35	0
58	MG	DA	3120	1/1	0.94	0.11	-1.08	8,8,8,8	0
58	MG	CA	3013	1/1	0.97	0.15	-1.16	0,0,0,0	0
58	MG	DA	3005	1/1	0.87	0.10	-1.16	25,25,25,25	0
58	MG	BA	1616	1/1	0.95	0.11	-1.19	0,0,0,0	0
58	MG	BA	1614	1/1	0.90	0.07	-1.27	19,19,19,19	0
58	MG	AA	1616	1/1	0.94	0.09	-1.28	11,11,11,11	0
58	MG	AA	1632	1/1	0.92	0.07	-1.29	15,15,15,15	0
58	MG	DA	3153	1/1	0.99	0.10	-1.33	11,11,11,11	0
58	MG	DA	3077	1/1	0.94	0.05	-1.35	12,12,12,12	0
58	MG	CA	3074	1/1	0.97	0.15	-1.38	0,0,0,0	0
58	MG	CA	3054	1/1	0.98	0.14	-1.48	0,0,0,0	0
58	MG	DA	3008	1/1	0.98	0.10	-1.53	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	CA	3117	1/1	0.89	0.14	-1.60	5,5,5,5	0
58	MG	DA	3038	1/1	0.93	0.12	-1.61	0,0,0,0	0
58	MG	DA	3097	1/1	0.97	0.08	-1.67	13,13,13,13	0
58	MG	DA	3036	1/1	0.90	0.08	-1.73	21,21,21,21	0
58	MG	CA	3113	1/1	0.97	0.12	-1.86	0,0,0,0	0
59	ZN	C4	101	1/1	0.99	0.07	-1.89	0,0,0,0	0
58	MG	AA	1617	1/1	0.88	0.05	-1.92	21,21,21,21	0
58	MG	DA	3078	1/1	0.82	0.09	-1.96	15,15,15,15	0
59	ZN	D4	101	1/1	0.99	0.06	-1.96	41,41,41,41	0
58	MG	BA	1603	1/1	0.93	0.09	-1.96	13,13,13,13	0
58	MG	CA	3033	1/1	0.98	0.14	-2.17	0,0,0,0	0
58	MG	CA	3137	1/1	0.96	0.09	-2.28	4,4,4,4	0
58	MG	BA	1601	1/1	0.98	0.08	-2.30	2,2,2,2	0
58	MG	CA	3023	1/1	0.97	0.13	-2.34	0,0,0,0	0
58	MG	CA	3098	1/1	0.95	0.14	-2.35	0,0,0,0	0
58	MG	DA	3073	1/1	0.97	0.11	-2.44	6,6,6,6	0
58	MG	DA	3012	1/1	0.96	0.11	-2.53	0,0,0,0	0
58	MG	DA	3018	1/1	0.96	0.07	-2.53	6,6,6,6	0
58	MG	DA	3105	1/1	0.96	0.11	-2.56	0,0,0,0	0
58	MG	DA	3107	1/1	0.98	0.09	-2.56	9,9,9,9	0
58	MG	CA	3102	1/1	0.92	0.15	-2.59	0,0,0,0	0
58	MG	CA	3133	1/1	0.99	0.05	-2.60	0,0,0,0	0
58	MG	DA	3071	1/1	0.92	0.08	-2.62	0,0,0,0	0
58	MG	DA	3070	1/1	0.92	0.08	-2.66	0,0,0,0	0
58	MG	DA	3112	1/1	0.94	0.09	-2.67	5,5,5,5	0
58	MG	DA	3027	1/1	0.95	0.10	-2.68	14,14,14,14	0
58	MG	DA	3132	1/1	0.96	0.05	-2.74	6,6,6,6	0
58	MG	CA	3069	1/1	0.98	0.14	-2.82	0,0,0,0	0
58	MG	CA	3097	1/1	0.98	0.12	-2.89	0,0,0,0	0
58	MG	DA	3028	1/1	0.95	0.11	-2.91	0,0,0,0	0
58	MG	BA	1630	1/1	0.81	0.07	-2.92	41,41,41,41	0
58	MG	CA	3051	1/1	0.95	0.09	-3.07	3,3,3,3	0
58	MG	CA	3024	1/1	0.93	0.11	-3.15	0,0,0,0	0
58	MG	DA	3134	1/1	0.99	0.07	-3.22	0,0,0,0	0
58	MG	CA	3059	1/1	0.95	0.07	-3.30	4,4,4,4	0
58	MG	CA	3022	1/1	0.99	0.14	-3.37	0,0,0,0	0
58	MG	CA	3108	1/1	0.97	0.10	-3.50	0,0,0,0	0
58	MG	CA	3029	1/1	0.98	0.13	-3.51	0,0,0,0	0
58	MG	DA	3021	1/1	0.95	0.08	-3.55	3,3,3,3	0
58	MG	AA	1629	1/1	0.99	0.07	-3.65	0,0,0,0	0
58	MG	DA	3114	1/1	0.94	0.08	-3.66	14,14,14,14	0
58	MG	CA	3063	1/1	0.95	0.12	-3.80	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	DA	3024	1/1	0.98	0.07	-3.82	0,0,0,0	0
58	MG	DA	3129	1/1	0.99	0.08	-3.89	0,0,0,0	0
58	MG	BA	1619	1/1	0.98	0.08	-3.98	0,0,0,0	0
58	MG	DA	3053	1/1	0.99	0.06	-3.98	0,0,0,0	0
58	MG	AA	1630	1/1	0.92	0.09	-4.05	16,16,16,16	0
58	MG	CA	3028	1/1	0.92	0.14	-4.11	21,21,21,21	0
58	MG	AA	1618	1/1	0.96	0.07	-4.12	21,21,21,21	0
58	MG	DA	3079	1/1	0.92	0.08	-4.24	27,27,27,27	0
58	MG	DA	3023	1/1	0.97	0.06	-4.26	0,0,0,0	0
58	MG	AA	1642	1/1	0.98	0.06	-4.36	1,1,1,1	0
58	MG	DA	3068	1/1	0.97	0.06	-4.36	6,6,6,6	0
58	MG	DA	3104	1/1	0.97	0.09	-4.39	0,0,0,0	0
58	MG	CA	3008	1/1	0.97	0.09	-4.40	0,0,0,0	0
58	MG	CA	3056	1/1	0.94	0.08	-4.42	10,10,10,10	0
58	MG	CA	3125	1/1	0.96	0.09	-4.55	0,0,0,0	0
58	MG	DA	3124	1/1	0.94	0.05	-4.59	0,0,0,0	0
58	MG	DA	3046	1/1	0.96	0.07	-4.60	1,1,1,1	0
58	MG	CA	3170	1/1	0.97	0.07	-4.65	0,0,0,0	0
58	MG	BA	1635	1/1	0.92	0.08	-4.78	21,21,21,21	0
58	MG	AA	1613	1/1	0.92	0.06	-4.95	2,2,2,2	0
58	MG	DA	3096	1/1	0.95	0.06	-5.02	13,13,13,13	0
58	MG	AA	1641	1/1	0.93	0.09	-5.04	0,0,0,0	0
58	MG	CB	201	1/1	0.94	0.05	-5.10	0,0,0,0	0
58	MG	BA	1617	1/1	0.94	0.06	-5.28	13,13,13,13	0
58	MG	DA	3110	1/1	0.94	0.05	-5.33	18,18,18,18	0
58	MG	BA	1607	1/1	0.97	0.06	-5.37	1,1,1,1	0
58	MG	CA	3135	1/1	0.94	0.12	-5.43	0,0,0,0	0
58	MG	CA	3080	1/1	0.93	0.06	-5.51	1,1,1,1	0
58	MG	CA	3043	1/1	0.98	0.07	-5.54	0,0,0,0	0
58	MG	DA	3058	1/1	0.98	0.07	-5.64	6,6,6,6	0
58	MG	CA	3071	1/1	0.96	0.07	-5.65	0,0,0,0	0
58	MG	BA	1632	1/1	0.94	0.04	-5.81	18,18,18,18	0
58	MG	BA	1634	1/1	0.93	0.05	-6.08	10,10,10,10	0
58	MG	DA	3050	1/1	0.89	0.06	-6.39	0,0,0,0	0
58	MG	CA	3072	1/1	0.98	0.07	-6.43	0,0,0,0	0
58	MG	AA	1625	1/1	0.94	0.07	-6.68	6,6,6,6	0
58	MG	BA	1626	1/1	0.94	0.06	-6.83	14,14,14,14	0
58	MG	DA	3065	1/1	0.93	0.08	-6.93	0,0,0,0	0
58	MG	BA	1612	1/1	0.94	0.05	-7.13	18,18,18,18	0
58	MG	DA	3002	1/1	0.97	0.05	-7.26	1,1,1,1	0
58	MG	BA	1610	1/1	0.97	0.03	-7.43	0,0,0,0	0
58	MG	AA	1609	1/1	0.98	0.05	-7.63	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	DA	3049	1/1	0.98	0.05	-8.10	0,0,0,0	0
58	MG	BA	1621	1/1	0.98	0.05	-8.76	12,12,12,12	0
58	MG	CA	3111	1/1	0.96	0.04	-9.72	6,6,6,6	0
58	MG	CA	3035	1/1	0.94	0.07	-10.28	1,1,1,1	0
58	MG	CA	3009	1/1	0.95	0.11	-10.36	0,0,0,0	0
58	MG	CA	3002	1/1	0.93	0.07	-10.61	0,0,0,0	0
58	MG	CA	3119	1/1	0.99	0.02	-12.88	8,8,8,8	0
58	MG	DA	3022	1/1	0.98	0.07	-13.69	0,0,0,0	0
58	MG	CA	3037	1/1	0.97	0.06	-15.61	11,11,11,11	0
58	MG	CA	3127	1/1	0.95	0.12	-	0,0,0,0	0
58	MG	CA	3103	1/1	0.97	0.09	-	0,0,0,0	0
58	MG	CA	3168	1/1	0.95	0.20	-	0,0,0,0	0
58	MG	CB	202	1/1	0.96	0.10	-	0,0,0,0	0
58	MG	CA	3173	1/1	0.95	0.25	-	0,0,0,0	0
58	MG	CA	3091	1/1	0.92	0.08	-	3,3,3,3	0
58	MG	BA	1637	1/1	0.95	0.16	-	19,19,19,19	0
58	MG	DA	3166	1/1	0.96	0.20	-	9,9,9,9	0
58	MG	AA	1605	1/1	0.99	0.07	-	0,0,0,0	0
58	MG	CA	3055	1/1	0.98	0.10	-	6,6,6,6	0
58	MG	DA	3130	1/1	0.99	0.11	-	0,0,0,0	0
58	MG	CA	3093	1/1	0.96	0.12	-	11,11,11,11	0
58	MG	AA	1650	1/1	0.97	0.11	-	0,0,0,0	0
58	MG	CA	3156	1/1	0.98	0.29	-	0,0,0,0	0
58	MG	DA	3035	1/1	0.98	0.10	-	0,0,0,0	0
58	MG	CA	3136	1/1	0.96	0.09	-	0,0,0,0	0
58	MG	CA	3085	1/1	0.95	0.21	-	12,12,12,12	0
58	MG	DA	3081	1/1	0.97	0.06	-	0,0,0,0	0
58	MG	CA	3038	1/1	0.99	0.20	-	0,0,0,0	0
58	MG	CA	3058	1/1	0.95	0.10	-	10,10,10,10	0
58	MG	DA	3121	1/1	0.96	0.07	-	7,7,7,7	0
58	MG	AA	1637	1/1	0.91	0.09	-	1,1,1,1	0
58	MG	BA	1609	1/1	0.90	0.09	-	26,26,26,26	0
58	MG	CA	3011	1/1	0.97	0.20	-	0,0,0,0	0
58	MG	DA	3062	1/1	0.93	0.09	-	0,0,0,0	0
58	MG	CA	3149	1/1	0.98	0.32	-	0,0,0,0	0
58	MG	BA	1639	1/1	0.95	0.06	-	0,0,0,0	0
58	MG	DA	3085	1/1	0.94	0.20	-	0,0,0,0	0
58	MG	CA	3118	1/1	0.98	0.07	-	0,0,0,0	0
58	MG	CA	3048	1/1	0.91	0.09	-	13,13,13,13	0
58	MG	CA	3193	1/1	0.96	0.25	-	0,0,0,0	0
58	MG	DA	3025	1/1	0.88	0.20	-	16,16,16,16	0
58	MG	BA	1618	1/1	0.87	0.19	-	4,4,4,4	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	BA	1656	1/1	0.96	0.19	-	9,9,9,9	0
58	MG	DA	3044	1/1	0.94	0.05	-	11,11,11,11	0
58	MG	AA	1639	1/1	0.86	0.10	-	22,22,22,22	0
58	MG	BA	1602	1/1	0.82	0.08	-	21,21,21,21	0
58	MG	DA	3161	1/1	0.93	0.09	-	15,15,15,15	0
58	MG	DA	3014	1/1	0.93	0.11	-	12,12,12,12	0
58	MG	CA	3166	1/1	0.96	0.14	-	0,0,0,0	0
58	MG	BA	1627	1/1	0.89	0.12	-	35,35,35,35	0
58	MG	CA	3010	1/1	0.98	0.11	-	0,0,0,0	0
58	MG	AA	1640	1/1	0.74	0.19	-	34,34,34,34	0
58	MG	DA	3033	1/1	0.94	0.12	-	0,0,0,0	0
58	MG	DA	3056	1/1	0.97	0.05	-	5,5,5,5	0
58	MG	CA	3099	1/1	0.88	0.85	-	53,53,53,53	0
58	MG	CA	3021	1/1	0.96	0.10	-	0,0,0,0	0
58	MG	AA	1620	1/1	0.83	0.07	-	10,10,10,10	0
58	MG	DA	3140	1/1	0.97	0.28	-	0,0,0,0	0
58	MG	AA	1664	1/1	0.98	0.11	-	4,4,4,4	0
58	MG	CA	3178	1/1	0.94	0.13	-	0,0,0,0	0
58	MG	AA	1654	1/1	0.93	0.16	-	5,5,5,5	0
58	MG	AA	1612	1/1	0.96	0.05	-	0,0,0,0	0
58	MG	DA	3020	1/1	0.98	0.06	-	0,0,0,0	0
58	MG	CA	3046	1/1	0.95	0.06	-	0,0,0,0	0
58	MG	DA	3080	1/1	0.85	0.09	-	1,1,1,1	0
58	MG	CA	3177	1/1	0.96	0.13	-	0,0,0,0	0
58	MG	AA	1665	1/1	0.95	0.08	-	0,0,0,0	0
58	MG	CA	3128	1/1	0.98	0.14	-	0,0,0,0	0
58	MG	CA	3143	1/1	0.99	0.28	-	0,0,0,0	0
58	MG	BA	1648	1/1	0.96	0.17	-	0,0,0,0	0
58	MG	DA	3143	1/1	0.98	0.21	-	0,0,0,0	0
58	MG	DA	3119	1/1	0.94	0.15	-	44,44,44,44	0
58	MG	DA	3162	1/1	0.94	0.20	-	4,4,4,4	0
58	MG	DA	3037	1/1	0.95	0.18	-	0,0,0,0	0
58	MG	DA	3098	1/1	0.65	0.54	-	49,49,49,49	0
58	MG	BA	1628	1/1	0.99	0.08	-	25,25,25,25	0
58	MG	AA	1651	1/1	0.97	0.24	-	0,0,0,0	0
58	MG	AA	1649	1/1	0.96	0.23	-	0,0,0,0	0
58	MG	BA	1622	1/1	0.94	0.05	-	4,4,4,4	0
58	MG	DA	3059	1/1	0.94	0.11	-	6,6,6,6	0
58	MG	AA	1671	1/1	0.94	0.17	-	6,6,6,6	0
58	MG	AA	1610	1/1	0.97	0.07	-	32,32,32,32	0
58	MG	DA	3011	1/1	0.98	0.08	-	0,0,0,0	0
58	MG	AA	1655	1/1	0.92	0.15	-	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	AA	1626	1/1	0.85	0.10	-	0,0,0,0	0
58	MG	CA	3073	1/1	0.98	0.12	-	0,0,0,0	0
58	MG	DA	3003	1/1	0.94	0.07	-	8,8,8,8	0
58	MG	DA	3084	1/1	0.87	0.12	-	32,32,32,32	0
58	MG	AA	1669	1/1	0.90	0.14	-	10,10,10,10	0
58	MG	CA	3164	1/1	0.92	0.24	-	0,0,0,0	0
58	MG	DA	3087	1/1	0.90	0.05	-	20,20,20,20	0
58	MG	CA	3092	1/1	0.90	0.09	-	16,16,16,16	0
58	MG	DA	3115	1/1	0.60	0.18	-	27,27,27,27	0
58	MG	DA	3102	1/1	0.90	0.09	-	12,12,12,12	0
58	MG	CA	3057	1/1	0.98	0.04	-	0,0,0,0	0
58	MG	CA	3189	1/1	0.98	0.14	-	0,0,0,0	0
58	MG	CA	3154	1/1	0.94	0.29	-	0,0,0,0	0
58	MG	CA	3122	1/1	1.00	0.11	-	0,0,0,0	0
58	MG	CA	3031	1/1	0.97	0.22	-	0,0,0,0	0
58	MG	DA	3118	1/1	0.95	0.10	-	7,7,7,7	0
58	MG	CA	3150	1/1	0.96	0.10	-	0,0,0,0	0
58	MG	DA	3095	1/1	0.92	0.11	-	10,10,10,10	0
58	MG	DA	3010	1/1	0.94	0.09	-	7,7,7,7	0
58	MG	DA	3026	1/1	0.94	0.09	-	0,0,0,0	0
58	MG	CA	3006	1/1	0.94	0.07	-	1,1,1,1	0
58	MG	DL	201	1/1	0.93	0.05	-	10,10,10,10	0
58	MG	CA	3174	1/1	0.98	0.31	-	0,0,0,0	0
58	MG	CA	3115	1/1	0.97	0.06	-	0,0,0,0	0
58	MG	DA	3006	1/1	0.91	0.05	-	10,10,10,10	0
58	MG	BA	1652	1/1	0.95	0.10	-	1,1,1,1	0
58	MG	DB	201	1/1	0.95	0.05	-	24,24,24,24	0
58	MG	CA	3034	1/1	0.95	0.20	-	0,0,0,0	0
58	MG	AA	1624	1/1	0.96	0.06	-	10,10,10,10	0
58	MG	CA	3001	1/1	0.95	0.10	-	0,0,0,0	0
58	MG	DA	3094	1/1	0.96	0.08	-	43,43,43,43	0
58	MG	DA	3034	1/1	0.94	0.06	-	11,11,11,11	0
58	MG	AA	1638	1/1	0.98	0.06	-	12,12,12,12	0
58	MG	DA	3041	1/1	0.98	0.04	-	6,6,6,6	0
58	MG	AA	1661	1/1	0.97	0.15	-	15,15,15,15	0
58	MG	BA	1620	1/1	0.96	0.07	-	19,19,19,19	0
58	MG	AA	1615	1/1	0.97	0.08	-	9,9,9,9	0
58	MG	DA	3004	1/1	0.93	0.10	-	30,30,30,30	0
58	MG	AA	1643	1/1	0.96	0.27	-	0,0,0,0	0
58	MG	BA	1613	1/1	0.95	0.13	-	0,0,0,0	0
58	MG	CA	3160	1/1	0.94	0.32	-	0,0,0,0	0
58	MG	DA	3117	1/1	0.95	0.05	-	5,5,5,5	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	BA	1615	1/1	0.94	0.18	-	9,9,9,9	0
58	MG	DA	3127	1/1	0.98	0.05	-	0,0,0,0	0
58	MG	CA	3049	1/1	0.97	0.07	-	0,0,0,0	0
58	MG	DA	3147	1/1	0.97	0.18	-	0,0,0,0	0
58	MG	CA	3162	1/1	0.98	0.28	-	0,0,0,0	0
58	MG	DA	3111	1/1	0.95	0.08	-	1,1,1,1	0
58	MG	CA	3191	1/1	0.94	0.20	-	0,0,0,0	0
58	MG	AA	1648	1/1	0.96	0.12	-	4,4,4,4	0
58	MG	DA	3076	1/1	0.95	0.09	-	5,5,5,5	0
58	MG	DA	3007	1/1	0.99	0.19	-	26,26,26,26	0
58	MG	CA	3040	1/1	0.94	0.16	-	0,0,0,0	0
58	MG	CA	3015	1/1	0.79	0.25	-	36,36,36,36	0
58	MG	BA	1624	1/1	0.89	0.07	-	1,1,1,1	0
58	MG	AA	1621	1/1	0.97	0.03	-	10,10,10,10	0
58	MG	CA	3060	1/1	0.97	0.04	-	4,4,4,4	0
58	MG	CA	3134	1/1	0.89	0.32	-	14,14,14,14	0
58	MG	DA	3159	1/1	0.98	0.26	-	3,3,3,3	0
58	MG	CA	3018	1/1	0.99	0.18	-	0,0,0,0	0
58	MG	AA	1659	1/1	0.92	0.08	-	12,12,12,12	0
58	MG	AA	1603	1/1	0.85	0.08	-	28,28,28,28	0
58	MG	CA	3053	1/1	0.97	0.08	-	0,0,0,0	0
58	MG	CA	3100	1/1	0.93	0.10	-	0,0,0,0	0
58	MG	CA	3141	1/1	0.98	0.27	-	0,0,0,0	0
58	MG	AA	1601	1/1	0.82	0.10	-	44,44,44,44	0
58	MG	DA	3165	1/1	0.87	0.23	-	0,0,0,0	0
58	MG	DA	3030	1/1	0.92	0.12	-	0,0,0,0	0
58	MG	CA	3078	1/1	0.98	0.07	-	0,0,0,0	0
58	MG	AA	1657	1/1	0.96	0.17	-	2,2,2,2	0
58	MG	CA	3081	1/1	0.95	0.07	-	0,0,0,0	0
58	MG	CA	3171	1/1	0.95	0.14	-	0,0,0,0	0
58	MG	CA	3185	1/1	0.93	0.28	-	0,0,0,0	0
58	MG	BA	1608	1/1	0.92	0.15	-	18,18,18,18	0
58	MG	DA	3061	1/1	0.81	0.19	-	24,24,24,24	0
58	MG	CA	3179	1/1	0.96	0.14	-	0,0,0,0	0
58	MG	AA	1614	1/1	0.96	0.05	-	12,12,12,12	0
58	MG	AA	1634	1/1	0.90	0.05	-	2,2,2,2	0
58	MG	CA	3086	1/1	0.96	0.16	-	0,0,0,0	0
58	MG	CA	3142	1/1	0.99	0.41	-	0,0,0,0	0
58	MG	CA	3065	1/1	0.97	0.09	-	0,0,0,0	0
58	MG	CA	3007	1/1	0.96	0.04	-	0,0,0,0	0
58	MG	DA	3060	1/1	0.95	0.13	-	5,5,5,5	0
58	MG	DA	3067	1/1	0.97	0.07	-	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	CA	3088	1/1	0.98	0.10	-	0,0,0,0	0
58	MG	DA	3031	1/1	0.97	0.11	-	0,0,0,0	0
58	MG	DA	3158	1/1	0.99	0.14	-	0,0,0,0	0
58	MG	CA	3083	1/1	0.98	0.04	-	10,10,10,10	0
58	MG	CA	3032	1/1	0.95	0.07	-	0,0,0,0	0
58	MG	BA	1642	1/1	0.96	0.23	-	6,6,6,6	0
58	MG	CA	3079	1/1	0.97	0.05	-	3,3,3,3	0
58	MG	CA	3181	1/1	0.96	0.15	-	0,0,0,0	0
58	MG	DA	3069	1/1	0.97	0.09	-	41,41,41,41	0
58	MG	CA	3144	1/1	0.98	0.33	-	0,0,0,0	0
58	MG	DA	3055	1/1	0.71	0.13	-	28,28,28,28	0
58	MG	CA	3075	1/1	0.96	0.07	-	0,0,0,0	0
58	MG	DA	3082	1/1	0.95	0.05	-	7,7,7,7	0
58	MG	CA	3169	1/1	0.95	0.22	-	7,7,7,7	0
58	MG	AA	1619	1/1	0.94	0.16	-	32,32,32,32	0
58	MG	BA	1623	1/1	0.97	0.08	-	3,3,3,3	0
58	MG	DA	3045	1/1	0.95	0.09	-	0,0,0,0	0
58	MG	AA	1658	1/1	0.87	0.19	-	16,16,16,16	0
58	MG	CA	3045	1/1	0.95	0.10	-	0,0,0,0	0
58	MG	DA	3113	1/1	0.95	0.12	-	0,0,0,0	0
58	MG	CA	3094	1/1	0.96	0.05	-	3,3,3,3	0
58	MG	CA	3112	1/1	0.93	0.10	-	4,4,4,4	0
58	MG	DA	3048	1/1	0.98	0.06	-	0,0,0,0	0
58	MG	CA	3047	1/1	0.98	0.09	-	0,0,0,0	0
58	MG	AA	1660	1/1	0.91	0.12	-	15,15,15,15	0
58	MG	AA	1635	1/1	0.91	0.09	-	18,18,18,18	0
58	MG	DA	3123	1/1	0.98	0.05	-	6,6,6,6	0
58	MG	CA	3076	1/1	0.93	0.15	-	0,0,0,0	0
58	MG	AA	1667	1/1	0.92	0.26	-	13,13,13,13	0
58	MG	CA	3014	1/1	0.88	0.14	-	12,12,12,12	0
58	MG	DB	203	1/1	0.88	0.06	-	16,16,16,16	0
58	MG	AA	1645	1/1	0.88	0.24	-	8,8,8,8	0
58	MG	AA	1662	1/1	0.87	0.10	-	8,8,8,8	0
58	MG	CA	3052	1/1	0.97	0.12	-	0,0,0,0	0
58	MG	CB	204	1/1	0.98	0.39	-	0,0,0,0	0
58	MG	CA	3158	1/1	0.97	0.34	-	0,0,0,0	0
58	MG	DA	3149	1/1	0.95	0.18	-	0,0,0,0	0
58	MG	DA	3009	1/1	0.94	0.09	-	4,4,4,4	0
58	MG	CB	203	1/1	0.98	0.04	-	5,5,5,5	0
58	MG	DA	3083	1/1	0.65	0.22	-	31,31,31,31	0
58	MG	BA	1641	1/1	0.88	0.09	-	20,20,20,20	0
58	MG	DA	3099	1/1	0.95	0.07	-	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	DA	3100	1/1	0.96	0.06	-	4,4,4,4	0
58	MG	DA	3043	1/1	0.97	0.05	-	6,6,6,6	0
58	MG	DA	3039	1/1	0.98	0.09	-	3,3,3,3	0
58	MG	DA	3148	1/1	0.99	0.27	-	0,0,0,0	0
58	MG	DA	3128	1/1	0.96	0.11	-	0,0,0,0	0
58	MG	CA	3044	1/1	0.95	0.06	-	0,0,0,0	0
58	MG	DA	3137	1/1	0.97	0.46	-	0,0,0,0	0
58	MG	DA	3163	1/1	0.98	0.09	-	0,0,0,0	0
58	MG	DA	3090	1/1	0.86	0.08	-	15,15,15,15	0
58	MG	DA	3015	1/1	0.88	0.18	-	23,23,23,23	0
58	MG	CA	3116	1/1	0.93	0.22	-	10,10,10,10	0
58	MG	CA	3039	1/1	0.98	0.11	-	0,0,0,0	0
58	MG	CA	3104	1/1	0.97	0.06	-	0,0,0,0	0
58	MG	DA	3093	1/1	0.96	0.08	-	2,2,2,2	0
58	MG	DA	3106	1/1	0.98	0.17	-	0,0,0,0	0
58	MG	CA	3082	1/1	0.86	0.12	-	0,0,0,0	0
58	MG	DA	3088	1/1	0.74	0.10	-	12,12,12,12	0
58	MG	DA	3160	1/1	0.91	0.12	-	0,0,0,0	0
58	MG	CA	3124	1/1	0.96	0.09	-	0,0,0,0	0
58	MG	BA	1654	1/1	0.96	0.09	-	22,22,22,22	0
58	MG	CA	3187	1/1	0.93	0.16	-	0,0,0,0	0
58	MG	AA	1623	1/1	0.87	0.07	-	24,24,24,24	0
58	MG	CA	3062	1/1	0.80	0.46	-	46,46,46,46	0
58	MG	CA	3114	1/1	0.91	0.10	-	0,0,0,0	0
58	MG	DA	3089	1/1	0.98	0.08	-	24,24,24,24	0
58	MG	CA	3020	1/1	0.98	0.12	-	0,0,0,0	0
58	MG	DA	3126	1/1	0.94	0.13	-	0,0,0,0	0
58	MG	CA	3070	1/1	0.96	0.12	-	25,25,25,25	0
58	MG	DA	3042	1/1	0.96	0.06	-	5,5,5,5	0
58	MG	DA	3074	1/1	0.99	0.13	-	0,0,0,0	0
58	MG	BA	1611	1/1	0.92	0.11	-	13,13,13,13	0
58	MG	CA	3068	1/1	0.99	0.12	-	0,0,0,0	0
58	MG	BA	1605	1/1	0.92	0.06	-	21,21,21,21	0
58	MG	CA	3026	1/1	0.91	0.33	-	30,30,30,30	0
58	MG	DA	3064	1/1	0.87	0.10	-	0,0,0,0	0
58	MG	DA	3052	1/1	0.98	0.05	-	0,0,0,0	0
58	MG	DA	3092	1/1	0.92	0.25	-	34,34,34,34	0
58	MG	CA	3042	1/1	0.97	0.10	-	0,0,0,0	0
58	MG	DA	3016	1/1	0.93	0.08	-	1,1,1,1	0
58	MG	DA	3103	1/1	0.90	0.08	-	0,0,0,0	0
58	MG	AA	1608	1/1	0.95	0.20	-	0,0,0,0	0
58	MG	DA	3164	1/1	0.97	0.15	-	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	BA	1644	1/1	0.97	0.09	-	0,0,0,0	0
58	MG	BA	1604	1/1	0.97	0.07	-	13,13,13,13	0
58	MG	BA	1651	1/1	0.97	0.14	-	7,7,7,7	0
58	MG	BA	1633	1/1	0.94	0.12	-	11,11,11,11	0
58	MG	AA	1663	1/1	0.95	0.10	-	6,6,6,6	0
58	MG	CA	3077	1/1	0.98	0.07	-	0,0,0,0	0
58	MG	CA	3190	1/1	0.99	0.23	-	0,0,0,0	0
58	MG	DA	3146	1/1	0.97	0.18	-	0,0,0,0	0
58	MG	CA	3067	1/1	0.96	0.13	-	0,0,0,0	0
58	MG	DA	3032	1/1	0.98	0.08	-	0,0,0,0	0
58	MG	CA	3148	1/1	0.98	0.47	-	0,0,0,0	0
58	MG	CA	3183	1/1	0.97	0.18	-	0,0,0,0	0
58	MG	AA	1606	1/1	0.91	0.06	-	6,6,6,6	0
58	MG	CA	3182	1/1	0.99	0.30	-	0,0,0,0	0
58	MG	CA	3061	1/1	0.95	0.12	-	9,9,9,9	0
58	MG	DA	3001	1/1	0.96	0.05	-	0,0,0,0	0
58	MG	DA	3135	1/1	0.94	0.08	-	11,11,11,11	0
58	MG	DA	3072	1/1	0.97	0.09	-	0,0,0,0	0
58	MG	CA	3139	1/1	0.99	0.42	-	0,0,0,0	0
58	MG	BA	1643	1/1	0.96	0.14	-	3,3,3,3	0
58	MG	DA	3150	1/1	0.96	0.15	-	0,0,0,0	0
58	MG	CA	3151	1/1	0.99	0.32	-	0,0,0,0	0
58	MG	AA	1646	1/1	0.96	0.17	-	0,0,0,0	0
58	MG	CA	3027	1/1	0.95	0.14	-	0,0,0,0	0
58	MG	CA	3172	1/1	0.96	0.17	-	0,0,0,0	0
58	MG	AA	1672	1/1	0.96	0.21	-	3,3,3,3	0
58	MG	CA	3176	1/1	0.97	0.14	-	10,10,10,10	0
58	MG	AA	1647	1/1	0.96	0.23	-	1,1,1,1	0
58	MG	AA	1628	1/1	0.98	0.04	-	1,1,1,1	0
58	MG	DA	3091	1/1	0.71	0.26	-	50,50,50,50	0
58	MG	BA	1647	1/1	0.98	0.06	-	0,0,0,0	0
58	MG	DA	3125	1/1	0.98	0.07	-	0,0,0,0	0
58	MG	AA	1631	1/1	0.82	0.17	-	35,35,35,35	0
58	MG	CA	3129	1/1	0.93	0.12	-	0,0,0,0	0
58	MG	AA	1644	1/1	0.84	0.19	-	5,5,5,5	0
58	MG	CA	3140	1/1	0.96	0.52	-	0,0,0,0	0
58	MG	DB	202	1/1	0.96	0.04	-	9,9,9,9	0
58	MG	CQ	201	1/1	0.97	0.31	-	0,0,0,0	0
58	MG	DQ	801	1/1	0.97	0.26	-	0,0,0,0	0
58	MG	CA	3003	1/1	0.96	0.06	-	0,0,0,0	0
58	MG	CA	3138	1/1	0.92	0.43	-	0,0,0,0	0
58	MG	CA	3095	1/1	0.98	0.16	-	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	AA	1633	1/1	0.96	0.04	-	3,3,3,3	0
58	MG	DA	3047	1/1	0.91	0.05	-	28,28,28,28	0
58	MG	CA	3180	1/1	0.95	0.19	-	6,6,6,6	0
58	MG	CA	3030	1/1	0.94	0.11	-	0,0,0,0	0
58	MG	DA	3019	1/1	0.92	0.11	-	0,0,0,0	0
58	MG	CA	3107	1/1	0.98	0.17	-	0,0,0,0	0
58	MG	AA	1653	1/1	0.95	0.15	-	1,1,1,1	0
58	MG	BA	1625	1/1	0.93	0.06	-	0,0,0,0	0
58	MG	CA	3019	1/1	0.89	0.09	-	0,0,0,0	0
58	MG	DA	3156	1/1	0.94	0.23	-	3,3,3,3	0
58	MG	AA	1668	1/1	0.97	0.09	-	0,0,0,0	0
58	MG	DA	3029	1/1	0.99	0.05	-	0,0,0,0	0
58	MG	CA	3004	1/1	0.97	0.05	-	11,11,11,11	0
58	MG	BA	1649	1/1	0.92	0.15	-	11,11,11,11	0
58	MG	CA	3192	1/1	0.98	0.11	-	0,0,0,0	0
58	MG	AA	1627	1/1	0.94	0.14	-	19,19,19,19	0
58	MG	CA	3157	1/1	0.97	0.21	-	0,0,0,0	0
58	MG	BA	1650	1/1	0.98	0.21	-	5,5,5,5	0
58	MG	AA	1602	1/1	0.95	0.11	-	17,17,17,17	0
58	MG	CA	3090	1/1	0.96	0.08	-	1,1,1,1	0
58	MG	BA	1655	1/1	0.91	0.11	-	9,9,9,9	0
58	MG	CA	3123	1/1	0.98	0.20	-	0,0,0,0	0
58	MG	CA	3087	1/1	0.99	0.12	-	0,0,0,0	0
58	MG	DA	3133	1/1	0.91	0.17	-	16,16,16,16	0
58	MG	CA	3005	1/1	0.99	0.05	-	14,14,14,14	0
58	MG	CA	3167	1/1	0.97	0.30	-	0,0,0,0	0
58	MG	BA	1636	1/1	0.86	0.10	-	42,42,42,42	0
58	MG	DA	3144	1/1	0.97	0.07	-	0,0,0,0	0
58	MG	BA	1638	1/1	0.96	0.09	-	27,27,27,27	0
58	MG	AA	1670	1/1	0.92	0.27	-	11,11,11,11	0
58	MG	CA	3016	1/1	0.99	0.12	-	0,0,0,0	0
58	MG	BA	1653	1/1	0.91	0.09	-	7,7,7,7	0
58	MG	CA	3120	1/1	0.94	0.12	-	2,2,2,2	0
58	MG	CA	3126	1/1	0.95	0.13	-	0,0,0,0	0
58	MG	DA	3075	1/1	0.93	0.12	-	8,8,8,8	0
58	MG	CA	3101	1/1	0.95	0.11	-	0,0,0,0	0
58	MG	CA	3089	1/1	0.90	0.08	-	19,19,19,19	0
58	MG	CA	3184	1/1	0.97	0.22	-	0,0,0,0	0
58	MG	AA	1611	1/1	0.85	0.09	-	0,0,0,0	0
58	MG	AA	1652	1/1	0.98	0.12	-	13,13,13,13	0
58	MG	DA	3138	1/1	0.92	0.45	-	0,0,0,0	0
58	MG	BA	1629	1/1	0.92	0.06	-	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	BA	1645	1/1	0.93	0.08	-	8,8,8,8	0
58	MG	DA	3054	1/1	0.98	0.09	-	0,0,0,0	0
58	MG	DA	3122	1/1	0.95	0.15	-	0,0,0,0	0
58	MG	DA	3051	1/1	0.97	0.07	-	0,0,0,0	0
58	MG	CA	3194	1/1	0.94	0.19	-	0,0,0,0	0
58	MG	DA	3086	1/1	0.98	0.15	-	0,0,0,0	0
58	MG	DA	3066	1/1	0.95	0.05	-	0,0,0,0	0
58	MG	CA	3036	1/1	0.98	0.16	-	0,0,0,0	0
58	MG	DA	3141	1/1	0.99	0.23	-	0,0,0,0	0
58	MG	DA	3155	1/1	0.98	0.18	-	1,1,1,1	0
58	MG	CA	3096	1/1	0.99	0.06	-	0,0,0,0	0
58	MG	AA	1666	1/1	0.90	0.16	-	13,13,13,13	0
58	MG	CA	3146	1/1	0.96	0.33	-	0,0,0,0	0
58	MG	BA	1606	1/1	0.97	0.12	-	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.