



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:38 PM GMT

PDB ID : 4V56
Title : Crystal structure of the bacterial ribosome from Escherichia coli in complex with spectinomycin.
Authors : Borovinskaya, M.A.; Shoji, S.; Holton, J.M.; Fredrick, K.; Cate, J.H.D.
Deposited on : 2007-07-21
Resolution : 3.93 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:

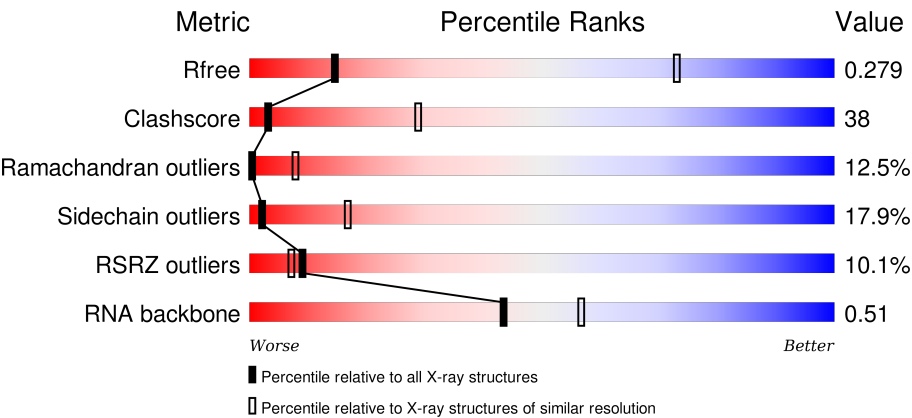
MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.93 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	1007 (4.34-3.54)
Clashscore	102246	1042 (4.30-3.58)
Ramachandran outliers	100387	1000 (4.30-3.58)
Sidechain outliers	100360	1021 (4.32-3.56)
RSRZ outliers	91569	1011 (4.34-3.54)
RNA backbone	2183	1079 (5.04-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	1542	<div><div></div><div><div></div><div>19%</div><div>63%</div><div>16%</div><div>..</div></div></div>
1	CA	1542	<div><div></div><div><div></div><div>20%</div><div>63%</div><div>16%</div><div>.</div></div></div>
2	AC	232	<div><div>7%</div><div></div><div><div></div><div>19%</div><div>46%</div><div>22%</div><div>.</div><div>11%</div></div></div>
2	CC	232	<div><div></div><div><div></div><div>13%</div><div>22%</div><div>48%</div><div>18%</div><div>11%</div></div></div>

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Mol	Chain	Length	Quality of chain
3	AD	205	
3	CD	205	
4	AE	166	
4	CE	166	
5	AF	135	
5	CF	135	
6	AG	178	
6	CG	178	
7	AH	129	
7	CH	129	
8	AI	129	
8	CI	129	
9	AJ	103	
9	CJ	103	
10	AK	128	
10	CK	128	
11	AL	123	
11	CL	123	
12	AM	117	
12	CM	117	
13	AP	82	
13	CP	82	
14	AQ	83	
14	CQ	83	
15	AR	74	

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Mol	Chain	Length	Quality of chain
15	CR	74	
16	AS	91	
16	CS	91	
17	AT	86	
17	CT	86	
18	AB	240	
18	CB	240	
19	AU	70	
19	CU	70	
20	AO	89	
20	CO	89	
21	AN	100	
21	CN	100	
22	BA	120	
22	DA	120	
23	BB	2904	
23	DB	2904	
24	BI	141	
24	DI	141	
25	BC	272	
25	DC	272	
26	BD	209	
26	DD	209	
27	BK	123	
27	DK	123	

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

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

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
53	MG	BB	3087	-	-	-	X
53	MG	CA	1612	-	-	-	X
53	MG	CA	1654	-	-	-	X
53	MG	DB	3026	-	-	-	X

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 284033 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

- Molecule 2 is a protein called 30S ribosomal protein S3.

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

- Molecule 3 is a protein called 30S ribosomal protein S4.

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

- Molecule 4 is a protein called 30S ribosomal protein S5.

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

- Molecule 5 is a protein called 30S ribosomal protein S6.

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

- Molecule 6 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AG	150	Total	C	N	O	S	0	0	0
			1174	730	226	214	4			
6	CG	152	Total	C	N	O	S	0	0	0
			1196	745	230	217	4			

- Molecule 7 is a protein called 30S ribosomal protein S8.

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

- Molecule 8 is a protein called 30S ribosomal protein S9.

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

- Molecule 9 is a protein called 30S ribosomal protein S10.

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

- Molecule 10 is a protein called 30S ribosomal protein S11.

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

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

- Molecule 11 is a protein called 30S ribosomal protein S12.

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

- Molecule 12 is a protein called 30S ribosomal protein S13.

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

- Molecule 13 is a protein called 30S ribosomal protein S16.

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

- Molecule 14 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AQ	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			
14	CQ	81	Total	C	N	O	S	0	0	0
			657	417	122	115	3			

- Molecule 15 is a protein called 30S ribosomal protein S18.

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

- Molecule 16 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AS	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			
16	CS	80	Total	C	N	O	S	0	0	0
			644	413	121	108	2			

- Molecule 17 is a protein called 30S ribosomal protein S20.

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

- Molecule 18 is a protein called 30S ribosomal protein S2.

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

- Molecule 19 is a protein called 30S ribosomal protein S21.

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

- Molecule 20 is a protein called 30S ribosomal protein S15.

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

- Molecule 21 is a protein called 30S ribosomal protein S14.

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

- Molecule 22 is a RNA chain called 5S rRNA.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	120	U	-	INSERTION	GB 85674274
DA	120	U	-	INSERTION	GB 85674274

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

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BB	2903	U	-	INSERTION	GB 85674274
BB	2904	U	-	INSERTION	GB 85674274
DB	2903	U	-	INSERTION	GB 85674274
DB	2904	U	-	INSERTION	GB 85674274

- Molecule 24 is a protein called 50S ribosomal protein L11.

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

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

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

- Molecule 26 is a protein called 50S ribosomal protein L3.

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

- Molecule 27 is a protein called 50S ribosomal protein L14.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

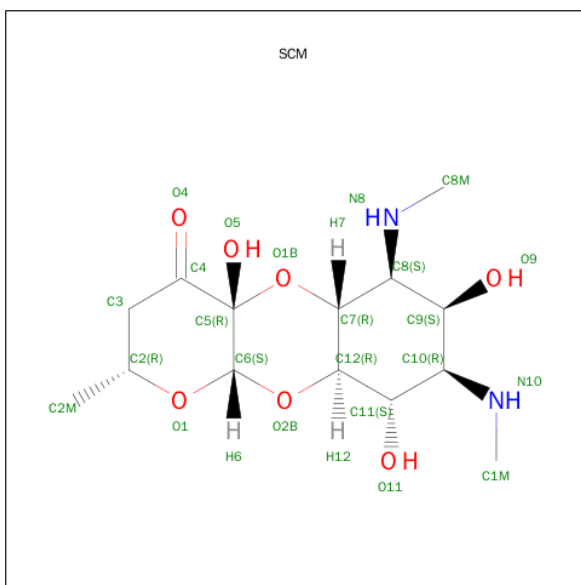
- Molecule 52 is a protein called 50S ribosomal protein L27.

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

- Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
53	BB	110	Total	Mg	0	0
			110	110		
53	CA	58	Total	Mg	0	0
			58	58		
53	AA	60	Total	Mg	0	0
			60	60		
53	CE	1	Total	Mg	0	0
			1	1		
53	DN	1	Total	Mg	0	0
			1	1		
53	DB	110	Total	Mg	0	0
			110	110		

- Molecule 54 is SPECTINOMYCIN (three-letter code: SCM) (formula: C₁₄H₂₄N₂O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
54	AA	1	Total	C	N	O	0	0
			23	14	2	7		
54	CA	1	Total	C	N	O	0	0
			23	14	2	7		

- Molecule 55 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 56 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AA	288	Total	O	0	0
			288	288		
56	AE	3	Total	O	0	0
			3	3		
56	AK	1	Total	O	0	0
			1	1		
56	AL	4	Total	O	0	0
			4	4		
56	AP	1	Total	O	0	0
			1	1		

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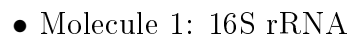
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AT	1	Total 1	O 1	0	0
56	AN	2	Total 2	O 2	0	0
56	BB	494	Total 494	O 494	0	0
56	BC	4	Total 4	O 4	0	0
56	BE	3	Total 3	O 3	0	0
56	BL	4	Total 4	O 4	0	0
56	BH	1	Total 1	O 1	0	0
56	BT	1	Total 1	O 1	0	0
56	CA	275	Total 275	O 275	0	0
56	CE	4	Total 4	O 4	0	0
56	CK	1	Total 1	O 1	0	0
56	CL	5	Total 5	O 5	0	0
56	CP	1	Total 1	O 1	0	0
56	CT	2	Total 2	O 2	0	0
56	CN	5	Total 5	O 5	0	0
56	DB	500	Total 500	O 500	0	0
56	DC	3	Total 3	O 3	0	0
56	DD	1	Total 1	O 1	0	0
56	DP	1	Total 1	O 1	0	0
56	DE	1	Total 1	O 1	0	0
56	DL	3	Total 3	O 3	0	0

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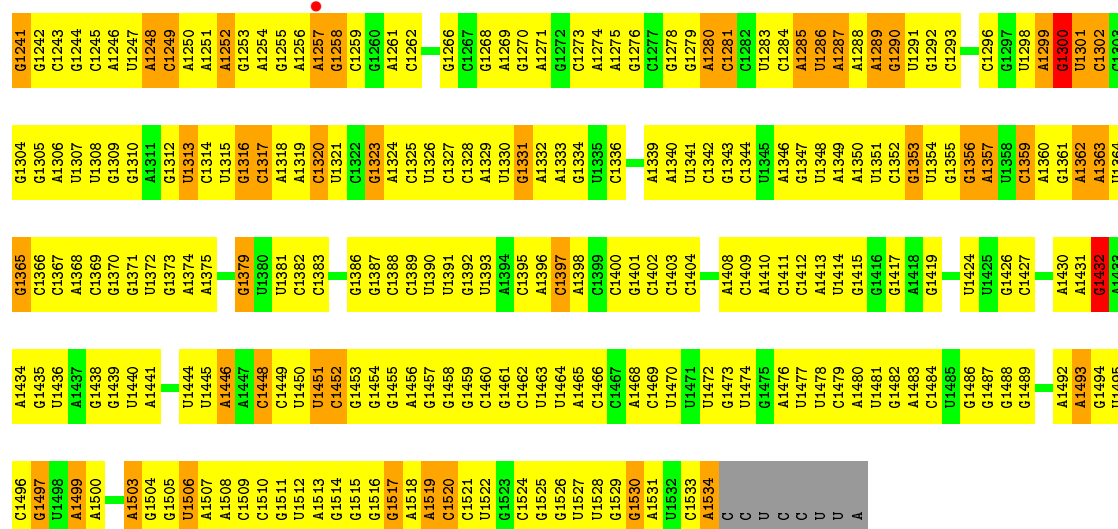
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	DJ	1	Total 1	O 1	0	0
56	DN	2	Total 2	O 2	0	0
56	DR	1	Total 1	O 1	0	0

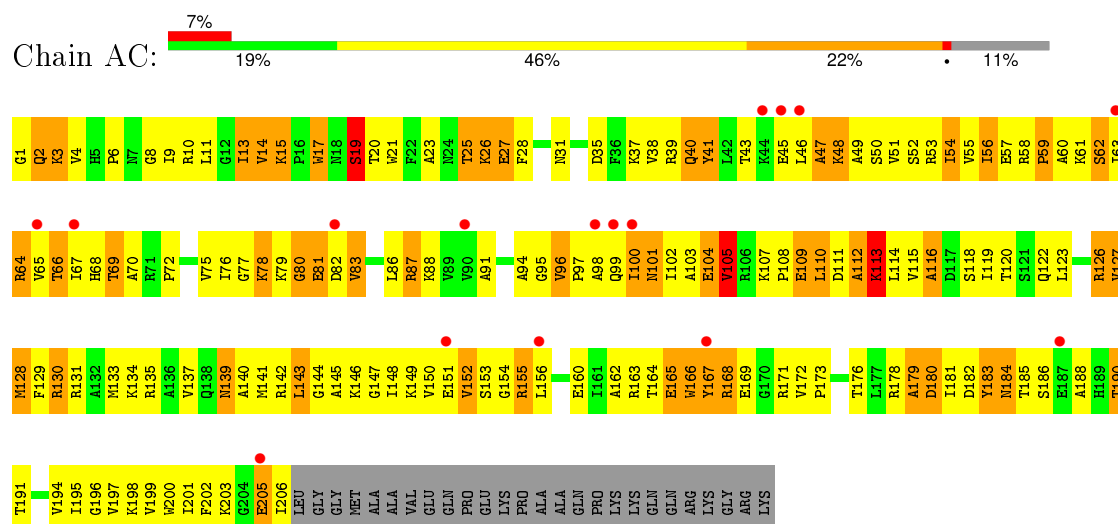


U133	A65	A
G134	A66	A
C135	C67	A
U136	G68	U
U137	G69	U5
G138	U70	G6
	A71	A7
A143	A72	A8
G144	C73	G9
G145	A74	A10
	G75	
G148	G76	U13
A149	A77	U14
U150	A78	G15
A151	G79	A16
A152	A80	U17
C153	A81	C18
U154	G82	A19
	C83	U20
U157	U84	G21
G158	U85	G22
G159	G86	C23
A160	C87	U24
A161	U88	C25
A162	U89	A26
C163	C90	G27
G164	U91	A28
	U92	
A167	U93	A32
G168	G94	A33
C169	C95	C34
		G35
A174	A98	C36
C175	C99	
C176	G100	G39
G177	A101	C40
C178	G102	G41
A179	U103	G42
U180	G104	C43
A181	G105	A44
A182	C106	G45
C183	G107	G46
G184	G108	C47
		C48
U185	G112	U49
C186	G113	A50
G187	U114	A51
C188	G115	C52
A189		A53
A190		C54
G191	A120	A55
A192	U121	U56
C193	G122	G57
C194	U123	C58
A195	C124	C59
A196	U125	A60
A197	G126	G61
G198		U62
	A130	C63
	U131	G64
	C132	
G201		

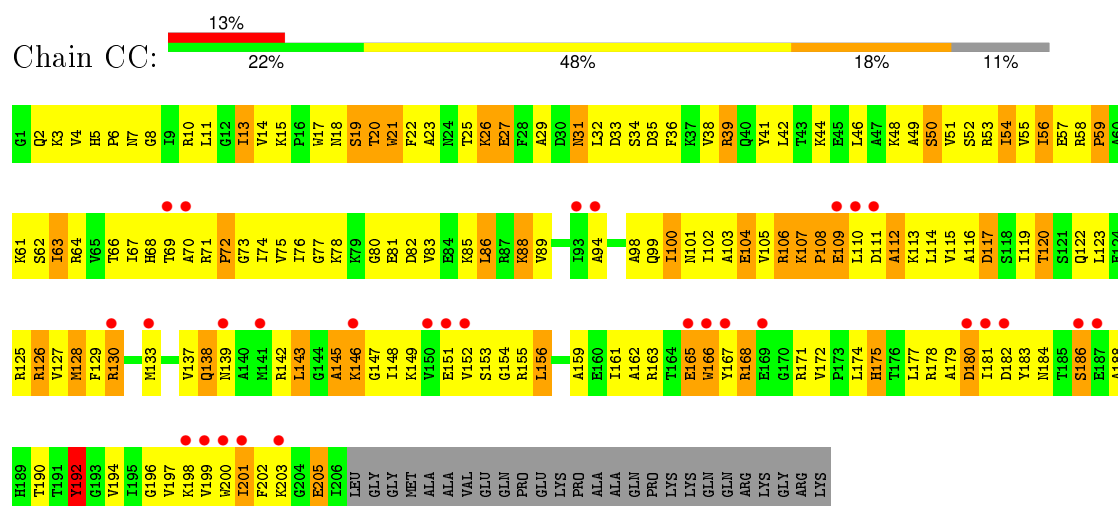
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A1176	C1112	U1049	U986	A923	G858	U793	G725	G661	U998	G538	C475	C403	A336	C267	G204
G1177	G1113	G1050	G987	C924	A859	A794		U662	C599	A539	C476	U405	A337	U268	A205
G1178	C1114	G1051	G988	C925	A860	C795	A728	A663	A600	G540	C477	U406	A338	C269	C206
A1179	U1115	U1052	U989	G926	G861	C796	A729	G664	G601	G541	A479	U407	C341	A270	U209
A1180	U1116	G1053	C990	G927	G862	C797	A730	A665	A602	G542	U480	U408	C342	C271	C210
G1181	A1117	C1054	U991	G928	U863	U798	G731	G666	U603	U543	U481	U409	C343	C272	G211
G1182	U1118	A1055	U992	G929	A864		G732	G667	G604	G544	A482	U410	U344	U273	G212
A1183	C1119	U1056	G993	C930	A865	G803	G733	G668	G606	G545	G483	U411	U345	A274	G213
G1184	U1121	G1058	A994	G931	C866	U804	G734		G607	A546	C484	A412	C346	G275	C214
	C995	G967	C995	C932	G867	U805	G735	U672	G608	A547	G485	A413	C347	A279	C215
G1190	U1122	C1059	A996	G933	C868	C806	G736	A673	A608	G548	U486	A414		C280	U216
G1191	U1060	U997	U997	C934	G869	A807	C737	G674	A609	C549	U487	A415	C352	G281	C217
C1192	G1124	G1061	A985	A985			C738	A675		G550				A282	U218
G1193	U1125	U1062	C936	C936	G874	C808	C739	A676	C612	U551	C488	U420	C353	U282	U219
	U1126	C1063	A937	A937	U875	G809	U740	A677	C613	U552	C489	U421	A354	U283	U218
A1196	G1127	G1064	A938	A938	C876	C810	G741	U678	G614	A553	C490	U422	C355	C284	G220
A1197	C1128	U1065	G939	G939	G877	C811		C679	G615	A554	C491	U423	C356	C285	C221
G1198	U1066	C1066	C940	C940	A878	G812	G745	C680	G616	U555	C492	G423		C286	C222
U1199	C1129	A1004	G941	G941	A879	U813	A746	A681	G617	C556	A493	G424	G361	U287	A223
	C1132	G1068	G942	G942	C880	A814	A747	G682	C618	C557	G494	G425	G362	U288	U224
A1201	G1133	C1069	A946	A946	G881	A815	G748	U683	U619	G558	A495	U426	A363	G289	C225
U1202	G1134	U1070	G882	G882	C882	A816	A749	U684	C620	A559	A496	U427	A364		G226
C1203	U1135	C1071	G947	G947	C883	C817	C750	G685	A621	U560				G292	
	C1136	G1072	C948	C948	U884	G818		U686	A622	A561	U499	U429	A366		U228
G1206	G1137	U1073	A949	A949	G885	A819	A753	A687	G623	U562	A430	U430	U367	C295	G230
G1207	U1138	G1074	U950	U950		U820	G754	G688	U625	A563	A431	U431	U368	U296	U231
C1208	G1139	U1075	G951	G951	A889	G821	G755			A564	A432	U432	C369	C297	G232
C1209	C1140	A1014	U952	U952	G890	U822		G691	U632	U570	A502	U433	C370	A298	G233
C1210	U1141	G1015	G953	G953	U891	C823	U757	U692	G634	A572	C504	U434	A371	C299	C234
U1211	G1142	G1079	G954	G954	A892	G824	G758	G693	A629	G567	A435	U435	C372	A300	C235
	G1143	A1080	U955	U955	C893	A825		A694	A630	C568		C436	A373	G301	A236
A1212	A1144	A1081	U956	U956	G894	C826	G761	A695	C631	C569	A509	U437	A374	G302	G237
C1214	A1145	A1082	U957	U957	G895	U827	U762	A696	U632	U571	A510	U438	A303	A303	G238
G1215	A1146	U1083	A958	A958	C896	U828	G763	U697	G633	G570	C511	U439	U375	U304	U239
A1216	G1147	G1084	A959	A959	C897	G829	C764	G698	C534	A573	U512		G377	G305	G240
G1217	U1148	U1085	U960	U960	G898		G765	C699	A635	A573	C513	U440	C378	A306	G241
U1218	C1149	U1086	U961	U961	G899	G832	A766	G700	U636	A574	C514	G449	C379	C307	G242
A1219	A1150	G1087	G962	G962	A900	G833	U767	U701	C537	C575	G515	G450	G380	C308	A243
G1220	A1151	G1088	G963	G963	A901	U834	A768	A702	U638	C576	U516	A451	C381	A309	U244
G1221		G1089	A964	A964	G902	U835	G769	G703	G639	G577	C517	A452	A382	G310	U245
G1222	A1155	U1090	U965	U965	G903	G836	C770	A704	A640	C578	C518	G453	A383	C311	G246
U1224	G1156	G966	G966	G966	U904	U837	G771	G705	U641	A579	C519	G454	A384	C312	G247
	A1157	U1091	C967	C967	U905	G838	U772	A706	A642	C580	C520	G455	A385	A313	
A1225	C1158	G1094	A968	A968	A906	C839	G773	U707	C643	G581	C522	A456	C386	C314	A250
C1226	U1159	U1095	A969	A969	A907	C840		G708	U644	C582	C523	G457	U387	A315	G251
A1227	G1160	C1096	C970	C970	A908	C841	G776	U709	G645	A583	A524	A461	C388	A316	U252
C1228		C1097	G971	G971	A909	U842	A777	G710	G646	G584	C525	U462	A389	U317	A253
A1229	A1163	C1098	C972	C972	C910	U843	G778	G711	C647	G585	C526	U463	G318	G318	G254
C1230	G1164	G1099	G973	G973	U911	G844	C779	A712	A648	C586	C527	U464	C391		G255
G1231	U1165	C1100	A974	A974	C912	A845	A780	G713	A649	G587	G528	U465	C392	A321	U256
U1232	G1166	A1101	A975	A975	A913	G846	A781	G714	G650	U589	C529	A466	A393	C322	G257
G1233	A1167	A1102	G976	G976	A914	G847	A782	A715	C651	U590	G530	U467	C394	C328	G258
C1234	U1168	C1103	U1040	U1040	A915	C848	G783	A716	U652	U591	G531	U468	C395	A329	G259
U1235	A1169	G1104	A977	A977	U916		A784		U653	U591	U531	A468	C396	A330	G260
A1236	C1170	G1105	A978	A978	U917	G851	G785	C719	G592	G592	A532	C469	A397	C330	U261
C1237	A1171	C979	C979	C979	G917	G852		G720	U593	U593	A533	C470	U398	G331	A262
A1238	U1172	G1108	U981	U981	A918	G853	A789	G721	U594	U594	U534	U471	C399	G332	A263
	G1173	C1109			U920	U854	U790	A790	C658	A590	A535	U472	C400	U333	C264
U1240	G1174	A1110	C984	C984	U921		G791	U723	U659	A596	C536	U473	C401	C334	G265



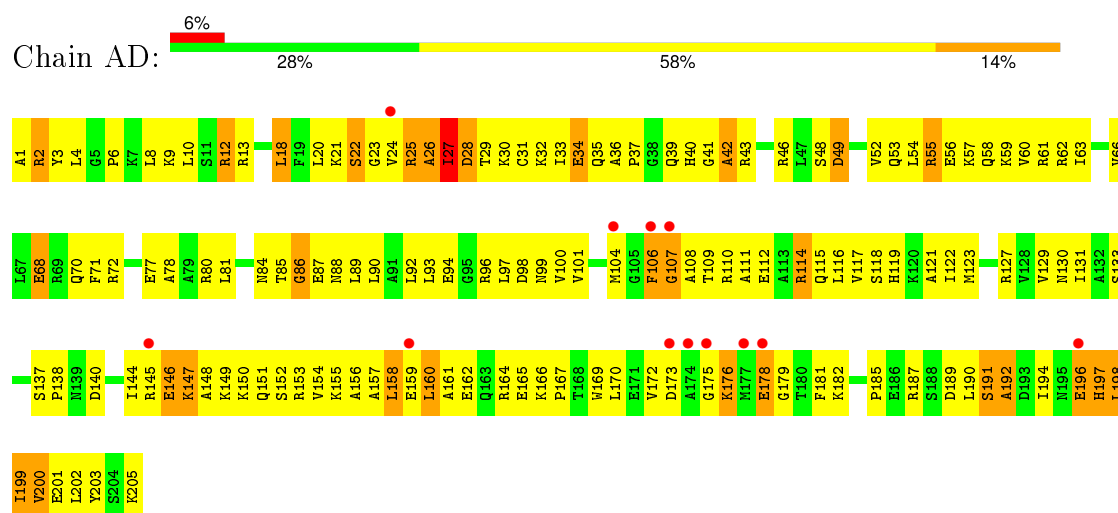
• Molecule 2: 30S ribosomal protein S3



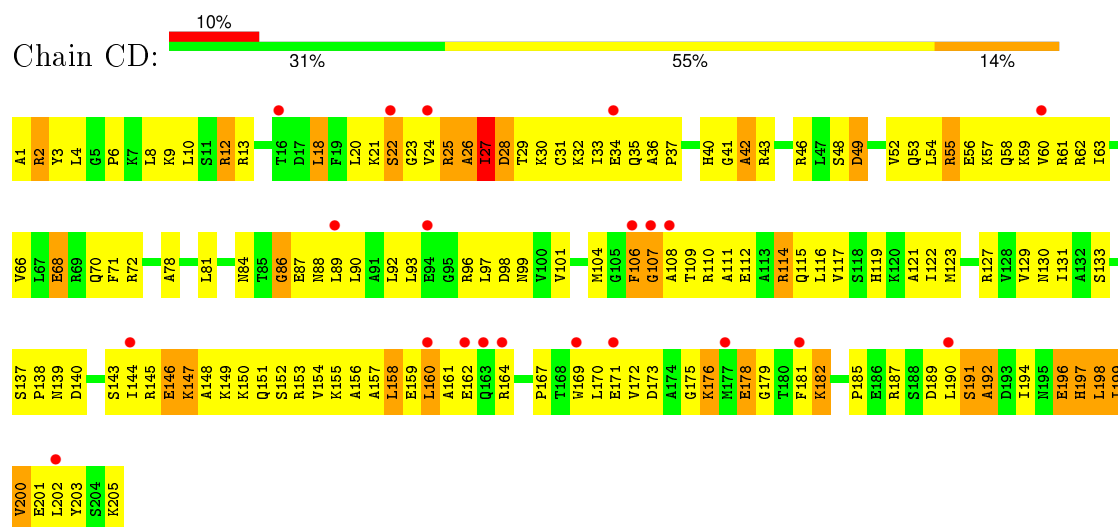
• Molecule 2: 30S ribosomal protein S3



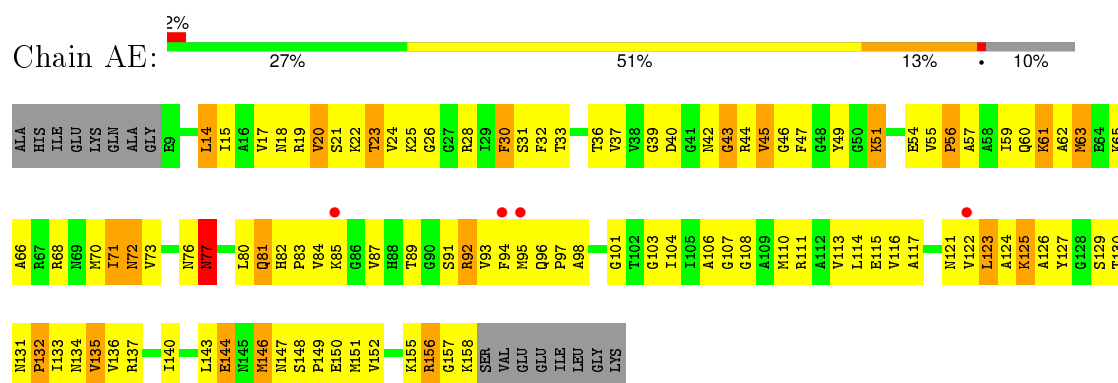
• Molecule 3: 30S ribosomal protein S4



• Molecule 3: 30S ribosomal protein S4

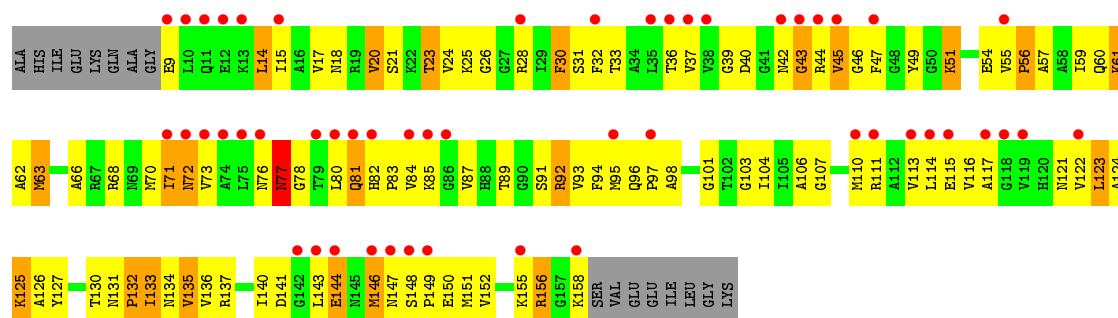


• Molecule 4: 30S ribosomal protein S5

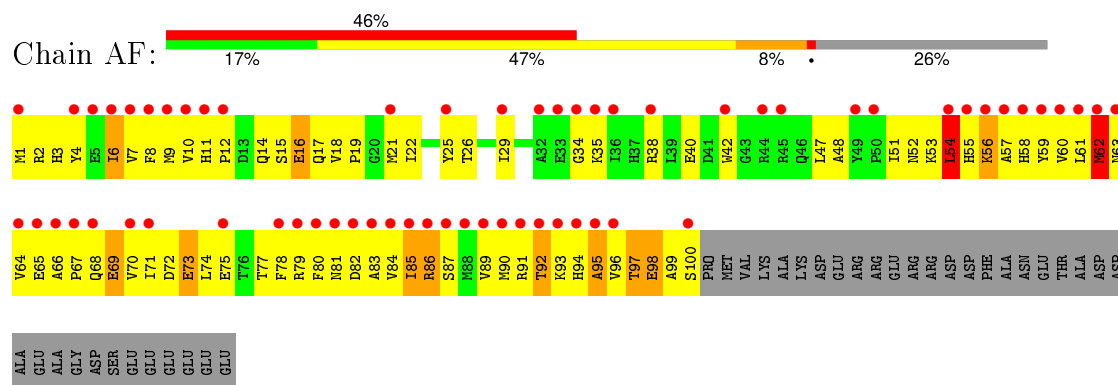


• Molecule 4: 30S ribosomal protein S5

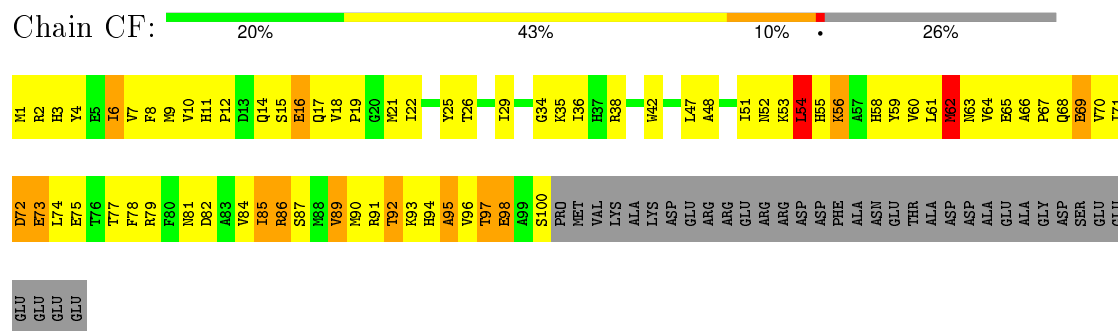




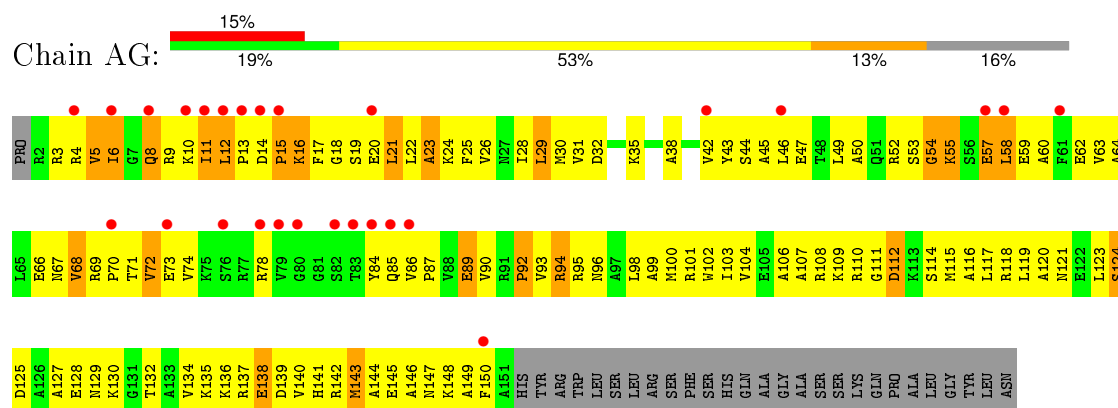
• Molecule 5: 30S ribosomal protein S6



• Molecule 5: 30S ribosomal protein S6

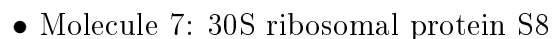


• Molecule 6: 30S ribosomal protein S7

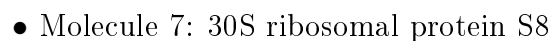


• Molecule 6: 30S ribosomal protein S7

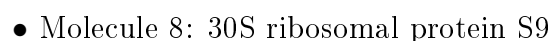
Category	Percentage
Very bad	22%
Bad	47%
Good	16%
Very good	15%



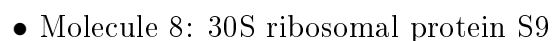
Frequency	Percentage
Daily	12%
Often	40%
Sometimes	53%
Never	8%



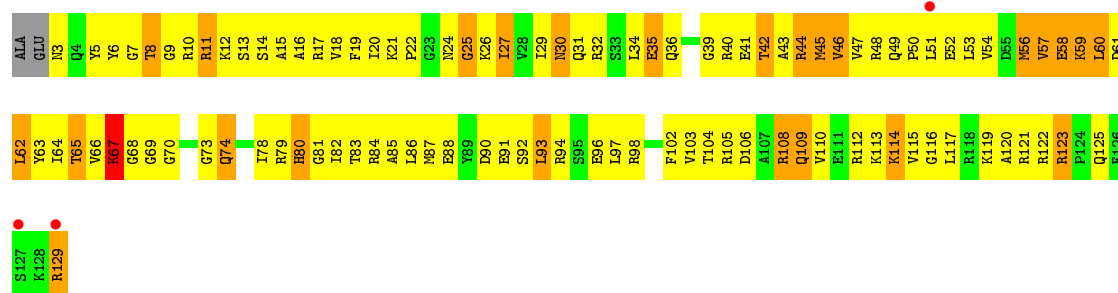
Frequency	Percentage
Daily	21%
Often	39%
Sometimes	53%
Never	8%



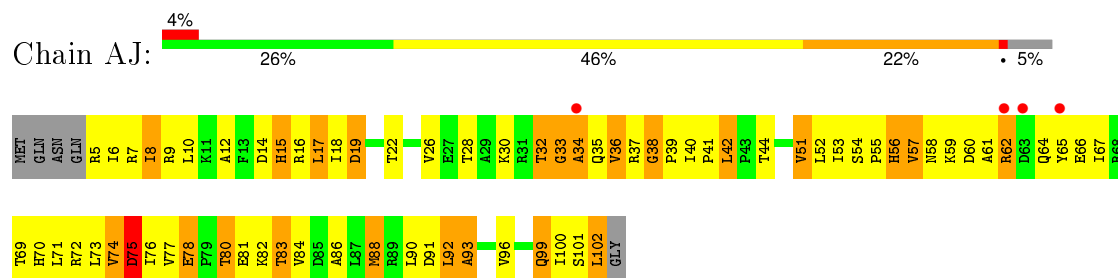
Response	Percentage
Yes	19%
No	10%
Don't know	64%
Other	23%



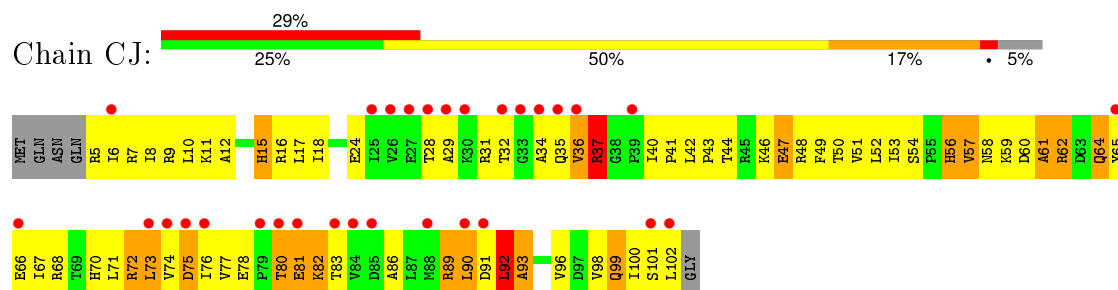
Frequency	Percentage
Never	2%
Almost never	19%
Often	60%
Very often	19%
Other	...



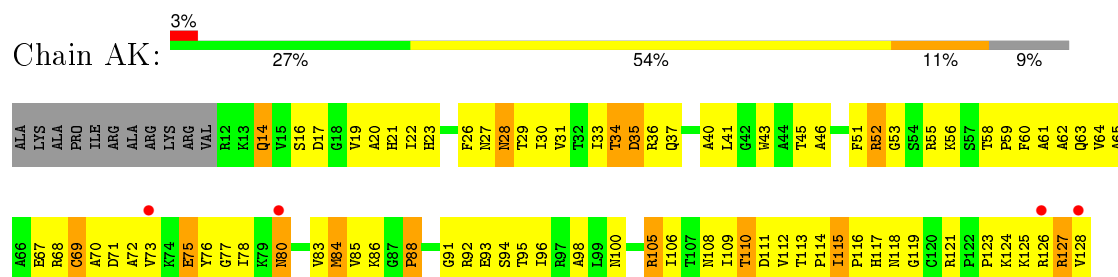
- Molecule 9: 30S ribosomal protein S10



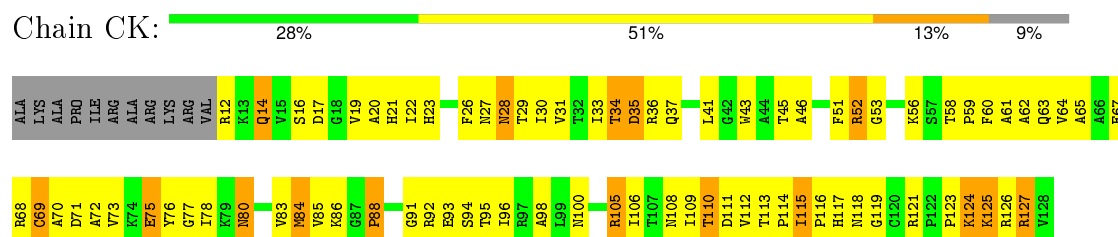
- Molecule 9: 30S ribosomal protein S10



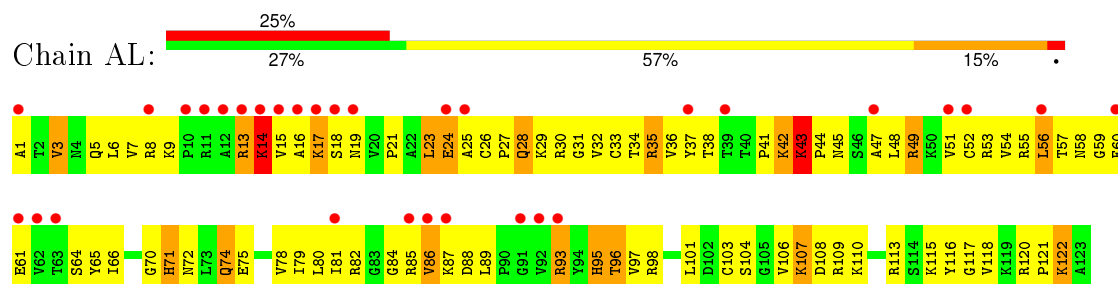
- Molecule 10: 30S ribosomal protein S11



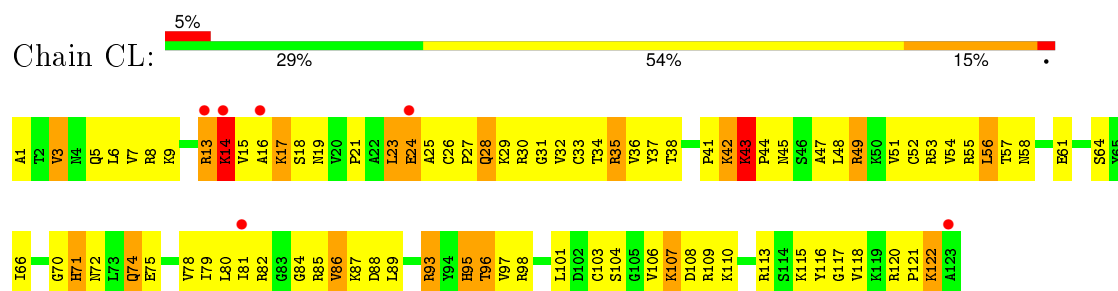
- Molecule 10: 30S ribosomal protein S11



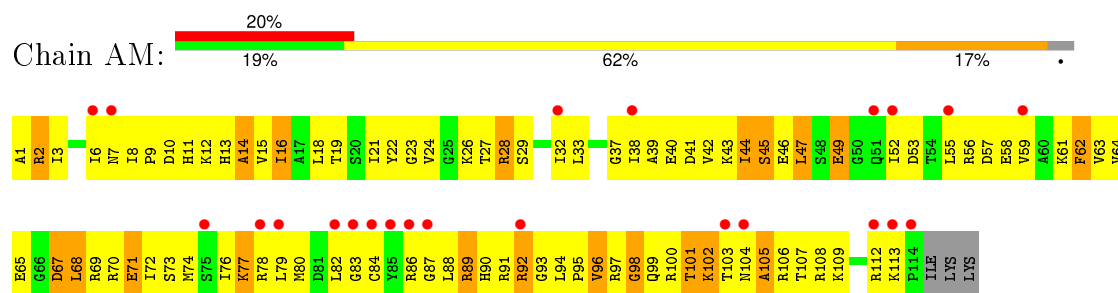
- Molecule 11: 30S ribosomal protein S12



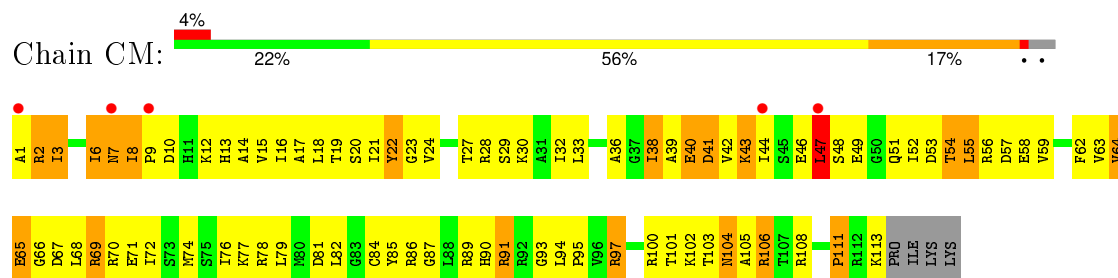
- Molecule 11: 30S ribosomal protein S12



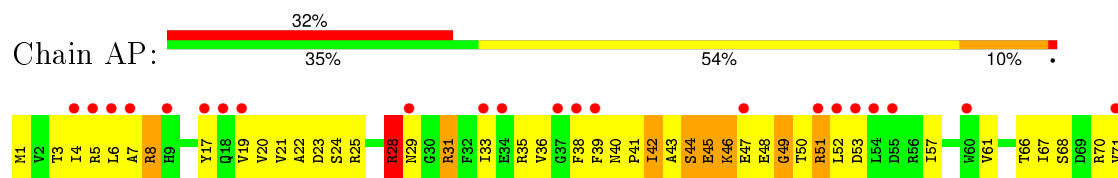
- Molecule 12: 30S ribosomal protein S13

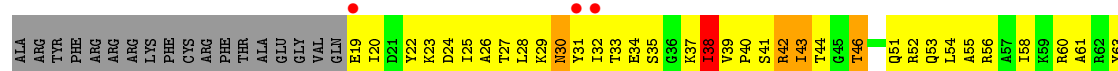


- Molecule 12: 30S ribosomal protein S13



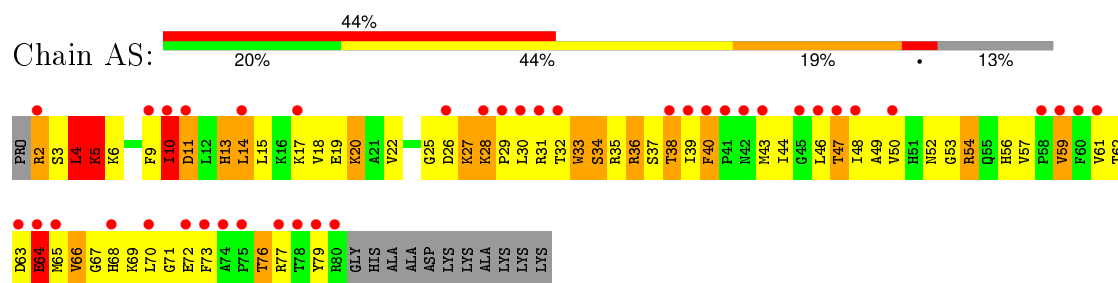
- Molecule 13: 30S ribosomal protein S16



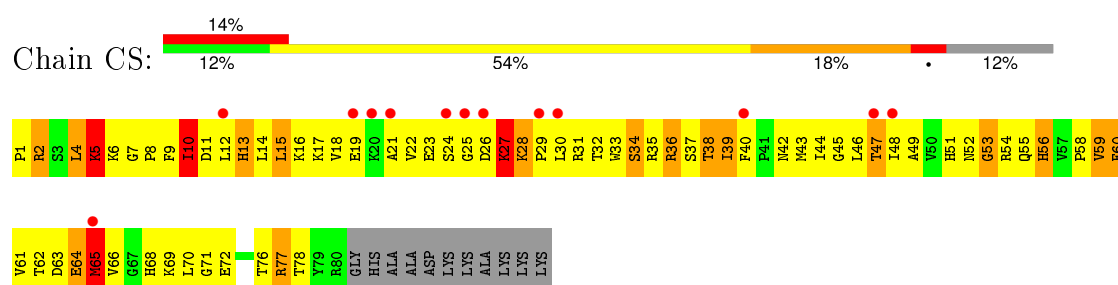




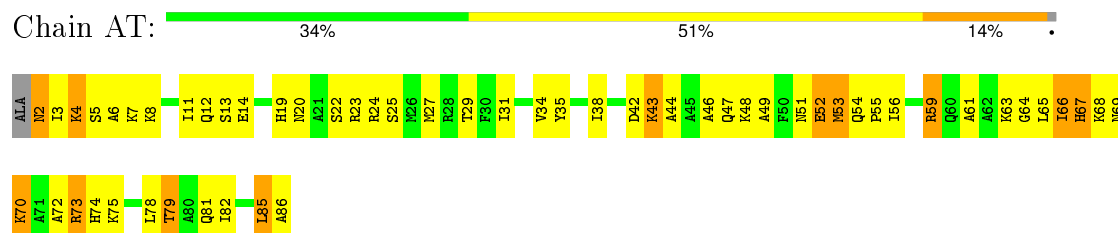
- Molecule 16: 30S ribosomal protein S19



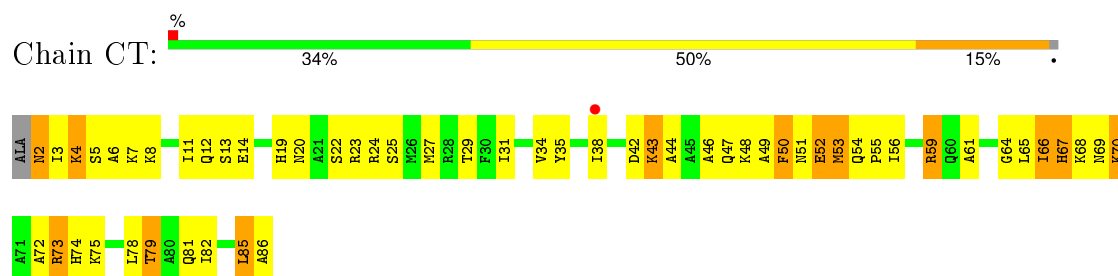
- Molecule 16: 30S ribosomal protein S19



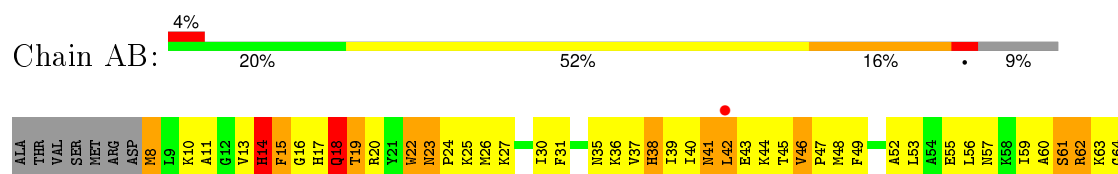
- Molecule 17: 30S ribosomal protein S20



- Molecule 17: 30S ribosomal protein S20



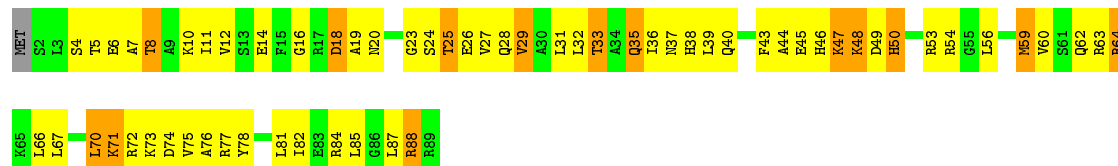
- Molecule 18: 30S ribosomal protein S2





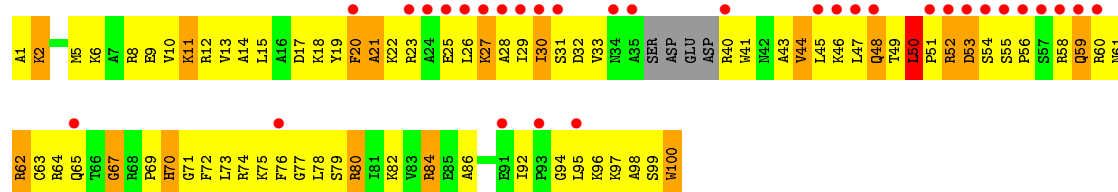
- Molecule 20: 30S ribosomal protein S15

Chain CO: 29% 54% 16%



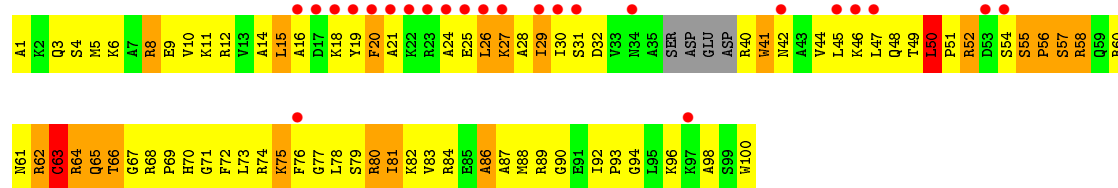
- Molecule 21: 30S ribosomal protein S14

Chain AN: 20% 32% 58% 17%



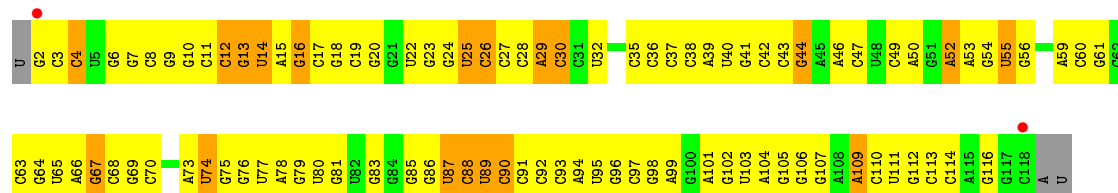
- Molecule 21: 30S ribosomal protein S14

Chain CN: 17% 24% 57% 20%



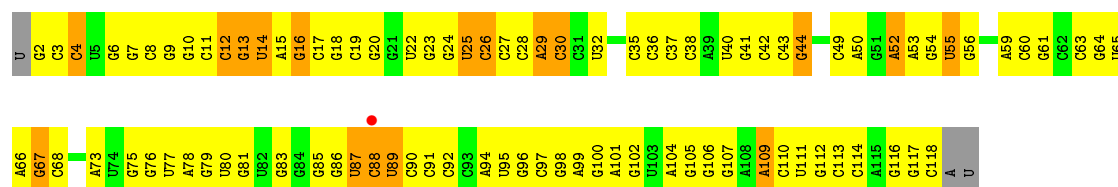
- Molecule 22: 5S rRNA

Chain BA: 2% 17% 65% 16%

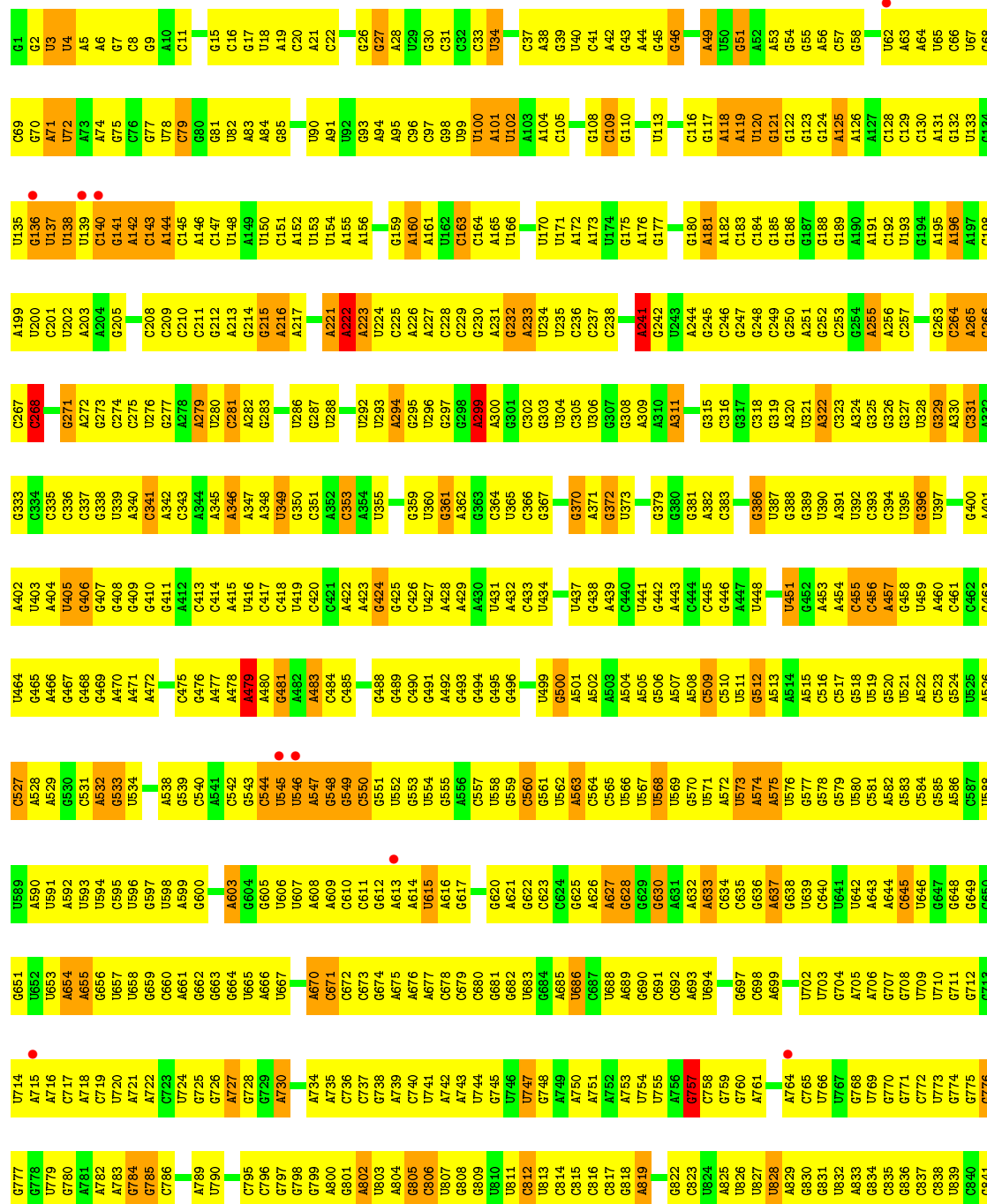


- Molecule 22: 5S rRNA

Chain DA: 21% 63% 14%



Molecule 23: 23S rRNA



C1748	C1749	U1683	A1618	A1551	U1485	G1423	A1359	G1292	G1228	U1159	A1096	U1032	C968	U942
G1686	G1685	G1684	G1619	A1552	U1486	G1424	G1360	C1293	C1229	G1160	U1097	U1033	G969	G843
U1750	C1686	C1685	G1623	A1553	U1487	G1425	G1361	U1294	U1230	G1163	G1099	G1034	G970	A844
G1752	G1687	G1688	U1624	U1554	C1488	G1426	C1362	G1296	U1231	C1164	C1109	U1035	G971	A845
G1753	G1688	A1689	C1625	G1558	C1489	C1427	A1365	C1297	U1234	A1165	U1101	G1037	A973	U847
A1754	U1689	A1690	A1626	U1559	G1490	G1428	A1366	G1300	G1235	G1166	C1102	G1038	G974	C848
G1756	C1691	C1493	U1629	U1560	C1493	G1429	G1367	A1301	G1236	G1167	C1103	A1039	A975	A849
A1757	A1692	A1495	A1630	U1561	A1494	A1430	G1368	A1302	A1237	G1170	U1105	A1040	U912	U850
U1758	U1693	A1496	A1631	U1562	A1495	A1431	G1369	A1302	G1238	C1171	G1106	G1041	G914	C851
G1694	G1694	G1501	A1632	U1564	A1496	A1432	G1370	C1306	G1239	G1172	C1107	G1042	C915	U852
C1760	C1695	A1502	A1633	C1565	G1501	A1434	G1371	A1307	U1240	U1173	U1108	C1043	A916	C853
C1761	A1634	A1502	A1634	U1566	A1502	G1435	U1372	U1241	U1241	U1174	A1046	C1044	A917	C854
A1762	A1695	A1503	A1635	U1567	A1503	G1436	A1373	U1242	U1242	U1175	C1109	G1045	A918	G855
G1763	U1696	A1504	U1636	U1568	A1504	C1437	G1374	G1309	C1243	A1176	G1110	A1046	U919	G856
C1765	A1637	A1505	A1637	U1569	A1505	A1439	U1375	G1310	G1245	U1177	G1112	G1047	A920	G857
U1766	C1638	A1506	C1638	A1570	U1506	U1440	U1379	U1312	U1255	C1178	A1050	A1050	C922	G858
A1705	A1507	C1507	C1639	A1571	C1507	G1441	G1380	U1313	U1256	U1179	G1115	G1051	G923	U860
C1706	A1640	A1572	A1641	U1573	A1508	U1442	G1381	U1314	U1249	U1180	G1116	C1052	G924	A861
G1768	A1641	U1573	A1641	U1573	A1509	U1443	G1382	C1315	U1250	U1181	G1117	C1053	A925	G862
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A1772	U1647	C1577	U1647	U1578	A1514	C1447	A1387	U1325	U1260	G1192	G1128	G1063	C935	G874
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U1775	A1650	G1581	A1650	U1581	C1518	G1450	G1389	A1328	U1263	G1195	U1131	U1066	G938	A877
C1776	G1651	G1651	G1651	U1582	A1520	A1453	U1390	G1329	U1263	C1196	A1067	C1006	G939	A878
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U1778	G1653	C1585	G1653	U1584	A1522	U1457	A1393	U1327	U1267	U1198	A1136	C1007	A941	G
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U1780	U1655	C1586	U1655	C1586	A1524	U1459	U1397	U1330	U1269	C1200	G1136	G1071	A943	G
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A1785	G1659	A1590	G1659	A1590	G1527	C1463	C1403	G1338	U1273	A1206	U1141	U1078	A947	U
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C1790	U1662	A1593	U1662	A1593	A1530	G1466	U1406	G1344	U1276	C1211	G1144	A1086	G956	U
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G1792	A1664	C1595	A1664	C1595	A1533	U1468	G1408	G1346	G1280	C1219	C1150	A1088	U958	A
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G1797	U1669	C1600	U1669	C1600	G1537	U1473	U1415	U1349	G1285	C1219	C1150	A1086	G1023	U
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G1799	U1671	U1602	U1671	U1602	U1539	U1475	U1417	C1351	U1287	C1221	C1152	A1088	G1025	C
C1800	A1672	A1603	A1672	A1603	G1540	U1476	U1418	A1352	U1288	U1222	C1153	A1089	G1026	A960
A1801	G1673	G1673	G1673	G1673	C1541	U1477	U1419	A1354	G1289	C1225	G1154	A1090	G1027	C861
A1802	U1674	C1607	U1674	C1607	U1542	U1478	U1420	U1355	U1290	G1157	C1158	A1091	A1028	G962
A1803	A1675	A1608	A1675	A1608	U1543	U1479	U1421	G1356	C1291	A1226	C1159	A1092	A1029	U963
C1804	C1676	A1609	C1676	A1609	A1544	G1479	G1416	C1357	U1291	C1227	G1158	A1095	G1031	C903
A1805	A1677	A1610	A1677	A1610	A1545	U1480	U1418	A1358	G1288	G1225	C1159	A1096	G1030	C901
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A1808	U1680	A1681	U1680	A1681	A1549	G1483	A1420	G1356	C1291	G1227	C1158	A1095	G1031	C903
U1809	A1745	A1616	A1745	A1616	A1549	U1484	G1422	G1356	C1291	G1227	C1158	A1095	G1031	C903
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G2865	C2736	U2742	U2662	U2594	U2528	A2458	U2393	U2329	U2262	C	U2135	C2070	A1999	A1938	A1872
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C2876	U2747	U2753	U2673	U2605	U2539	A2469	U2404	U2340	U2273	C	U2146	C2081	C2001		
G2877	A2748	U2754	U2674	U2606	U2540	A2470	U2405	U2341	U2274	C	U2147	C2082	C2001		
U2878	G2749	U2755	U2675	U2607	U2541	A2471	U2406	U2342	U2275	C	U2148	C2083	C2001		
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G2881	G2752	U2758	U2678	U2610	U2544	A2474	U2409	U2345	U2278	C	U2151	C2086	C2001		
U2882	U2753	U2759	U2679	U2611	U2545	A2475	U2410	U2346	U2279	C	U2152	C2087	C2001		
C2883	A2754	U2760	U2680	U2612	U2546	A2476	U2411	U2347	U2280	C	U2153	C2088	C2001		
U2884	G2755	U2761	U2681	U2613	U2547	A2477	U2412	U2348	U2281	C	U2154	C2089	C2001		
G2885	U2756	U2762	U2682	U2614	U2548	A2478	U2413	U2349	U2282	C	U2155	C2090	C2001		
C2886	A2757	U2763	U2683	U2615	U2549	A2479	U2414	U2350	U2283	C	U2156	C2091	C2001		
U2887	G2758	U2764	U2684	U2616	U2550	A2480	U2415	U2351	U2284	C	U2157	C2092	C2001		
G2888	U2759	U2765	U2685	U2617	U2551	A2481	U2416	U2352	U2285	C	U2158	C2093	C2001		
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C2877
U2878
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C2880
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• Molecule 23: 23S rRNA

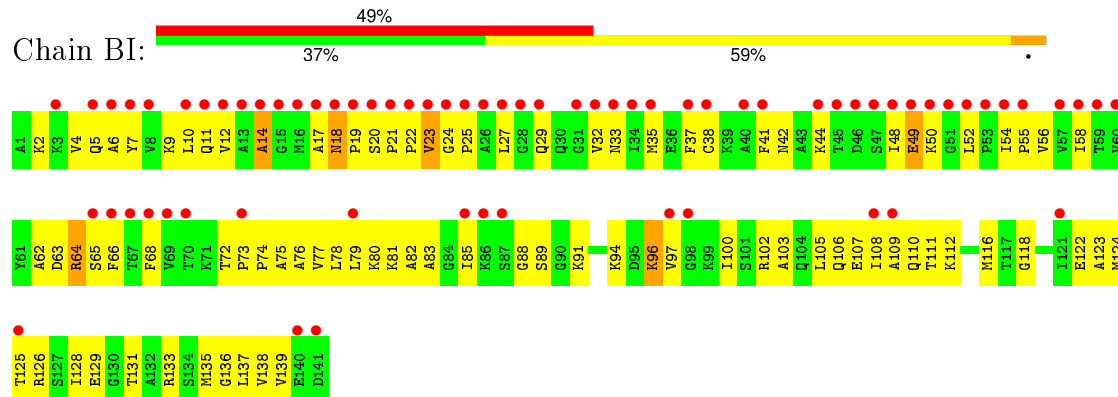
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U842	G777	A716	A654	U589	A466	C334	U202	G136	C69	U3
G843	G778	G717	A655	A590	G467	C335	G273	U137	G70	U4
U844	U779	A718	G556	U591	G468	C336	A204	U138	A71	A5
G845	G780	C719	U857	A592	G469	C337	G205	U139	U72	A6
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U847	A782	A721	G659	U594	A471	U339	C209	G141	A74	C8
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G784	G784	G723	A661	U596		G341	C210	C143	G76	A10
G785	U724	U725	G662	G597	C475	A342	C211	A144	G77	C11
U850	G786	G726	G663	U598	G476	C343	C212	G145	U78	
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C853	U790	G728	A666		A479	C414	G283	G215	G81	C16
C854	G791	G729	U667	A603	A480	A415	G285	A216	U82	G17
G855		A730		G603	U481	U416	U286	A217	A83	U18
G856	U794	G731	A670	U607	A482	C417	G287		A84	A19
G857	G795	C732	C671	A608	U545	C418	U288	A221	G85	C20
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G859	G797	A734	G673	C610	C484	C353	U290	A223	U90	C22
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G861	G799	G736	A675	G612	C486	U355	U292	C225	U92	
G862	A800	C737	A676	C550		G356	U293	A226	G93	G26
G863	G801	A743	A677	C551	G489	C424	U295	A227	A94	G27
G864	A802	G738	C678	A614	C490	C426	G295	C228	A161	A28
C865	U803	A740	C679	U615	G491	U427	U296	U162	U162	U29
A866	A804	C739	C679	A616	A492	A428	U360	C163	G96	G30
	G805	A741	C680	G820	G493	A428	U360	G297	C97	C31
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C873	G809	G745	C684	C623		A432	C364	U234	A101	U34
G874	U810	U746	A685	C624	U499	C433	U365	U235	U102	
U811	G825	U747	U686	G625	C560	U434	G366	C236	A103	A38
U812	U811	G748	C687	A626	A501	U437	G367	U304	A104	G39
G876	C812	A749	U688	A627	A502	U437	A368	C305	C105	U40
U877	U813	A750	A689	G628	A503	G438	U369	U306	G106	C41
G878	A878	A751	G690	G629	A504	A439	A371	G307	G107	C41
G	G	C815	C691	G630	A505	C440	A371	G308	G108	A42
G	C816	A753	C692	A631	A506	U441	G372	A309	G109	G43
G	C817	U754	C692	A632	U567	G442	U373	G177	G110	A44
G	C818	U755	G693	A633	A508	A443	U373	G178	A111	G45
G	A819	G	U694	A634	A508	A443		C246	A112	
U	G756	C	G695	C634	C509	C444	G379	G247		G46
U	G757	C	G696	C635	C510	C445	G380	G248	G180	
C	G758	C	G697	U570	C510	C446	G381	C249	A182	A49
A	C823	C	C698	A636	U571	G446	A382	G250	C183	U50
U	U824	U	A699	A572	A512	U447	C382	A251	C184	G51
C	A825	C		G638	A513	U448	C383	G252	G185	A52
C				U639	A574			C253	A113	
C	U702			C640	A575	U451	G386	A119	G186	A53
C	G703			U641	A576	G452	U387	U120		G54
C	G704			U642	C517	A453	G388	G121	G189	G55
A	A705			A643	C517	A454	A322	G122	G190	A56
C	A706			A644	U519	C455	C323	G123	A191	C57
U	G707			C845	C520	C456	A324	G124	G192	G58
C	G708			U646	U580	A457	G325		C192	
A	U709			C647	C581	A458	G326		U193	
C	G710			G648	A582	C459	G327	A125	G194	U62
C	G711			G649	C523	C394	A328	A126	G194	A63
C	C772			U650	C584	U395	G329	A127	A195	A64
C	U773			C650	U525	C461	G330	G132	G196	U65
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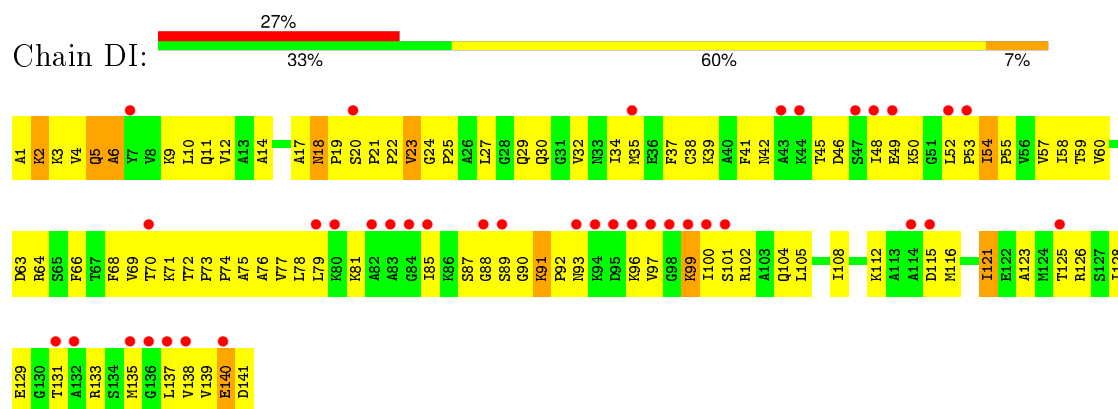
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G1828	A1705	A1705	A1637	A1570	U1506	G1442	G1381	U1316	U1249	G1179	U1114	G1043		U913
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	C1795	G1732	G1666	A1598	A1535	A1469	U1409	C1345	G1279	G1212	C1146		C1007	G942
	U1796	G1733		U1599	C1536	A1470	U1410	G1346	G1280	A1213	A1147	A1080	A1008	A943
	G1797	A1734	A1669	G1600	G1537	G1471	U1411	A1347	G1281	G1214	U1148	U1081	A1009	G944
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	A1801	G1738	G1673	G1603	C1541	G1475	U1415	C1351	A1285	G1220	C1152	A1085	C1013	C948
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WORLDWIDE
PDB
PROTEIN DATA BANK

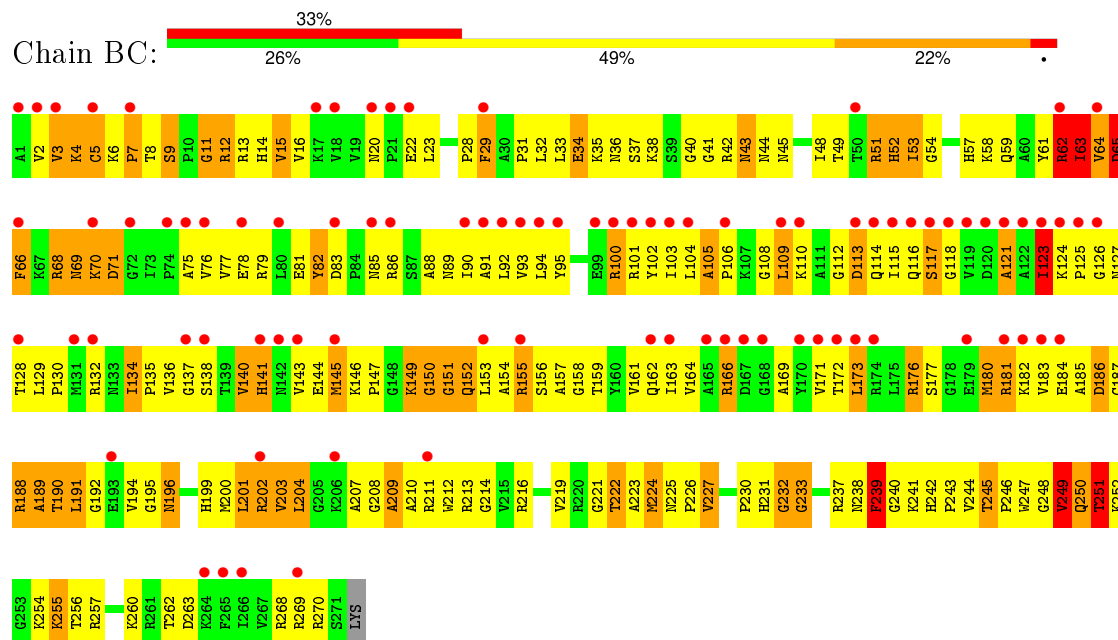
- Molecule 24: 50S ribosomal protein L11



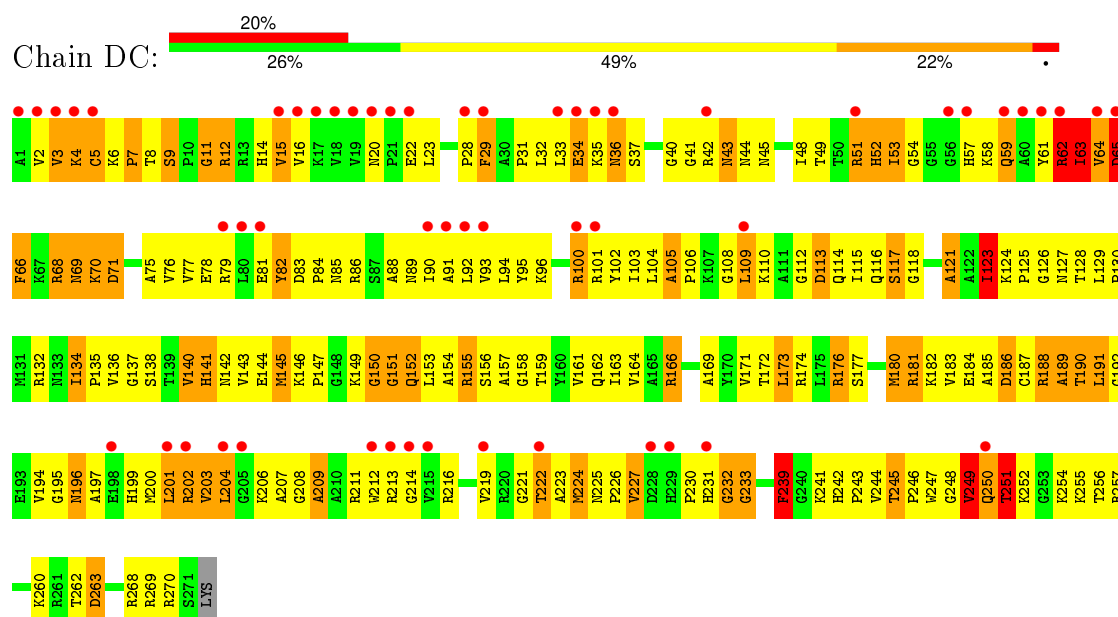
- Molecule 24: 50S ribosomal protein L11



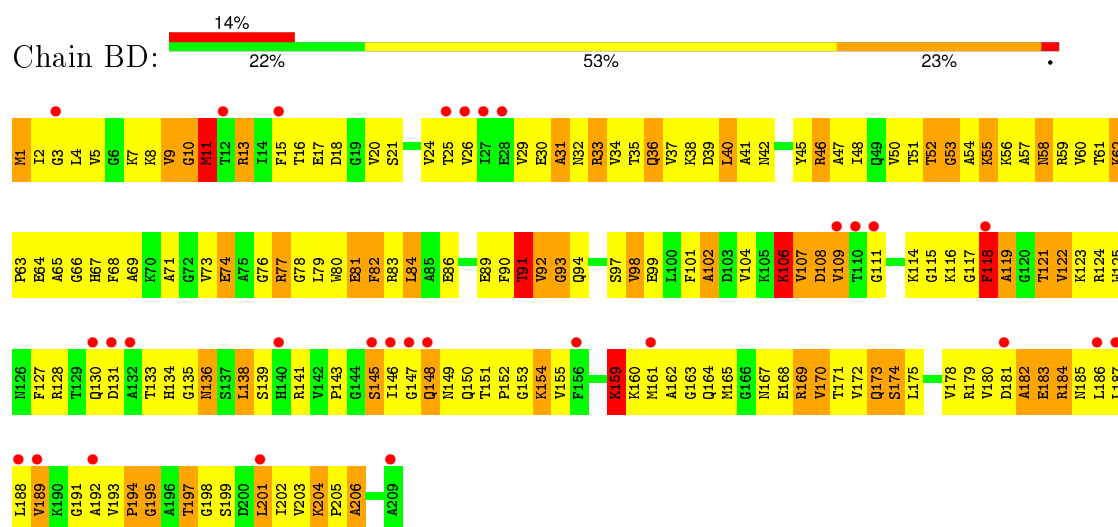
- Molecule 25: 50S ribosomal protein L2



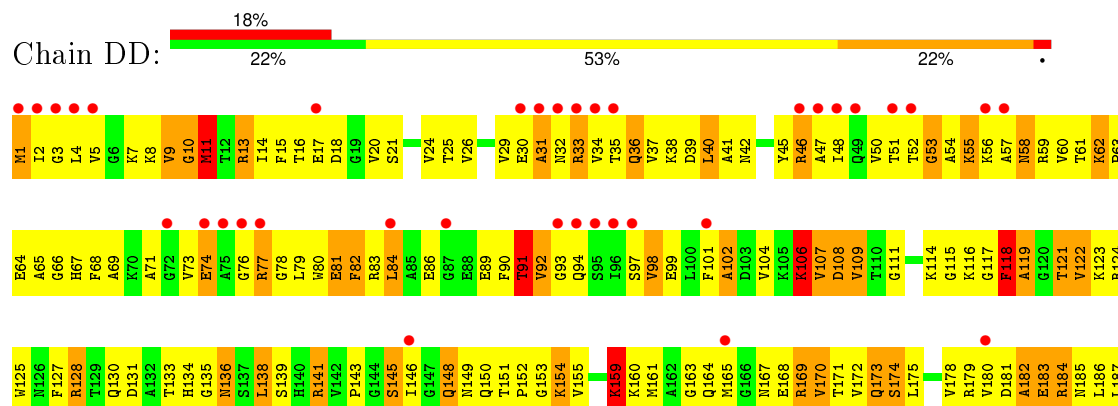
- Molecule 25: 50S ribosomal protein L2

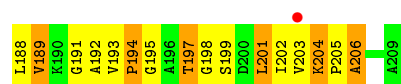


• Molecule 26: 50S ribosomal protein L3

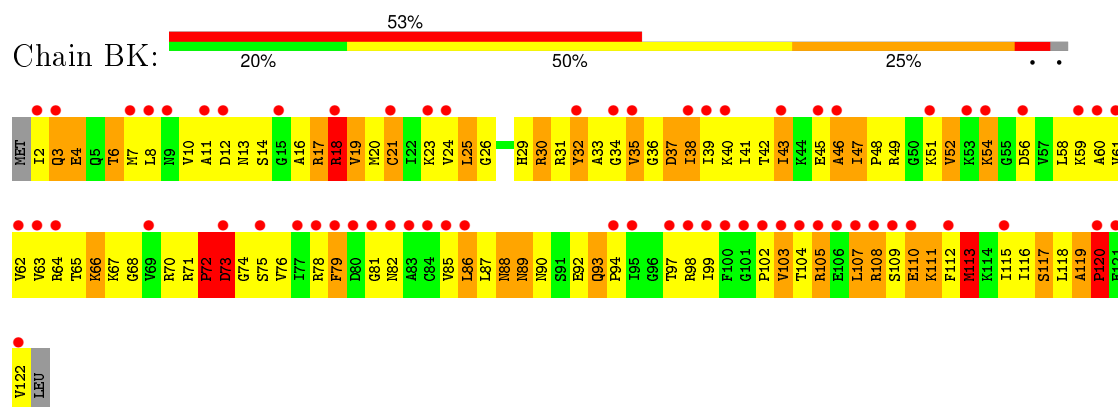


• Molecule 26: 50S ribosomal protein L3

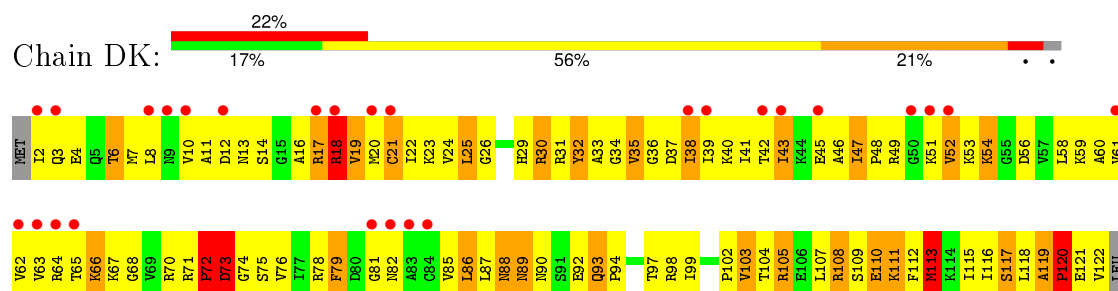




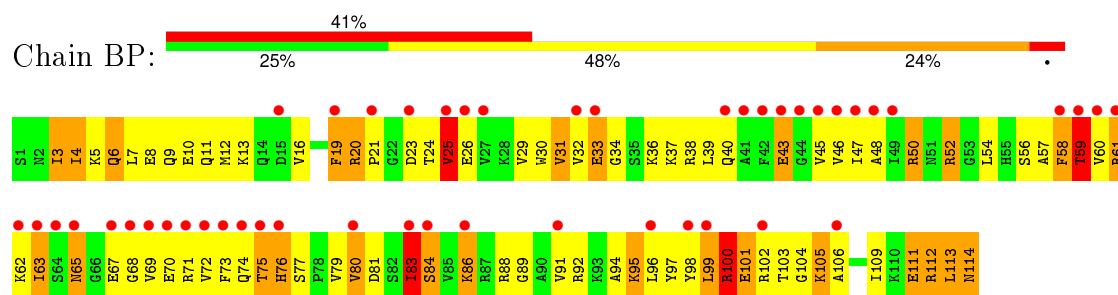
- Molecule 27: 50S ribosomal protein L14



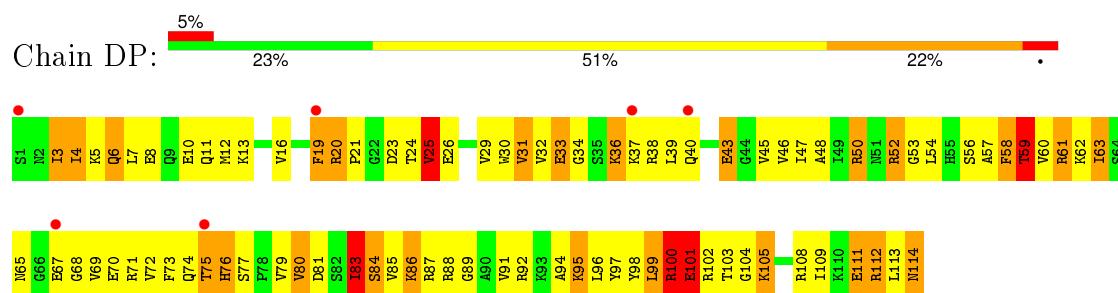
- Molecule 27: 50S ribosomal protein L14



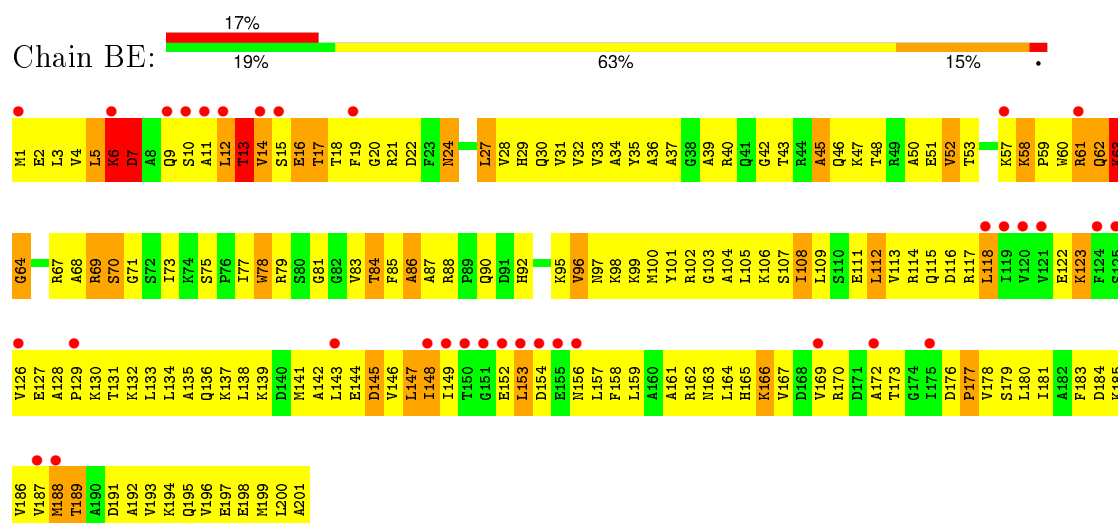
- Molecule 28: 50S ribosomal protein L19



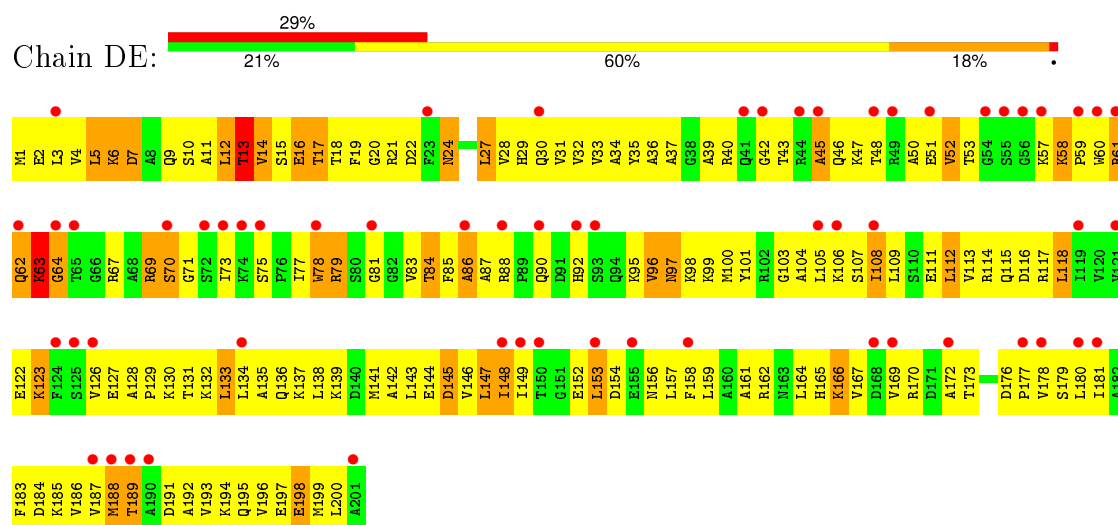
- Molecule 28: 50S ribosomal protein L19



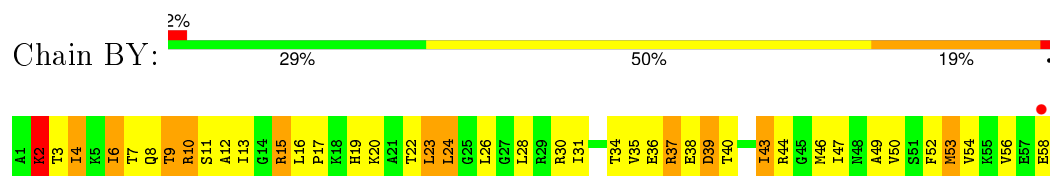
- Molecule 29: 50S ribosomal protein L4



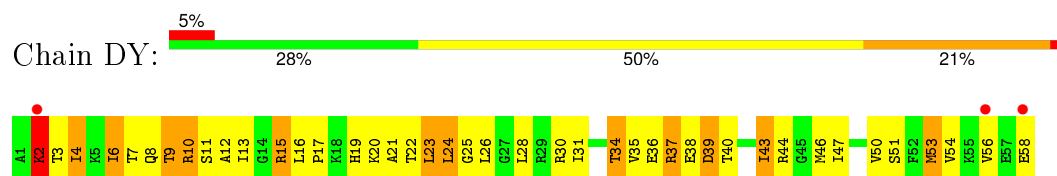
- Molecule 29: 50S ribosomal protein L4



- Molecule 30: 50S ribosomal protein L30

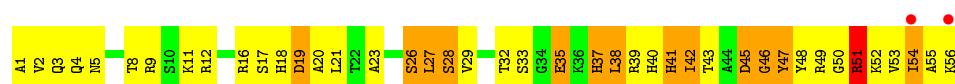


- Molecule 30: 50S ribosomal protein L30

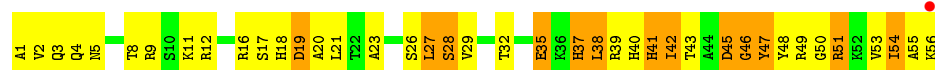


- Molecule 31: 50S ribosomal protein L32

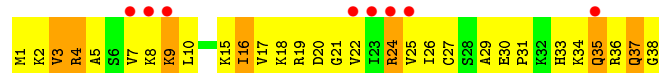




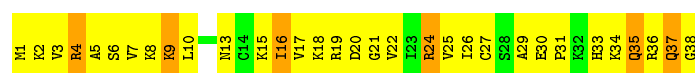
- Molecule 31: 50S ribosomal protein L32



- Molecule 32: 50S ribosomal protein L36



- Molecule 32: 50S ribosomal protein L36



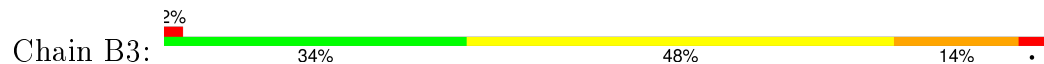
- Molecule 33: 50S ribosomal protein L33



- Molecule 33: 50S ribosomal protein L33

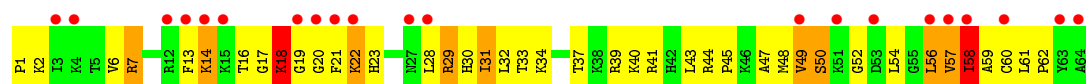


- Molecule 34: 50S ribosomal protein L35

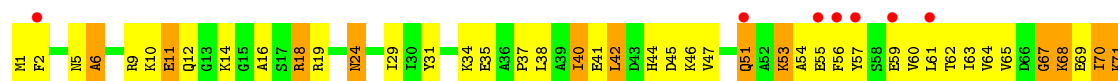


- Molecule 34: 50S ribosomal protein L35

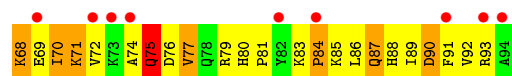
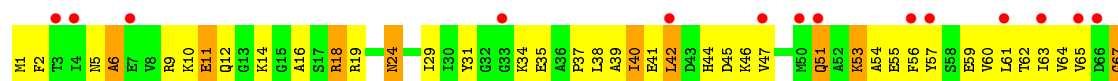




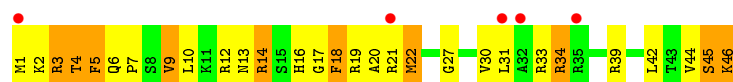
- Molecule 35: 50S ribosomal protein L25



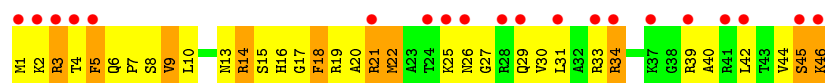
- Molecule 35: 50S ribosomal protein L25



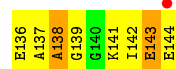
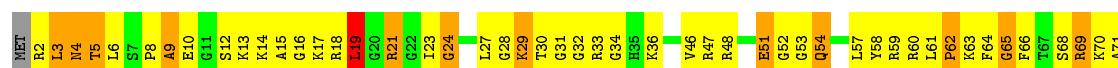
- Molecule 36: 50S ribosomal protein L34



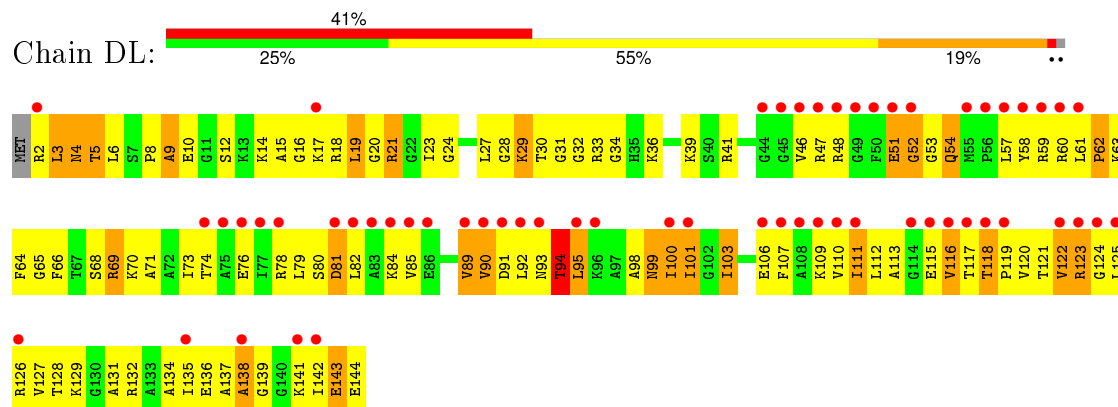
- Molecule 36: 50S ribosomal protein L34



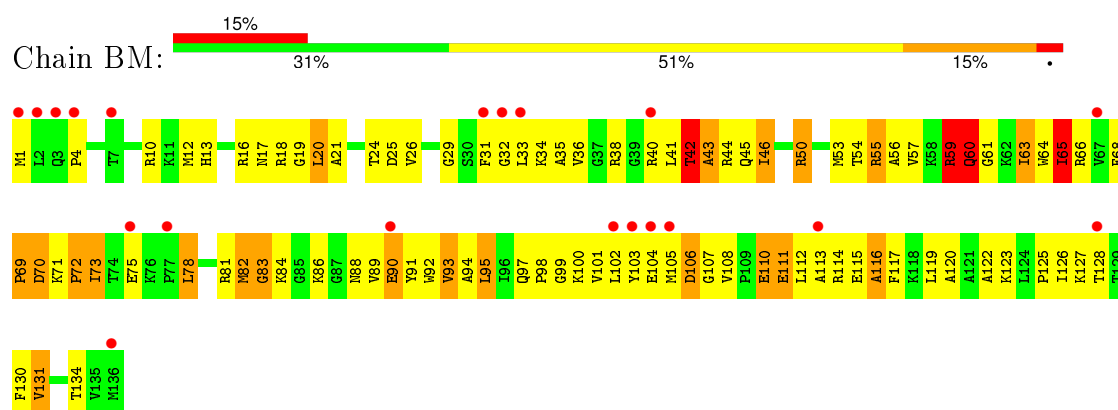
- Molecule 37: 50S ribosomal protein L15



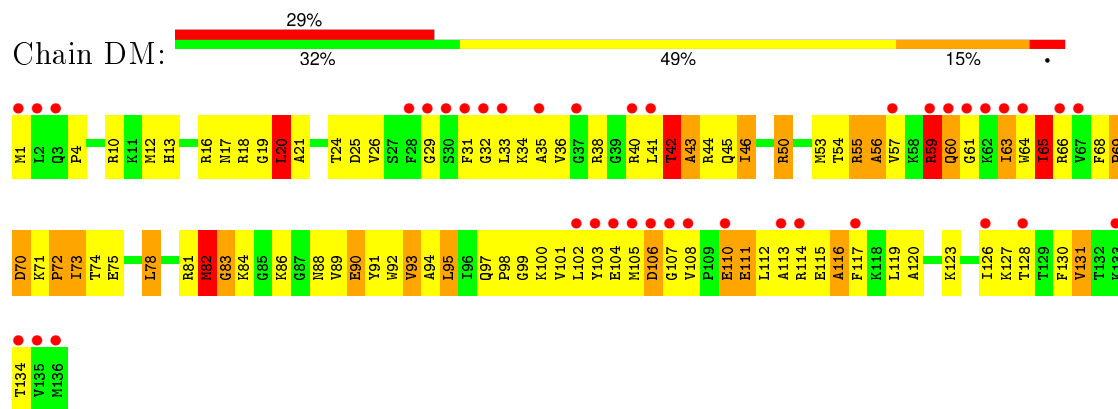
- Molecule 37: 50S ribosomal protein L15



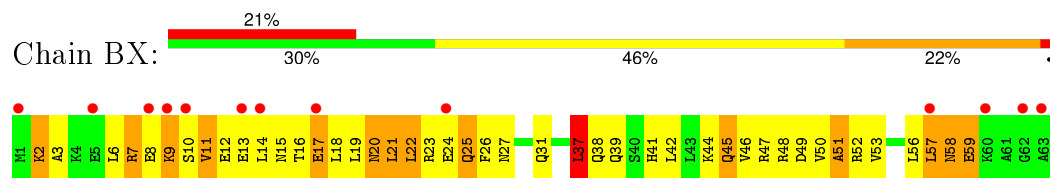
- Molecule 38: 50S ribosomal protein L16



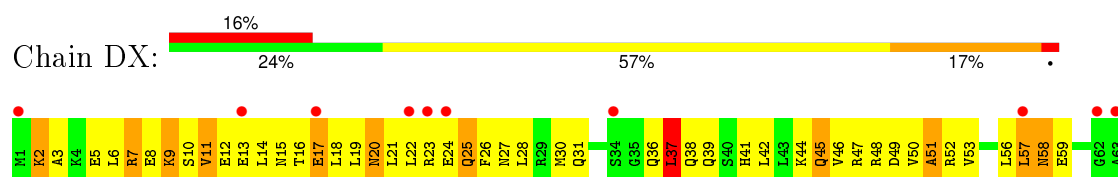
- Molecule 38: 50S ribosomal protein L16



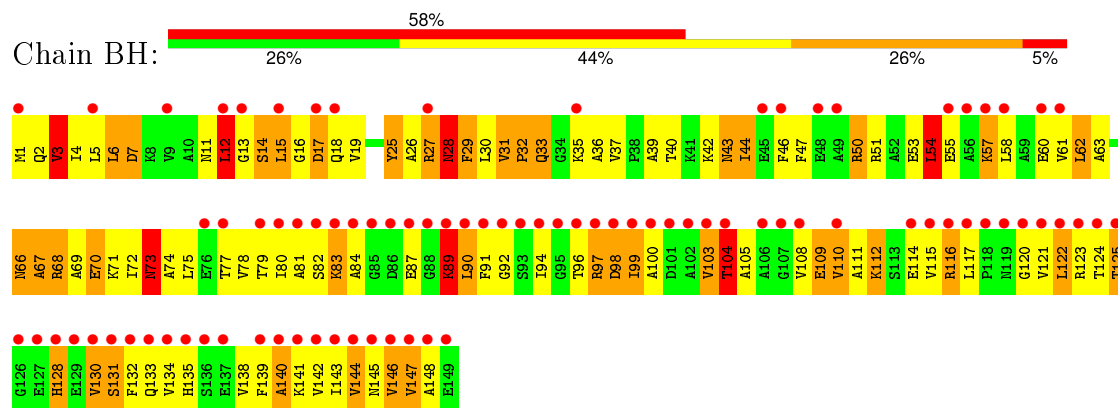
- Molecule 39: 50S ribosomal protein L29



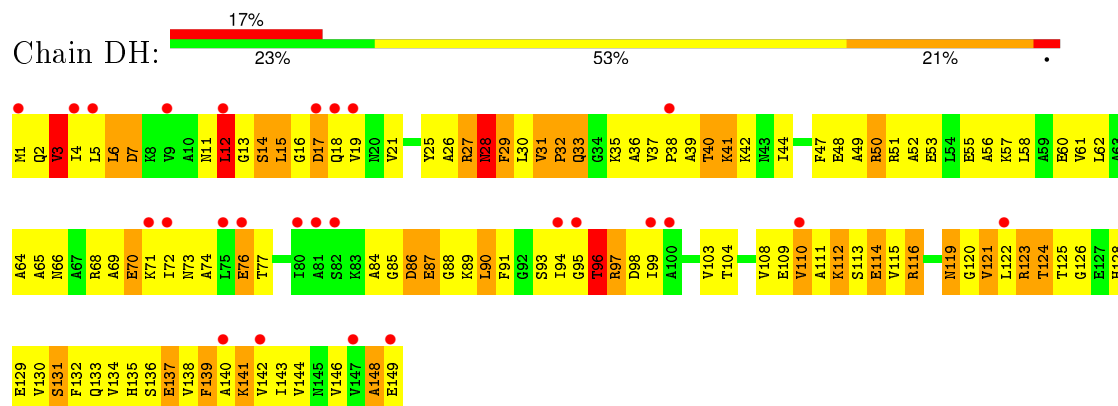
- Molecule 39: 50S ribosomal protein L29



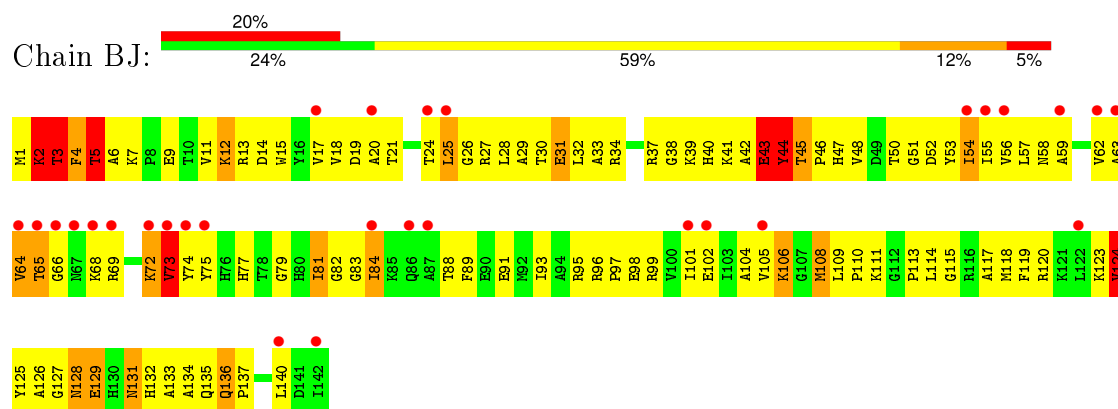
• Molecule 40: 50S ribosomal protein L9



• Molecule 40: 50S ribosomal protein L9

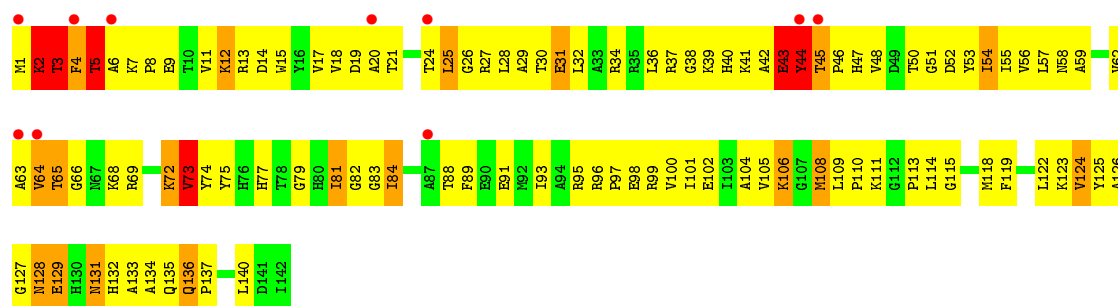


• Molecule 41: 50S ribosomal protein L13

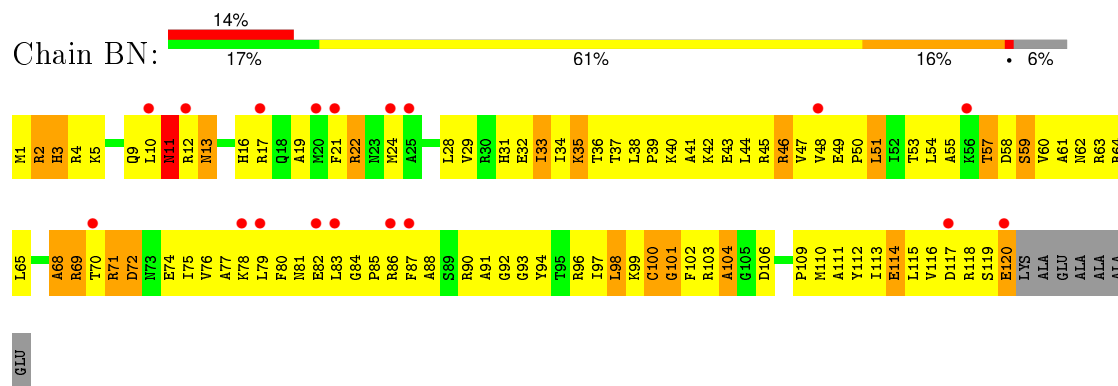


• Molecule 41: 50S ribosomal protein L13

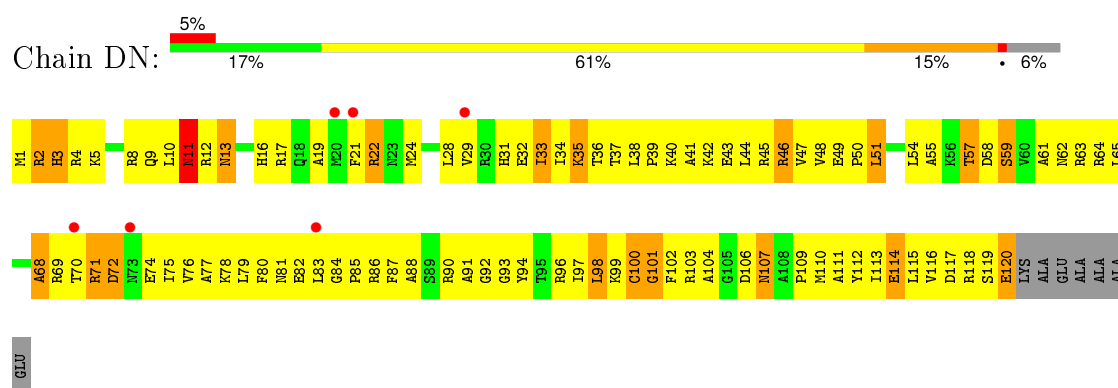




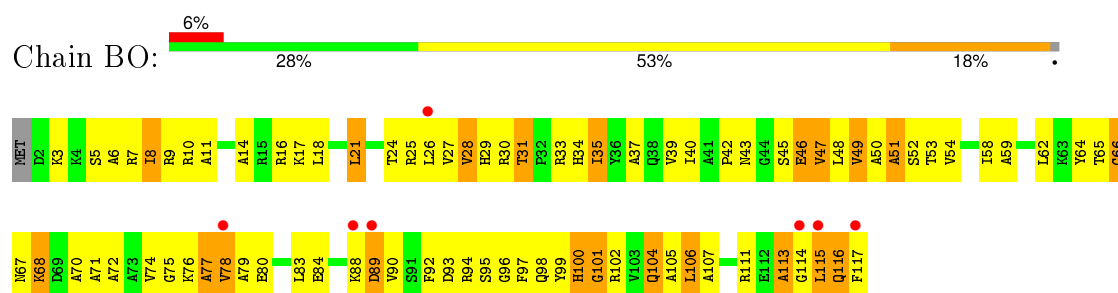
• Molecule 42: 50S ribosomal protein L17



• Molecule 42: 50S ribosomal protein L17

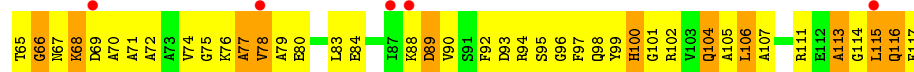


• Molecule 43: 50S ribosomal protein L18



• Molecule 43: 50S ribosomal protein L18

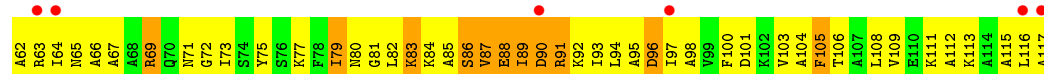
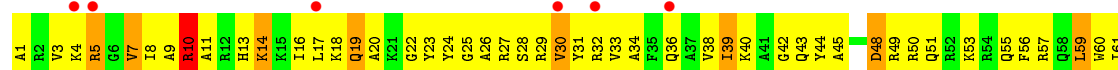




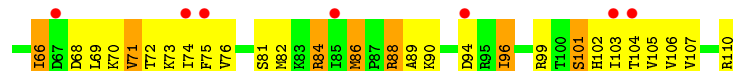
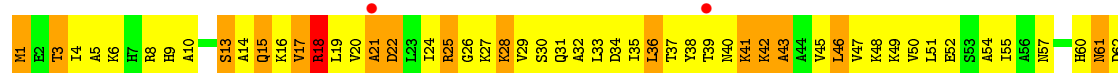
• Molecule 44: 50S ribosomal protein L20



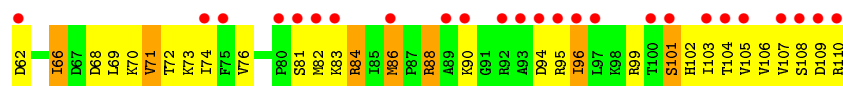
• Molecule 44: 50S ribosomal protein L20



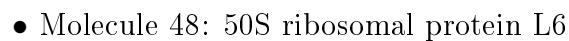
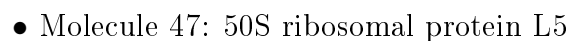
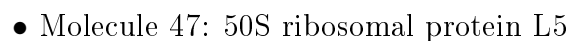
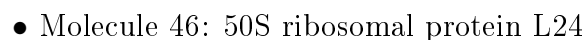
• Molecule 45: 50S ribosomal protein L22

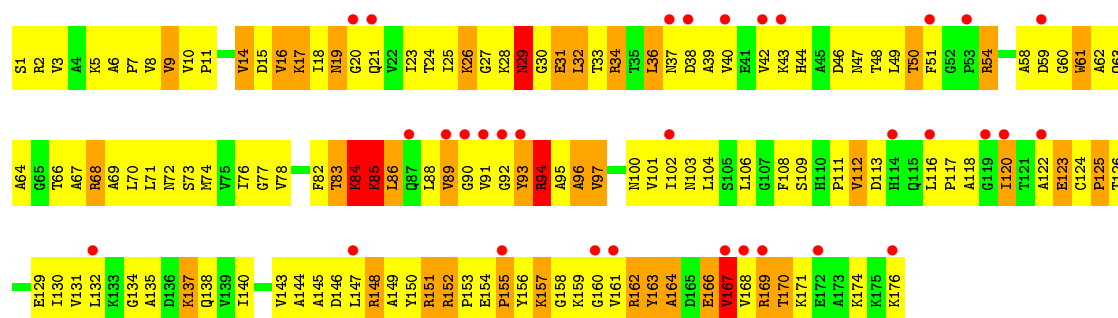


• Molecule 45: 50S ribosomal protein L22

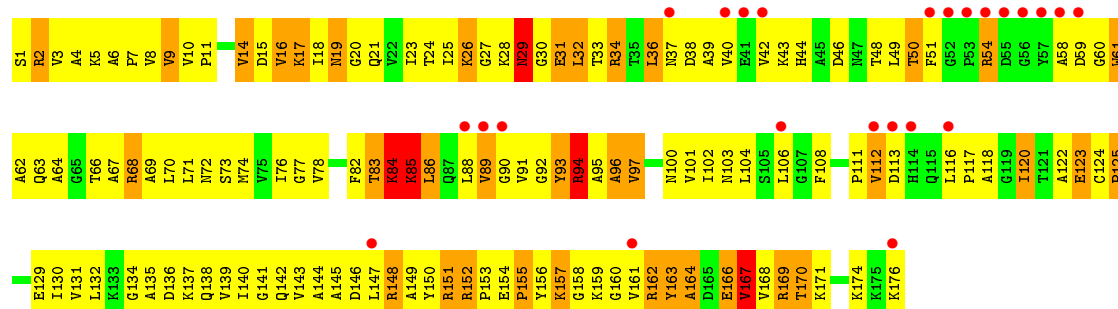


• Molecule 46: 50S ribosomal protein L24

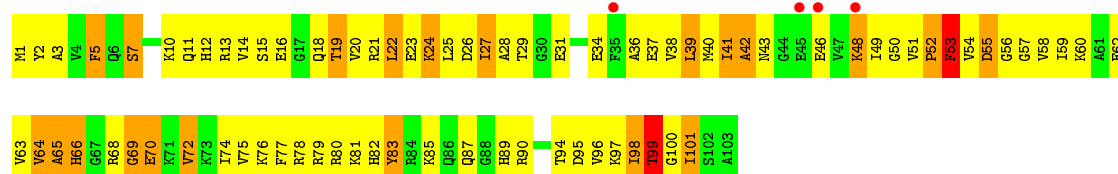




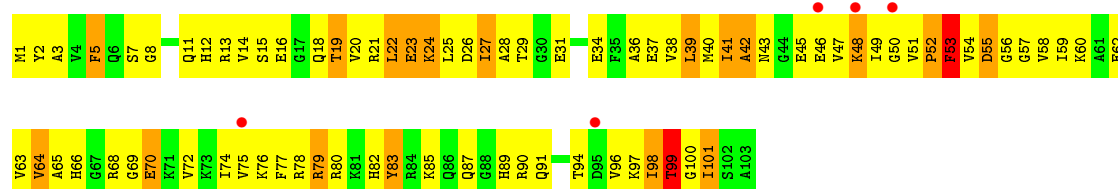
• Molecule 48: 50S ribosomal protein L6



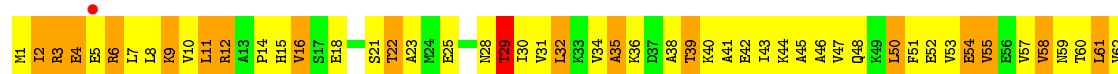
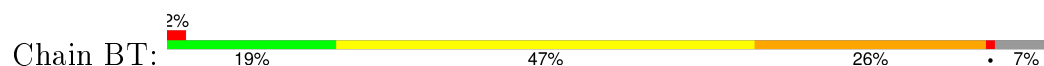
• Molecule 49: 50S ribosomal protein L21

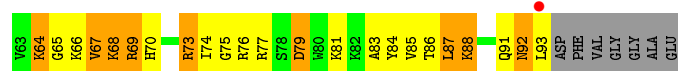


• Molecule 49: 50S ribosomal protein L21

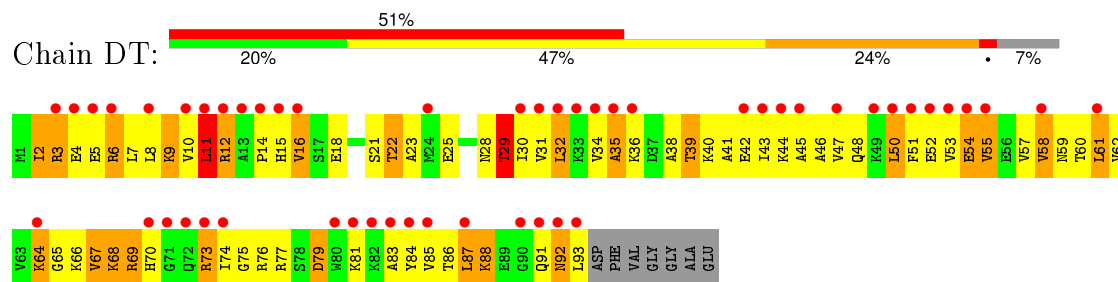


• Molecule 50: 50S ribosomal protein L23

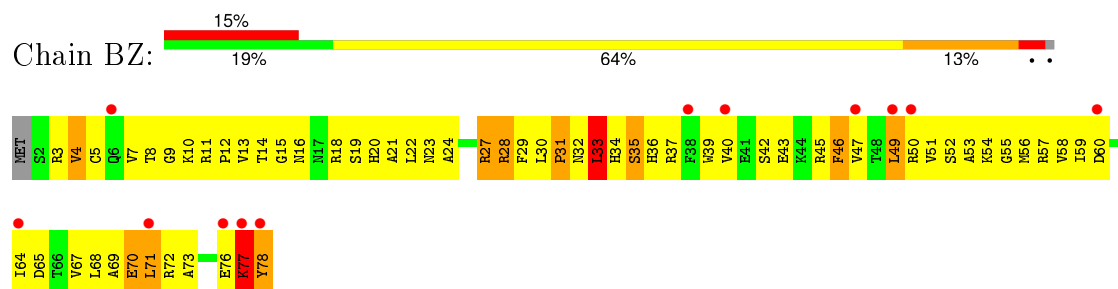




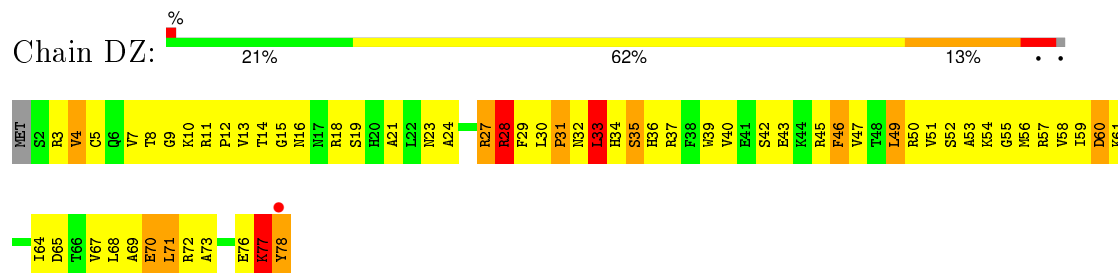
- Molecule 50: 50S ribosomal protein L23



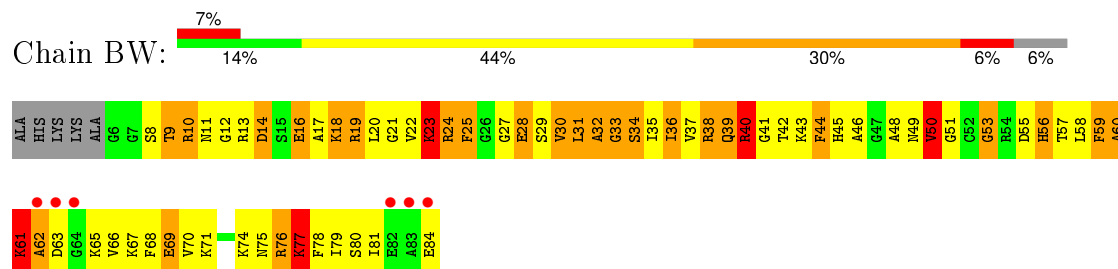
- Molecule 51: 50S ribosomal protein L28



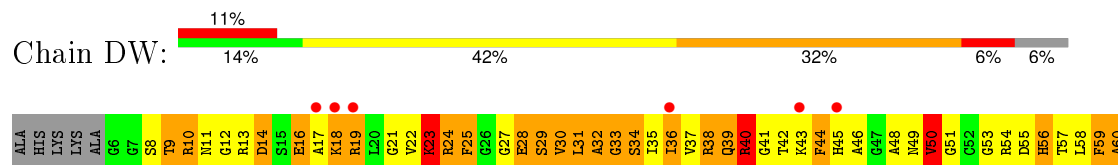
- Molecule 51: 50S ribosomal protein L28

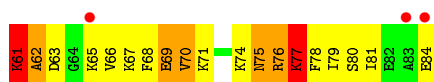


- Molecule 52: 50S ribosomal protein L27



- Molecule 52: 50S ribosomal protein L27





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.85Å 379.20Å 739.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.00 – 3.93 182.94 – 3.94	Depositor EDS
% Data completeness (in resolution range)	(Not available) (70.00-3.93) 75.9 (182.94-3.94)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 3.89Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.258 , 0.311 0.231 , 0.279	Depositor DCC
R_{free} test set	19244 reflections (5.18%)	DCC
Wilson B-factor (Å ²)	149.7	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 71.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 390843 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	284033	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% 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: SCM, 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	0.27	2/36762 (0.0%)	0.76	12/57350 (0.0%)
1	CA	0.31	1/36762 (0.0%)	0.77	11/57350 (0.0%)
2	AC	0.23	0/1651	0.45	0/2225
2	CC	0.23	0/1651	0.46	0/2225
3	AD	0.23	0/1665	0.44	0/2227
3	CD	0.23	0/1665	0.44	0/2227
4	AE	0.23	0/1118	0.45	0/1504
4	CE	0.23	0/1118	0.45	0/1504
5	AF	0.24	0/835	0.45	0/1128
5	CF	0.24	0/835	0.45	0/1128
6	AG	0.23	0/1187	0.45	0/1591
6	CG	0.23	0/1211	0.45	0/1624
7	AH	0.23	0/989	0.44	0/1326
7	CH	0.23	0/989	0.44	0/1326
8	AI	0.24	0/1034	0.44	0/1375
8	CI	0.24	0/1034	0.45	0/1375
9	AJ	0.22	0/796	0.48	0/1077
9	CJ	0.22	0/796	0.48	0/1077
10	AK	0.24	0/893	0.44	0/1205
10	CK	0.24	0/893	0.44	0/1205
11	AL	0.22	0/969	0.48	0/1300
11	CL	0.22	0/969	0.48	0/1300
12	AM	0.21	0/892	0.45	0/1193
12	CM	0.21	0/884	0.45	0/1181
13	AP	0.25	0/659	0.45	0/884
13	CP	0.25	0/648	0.44	0/870
14	AQ	0.23	0/657	0.46	0/881
14	CQ	0.24	0/666	0.46	0/892
15	AR	0.23	0/462	0.46	0/621
15	CR	0.23	0/462	0.46	0/621
16	AS	0.25	0/652	0.46	0/877
16	CS	0.25	0/660	0.49	0/888

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AT	0.23	0/671	0.40	0/888
17	CT	0.23	0/671	0.40	0/888
18	AB	0.25	0/1735	0.45	0/2338
18	CB	0.25	0/1735	0.45	0/2338
19	AU	0.26	0/430	0.46	0/570
19	CU	0.25	0/430	0.46	0/570
20	AO	0.22	0/722	0.45	0/964
20	CO	0.23	0/722	0.44	0/964
21	AN	0.24	0/785	0.44	0/1043
21	CN	0.24	0/785	0.46	0/1043
22	BA	0.23	0/2803	0.74	1/4371 (0.0%)
22	DA	0.24	0/2803	0.75	1/4371 (0.0%)
23	BB	0.28	5/68314 (0.0%)	0.77	33/106569 (0.0%)
23	DB	0.28	5/68314 (0.0%)	0.77	33/106569 (0.0%)
24	BI	0.24	0/1046	0.46	0/1410
24	DI	0.25	0/1046	0.47	0/1410
25	BC	0.22	0/2121	0.47	0/2852
25	DC	0.22	0/2121	0.47	0/2852
26	BD	0.24	0/1586	0.48	0/2134
26	DD	0.24	0/1586	0.48	0/2134
27	BK	0.24	0/939	0.53	0/1258
27	DK	0.24	0/939	0.53	0/1258
28	BP	0.24	0/929	0.49	0/1242
28	DP	0.24	0/929	0.49	0/1242
29	BE	0.24	0/1571	0.48	0/2113
29	DE	0.24	0/1571	0.48	0/2113
30	BY	0.24	0/453	0.49	0/605
30	DY	0.23	0/453	0.49	0/605
31	B0	0.23	0/450	0.51	0/599
31	D0	0.23	0/450	0.51	0/599
32	B4	0.22	0/303	0.49	0/397
32	D4	0.23	0/303	0.49	0/397
33	B1	0.27	0/416	0.48	0/554
33	D1	0.27	0/416	0.48	0/554
34	B3	0.24	0/513	0.46	0/676
34	D3	0.24	0/513	0.46	0/676
35	BV	0.25	0/766	0.43	0/1025
35	DV	0.25	0/766	0.43	0/1025
36	B2	0.26	0/380	0.47	0/498
36	D2	0.26	0/380	0.47	0/498
37	BL	0.24	0/1054	0.48	0/1403
37	DL	0.24	0/1054	0.48	0/1403
38	BM	0.25	0/1093	0.47	0/1460

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DM	0.25	0/1093	0.47	0/1460
39	BX	0.24	0/510	0.50	0/677
39	DX	0.23	0/510	0.50	0/677
40	BH	0.25	0/1122	0.47	0/1515
40	DH	0.25	0/1122	0.47	0/1515
41	BJ	0.23	0/1152	0.47	0/1551
41	DJ	0.23	0/1152	0.47	0/1551
42	BN	0.24	0/973	0.49	0/1301
42	DN	0.24	0/973	0.49	0/1301
43	BO	0.23	0/902	0.47	0/1209
43	DO	0.23	0/902	0.47	0/1209
44	BQ	0.25	0/960	0.47	0/1278
44	DQ	0.25	0/960	0.47	0/1278
45	BS	0.22	0/864	0.50	0/1156
45	DS	0.22	0/864	0.50	0/1156
46	BU	0.25	0/787	0.45	0/1051
46	DU	0.25	0/787	0.45	0/1051
47	BF	0.26	0/1444	0.49	0/1937
47	DF	0.26	0/1444	0.49	0/1937
48	BG	0.23	0/1343	0.47	0/1816
48	DG	0.23	0/1343	0.47	0/1816
49	BR	0.26	0/829	0.48	0/1107
49	DR	0.25	0/829	0.48	0/1107
50	BT	0.23	0/744	0.51	0/994
50	DT	0.23	0/744	0.51	0/994
51	BZ	0.25	0/635	0.49	0/848
51	DZ	0.25	0/635	0.50	0/848
52	BW	0.28	0/603	0.49	0/797
52	DW	0.28	0/603	0.49	0/797
All	All	0.27	13/306360 (0.0%)	0.70	91/457969 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	15
1	CA	0	19
23	BB	0	37
23	DB	0	37
All	All	0	108

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	DB	1086	A	C5-C6	-16.20	1.26	1.41
23	BB	1086	A	C5-C6	-16.10	1.26	1.41
23	DB	1088	A	C6-N1	-10.51	1.28	1.35
23	BB	1088	A	C6-N1	-10.50	1.28	1.35
23	BB	1060	U	C2-N3	7.92	1.43	1.37

The worst 5 of 91 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	DB	2204	G	O5'-P-OP1	-30.02	74.68	110.70
23	BB	2204	G	O5'-P-OP2	-28.49	76.52	110.70
23	DB	2791	G	O5'-P-OP2	-28.43	76.59	110.70
23	BB	2791	G	O5'-P-OP1	-27.42	77.80	110.70
23	DB	2204	G	O5'-P-OP2	17.65	131.88	110.70

There are no chirality outliers.

5 of 108 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	187	G	Sidechain
1	AA	281	G	Sidechain
1	AA	437	U	Sidechain
1	AA	438	U	Sidechain
1	AA	450	G	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32831	0	16521	1458	0
1	CA	32831	0	16521	1414	0
2	AC	1624	0	1699	205	0
2	CC	1624	0	1699	191	0
3	AD	1643	0	1710	179	0
3	CD	1643	0	1710	177	0
4	AE	1105	0	1148	129	0

Continued on next page...

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	CE	1105	0	1148	121	0
5	AF	817	0	808	89	0
5	CF	817	0	808	91	0
6	AG	1174	0	1230	146	0
6	CG	1196	0	1246	133	0
7	AH	979	0	1034	89	0
7	CH	979	0	1034	91	0
8	AI	1022	0	1070	180	0
8	CI	1022	0	1070	146	0
9	AJ	786	0	828	85	0
9	CJ	786	0	828	103	0
10	AK	877	0	887	110	0
10	CK	877	0	887	100	0
11	AL	955	0	1019	96	0
11	CL	955	0	1019	97	0
12	AM	883	0	944	135	0
12	CM	876	0	937	138	0
13	AP	649	0	666	65	0
13	CP	638	0	656	66	0
14	AQ	648	0	691	63	0
14	CQ	657	0	702	62	0
15	AR	455	0	478	35	0
15	CR	455	0	478	37	0
16	AS	637	0	665	97	0
16	CS	644	0	675	115	0
17	AT	665	0	714	60	0
17	CT	665	0	714	61	0
18	AB	1704	0	1732	209	0
18	CB	1704	0	1732	229	0
19	AU	425	0	449	57	0
19	CU	425	0	449	54	0
20	AO	714	0	734	63	0
20	CO	714	0	734	62	0
21	AN	774	0	827	102	0
21	CN	774	0	827	114	0
22	BA	2507	0	1270	116	0
22	DA	2507	0	1270	111	0
23	BB	60995	0	30679	2412	0
23	DB	60995	0	30678	2455	0
24	BI	1032	0	1088	109	0
24	DI	1032	0	1088	168	0
25	BC	2082	0	2157	234	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	DC	2082	0	2157	239	0
26	BD	1565	0	1616	234	0
26	DD	1565	0	1616	239	0
27	BK	930	0	1000	153	0
27	DK	930	0	1000	154	0
28	BP	917	0	965	126	0
28	DP	917	0	965	132	0
29	BE	1552	0	1619	208	0
29	DE	1552	0	1619	202	0
30	BY	449	0	491	59	0
30	DY	449	0	491	53	0
31	B0	444	0	461	48	0
31	D0	444	0	461	44	0
32	B4	302	0	340	42	0
32	D4	302	0	340	43	0
33	B1	409	0	440	54	0
33	D1	409	0	440	50	0
34	B3	504	0	574	47	0
34	D3	504	0	574	52	0
35	BV	753	0	780	83	0
35	DV	753	0	780	86	0
36	B2	377	0	418	37	0
36	D2	377	0	418	43	0
37	BL	1045	0	1117	138	0
37	DL	1045	0	1117	144	0
38	BM	1074	0	1157	123	0
38	DM	1074	0	1157	119	0
39	BX	509	0	543	46	0
39	DX	509	0	543	50	0
40	BH	1111	0	1148	172	0
40	DH	1111	0	1148	147	0
41	BJ	1129	0	1162	134	0
41	DJ	1129	0	1162	141	0
42	BN	960	0	1000	137	0
42	DN	960	0	1000	133	0
43	BO	892	0	923	91	0
43	DO	892	0	923	94	0
44	BQ	947	0	1022	150	0
44	DQ	947	0	1022	143	0
45	BS	857	0	922	97	0
45	DS	857	0	922	98	0
46	BU	779	0	834	116	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	DU	779	0	834	114	0
47	BF	1420	0	1460	264	0
47	DF	1420	0	1460	249	0
48	BG	1323	0	1374	187	0
48	DG	1323	0	1374	178	0
49	BR	816	0	839	105	0
49	DR	816	0	839	112	0
50	BT	738	0	807	115	0
50	DT	738	0	807	110	0
51	BZ	625	0	652	75	0
51	DZ	625	0	652	71	0
52	BW	596	0	610	122	0
52	DW	596	0	610	130	0
53	AA	60	0	0	0	0
53	BB	110	0	0	0	0
53	CA	58	0	0	0	0
53	CE	1	0	0	0	0
53	DB	110	0	0	0	0
53	DN	1	0	0	0	0
54	AA	23	0	24	2	0
54	CA	23	0	24	1	0
55	B4	1	0	0	0	0
55	D4	1	0	0	0	0
56	AA	288	0	0	6	0
56	AE	3	0	0	1	0
56	AK	1	0	0	0	0
56	AL	4	0	0	0	0
56	AN	2	0	0	0	0
56	AP	1	0	0	0	0
56	AT	1	0	0	0	0
56	BB	494	0	0	4	0
56	BC	4	0	0	0	0
56	BE	3	0	0	0	0
56	BH	1	0	0	0	0
56	BL	4	0	0	0	0
56	BT	1	0	0	0	0
56	CA	275	0	0	4	0
56	CE	4	0	0	0	0
56	CK	1	0	0	0	0
56	CL	5	0	0	0	0
56	CN	5	0	0	0	0
56	CP	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	CT	2	0	0	0	0
56	DB	500	0	0	9	0
56	DC	3	0	0	0	0
56	DD	1	0	0	0	0
56	DE	1	0	0	0	0
56	DJ	1	0	0	0	0
56	DL	3	0	0	0	0
56	DN	2	0	0	0	0
56	DP	1	0	0	0	0
56	DR	1	0	0	0	0
All	All	284033	0	190711	17874	0

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

The worst 5 of 17874 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:DB:1099:G:H8	24:DI:3:LYS:N	1.36	1.21
23:BB:855:G:H21	52:BW:23:LYS:HG2	1.11	1.13
23:DB:322:A:H5'	23:DB:340:A:H1'	1.32	1.12
2:AC:70:ALA:HA	2:AC:105:VAL:HG21	1.26	1.11
23:BB:1205:A:H62	29:BE:165:HIS:HB2	1.11	1.10

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	AC	204/232 (88%)	112 (55%)	56 (28%)	36 (18%)	0 3
2	CC	204/232 (88%)	134 (66%)	48 (24%)	22 (11%)	0 11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AD	203/205 (99%)	133 (66%)	58 (29%)	12 (6%)	2	28
3	CD	203/205 (99%)	132 (65%)	58 (29%)	13 (6%)	2	26
4	AE	148/166 (89%)	109 (74%)	30 (20%)	9 (6%)	2	27
4	CE	148/166 (89%)	108 (73%)	31 (21%)	9 (6%)	2	27
5	AF	98/135 (73%)	62 (63%)	27 (28%)	9 (9%)	1	16
5	CF	98/135 (73%)	64 (65%)	25 (26%)	9 (9%)	1	16
6	AG	148/178 (83%)	98 (66%)	44 (30%)	6 (4%)	3	36
6	CG	150/178 (84%)	101 (67%)	36 (24%)	13 (9%)	1	17
7	AH	127/129 (98%)	86 (68%)	35 (28%)	6 (5%)	3	33
7	CH	127/129 (98%)	85 (67%)	36 (28%)	6 (5%)	3	33
8	AI	125/129 (97%)	84 (67%)	25 (20%)	16 (13%)	0	7
8	CI	125/129 (97%)	89 (71%)	30 (24%)	6 (5%)	3	32
9	AJ	96/103 (93%)	61 (64%)	18 (19%)	17 (18%)	0	3
9	CJ	96/103 (93%)	62 (65%)	21 (22%)	13 (14%)	0	6
10	AK	115/128 (90%)	85 (74%)	26 (23%)	4 (4%)	4	42
10	CK	115/128 (90%)	84 (73%)	25 (22%)	6 (5%)	2	31
11	AL	121/123 (98%)	71 (59%)	34 (28%)	16 (13%)	0	6
11	CL	121/123 (98%)	72 (60%)	33 (27%)	16 (13%)	0	6
12	AM	112/117 (96%)	69 (62%)	36 (32%)	7 (6%)	2	27
12	CM	111/117 (95%)	77 (69%)	23 (21%)	11 (10%)	1	13
13	AP	80/82 (98%)	53 (66%)	18 (22%)	9 (11%)	0	9
13	CP	78/82 (95%)	53 (68%)	19 (24%)	6 (8%)	1	20
14	AQ	78/83 (94%)	61 (78%)	14 (18%)	3 (4%)	4	39
14	CQ	79/83 (95%)	62 (78%)	15 (19%)	2 (2%)	7	48
15	AR	53/74 (72%)	33 (62%)	17 (32%)	3 (6%)	2	28
15	CR	53/74 (72%)	33 (62%)	16 (30%)	4 (8%)	1	21
16	AS	77/91 (85%)	49 (64%)	21 (27%)	7 (9%)	1	16
16	CS	78/91 (86%)	51 (65%)	20 (26%)	7 (9%)	1	16
17	AT	83/86 (96%)	62 (75%)	16 (19%)	5 (6%)	2	27
17	CT	83/86 (96%)	63 (76%)	14 (17%)	6 (7%)	1	22
18	AB	216/240 (90%)	140 (65%)	53 (24%)	23 (11%)	0	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	CB	216/240 (90%)	135 (62%)	59 (27%)	22 (10%)	1	13
19	AU	49/70 (70%)	29 (59%)	13 (26%)	7 (14%)	0	5
19	CU	49/70 (70%)	29 (59%)	15 (31%)	5 (10%)	1	13
20	AO	86/89 (97%)	55 (64%)	24 (28%)	7 (8%)	1	18
20	CO	86/89 (97%)	50 (58%)	29 (34%)	7 (8%)	1	18
21	AN	92/100 (92%)	54 (59%)	29 (32%)	9 (10%)	1	14
21	CN	92/100 (92%)	45 (49%)	31 (34%)	16 (17%)	0	4
24	BI	139/141 (99%)	118 (85%)	16 (12%)	5 (4%)	4	41
24	DI	139/141 (99%)	115 (83%)	19 (14%)	5 (4%)	4	41
25	BC	269/272 (99%)	149 (55%)	68 (25%)	52 (19%)	0	3
25	DC	269/272 (99%)	147 (55%)	70 (26%)	52 (19%)	0	3
26	BD	207/209 (99%)	113 (55%)	58 (28%)	36 (17%)	0	4
26	DD	207/209 (99%)	114 (55%)	58 (28%)	35 (17%)	0	4
27	BK	119/123 (97%)	73 (61%)	24 (20%)	22 (18%)	0	3
27	DK	119/123 (97%)	73 (61%)	25 (21%)	21 (18%)	0	3
28	BP	112/114 (98%)	67 (60%)	28 (25%)	17 (15%)	0	5
28	DP	112/114 (98%)	66 (59%)	31 (28%)	15 (13%)	0	6
29	BE	199/201 (99%)	120 (60%)	49 (25%)	30 (15%)	0	5
29	DE	199/201 (99%)	123 (62%)	47 (24%)	29 (15%)	0	5
30	BY	56/58 (97%)	36 (64%)	16 (29%)	4 (7%)	1	23
30	DY	56/58 (97%)	36 (64%)	14 (25%)	6 (11%)	0	11
31	B0	54/56 (96%)	34 (63%)	10 (18%)	10 (18%)	0	3
31	D0	54/56 (96%)	35 (65%)	9 (17%)	10 (18%)	0	3
32	B4	36/38 (95%)	19 (53%)	13 (36%)	4 (11%)	0	10
32	D4	36/38 (95%)	19 (53%)	13 (36%)	4 (11%)	0	10
33	B1	48/54 (89%)	36 (75%)	8 (17%)	4 (8%)	1	18
33	D1	48/54 (89%)	35 (73%)	9 (19%)	4 (8%)	1	18
34	B3	62/64 (97%)	34 (55%)	20 (32%)	8 (13%)	0	7
34	D3	62/64 (97%)	35 (56%)	19 (31%)	8 (13%)	0	7
35	BV	92/94 (98%)	60 (65%)	25 (27%)	7 (8%)	1	20
35	DV	92/94 (98%)	61 (66%)	24 (26%)	7 (8%)	1	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	B2	44/46 (96%)	23 (52%)	16 (36%)	5 (11%)	0	9
36	D2	44/46 (96%)	23 (52%)	12 (27%)	9 (20%)	0	2
37	BL	141/144 (98%)	76 (54%)	37 (26%)	28 (20%)	0	2
37	DL	141/144 (98%)	76 (54%)	39 (28%)	26 (18%)	0	3
38	BM	134/136 (98%)	79 (59%)	39 (29%)	16 (12%)	0	8
38	DM	134/136 (98%)	82 (61%)	35 (26%)	17 (13%)	0	7
39	BX	61/63 (97%)	35 (57%)	20 (33%)	6 (10%)	1	14
39	DX	61/63 (97%)	35 (57%)	20 (33%)	6 (10%)	1	14
40	BH	147/149 (99%)	78 (53%)	42 (29%)	27 (18%)	0	3
40	DH	147/149 (99%)	91 (62%)	30 (20%)	26 (18%)	0	3
41	BJ	140/142 (99%)	85 (61%)	37 (26%)	18 (13%)	0	7
41	DJ	140/142 (99%)	85 (61%)	36 (26%)	19 (14%)	0	6
42	BN	118/127 (93%)	73 (62%)	33 (28%)	12 (10%)	1	13
42	DN	118/127 (93%)	74 (63%)	33 (28%)	11 (9%)	1	16
43	BO	114/117 (97%)	68 (60%)	28 (25%)	18 (16%)	0	5
43	DO	114/117 (97%)	66 (58%)	30 (26%)	18 (16%)	0	5
44	BQ	115/117 (98%)	76 (66%)	29 (25%)	10 (9%)	1	17
44	DQ	115/117 (98%)	76 (66%)	30 (26%)	9 (8%)	1	20
45	BS	108/110 (98%)	59 (55%)	34 (32%)	15 (14%)	0	6
45	DS	108/110 (98%)	60 (56%)	33 (31%)	15 (14%)	0	6
46	BU	100/103 (97%)	58 (58%)	25 (25%)	17 (17%)	0	4
46	DU	100/103 (97%)	57 (57%)	24 (24%)	19 (19%)	0	3
47	BF	176/178 (99%)	91 (52%)	51 (29%)	34 (19%)	0	3
47	DF	176/178 (99%)	93 (53%)	49 (28%)	34 (19%)	0	3
48	BG	174/176 (99%)	100 (58%)	42 (24%)	32 (18%)	0	3
48	DG	174/176 (99%)	101 (58%)	42 (24%)	31 (18%)	0	3
49	BR	101/103 (98%)	57 (56%)	26 (26%)	18 (18%)	0	3
49	DR	101/103 (98%)	58 (57%)	26 (26%)	17 (17%)	0	4
50	BT	91/100 (91%)	40 (44%)	40 (44%)	11 (12%)	0	8
50	DT	91/100 (91%)	41 (45%)	39 (43%)	11 (12%)	0	8
51	BZ	75/78 (96%)	53 (71%)	16 (21%)	6 (8%)	1	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	DZ	75/78 (96%)	54 (72%)	14 (19%)	7 (9%)	1	16
52	BW	77/84 (92%)	29 (38%)	24 (31%)	24 (31%)	0	0
52	DW	77/84 (92%)	27 (35%)	26 (34%)	24 (31%)	0	0
All	All	11241/11914 (94%)	6932 (62%)	2908 (26%)	1401 (12%)	0	8

5 of 1401 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AC	14	VAL
2	AC	19	SER
2	AC	26	LYS
2	AC	47	ALA
2	AC	54	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AC	170/189 (90%)	139 (82%)	31 (18%)	2	16
2	CC	170/189 (90%)	134 (79%)	36 (21%)	1	10
3	AD	172/172 (100%)	145 (84%)	27 (16%)	3	23
3	CD	172/172 (100%)	146 (85%)	26 (15%)	3	25
4	AE	113/125 (90%)	93 (82%)	20 (18%)	2	17
4	CE	113/125 (90%)	93 (82%)	20 (18%)	2	17
5	AF	87/116 (75%)	76 (87%)	11 (13%)	5	31
5	CF	87/116 (75%)	75 (86%)	12 (14%)	4	29
6	AG	123/146 (84%)	102 (83%)	21 (17%)	2	19
6	CG	125/146 (86%)	98 (78%)	27 (22%)	1	10
7	AH	104/104 (100%)	95 (91%)	9 (9%)	13	49
7	CH	104/104 (100%)	95 (91%)	9 (9%)	13	49
8	AI	105/106 (99%)	78 (74%)	27 (26%)	0	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	CI	105/106 (99%)	79 (75%)	26 (25%)	1	7
9	AJ	86/90 (96%)	73 (85%)	13 (15%)	3	25
9	CJ	86/90 (96%)	72 (84%)	14 (16%)	3	21
10	AK	90/98 (92%)	73 (81%)	17 (19%)	2	14
10	CK	90/98 (92%)	73 (81%)	17 (19%)	2	14
11	AL	103/103 (100%)	87 (84%)	16 (16%)	3	24
11	CL	103/103 (100%)	87 (84%)	16 (16%)	3	24
12	AM	92/95 (97%)	72 (78%)	20 (22%)	1	10
12	CM	91/95 (96%)	75 (82%)	16 (18%)	2	18
13	AP	65/65 (100%)	61 (94%)	4 (6%)	23	62
13	CP	65/65 (100%)	61 (94%)	4 (6%)	23	62
14	AQ	74/77 (96%)	63 (85%)	11 (15%)	4	25
14	CQ	75/77 (97%)	63 (84%)	12 (16%)	3	22
15	AR	48/64 (75%)	41 (85%)	7 (15%)	4	26
15	CR	48/64 (75%)	40 (83%)	8 (17%)	3	20
16	AS	70/78 (90%)	49 (70%)	21 (30%)	0	4
16	CS	71/78 (91%)	51 (72%)	20 (28%)	0	4
17	AT	65/65 (100%)	51 (78%)	14 (22%)	1	10
17	CT	65/65 (100%)	51 (78%)	14 (22%)	1	10
18	AB	180/198 (91%)	141 (78%)	39 (22%)	1	10
18	CB	180/198 (91%)	133 (74%)	47 (26%)	0	6
19	AU	44/60 (73%)	31 (70%)	13 (30%)	0	4
19	CU	44/60 (73%)	32 (73%)	12 (27%)	0	5
20	AO	76/77 (99%)	65 (86%)	11 (14%)	4	26
20	CO	76/77 (99%)	61 (80%)	15 (20%)	1	13
21	AN	79/83 (95%)	63 (80%)	16 (20%)	1	12
21	CN	79/83 (95%)	64 (81%)	15 (19%)	2	14
24	BI	109/109 (100%)	108 (99%)	1 (1%)	84	93
24	DI	109/109 (100%)	103 (94%)	6 (6%)	27	66
25	BC	216/217 (100%)	180 (83%)	36 (17%)	3	20
25	DC	216/217 (100%)	181 (84%)	35 (16%)	3	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	BD	164/164 (100%)	134 (82%)	30 (18%)	2	16
26	DD	164/164 (100%)	133 (81%)	31 (19%)	2	14
27	BK	102/104 (98%)	76 (74%)	26 (26%)	1	6
27	DK	102/104 (98%)	78 (76%)	24 (24%)	1	8
28	BP	99/99 (100%)	77 (78%)	22 (22%)	1	10
28	DP	99/99 (100%)	77 (78%)	22 (22%)	1	10
29	BE	165/165 (100%)	143 (87%)	22 (13%)	5	30
29	DE	165/165 (100%)	143 (87%)	22 (13%)	5	30
30	BY	48/48 (100%)	39 (81%)	9 (19%)	2	15
30	DY	48/48 (100%)	39 (81%)	9 (19%)	2	15
31	B0	47/47 (100%)	36 (77%)	11 (23%)	1	8
31	D0	47/47 (100%)	37 (79%)	10 (21%)	1	10
32	B4	34/34 (100%)	30 (88%)	4 (12%)	6	35
32	D4	34/34 (100%)	31 (91%)	3 (9%)	12	48
33	B1	45/48 (94%)	39 (87%)	6 (13%)	5	30
33	D1	45/48 (94%)	39 (87%)	6 (13%)	5	30
34	B3	51/51 (100%)	45 (88%)	6 (12%)	6	35
34	D3	51/51 (100%)	45 (88%)	6 (12%)	6	35
35	BV	78/78 (100%)	64 (82%)	14 (18%)	2	17
35	DV	78/78 (100%)	64 (82%)	14 (18%)	2	17
36	B2	38/38 (100%)	32 (84%)	6 (16%)	3	23
36	D2	38/38 (100%)	33 (87%)	5 (13%)	5	30
37	BL	102/103 (99%)	89 (87%)	13 (13%)	5	31
37	DL	102/103 (99%)	90 (88%)	12 (12%)	6	35
38	BM	109/109 (100%)	86 (79%)	23 (21%)	1	11
38	DM	109/109 (100%)	86 (79%)	23 (21%)	1	11
39	BX	55/55 (100%)	43 (78%)	12 (22%)	1	10
39	DX	55/55 (100%)	45 (82%)	10 (18%)	2	16
40	BH	114/114 (100%)	81 (71%)	33 (29%)	0	4
40	DH	114/114 (100%)	89 (78%)	25 (22%)	1	10
41	BJ	116/116 (100%)	95 (82%)	21 (18%)	2	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	DJ	116/116 (100%)	96 (83%)	20 (17%)	2	19
42	BN	100/103 (97%)	87 (87%)	13 (13%)	5	31
42	DN	100/103 (97%)	87 (87%)	13 (13%)	5	31
43	BO	86/87 (99%)	72 (84%)	14 (16%)	3	21
43	DO	86/87 (99%)	72 (84%)	14 (16%)	3	21
44	BQ	89/89 (100%)	74 (83%)	15 (17%)	2	20
44	DQ	89/89 (100%)	74 (83%)	15 (17%)	2	20
45	BS	93/93 (100%)	80 (86%)	13 (14%)	4	28
45	DS	93/93 (100%)	80 (86%)	13 (14%)	4	28
46	BU	83/84 (99%)	69 (83%)	14 (17%)	2	20
46	DU	83/84 (99%)	69 (83%)	14 (17%)	2	20
47	BF	149/149 (100%)	117 (78%)	32 (22%)	1	10
47	DF	149/149 (100%)	116 (78%)	33 (22%)	1	10
48	BG	137/137 (100%)	112 (82%)	25 (18%)	2	16
48	DG	137/137 (100%)	112 (82%)	25 (18%)	2	16
49	BR	84/84 (100%)	71 (84%)	13 (16%)	3	24
49	DR	84/84 (100%)	73 (87%)	11 (13%)	5	30
50	BT	80/84 (95%)	59 (74%)	21 (26%)	0	6
50	DT	80/84 (95%)	60 (75%)	20 (25%)	1	7
51	BZ	67/68 (98%)	53 (79%)	14 (21%)	1	11
51	DZ	67/68 (98%)	53 (79%)	14 (21%)	1	11
52	BW	59/62 (95%)	42 (71%)	17 (29%)	0	4
52	DW	59/62 (95%)	42 (71%)	17 (29%)	0	4
All	All	9333/9700 (96%)	7661 (82%)	1672 (18%)	2	17

5 of 1672 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
48	BG	84	LYS
13	CP	28	ARG
46	DU	51	LEU
49	BR	66	HIS
3	CD	147	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 332 such sidechains are listed below:

Mol	Chain	Res	Type
47	BF	126	ASN
5	CF	17	GLN
46	DU	26	ASN
48	BG	127	GLN
3	CD	35	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1529/1542 (99%)	292 (19%)	25 (1%)
1	CA	1529/1542 (99%)	282 (18%)	21 (1%)
22	BA	116/120 (96%)	21 (18%)	1 (0%)
22	DA	116/120 (96%)	19 (16%)	1 (0%)
23	BB	2837/2904 (97%)	456 (16%)	18 (0%)
23	DB	2837/2904 (97%)	469 (16%)	20 (0%)
All	All	8964/9132 (98%)	1539 (17%)	86 (0%)

5 of 1539 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	7	A
1	AA	9	G
1	AA	14	U
1	AA	32	A
1	AA	39	G

5 of 86 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	BB	2425	A
1	CA	279	A
23	DB	2336	A
23	BB	2430	A
23	BB	2894	G

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 344 ligands modelled in this entry, 342 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
54	SCM	AA	1661	-	23,25,25	1.63	7 (30%)	22,39,39	0.99	1 (4%)
54	SCM	CA	1659	-	23,25,25	1.58	6 (26%)	22,39,39	1.07	1 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	SCM	AA	1661	-	-	0/4/57/57	0/3/3/3
54	SCM	CA	1659	-	-	0/4/57/57	0/3/3/3

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	CA	1659	SCM	O2B-C12	2.00	1.47	1.43
54	AA	1661	SCM	O5-C5	2.18	1.43	1.39
54	AA	1661	SCM	O2B-C12	2.18	1.47	1.43
54	CA	1659	SCM	C12-C7	2.22	1.57	1.52
54	CA	1659	SCM	C3-C4	2.23	1.54	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	CA	1659	SCM	C2M-C2-C3	-2.98	108.11	113.45
54	AA	1661	SCM	C2M-C2-C3	-2.77	108.49	113.45

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	AA	1661	SCM	2	0
54	CA	1659	SCM	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1530/1542 (99%)	-0.71	9 (0%) 90 86	12, 77, 142, 179	0
1	CA	1530/1542 (99%)	-0.70	2 (0%) 95 95	5, 57, 124, 180	0
2	AC	206/232 (88%)	0.25	16 (7%) 16 11	5, 70, 115, 162	0
2	CC	206/232 (88%)	0.55	29 (14%) 4 4	5, 71, 111, 150	0
3	AD	205/205 (100%)	-0.02	12 (5%) 26 17	5, 79, 127, 173	0
3	CD	205/205 (100%)	0.59	21 (10%) 9 7	5, 66, 125, 166	0
4	AE	150/166 (90%)	0.08	4 (2%) 58 46	5, 68, 122, 157	0
4	CE	150/166 (90%)	1.50	51 (34%) 0 1	5, 67, 121, 180	0
5	AF	100/135 (74%)	2.52	62 (62%) 0 1	10, 81, 133, 147	0
5	CF	100/135 (74%)	-0.44	0 100 100	5, 73, 131, 172	0
6	AG	150/178 (84%)	0.76	27 (18%) 2 2	16, 89, 125, 143	0
6	CG	152/178 (85%)	-0.51	0 100 100	6, 79, 125, 172	0
7	AH	129/129 (100%)	0.40	16 (12%) 5 5	19, 77, 130, 158	0
7	CH	129/129 (100%)	0.77	27 (20%) 1 2	5, 62, 116, 158	0
8	AI	127/129 (98%)	0.78	25 (19%) 1 2	6, 83, 117, 155	0
8	CI	127/129 (98%)	0.04	3 (2%) 62 50	5, 80, 122, 157	0
9	AJ	98/103 (95%)	0.51	4 (4%) 41 30	9, 79, 126, 147	0
9	CJ	98/103 (95%)	1.29	30 (30%) 1 1	16, 82, 113, 137	0
10	AK	117/128 (91%)	0.26	4 (3%) 49 37	5, 72, 117, 155	0
10	CK	117/128 (91%)	-0.51	0 100 100	5, 67, 123, 136	0
11	AL	123/123 (100%)	1.02	31 (25%) 1 1	6, 79, 123, 158	0
11	CL	123/123 (100%)	0.28	6 (4%) 33 24	5, 54, 103, 151	0
12	AM	114/117 (97%)	0.96	23 (20%) 1 2	23, 96, 137, 169	0
12	CM	113/117 (96%)	-0.19	5 (4%) 38 27	22, 96, 142, 162	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AP	82/82 (100%)	1.49	26 (31%) 1 1	15, 82, 130, 163	0
13	CP	80/82 (97%)	0.07	6 (7%) 17 12	5, 58, 126, 180	0
14	AQ	80/83 (96%)	1.26	24 (30%) 1 1	15, 92, 145, 154	0
14	CQ	81/83 (97%)	0.28	3 (3%) 45 34	5, 72, 119, 149	0
15	AR	55/74 (74%)	0.83	8 (14%) 3 4	5, 73, 129, 164	0
15	CR	55/74 (74%)	0.26	3 (5%) 29 20	5, 66, 127, 143	0
16	AS	79/91 (86%)	1.98	40 (50%) 0 1	52, 98, 142, 167	0
16	CS	80/91 (87%)	0.53	13 (16%) 2 3	41, 95, 133, 159	0
17	AT	85/86 (98%)	-0.65	0 100 100	19, 88, 126, 156	0
17	CT	85/86 (98%)	-0.25	1 (1%) 81 72	5, 66, 113, 154	0
18	AB	218/240 (90%)	-0.05	10 (4%) 36 26	12, 81, 120, 160	0
18	CB	218/240 (90%)	0.94	50 (22%) 1 1	5, 87, 133, 163	0
19	AU	51/70 (72%)	0.80	8 (15%) 3 3	20, 94, 139, 153	0
19	CU	51/70 (72%)	0.14	3 (5%) 26 17	57, 96, 137, 171	0
20	AO	88/89 (98%)	1.02	12 (13%) 4 4	5, 73, 118, 177	0
20	CO	88/89 (98%)	-0.45	0 100 100	5, 56, 108, 135	0
21	AN	96/100 (96%)	1.34	32 (33%) 0 1	5, 84, 128, 155	0
21	CN	96/100 (96%)	1.15	24 (25%) 1 1	5, 75, 129, 145	0
22	BA	117/120 (97%)	0.11	2 (1%) 73 62	35, 77, 125, 167	0
22	DA	117/120 (97%)	-0.50	1 (0%) 85 79	31, 87, 133, 176	0
23	BB	2841/2904 (97%)	-0.40	22 (0%) 87 82	5, 60, 136, 180	0
23	DB	2841/2904 (97%)	-0.46	22 (0%) 87 82	5, 51, 136, 180	0
24	BI	141/141 (100%)	2.65	69 (48%) 0 1	60, 135, 178, 180	0
24	DI	141/141 (100%)	1.31	38 (26%) 1 1	66, 135, 180, 180	0
25	BC	271/272 (99%)	1.42	89 (32%) 0 1	5, 61, 109, 132	0
25	DC	271/272 (99%)	0.82	54 (19%) 1 2	5, 45, 99, 144	0
26	BD	209/209 (100%)	0.51	29 (13%) 4 4	5, 71, 118, 148	0
26	DD	209/209 (100%)	0.92	37 (17%) 2 2	5, 60, 110, 168	0
27	BK	121/123 (98%)	2.09	65 (53%) 0 1	5, 75, 125, 159	0
27	DK	121/123 (98%)	1.06	27 (22%) 1 1	5, 45, 112, 150	0
28	BP	114/114 (100%)	1.55	47 (41%) 0 1	7, 82, 125, 155	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DP	114/114 (100%)	0.42	6 (5%) 30 22	5, 64, 118, 139	0
29	BE	201/201 (100%)	0.83	34 (16%) 2 3	5, 65, 128, 164	0
29	DE	201/201 (100%)	1.24	59 (29%) 1 1	5, 73, 123, 160	0
30	BY	58/58 (100%)	-0.23	1 (1%) 73 62	5, 75, 129, 160	0
30	DY	58/58 (100%)	-0.20	3 (5%) 31 23	5, 72, 116, 147	0
31	B0	56/56 (100%)	0.06	2 (3%) 46 35	5, 78, 118, 147	0
31	D0	56/56 (100%)	0.21	1 (1%) 71 61	5, 62, 129, 153	0
32	B4	38/38 (100%)	0.96	8 (21%) 1 2	27, 81, 131, 145	0
32	D4	38/38 (100%)	-0.32	0 100 100	5, 67, 106, 117	0
33	B1	50/54 (92%)	0.64	4 (8%) 15 10	17, 70, 120, 134	0
33	D1	50/54 (92%)	0.35	5 (10%) 9 7	17, 73, 116, 137	0
34	B3	64/64 (100%)	-0.20	1 (1%) 74 63	5, 68, 103, 129	0
34	D3	64/64 (100%)	1.36	21 (32%) 0 1	5, 55, 86, 122	0
35	BV	94/94 (100%)	0.65	13 (13%) 4 4	5, 81, 126, 152	0
35	DV	94/94 (100%)	0.96	23 (24%) 1 1	5, 88, 120, 160	0
36	B2	46/46 (100%)	0.79	5 (10%) 7 6	5, 53, 104, 141	0
36	D2	46/46 (100%)	1.64	20 (43%) 0 1	9, 48, 110, 141	0
37	BL	143/144 (99%)	-0.13	2 (1%) 78 68	5, 67, 121, 145	0
37	DL	143/144 (99%)	1.64	59 (41%) 0 1	5, 63, 111, 145	0
38	BM	136/136 (100%)	0.92	20 (14%) 3 3	7, 68, 121, 179	0
38	DM	136/136 (100%)	1.33	39 (28%) 1 1	5, 65, 117, 144	0
39	BX	63/63 (100%)	1.02	13 (20%) 1 2	16, 79, 128, 159	0
39	DX	63/63 (100%)	1.10	10 (15%) 3 3	16, 91, 144, 169	0
40	BH	149/149 (100%)	3.05	87 (58%) 0 1	7, 104, 149, 180	0
40	DH	149/149 (100%)	0.88	26 (17%) 2 2	5, 91, 131, 162	0
41	BJ	142/142 (100%)	0.96	29 (20%) 1 2	5, 77, 118, 140	0
41	DJ	142/142 (100%)	0.29	10 (7%) 19 13	5, 70, 119, 173	0
42	BN	120/127 (94%)	0.86	18 (15%) 3 3	5, 69, 111, 154	0
42	DN	120/127 (94%)	0.04	6 (5%) 32 24	5, 51, 94, 163	0
43	BO	116/117 (99%)	-0.06	7 (6%) 25 17	6, 80, 109, 172	0
43	DO	116/117 (99%)	0.92	21 (18%) 2 2	5, 83, 136, 158	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BQ	117/117 (100%)	-0.59	1 (0%) 85 79	5, 62, 115, 144	0
44	DQ	117/117 (100%)	0.48	12 (10%) 9 7	5, 60, 111, 154	0
45	BS	110/110 (100%)	0.41	9 (8%) 14 10	5, 62, 121, 148	0
45	DS	110/110 (100%)	1.43	36 (32%) 1 1	5, 64, 127, 156	0
46	BU	102/103 (99%)	0.86	16 (15%) 3 3	12, 80, 125, 157	0
46	DU	102/103 (99%)	-0.38	0 100 100	8, 94, 127, 149	0
47	BF	178/178 (100%)	0.75	33 (18%) 2 2	29, 100, 146, 180	0
47	DF	178/178 (100%)	2.24	88 (49%) 0 1	12, 93, 142, 163	0
48	BG	176/176 (100%)	0.78	32 (18%) 2 2	18, 94, 133, 171	0
48	DG	176/176 (100%)	0.42	24 (13%) 4 4	8, 90, 136, 166	0
49	BR	103/103 (100%)	-0.00	4 (3%) 43 32	5, 83, 123, 133	0
49	DR	103/103 (100%)	0.16	5 (4%) 33 24	10, 76, 135, 149	0
50	BT	93/100 (93%)	-0.05	2 (2%) 65 54	8, 83, 130, 165	0
50	DT	93/100 (93%)	2.28	51 (54%) 0 1	5, 84, 144, 172	0
51	BZ	77/78 (98%)	0.59	12 (15%) 3 3	5, 63, 120, 142	0
51	DZ	77/78 (98%)	0.04	1 (1%) 79 70	5, 56, 106, 120	0
52	BW	79/84 (94%)	0.48	6 (7%) 17 11	5, 75, 124, 180	0
52	DW	79/84 (94%)	0.71	9 (11%) 7 6	5, 71, 121, 166	0
All	All	20417/21046 (97%)	0.18	2066 (10%) 9 7	5, 70, 134, 180	0

The worst 5 of 2066 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
24	BI	17	ALA	14.5
23	BB	546	U	12.6
24	BI	18	ASN	12.5
40	BH	124	THR	12.3
24	BI	51	GLY	12.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
53	MG	CA	1612	1/1	0.84	0.28	10.75	93,93,93,93	0
53	MG	BB	3087	1/1	0.98	0.25	10.45	80,80,80,80	0
53	MG	CA	1654	1/1	0.91	0.22	4.60	105,105,105,105	0
53	MG	DB	3026	1/1	0.99	0.23	4.22	45,45,45,45	0
53	MG	CA	1656	1/1	0.99	0.14	2.00	38,38,38,38	0
53	MG	DB	3071	1/1	0.94	0.16	1.72	57,57,57,57	0
53	MG	DB	3097	1/1	0.99	0.17	1.64	41,41,41,41	0
53	MG	DB	3035	1/1	0.92	0.22	1.29	79,79,79,79	0
53	MG	BB	3001	1/1	0.92	0.19	1.19	5,5,5,5	0
53	MG	BB	3110	1/1	0.96	0.13	0.87	80,80,80,80	0
53	MG	DB	3030	1/1	0.97	0.19	0.72	47,47,47,47	0
53	MG	CA	1610	1/1	0.98	0.14	0.72	5,5,5,5	0
53	MG	DB	3089	1/1	0.96	0.13	0.49	79,79,79,79	0
53	MG	DB	3095	1/1	0.98	0.15	0.49	92,92,92,92	0
54	SCM	CA	1659	23/23	0.91	0.16	0.44	18,18,18,18	0
53	MG	CA	1621	1/1	0.98	0.16	0.41	80,80,80,80	0
53	MG	DB	3088	1/1	0.98	0.17	0.39	87,87,87,87	0
53	MG	BB	3098	1/1	0.97	0.15	0.25	14,14,14,14	0
53	MG	BB	3049	1/1	0.84	0.19	0.17	67,67,67,67	0
53	MG	BB	3011	1/1	0.98	0.15	0.07	5,5,5,5	0
53	MG	AA	1635	1/1	0.77	0.15	-0.02	80,80,80,80	0
54	SCM	AA	1661	23/23	0.97	0.10	-0.33	13,13,13,13	0
53	MG	DB	3069	1/1	0.97	0.23	-0.35	64,64,64,64	0
53	MG	DB	3010	1/1	0.97	0.14	-0.42	5,5,5,5	0
53	MG	DB	3077	1/1	0.98	0.13	-0.65	45,45,45,45	0
53	MG	DB	3102	1/1	0.99	0.23	-0.77	28,28,28,28	0
53	MG	AA	1643	1/1	0.98	0.09	-0.77	40,40,40,40	0
53	MG	DB	3007	1/1	0.97	0.12	-0.89	62,62,62,62	0
53	MG	DB	3047	1/1	0.98	0.15	-0.98	43,43,43,43	0
53	MG	DB	3109	1/1	0.94	0.04	-0.99	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	DB	3012	1/1	0.99	0.12	-1.02	9,9,9,9	0
53	MG	BB	3083	1/1	0.99	0.14	-1.03	30,30,30,30	0
53	MG	AA	1652	1/1	0.86	0.08	-1.08	84,84,84,84	0
53	MG	BB	3059	1/1	0.99	0.13	-1.08	10,10,10,10	0
53	MG	DB	3055	1/1	0.96	0.16	-1.09	44,44,44,44	0
53	MG	AA	1651	1/1	0.97	0.06	-1.12	35,35,35,35	0
53	MG	DB	3014	1/1	1.00	0.05	-1.12	21,21,21,21	0
53	MG	BB	3021	1/1	0.96	0.13	-1.12	52,52,52,52	0
53	MG	BB	3090	1/1	0.95	0.09	-1.14	88,88,88,88	0
53	MG	AA	1607	1/1	0.99	0.08	-1.17	57,57,57,57	0
53	MG	BB	3040	1/1	0.98	0.08	-1.22	12,12,12,12	0
53	MG	BB	3005	1/1	0.94	0.11	-1.22	5,5,5,5	0
53	MG	DB	3068	1/1	0.99	0.15	-1.24	5,5,5,5	0
53	MG	DB	3098	1/1	0.98	0.10	-1.24	5,5,5,5	0
55	ZN	D4	101	1/1	0.93	0.05	-1.26	62,62,62,62	0
53	MG	BB	3050	1/1	0.98	0.12	-1.29	53,53,53,53	0
53	MG	BB	3019	1/1	0.98	0.12	-1.40	21,21,21,21	0
53	MG	AA	1613	1/1	0.96	0.04	-1.46	58,58,58,58	0
53	MG	BB	3086	1/1	0.98	0.10	-1.54	5,5,5,5	0
53	MG	CA	1652	1/1	0.97	0.07	-1.57	49,49,49,49	0
55	ZN	B4	101	1/1	0.94	0.07	-1.64	67,67,67,67	0
53	MG	BB	3012	1/1	0.99	0.06	-1.65	67,67,67,67	0
53	MG	AA	1601	1/1	0.96	0.09	-1.68	36,36,36,36	0
53	MG	AA	1603	1/1	0.96	0.10	-1.73	57,57,57,57	0
53	MG	AA	1653	1/1	0.98	0.09	-1.75	21,21,21,21	0
53	MG	DB	3091	1/1	0.94	0.11	-1.82	90,90,90,90	0
53	MG	BB	3023	1/1	0.95	0.10	-1.90	5,5,5,5	0
53	MG	CA	1604	1/1	0.95	0.10	-1.96	20,20,20,20	0
53	MG	AA	1638	1/1	0.97	0.07	-1.98	51,51,51,51	0
53	MG	DB	3003	1/1	0.95	0.05	-1.98	30,30,30,30	0
53	MG	DB	3084	1/1	0.99	0.09	-2.04	29,29,29,29	0
53	MG	DB	3006	1/1	0.98	0.11	-2.09	10,10,10,10	0
53	MG	AA	1630	1/1	0.98	0.04	-2.16	88,88,88,88	0
53	MG	BB	3069	1/1	0.95	0.07	-2.22	5,5,5,5	0
53	MG	DB	3075	1/1	0.98	0.11	-2.26	44,44,44,44	0
53	MG	CA	1605	1/1	0.95	0.05	-2.27	12,12,12,12	0
53	MG	CA	1611	1/1	0.99	0.07	-2.27	28,28,28,28	0
53	MG	CA	1633	1/1	0.96	0.06	-2.29	23,23,23,23	0
53	MG	DB	3083	1/1	0.98	0.08	-2.30	27,27,27,27	0
53	MG	AA	1633	1/1	0.92	0.05	-2.30	65,65,65,65	0
53	MG	DB	3086	1/1	0.98	0.12	-2.30	18,18,18,18	0
53	MG	DB	3051	1/1	0.95	0.11	-2.35	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	AA	1629	1/1	0.97	0.06	-2.43	12,12,12,12	0
53	MG	AA	1609	1/1	0.98	0.06	-2.44	40,40,40,40	0
53	MG	BB	3085	1/1	0.99	0.07	-2.51	34,34,34,34	0
53	MG	BB	3035	1/1	0.88	0.07	-2.54	13,13,13,13	0
53	MG	BB	3062	1/1	0.98	0.08	-2.54	7,7,7,7	0
53	MG	CA	1636	1/1	1.00	0.04	-2.60	5,5,5,5	0
53	MG	DB	3107	1/1	0.99	0.04	-2.77	5,5,5,5	0
53	MG	DB	3067	1/1	0.94	0.06	-2.78	5,5,5,5	0
53	MG	BB	3096	1/1	0.97	0.07	-2.79	58,58,58,58	0
53	MG	BB	3079	1/1	0.94	0.07	-2.85	38,38,38,38	0
53	MG	DB	3044	1/1	0.98	0.05	-2.85	18,18,18,18	0
53	MG	DB	3056	1/1	0.98	0.06	-2.90	5,5,5,5	0
53	MG	BB	3081	1/1	0.92	0.10	-3.02	30,30,30,30	0
53	MG	CA	1624	1/1	0.99	0.07	-3.15	38,38,38,38	0
53	MG	DB	3087	1/1	0.98	0.08	-3.22	5,5,5,5	0
53	MG	BB	3066	1/1	0.99	0.04	-3.28	5,5,5,5	0
53	MG	BB	3094	1/1	0.98	0.06	-3.35	36,36,36,36	0
53	MG	BB	3065	1/1	0.97	0.06	-3.39	32,32,32,32	0
53	MG	BB	3013	1/1	0.97	0.10	-3.40	45,45,45,45	0
53	MG	BB	3103	1/1	0.98	0.08	-3.51	11,11,11,11	0
53	MG	CA	1655	1/1	0.99	0.03	-3.64	32,32,32,32	0
53	MG	BB	3108	1/1	0.93	0.06	-3.77	10,10,10,10	0
53	MG	BB	3088	1/1	0.96	0.06	-3.80	11,11,11,11	0
53	MG	DB	3009	1/1	0.98	0.07	-4.03	9,9,9,9	0
53	MG	CA	1627	1/1	0.92	0.07	-4.29	27,27,27,27	0
53	MG	DB	3019	1/1	0.98	0.06	-4.46	5,5,5,5	0
53	MG	BB	3002	1/1	0.98	0.06	-4.58	23,23,23,23	0
53	MG	AA	1654	1/1	0.95	0.07	-4.58	67,67,67,67	0
53	MG	BB	3056	1/1	0.98	0.03	-4.65	5,5,5,5	0
53	MG	DB	3002	1/1	0.98	0.05	-4.69	11,11,11,11	0
53	MG	DB	3034	1/1	0.91	0.08	-4.82	57,57,57,57	0
53	MG	DB	3079	1/1	0.97	0.06	-4.90	7,7,7,7	0
53	MG	CA	1601	1/1	0.98	0.06	-4.90	5,5,5,5	0
53	MG	AA	1610	1/1	0.99	0.06	-5.07	78,78,78,78	0
53	MG	CA	1635	1/1	0.98	0.06	-5.10	30,30,30,30	0
53	MG	AA	1619	1/1	0.97	0.04	-5.42	111,111,111,111	0
53	MG	AA	1641	1/1	0.99	0.02	-5.59	32,32,32,32	0
53	MG	BB	3074	1/1	0.98	0.06	-5.61	10,10,10,10	0
53	MG	BB	3029	1/1	0.99	0.05	-5.65	5,5,5,5	0
53	MG	BB	3048	1/1	0.98	0.04	-6.58	12,12,12,12	0
53	MG	BB	3032	1/1	0.96	0.07	-9.10	22,22,22,22	0
53	MG	DB	3001	1/1	0.96	0.06	-10.06	5,5,5,5	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	BB	3064	1/1	0.94	0.19	-	78,78,78,78	0
53	MG	DB	3096	1/1	0.95	0.11	-	26,26,26,26	0
53	MG	DB	3060	1/1	0.95	0.12	-	83,83,83,83	0
53	MG	DB	3070	1/1	0.98	0.06	-	33,33,33,33	0
53	MG	DB	3020	1/1	0.98	0.09	-	5,5,5,5	0
53	MG	BB	3076	1/1	0.96	0.12	-	35,35,35,35	0
53	MG	DB	3072	1/1	0.98	0.07	-	20,20,20,20	0
53	MG	DB	3101	1/1	0.99	0.10	-	26,26,26,26	0
53	MG	BB	3101	1/1	1.00	0.05	-	19,19,19,19	0
53	MG	BB	3099	1/1	0.95	0.06	-	41,41,41,41	0
53	MG	DB	3018	1/1	0.95	0.09	-	7,7,7,7	0
53	MG	BB	3106	1/1	0.98	0.12	-	10,10,10,10	0
53	MG	BB	3057	1/1	0.96	0.16	-	53,53,53,53	0
53	MG	DB	3046	1/1	0.98	0.04	-	23,23,23,23	0
53	MG	CA	1631	1/1	0.95	0.04	-	41,41,41,41	0
53	MG	BB	3037	1/1	0.87	0.13	-	45,45,45,45	0
53	MG	CE	201	1/1	0.92	0.08	-	109,109,109,109	0
53	MG	AA	1636	1/1	0.98	0.04	-	64,64,64,64	0
53	MG	CA	1637	1/1	0.94	0.17	-	98,98,98,98	0
53	MG	BB	3073	1/1	0.99	0.10	-	44,44,44,44	0
53	MG	AA	1602	1/1	0.93	0.13	-	85,85,85,85	0
53	MG	BB	3063	1/1	0.99	0.05	-	33,33,33,33	0
53	MG	DB	3100	1/1	0.96	0.17	-	19,19,19,19	0
53	MG	DB	3066	1/1	0.89	0.33	-	65,65,65,65	0
53	MG	DB	3008	1/1	0.98	0.06	-	13,13,13,13	0
53	MG	BB	3053	1/1	0.97	0.09	-	60,60,60,60	0
53	MG	DB	3092	1/1	0.98	0.15	-	10,10,10,10	0
53	MG	AA	1627	1/1	0.91	0.07	-	63,63,63,63	0
53	MG	AA	1655	1/1	0.89	0.14	-	88,88,88,88	0
53	MG	DB	3028	1/1	0.95	0.18	-	70,70,70,70	0
53	MG	AA	1648	1/1	0.99	0.06	-	6,6,6,6	0
53	MG	BB	3003	1/1	0.95	0.06	-	53,53,53,53	0
53	MG	DB	3062	1/1	0.98	0.23	-	58,58,58,58	0
53	MG	DB	3064	1/1	0.93	0.39	-	49,49,49,49	0
53	MG	AA	1615	1/1	0.96	0.35	-	96,96,96,96	0
53	MG	BB	3093	1/1	0.88	0.10	-	108,108,108,108	0
53	MG	DB	3054	1/1	0.97	0.15	-	21,21,21,21	0
53	MG	CA	1625	1/1	0.94	0.05	-	70,70,70,70	0
53	MG	DB	3073	1/1	0.99	0.07	-	50,50,50,50	0
53	MG	AA	1622	1/1	0.70	0.34	-	130,130,130,130	0
53	MG	DB	3057	1/1	0.97	0.05	-	48,48,48,48	0
53	MG	BB	3084	1/1	0.97	0.06	-	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	DB	3065	1/1	0.95	0.07	-	128,128,128,128	0
53	MG	AA	1625	1/1	0.82	0.39	-	79,79,79,79	1
53	MG	AA	1659	1/1	0.97	0.39	-	108,108,108,108	0
53	MG	AA	1616	1/1	0.97	0.09	-	5,5,5,5	0
53	MG	AA	1644	1/1	0.98	0.05	-	75,75,75,75	0
53	MG	DB	3090	1/1	0.98	0.09	-	14,14,14,14	0
53	MG	BB	3042	1/1	0.60	0.23	-	92,92,92,92	0
53	MG	BB	3100	1/1	0.97	0.20	-	116,116,116,116	0
53	MG	DB	3017	1/1	0.98	0.23	-	5,5,5,5	0
53	MG	DB	3032	1/1	0.90	0.16	-	73,73,73,73	0
53	MG	DB	3045	1/1	0.88	0.11	-	110,110,110,110	0
53	MG	DB	3022	1/1	0.94	0.06	-	11,11,11,11	0
53	MG	CA	1649	1/1	0.90	0.27	-	123,123,123,123	0
53	MG	BB	3022	1/1	0.98	0.12	-	32,32,32,32	0
53	MG	CA	1650	1/1	0.83	0.09	-	105,105,105,105	0
53	MG	BB	3039	1/1	0.97	0.15	-	41,41,41,41	0
53	MG	DB	3025	1/1	0.99	0.07	-	44,44,44,44	0
53	MG	CA	1617	1/1	0.93	0.18	-	88,88,88,88	0
53	MG	DB	3027	1/1	0.96	0.07	-	13,13,13,13	0
53	MG	DB	3104	1/1	0.92	0.12	-	29,29,29,29	0
53	MG	BB	3030	1/1	0.97	0.07	-	51,51,51,51	0
53	MG	BB	3007	1/1	0.98	0.14	-	68,68,68,68	0
53	MG	BB	3071	1/1	0.94	0.18	-	68,68,68,68	0
53	MG	CA	1645	1/1	0.92	0.10	-	55,55,55,55	0
53	MG	DB	3043	1/1	0.98	0.06	-	7,7,7,7	0
53	MG	AA	1647	1/1	0.85	0.82	-	113,113,113,113	0
53	MG	DB	3037	1/1	0.99	0.16	-	8,8,8,8	0
53	MG	BB	3051	1/1	0.91	0.13	-	107,107,107,107	0
53	MG	CA	1614	1/1	0.98	0.16	-	83,83,83,83	0
53	MG	BB	3058	1/1	0.99	0.06	-	15,15,15,15	0
53	MG	DB	3016	1/1	0.94	0.08	-	5,5,5,5	0
53	MG	BB	3041	1/1	0.99	0.08	-	5,5,5,5	0
53	MG	BB	3070	1/1	0.96	0.05	-	74,74,74,74	0
53	MG	CA	1638	1/1	0.97	0.10	-	86,86,86,86	0
53	MG	DB	3033	1/1	0.98	0.04	-	11,11,11,11	0
53	MG	BB	3044	1/1	0.98	0.09	-	45,45,45,45	0
53	MG	DB	3082	1/1	0.97	0.11	-	83,83,83,83	0
53	MG	CA	1623	1/1	0.96	0.10	-	11,11,11,11	0
53	MG	CA	1619	1/1	0.98	0.09	-	36,36,36,36	0
53	MG	DB	3052	1/1	0.77	0.29	-	105,105,105,105	0
53	MG	BB	3010	1/1	0.90	0.16	-	53,53,53,53	0
53	MG	AA	1618	1/1	0.95	0.08	-	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	DB	3094	1/1	0.79	0.14	-	100,100,100,100	0
53	MG	BB	3016	1/1	0.99	0.04	-	55,55,55,55	0
53	MG	BB	3061	1/1	0.98	0.08	-	24,24,24,24	0
53	MG	AA	1657	1/1	0.91	0.34	-	91,91,91,91	0
53	MG	DB	3105	1/1	0.99	0.04	-	40,40,40,40	0
53	MG	CA	1642	1/1	0.99	0.07	-	79,79,79,79	0
53	MG	DB	3074	1/1	0.98	0.07	-	26,26,26,26	0
53	MG	DB	3059	1/1	0.81	0.11	-	99,99,99,99	0
53	MG	DB	3011	1/1	0.99	0.10	-	5,5,5,5	0
53	MG	DB	3063	1/1	0.90	0.17	-	72,72,72,72	0
53	MG	AA	1639	1/1	0.98	0.04	-	93,93,93,93	0
53	MG	BB	3047	1/1	0.98	0.11	-	104,104,104,104	0
53	MG	AA	1631	1/1	0.97	0.12	-	5,5,5,5	0
53	MG	BB	3008	1/1	0.94	0.12	-	82,82,82,82	0
53	MG	BB	3036	1/1	0.96	0.20	-	51,51,51,51	0
53	MG	DB	3038	1/1	0.99	0.07	-	5,5,5,5	0
53	MG	AA	1604	1/1	0.99	0.09	-	38,38,38,38	0
53	MG	DB	3106	1/1	0.97	0.05	-	61,61,61,61	0
53	MG	CA	1613	1/1	0.88	0.49	-	126,126,126,126	0
53	MG	BB	3055	1/1	0.99	0.12	-	6,6,6,6	0
53	MG	BB	3034	1/1	0.96	0.12	-	86,86,86,86	0
53	MG	DB	3076	1/1	0.99	0.10	-	33,33,33,33	0
53	MG	CA	1644	1/1	0.86	0.14	-	57,57,57,57	0
53	MG	BB	3009	1/1	0.89	0.10	-	98,98,98,98	0
53	MG	DB	3050	1/1	0.92	0.11	-	80,80,80,80	0
53	MG	BB	3006	1/1	0.96	0.15	-	61,61,61,61	0
53	MG	BB	3068	1/1	0.90	0.19	-	13,13,13,13	0
53	MG	AA	1649	1/1	0.90	0.04	-	89,89,89,89	0
53	MG	CA	1646	1/1	0.82	0.11	-	139,139,139,139	0
53	MG	AA	1640	1/1	0.98	0.15	-	46,46,46,46	0
53	MG	AA	1612	1/1	0.91	0.08	-	61,61,61,61	0
53	MG	BB	3045	1/1	0.98	0.14	-	72,72,72,72	0
53	MG	CA	1634	1/1	0.91	0.11	-	74,74,74,74	0
53	MG	BB	3102	1/1	0.97	0.12	-	43,43,43,43	0
53	MG	AA	1634	1/1	0.99	0.03	-	72,72,72,72	0
53	MG	CA	1603	1/1	0.99	0.03	-	56,56,56,56	0
53	MG	BB	3015	1/1	0.95	0.10	-	25,25,25,25	0
53	MG	CA	1615	1/1	0.95	0.06	-	13,13,13,13	0
53	MG	CA	1626	1/1	0.98	0.08	-	8,8,8,8	0
53	MG	DB	3024	1/1	0.98	0.05	-	40,40,40,40	0
53	MG	BB	3107	1/1	0.99	0.21	-	46,46,46,46	0
53	MG	DB	3031	1/1	0.97	0.09	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	CA	1658	1/1	0.96	0.08	-	37,37,37,37	0
53	MG	DB	3041	1/1	0.96	0.08	-	40,40,40,40	0
53	MG	BB	3077	1/1	0.98	0.11	-	53,53,53,53	0
53	MG	AA	1645	1/1	0.94	0.20	-	70,70,70,70	0
53	MG	CA	1618	1/1	0.83	0.13	-	73,73,73,73	0
53	MG	DB	3015	1/1	0.99	0.06	-	42,42,42,42	0
53	MG	DB	3029	1/1	0.86	0.70	-	87,87,87,87	0
53	MG	BB	3072	1/1	0.99	0.10	-	35,35,35,35	0
53	MG	CA	1643	1/1	0.98	0.06	-	36,36,36,36	0
53	MG	BB	3075	1/1	0.97	0.09	-	40,40,40,40	0
53	MG	BB	3046	1/1	0.91	0.10	-	89,89,89,89	0
53	MG	BB	3078	1/1	0.95	0.19	-	27,27,27,27	0
53	MG	DB	3023	1/1	0.99	0.04	-	69,69,69,69	0
53	MG	CA	1606	1/1	0.88	0.14	-	106,106,106,106	0
53	MG	BB	3095	1/1	0.97	0.07	-	62,62,62,62	0
53	MG	DB	3021	1/1	0.99	0.04	-	16,16,16,16	0
53	MG	DB	3036	1/1	0.98	0.04	-	87,87,87,87	0
53	MG	CA	1608	1/1	0.91	0.05	-	76,76,76,76	0
53	MG	CA	1647	1/1	0.97	0.06	-	75,75,75,75	0
53	MG	DB	3080	1/1	0.99	0.10	-	62,62,62,62	0
53	MG	AA	1623	1/1	0.83	0.36	-	33,33,33,33	1
53	MG	BB	3026	1/1	0.98	0.10	-	65,65,65,65	0
53	MG	BB	3025	1/1	0.95	0.15	-	30,30,30,30	0
53	MG	BB	3020	1/1	0.94	0.31	-	6,6,6,6	0
53	MG	DB	3048	1/1	0.98	0.11	-	38,38,38,38	0
53	MG	DB	3040	1/1	0.99	0.05	-	5,5,5,5	0
53	MG	DB	3085	1/1	0.98	0.05	-	38,38,38,38	0
53	MG	DB	3099	1/1	0.98	0.13	-	58,58,58,58	0
53	MG	CA	1632	1/1	0.93	0.24	-	76,76,76,76	0
53	MG	AA	1646	1/1	0.85	0.10	-	84,84,84,84	0
53	MG	AA	1628	1/1	0.94	0.18	-	70,70,70,70	0
53	MG	AA	1642	1/1	0.90	0.13	-	49,49,49,49	0
53	MG	AA	1621	1/1	0.94	0.17	-	36,36,36,36	0
53	MG	DB	3053	1/1	0.95	0.07	-	65,65,65,65	0
53	MG	AA	1660	1/1	0.96	0.03	-	56,56,56,56	0
53	MG	DB	3061	1/1	0.98	0.04	-	66,66,66,66	0
53	MG	DB	3058	1/1	0.77	0.09	-	139,139,139,139	0
53	MG	DB	3004	1/1	0.98	0.08	-	8,8,8,8	0
53	MG	AA	1611	1/1	0.99	0.05	-	43,43,43,43	0
53	MG	DB	3049	1/1	1.00	0.14	-	42,42,42,42	0
53	MG	BB	3017	1/1	0.96	0.13	-	50,50,50,50	0
53	MG	BB	3067	1/1	0.97	0.17	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	CA	1641	1/1	0.96	0.10	-	42,42,42,42	0
53	MG	BB	3080	1/1	0.88	0.16	-	53,53,53,53	0
53	MG	CA	1629	1/1	0.91	0.17	-	67,67,67,67	0
53	MG	AA	1656	1/1	0.92	0.14	-	87,87,87,87	0
53	MG	BB	3038	1/1	0.96	0.07	-	92,92,92,92	0
53	MG	BB	3097	1/1	0.59	0.07	-	113,113,113,113	0
53	MG	BB	3089	1/1	0.98	0.12	-	72,72,72,72	0
53	MG	AA	1617	1/1	0.89	0.09	-	112,112,112,112	0
53	MG	DB	3110	1/1	0.95	0.12	-	84,84,84,84	0
53	MG	CA	1602	1/1	0.99	0.12	-	5,5,5,5	0
53	MG	CA	1609	1/1	0.92	0.10	-	85,85,85,85	0
53	MG	CA	1639	1/1	0.98	0.05	-	35,35,35,35	0
53	MG	CA	1657	1/1	0.99	0.05	-	73,73,73,73	0
53	MG	CA	1653	1/1	0.97	0.07	-	48,48,48,48	0
53	MG	AA	1608	1/1	0.56	0.13	-	123,123,123,123	0
53	MG	DB	3078	1/1	0.97	0.04	-	25,25,25,25	0
53	MG	AA	1624	1/1	0.70	0.24	-	83,83,83,83	0
53	MG	BB	3033	1/1	0.80	0.34	-	102,102,102,102	0
53	MG	AA	1632	1/1	0.96	0.22	-	96,96,96,96	0
53	MG	BB	3092	1/1	0.95	0.09	-	46,46,46,46	0
53	MG	CA	1640	1/1	0.84	0.11	-	62,62,62,62	0
53	MG	DN	201	1/1	0.92	0.51	-	145,145,145,145	0
53	MG	BB	3014	1/1	0.92	0.07	-	37,37,37,37	0
53	MG	CA	1630	1/1	0.99	0.10	-	37,37,37,37	0
53	MG	BB	3018	1/1	0.98	0.12	-	39,39,39,39	0
53	MG	BB	3031	1/1	0.97	0.18	-	60,60,60,60	0
53	MG	BB	3043	1/1	0.92	0.12	-	107,107,107,107	0
53	MG	CA	1651	1/1	0.85	0.08	-	101,101,101,101	0
53	MG	CA	1622	1/1	0.99	0.18	-	5,5,5,5	0
53	MG	CA	1648	1/1	0.88	0.07	-	104,104,104,104	0
53	MG	DB	3108	1/1	0.95	0.10	-	43,43,43,43	0
53	MG	BB	3105	1/1	0.99	0.18	-	5,5,5,5	0
53	MG	DB	3005	1/1	0.93	0.17	-	25,25,25,25	0
53	MG	BB	3082	1/1	0.97	0.15	-	18,18,18,18	0
53	MG	AA	1637	1/1	0.88	0.32	-	99,99,99,99	0
53	MG	CA	1628	1/1	0.92	0.11	-	52,52,52,52	0
53	MG	AA	1620	1/1	0.79	0.06	-	60,60,60,60	0
53	MG	DB	3081	1/1	0.99	0.06	-	41,41,41,41	0
53	MG	BB	3004	1/1	0.92	0.05	-	80,80,80,80	0
53	MG	DB	3039	1/1	0.98	0.08	-	62,62,62,62	0
53	MG	DB	3013	1/1	0.88	0.08	-	52,52,52,52	0
53	MG	AA	1614	1/1	0.84	0.18	-	119,119,119,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	CA	1607	1/1	0.97	0.06	-	5,5,5,5	0
53	MG	DB	3042	1/1	0.99	0.04	-	37,37,37,37	0
53	MG	BB	3028	1/1	0.99	0.24	-	9,9,9,9	0
53	MG	DB	3103	1/1	0.96	0.06	-	36,36,36,36	0
53	MG	AA	1605	1/1	0.92	0.10	-	50,50,50,50	0
53	MG	BB	3024	1/1	0.96	0.09	-	55,55,55,55	0
53	MG	BB	3091	1/1	0.98	0.10	-	5,5,5,5	0
53	MG	AA	1606	1/1	0.89	0.06	-	82,82,82,82	0
53	MG	BB	3109	1/1	0.98	0.10	-	11,11,11,11	0
53	MG	BB	3060	1/1	0.99	0.17	-	30,30,30,30	0
53	MG	CA	1620	1/1	0.99	0.10	-	72,72,72,72	0
53	MG	BB	3054	1/1	0.96	0.13	-	49,49,49,49	0
53	MG	AA	1658	1/1	0.94	0.04	-	120,120,120,120	0
53	MG	BB	3052	1/1	0.96	0.10	-	71,71,71,71	0
53	MG	DB	3093	1/1	0.98	0.05	-	59,59,59,59	0
53	MG	CA	1616	1/1	0.90	0.33	-	58,58,58,58	1
53	MG	BB	3104	1/1	0.95	0.17	-	26,26,26,26	0
53	MG	BB	3027	1/1	0.97	0.06	-	50,50,50,50	0
53	MG	AA	1626	1/1	0.88	0.20	-	36,36,36,36	1
53	MG	AA	1650	1/1	0.92	0.08	-	94,94,94,94	0

6.5 Other polymers

There are no such residues in this entry.