



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:36 PM GMT

PDB ID : 4V4Q
Title : Crystal structure of the bacterial ribosome from Escherichia coli at 3.5 Å resolution.
Authors : Schuwirth, B.S.; Borovinskaya, M.A.; Hau, C.W.; Zhang, W.; Vila-Sanjurjo, A.; Holton, J.M.; Cate, J.H.D.
Deposited on : 2005-08-30
Resolution : 3.46 Å(reported)

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

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

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

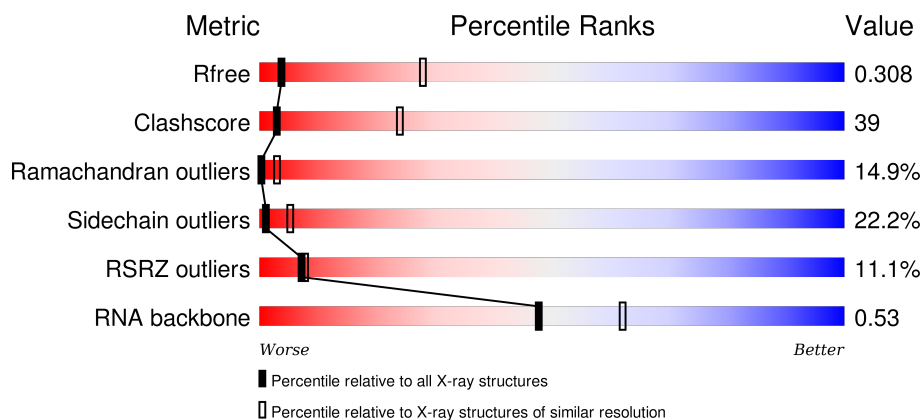
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.46 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	1000 (3.56-3.36)
Clashscore	102246	1090 (3.56-3.36)
Ramachandran outliers	100387	1057 (3.56-3.36)
Sidechain outliers	100360	1058 (3.56-3.36)
RSRZ outliers	91569	1005 (3.56-3.36)
RNA backbone	2183	1045 (4.10-2.80)

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>3%</div> <div>25%</div> <div>59%</div> <div>14%</div> <div>.</div> </div>
1	CA	1542	<div> <div>3%</div> <div>26%</div> <div>60%</div> <div>13%</div> <div>..</div> </div>
2	AC	232	<div> <div>3%</div> <div>26%</div> <div>49%</div> <div>13%</div> <div>.</div> <div>11%</div> </div>
2	CC	232	<div> <div>3%</div> <div>27%</div> <div>50%</div> <div>12%</div> <div>11%</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	AN	100	
13	CN	100	
14	AO	89	
14	CO	89	
15	AP	82	

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Mol	Chain	Length	Quality of chain
15	CP	82	
16	AQ	83	
16	CQ	83	
17	AR	74	
17	CR	74	
18	AS	91	
18	CS	91	
19	AT	86	
19	CT	86	
20	AB	240	
20	CB	240	
21	AU	71	
21	CU	71	
22	BA	120	
22	DA	120	
23	BB	2904	
23	DB	2904	
24	BV	94	
24	DV	94	
25	BC	273	
25	DC	273	
26	BD	209	
26	DD	209	
27	BE	201	
27	DE	201	

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Mol	Chain	Length	Quality of chain
28	BF	178	
28	DF	178	
29	BG	176	
29	DG	176	
30	BH	149	
30	DH	149	
31	BJ	142	
31	DJ	142	
32	BK	123	
32	DK	123	
33	BL	144	
33	DL	144	
34	BM	136	
34	DM	136	
35	BN	127	
35	DN	127	
36	BO	117	
36	DO	117	
37	BP	114	
37	DP	114	
38	BQ	117	
38	DQ	117	
39	BR	103	
39	DR	103	
40	BS	110	

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Mol	Chain	Length	Quality of chain
40	DS	110	
41	BT	100	
41	DT	100	
42	BU	103	
42	DU	103	
43	BW	84	
43	DW	84	
44	BX	63	
44	DX	63	
45	BY	58	
45	DY	58	
46	BZ	70	
46	DZ	70	
47	B0	56	
47	D0	56	
48	B1	54	
48	D1	54	
49	B2	46	
49	D2	46	
50	B3	64	
50	D3	64	
51	B4	38	
51	D4	38	
52	BI	141	
52	DI	141	

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	AA	1656	-	-	-	X

2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 284107 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

- Molecule 2 is a 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 S14.

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

- Molecule 14 is a protein called 30S ribosomal protein S15.

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

- Molecule 15 is a protein called 30S ribosomal protein S16.

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

- Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AQ	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			
16	CQ	81	Total	C	N	O	S	0	0	0
			656	417	122	114	3			

- Molecule 17 is a protein called 30S ribosomal protein S18.

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

- Molecule 18 is a protein called 30S ribosomal protein S19.

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

- Molecule 19 is a protein called 30S ribosomal protein S20.

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

- Molecule 20 is a protein called 30S ribosomal protein S2.

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

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

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

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

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			

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

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			

- Molecule 24 is a protein called 50S ribosomal protein L25.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BC	267	Total	C	N	O	S	0	0	0
			2053	1271	416	359	7			
25	DC	267	Total	C	N	O	S	0	0	0
			2053	1271	416	359	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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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 L4.

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

- Molecule 28 is a protein called 50S ribosomal protein L5.

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

- Molecule 29 is a protein called 50S ribosomal protein L6.

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

- Molecule 30 is a protein called 50S ribosomal protein L9.

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

- Molecule 31 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BJ	140	Total	C	N	O	S	0	0	0
			1112	704	210	194	4			
31	DJ	140	Total	C	N	O	S	0	0	0
			1112	704	210	194	4			

- Molecule 32 is a protein called 50S ribosomal protein L14.

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

- Molecule 33 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BL	144	Total	C	N	O	S	0	0	0
			1053	654	207	190	2			
33	DL	144	Total	C	N	O	S	0	0	0
			1053	654	207	190	2			

- Molecule 34 is a protein called 50S ribosomal protein L16.

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

- Molecule 35 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BN	127	Total	C	N	O	S	0	0	0
			1008	621	204	178	5			
35	DN	127	Total	C	N	O	S	0	0	0
			1008	621	204	178	5			

- Molecule 36 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BO	117	Total	C	N	O	S	0	0	0
			900	557	179	163	1			
36	DO	117	Total	C	N	O	S	0	0	0
			900	557	179	163	1			

- Molecule 37 is a protein called 50S ribosomal protein L19.

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

- Molecule 38 is a protein called 50S ribosomal protein L20.

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

- Molecule 39 is a protein called 50S ribosomal protein L21.

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

- Molecule 40 is a protein called 50S ribosomal protein L22.

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

- Molecule 41 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BT	99	Total	C	N	O	S	0	0	0
			777	491	145	139	2			
41	DT	99	Total	C	N	O	S	0	0	0
			777	491	145	139	2			

- Molecule 42 is a protein called 50S ribosomal protein L24.

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

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

- Molecule 43 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BW	84	Total	C	N	O	S			
			634	391	129	113	1	0	0	0
43	DW	84	Total	C	N	O	S			
			634	391	129	113	1	0	0	0

- Molecule 44 is a protein called 50S ribosomal protein L29.

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

- Molecule 45 is a protein called 50S ribosomal protein L30.

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

- Molecule 46 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BZ	70	Total	C	N	O	S			
			549	339	104	100	6	0	0	0
46	DZ	70	Total	C	N	O	S			
			549	339	104	100	6	0	0	0

- Molecule 47 is a protein called 50S ribosomal protein L32.

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

- Molecule 48 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
48	B1	54	Total	C	N	O	0	0	0
			441	284	81	76			
48	D1	54	Total	C	N	O	0	0	0
			441	284	81	76			

- Molecule 49 is a protein called 50S ribosomal protein L34.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L36.

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

- Molecule 52 is a protein called 50S ribosomal protein L11.

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
53	AP	1	Total Mg 1 1	0	0
53	BB	110	Total Mg 110 110	0	0
53	CA	62	Total Mg 62 62	0	0
53	AA	59	Total Mg 59 59	0	0
53	DN	1	Total Mg 1 1	0	0
53	DB	110	Total Mg 110 110	0	0

- Molecule 54 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	AA	290	Total O 290 290	0	0
54	AE	3	Total O 3 3	0	0
54	AK	2	Total O 2 2	0	0
54	AN	4	Total O 4 4	0	0
54	AP	1	Total O 1 1	0	0
54	BB	497	Total O 497 497	0	0
54	BC	1	Total O 1 1	0	0
54	BE	5	Total O 5 5	0	0
54	BH	1	Total O 1 1	0	0
54	BL	2	Total O 2 2	0	0
54	BN	1	Total O 1 1	0	0
54	CA	295	Total O 295 295	0	0
54	CE	3	Total O 3 3	0	0
54	CK	1	Total O 1 1	0	0

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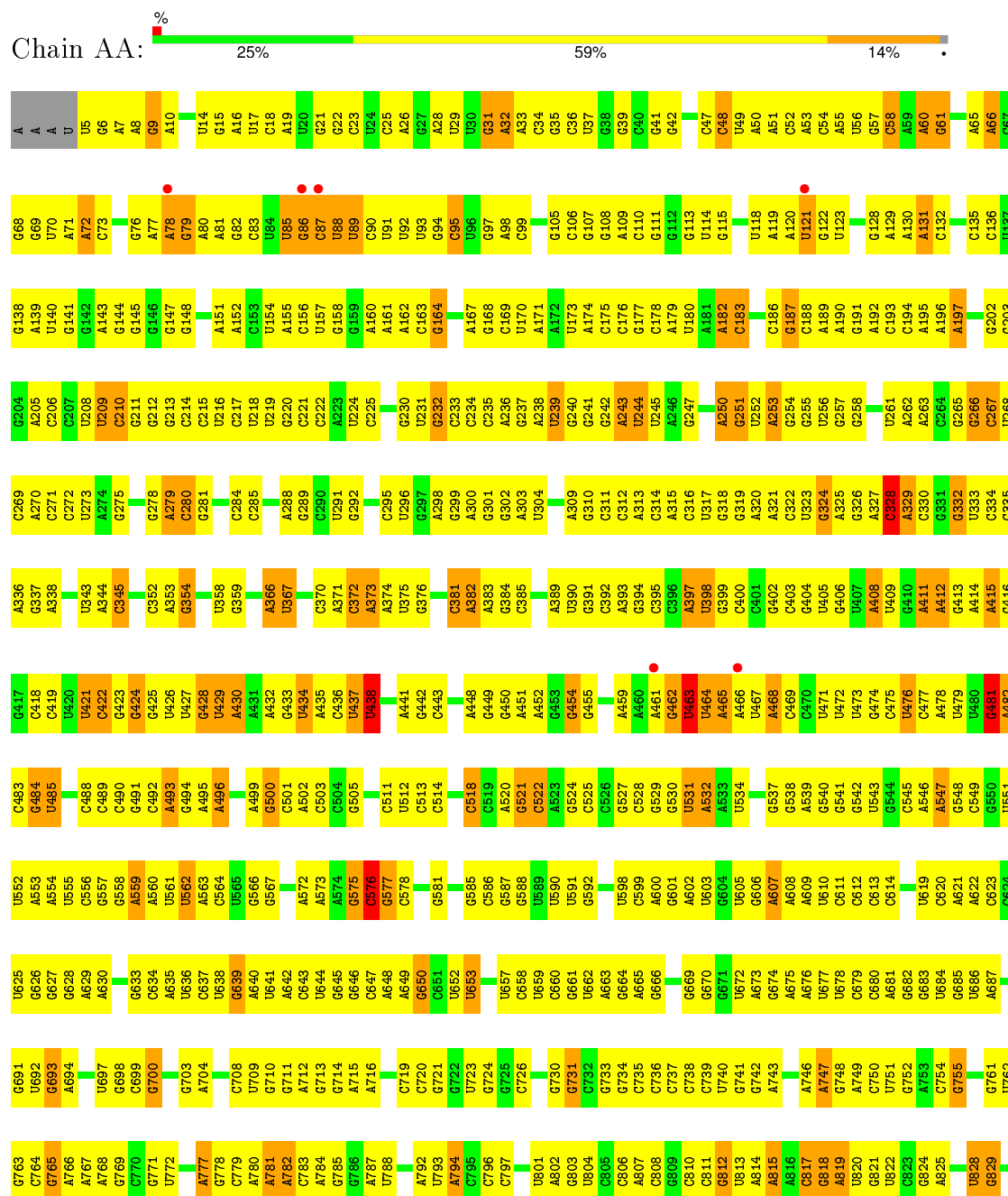
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	CL	4	Total 4	O 4	0	0
54	CN	2	Total 2	O 2	0	0
54	CP	1	Total 1	O 1	0	0
54	CT	2	Total 2	O 2	0	0
54	DB	499	Total 499	O 499	0	0
54	DC	1	Total 1	O 1	0	0
54	DD	1	Total 1	O 1	0	0
54	DE	3	Total 3	O 3	0	0
54	DJ	2	Total 2	O 2	0	0
54	DL	1	Total 1	O 1	0	0
54	DN	2	Total 2	O 2	0	0
54	DQ	1	Total 1	O 1	0	0
54	D2	2	Total 2	O 2	0	0

3 Residue-property plots

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

- Molecule 1: 16S ribosomal RNA



G1504	G1505	U1506	U1507	A1508	A1509	G1510	G1511	U1512	A1513	G1514	G1515	G1516	G1517	G1518	A1519	C1520	G1521	U1522	G1523	G1524	G1525	G1526	U1527	U1528	G1529	G1530
U1440	U1441	U1444	U1445	A1446	A1447	C1448	C1449	U1450	A1451	G1452	G1453	G1454	G1455	G1456	A1457	G1458	G1459	C1460	G1461	U1462	U1463	U1464	A1465	A1468	C1469	C1470
U1370	U1371	U1372	U1373	A1374	A1375	U1376	A1377	U1378	U1379	U1380	U1381	C1382	U1386	G1387	C1388	C1389	U1390	U1391	U1392	U1393	C1397	A1398	G1401	U1402	A1410	C1411
U1308	G1309	G1310	G1311	G1312	G1313	G1314	G1315	G1316	G1317	A1318	G1319	C1320	U1321	C1322	G1323	A1324	G1325	U1326	C1327	C1328	U1329	U1330	G1331	A1332	A1333	C1342
G1242	C1243	G1244	C1245	A1246	U1247	A1248	C1249	A1250	A1251	A1252	G1253	A1254	C1255	A1256	C1257	G1258	C1259	G1260	A1261	C1262	C1263	U1269	G1270	A1271	G1272	C1281
U1173	G1174	U1178	A1179	A1180	G1181	G1182	U1183	G1190	G1193	U1194	C1195	A1196	A1197	G1198	U1199	C1200	C1201	U1202	C1203	G1206	C1207	C1208	G1209	C1210	U1211	U1212
C1038	G1039	U1040	G1041	G1042	A1043	A1044	C1045	A1046	G1047	G1048	U1049	C1050	C1051	U1052	G1053	C1054	A1055	U1056	G1057	C1058	C1059	U1060	C1066	A1067	U1068	C1069
A978	C979	U980	U981	A982	A983	C984	C985	U986	G987	G988	U989	C990	U991	U992	G993	A994	C995	A996	U997	C998	C999	A1000	C996	U1001	G1002	G1003
C912	A913	A914	U915	U916	G917	A918	A919	U920	U921	G922	A923	C924	G925	G926	G927	G928	C929	C930	C931	C934	A935	C936	C937	A938	C939	C940
G832	G833	U834	U835	U836	U837	G838	C839	C840	U841	U842	U843	C844	A845	G846	G847	G848	C857	G858	G859	A860	G861	C862	U863	A864	C865	C866

● Molecule 1: 16S ribosomal RNA

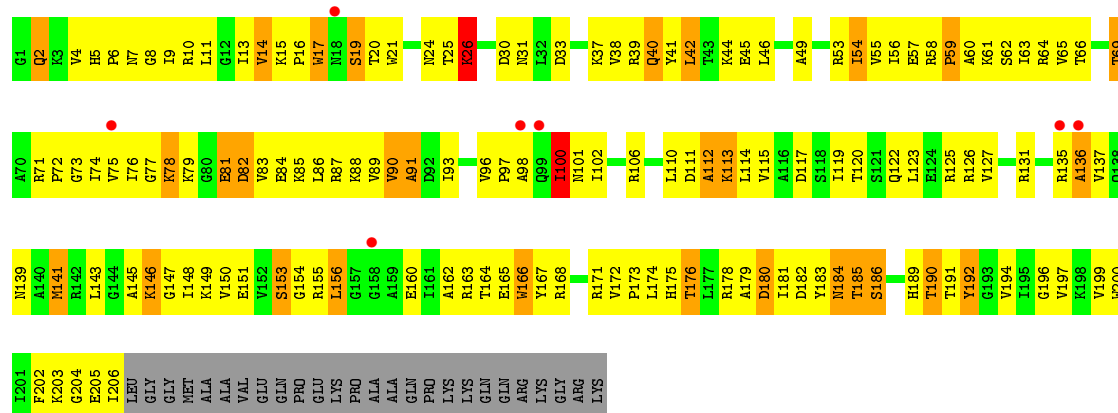


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G141	G142	A143	G144	G145	G146	G147	G148	U149	U150	A151	A152	A155	C156	U157	G158	G159	A160	A161	A162	C163	G164	A167	G168	C169	U170	U173	A174	C175	G176	G177	C178	A179	U180	A181	A182	C183	C186	G187	C188	A189	A190	G191	A192	C193	C194	A195	A196	A197	G202	G203	G204	A205	C206	C207				
A85	G69	U70	A71	A72	G75	G76	A77	A78	G79	C83	U84	U85	G86	C87	U88	U89	C90	U91	U92	U93	G94	C95	A98	C99	G105	C106	G107	G108	A109	C110	G111	G112	G113	U114	G115	U118	A119	A120	U121	G122	U123	A53	C54	A55	U56	G57	C58	A59	A60	G61	U62	A139	C63	G64				
A	A	A	U	U5	G6	A7	A8	G9	A10	G11	U12	U13	U14	U15	A16	U17	C18	G21	G22	C23	U24	C25	A26	G27	A28	U29	U30	G31	A32	A33	C34	G35	C36	U37	G38	C39	C40	G41	G42	C47	C48	U49	A50	A51	C52	A53	C54	A55	U56	G57	C58	A59	A60	G61	U62	A139	C63	G64

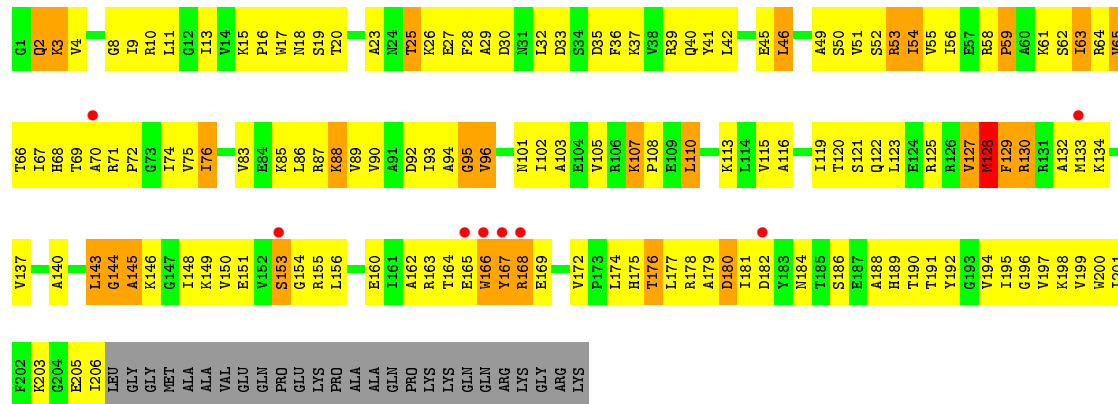
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U1308	G1242	A1178	A1112	A1044	U982	U920	C840	G769	G700	A630	U555	U485	U421	G352	G275
G1309	G1243	A1179	C1112	A983	U921	G922	C841	C770	G703	G633	C488	G423	G423	G354	G276
G1310	G1244	A1180	C1113	U1048	C984	G923	U842	G771	G704	G634	G489	G424	G424	G277	G277
G1312	G1245	A1181	C1114	U1049	C985	G924	U843	G772	A705	G635	G490	G425	G425	A279	A279
G1313	A1246	G1182	A1118	G1050	U986	C924	C844	G773	G706	A636	C490	U426	U426	C280	C280
U1314	U1247	U1183	U1118	C1051	G987	G925	A845	A777	G707	G637	A560	U427	U427	G360	G360
G1315	G1184	G988	C1119	U1052	G926	G926	G846	G778	A708	U638	A561	U428	U428	C384	C384
G1316	G1185	G989	U1120	C1053	G927	G927	C847	C779	G709	U639	A562	U429	U429	C285	C285
G1317	G1186	G990	U1121	C1054	G928	G928	C848	C780	G710	G639	A563	U430	U430	C370	C370
G1318	A1251	U991	U1122	A1055	G929	G929	C857	A781	G711	A642	G566	A431	A431	C371	C371
A1318	A1252	U992	U1123	U1056	C930	C930	G858	C782	G712	C643	G567	A432	A432	A288	A288
A1319	G1253	G993	G1124	G1057	C931	C931	G859	C783	G713	C644	G568	G433	G433	G289	G289
C1320	A1254	A994	U1125	U1058	G932	G932	A860	G785	A714	U645	C501	U434	U434	C372	C372
G1321	G1255	A1191	U1126	C1059	G933	G933	A861	G786	G715	U646	A572	A435	A435	A373	A373
G1322	A1256	C1192	G1127	U1060	C934	G934	G862	A792	A716	U647	A573	C436	C436	U296	U296
G1323	A1257	C1193	G1128	U1061	A935	A935	C863	A793	G719	U648	A574	C437	C437	U375	U375
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G1325	A1197	A1198	A1130	G1063	A937	A937	A864	A794	G721	U650	C504	U439	U439	A298	A298
U1326	G1198	G1199	G1131	U1064	A938	A938	A865	C795	G722	C651	C577	C440	C440	A441	A441
G1327	U1199	G1200	C1132	U1065	G939	G939	C866	C796	G723	U652	C578	C441	C441	A301	A301
C1328	C1200	C1200	G1133	C1066	C940	C940	C867	C797	G724	U653	C579	C442	C442	A302	A302
A1329	G1268	A1201	G1134	A1067	G941	G941	G869	U798	G725	C658	G585	C443	C443	A303	A303
G1288	U1202	U1135	U1135	G1068	A1005	A1005	U875	U801	G726	U659	G586	A444	A444	A382	A382
G1270	C1203	C1203	C1136	C1069	G1006	G1006	U876	A802	C726	U660	G587	A445	A445	A383	A383
A1271	A1204	A1204	C1137	U1070	U1007	U1007	A878	A803	G727	U661	U590	A446	A446	C384	C384
G1272	U1205	G1138	C1138	C1071	U1008	G947	C879	G803	G730	U662	U591	A447	A447	C385	C385
G1334	G1206	U1139	U1009	G1072	C1009	C948	C880	U804	G731	U663	C521	A448	A448	A386	A386
U1335	G1207	G1140	C1140	U1073	A949	A949	C881	C805	G732	U664	C522	A449	A449	A387	A387
G1336	C1208	C1141	C1141	G1074	U950	U950	C882	C806	G733	U665	C523	A450	A450	A388	A388
G1337	C1209	G1142	C1142	U1075	G951	G951	C883	A807	G734	U666	C524	A451	A451	A389	A389
G1338	G1210	G1143	U1143	U1076	U952	U952	C884	C808	G735	U667	C525	A452	A452	U390	U390
A1339	U1211	G1144	G1144	U1078	G953	G953	U885	G809	G736	U668	C526	A453	A453	A391	A391
G1342	G1212	A1213	A1145	G1079	G954	G954	C886	C810	G737	U669	C527	A454	A454	A392	A392
G1343	A1281	A1214	A1146	A1080	U955	U955	C887	C811	G738	U670	C528	A455	A455	A393	A393
C1344	U1283	G1215	G1147	A1081	U956	U956	G890	G812	C739	U671	C529	A456	A456	A394	A394
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A1285	C1217	U1150	C1149	U1083	A958	A958	G894	A814	U741	U673	G531	A458	A458	A396	A396
U1286	U1218	A1151	U1150	G1084	A959	A959	G895	A815	G742	U674	U531	A459	A459	A397	A397
A1287	A1219	A1152	U1085	U1085	A1022	U960	G896	A816	G743	U675	A532	A460	A460	U398	U398
A1288	A1220	A1152	U1086	U1086	U961	U961	C897	C817	A743	U676	A533	A461	A461	G399	G399
C1352	G1221	A1157	U1091	U1081	G1024	C962	C897	G818	A746	U677	G534	A462	A462	U400	U400
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U1354	U1223	U1159	A1093	A1093	G1026	A964	A901	U820	G748	U679	G536	A464	A464	A402	A402
G1355	U1224	G1160	G1094	C1028	U965	U965	G902	G821	A749	U680	G537	A465	A465	C403	C403
G1356	C1293	C1161	U1095	U1029	C967	G966	G903	G824	C750	U681	G538	C469	C469	U404	U404
A1357	G1294	G1162	C1096	U1030	A968	A968	U904	A825	U751	U682	G540	C470	C470	A405	A405
U1358	A1227	A1163	C1097	C1031	A969	A969	U905	G826	G752	U683	G541	U471	U471	U407	U407
C1359	G1296	G1164	C1098	G1032	C970	C970	A906	U828	A753	U684	G542	U472	U472	A408	A408
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A1360	U1298	G1166	G1100	G1034	C972	C972	A908	G830	G755	U686	G545	U474	U474	G410	G410
A1361	A1299	A1101	A1035	A1035	G973	G973	A909	A831	G756	U687	C546	U475	U475	A411	A411
A1362	G1234	A1170	A1102	A1102	A974	A974	C910	G832	U761	U688	G547	U476	U476	A412	A412
A1363	U1300	U1235	C1037	A1037	A975	A975	A914	G833	G762	U689	A621	C477	C477	A413	A413
U1364	A1301	C1172	C1038	G1104	G976	G976	A915	U834	G763	U690	A622	U478	U478	A414	A414
G1365	C1302	G1173	C1039	A1105	A977	A977	U916	U835	G764	U691	G548	U479	U479	A415	A415
G1367	G1303	G1174	U1039	A1106	A978	A978	U917	U836	G765	U692	G549	U480	U480	A416	A416
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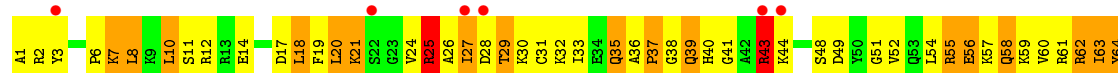
• Molecule 2: 30S ribosomal protein S3

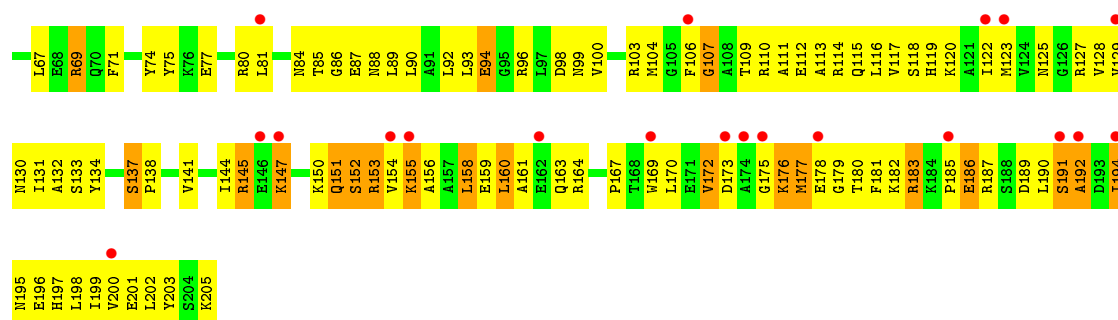


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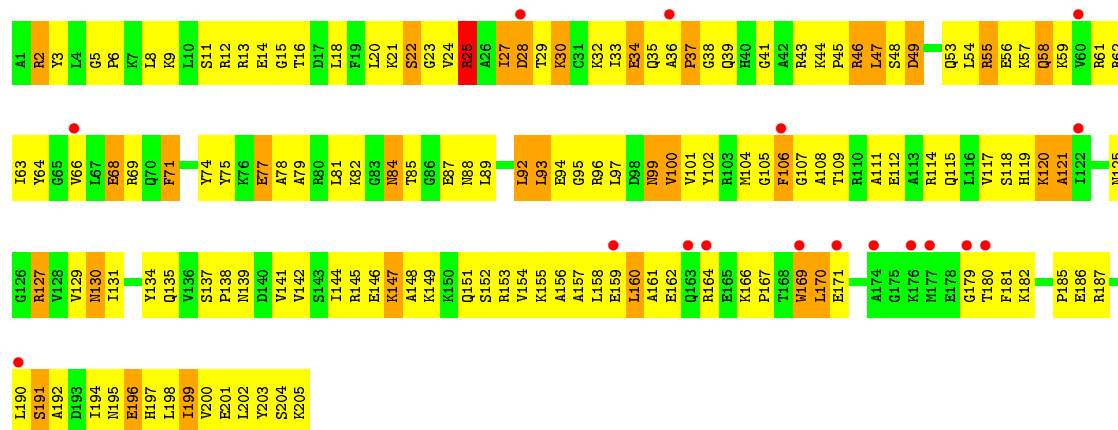


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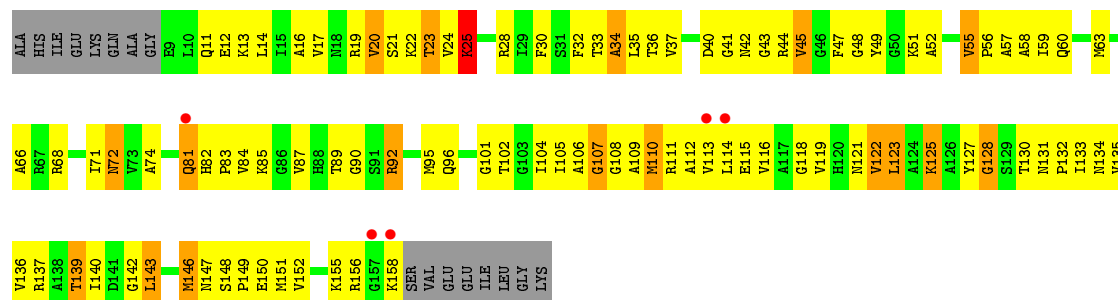




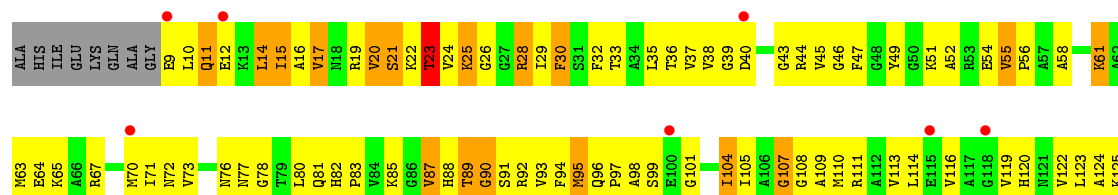
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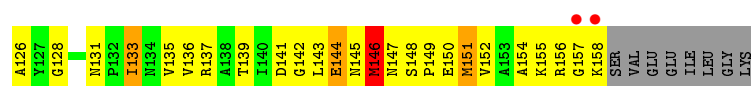


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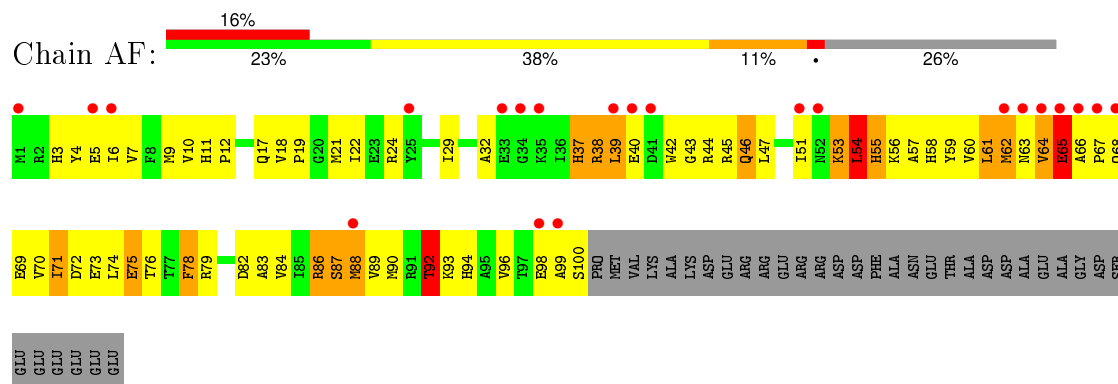


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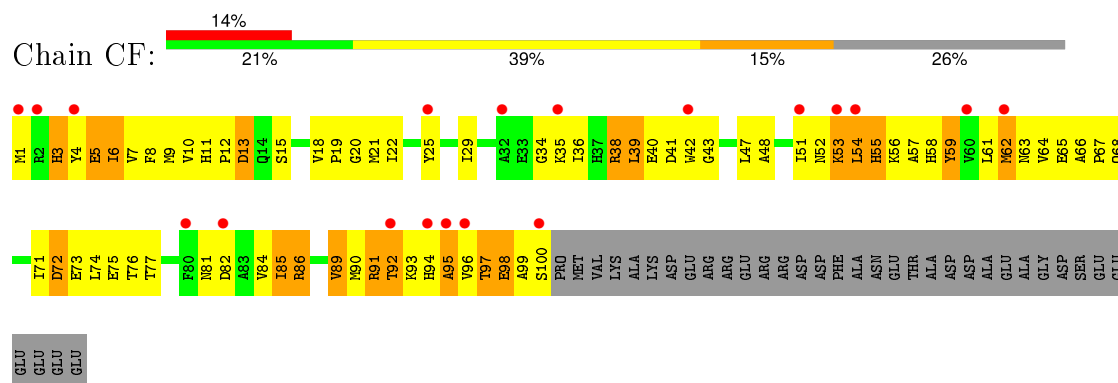




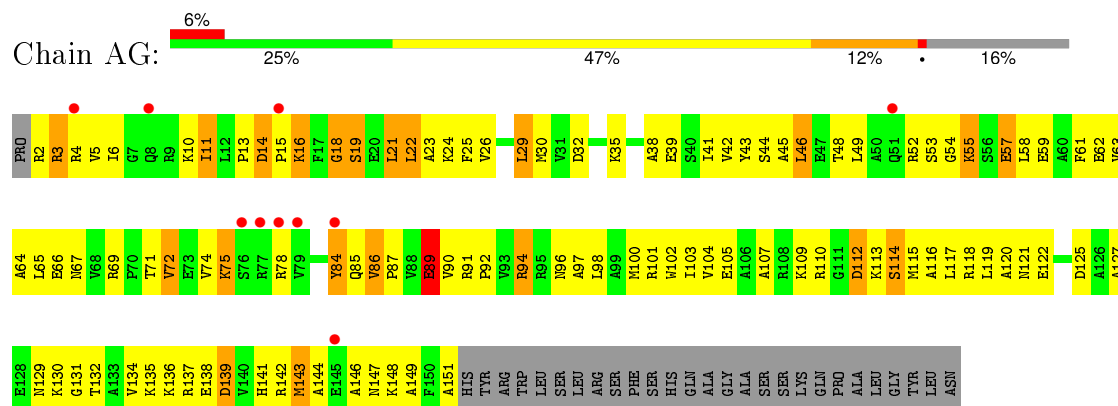
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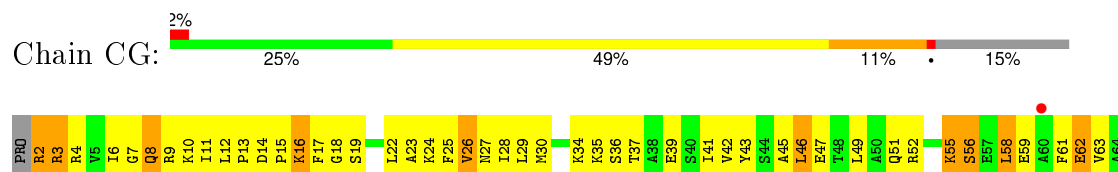
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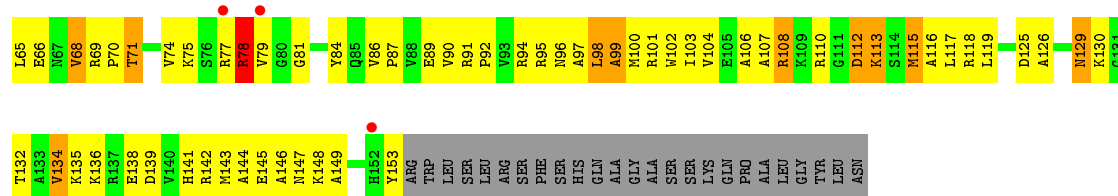


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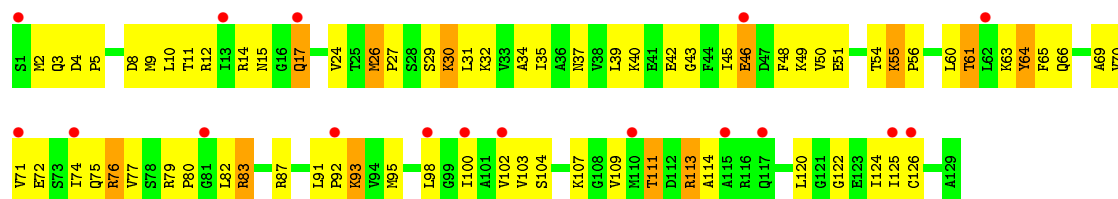


• Molecule 6: 30S ribosomal protein S7

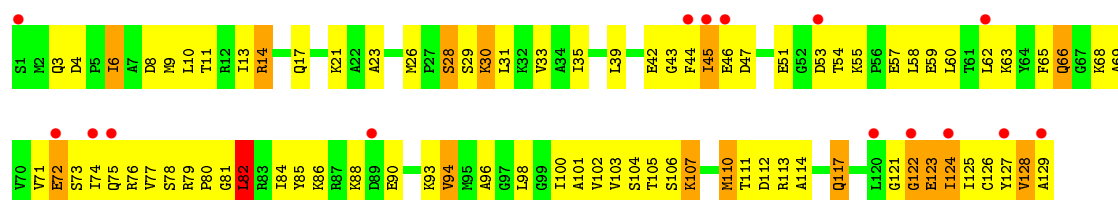




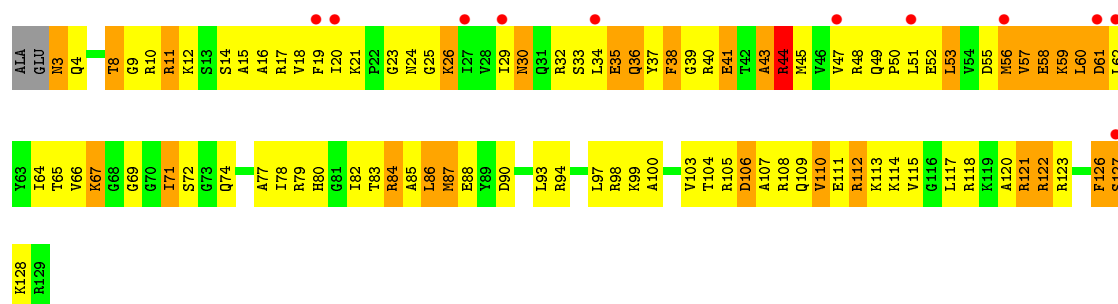
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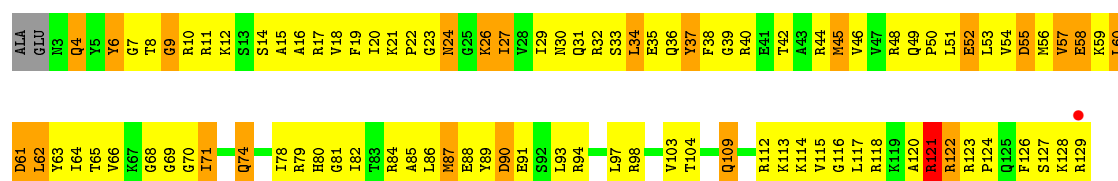
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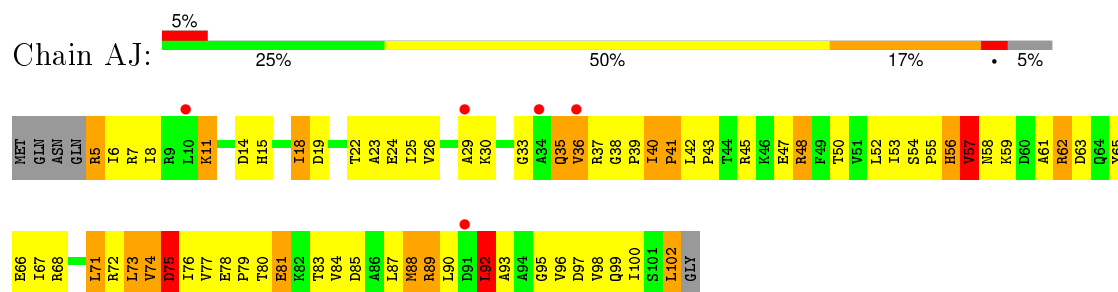
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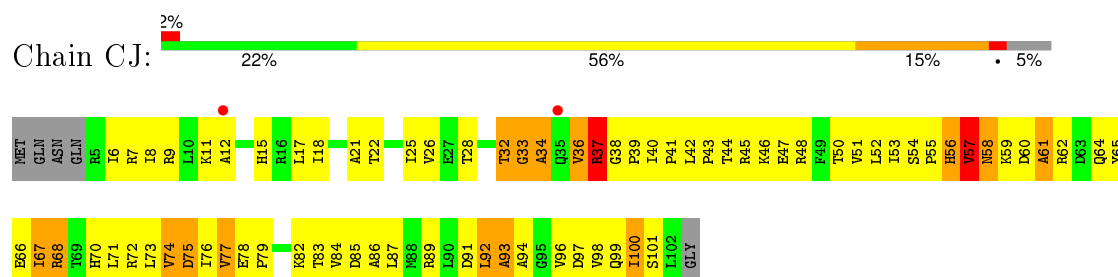
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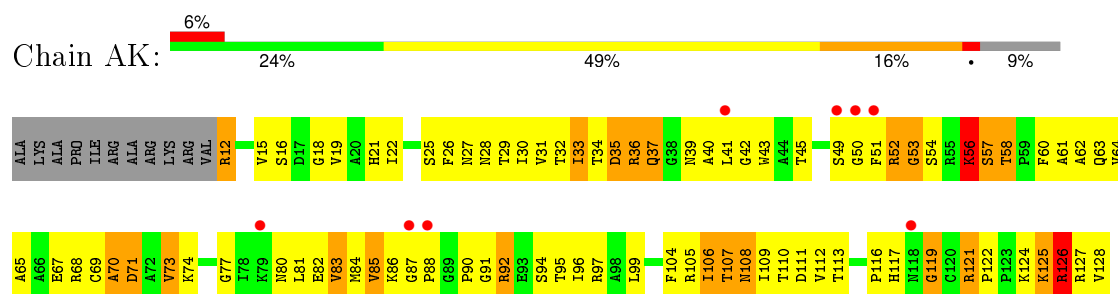
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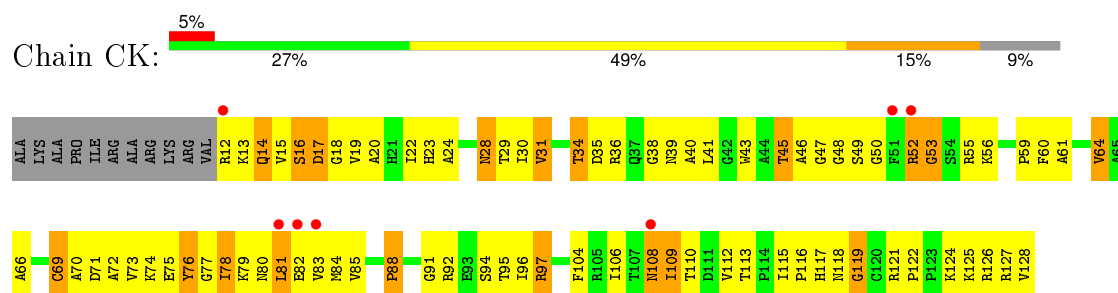
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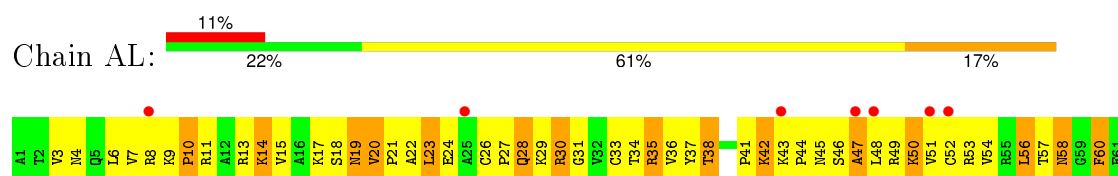
• Molecule 10: 30S ribosomal protein S11

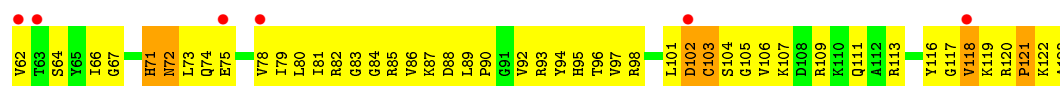


• Molecule 10: 30S ribosomal protein S11



• Molecule 11: 30S ribosomal protein S12



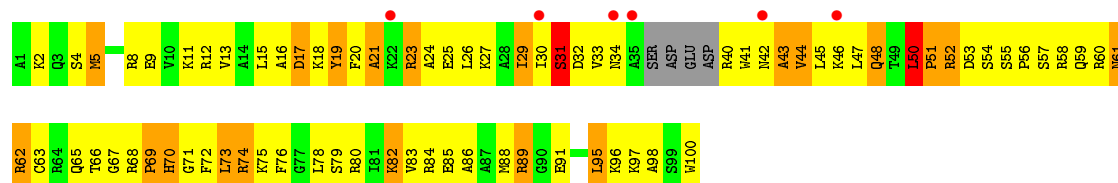


- Molecule 11: 30S ribosomal protein S12

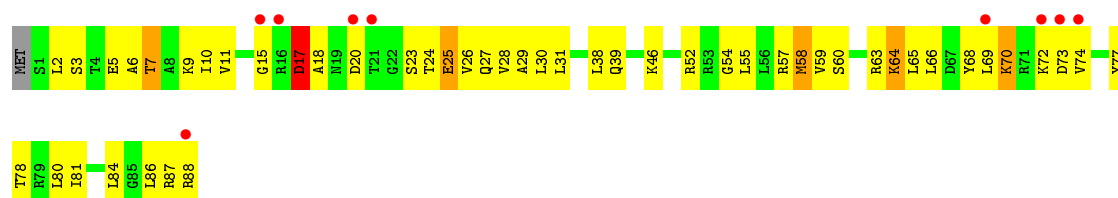


- Molecule 12: 30S ribosomal protein S13

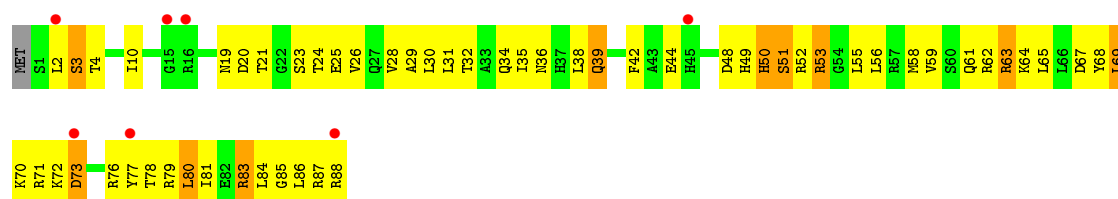




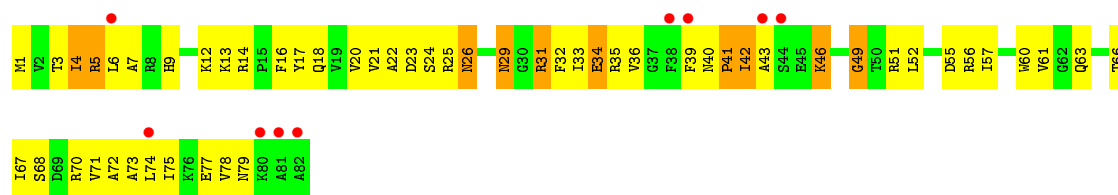
• Molecule 14: 30S ribosomal protein S15



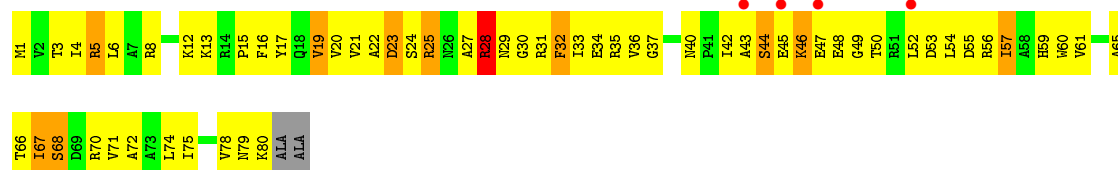
• Molecule 14: 30S ribosomal protein S15



• Molecule 15: 30S ribosomal protein S16

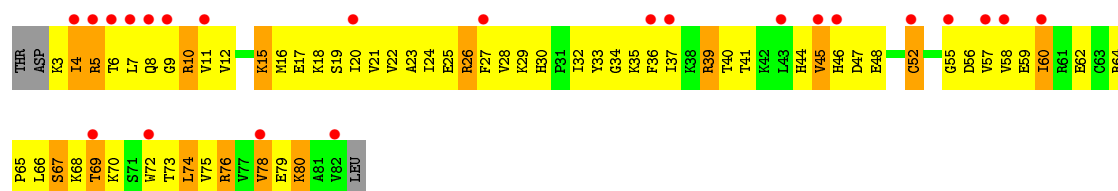


• Molecule 15: 30S ribosomal protein S16

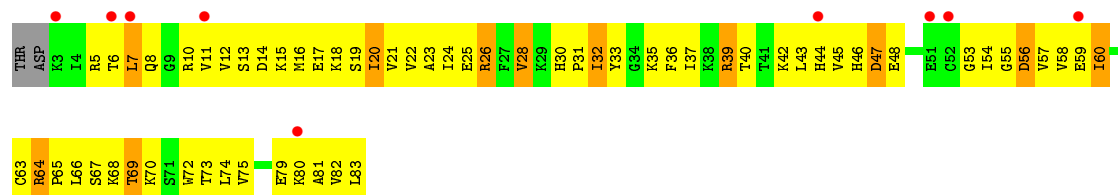


• Molecule 16: 30S ribosomal protein S17

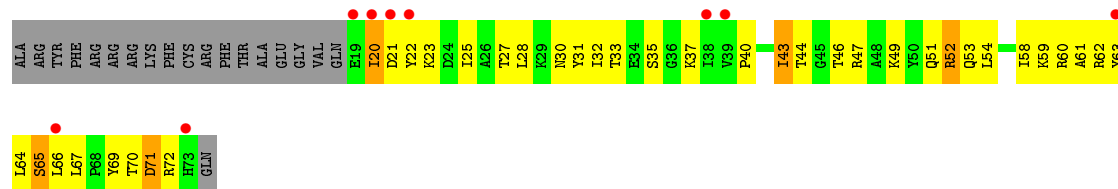




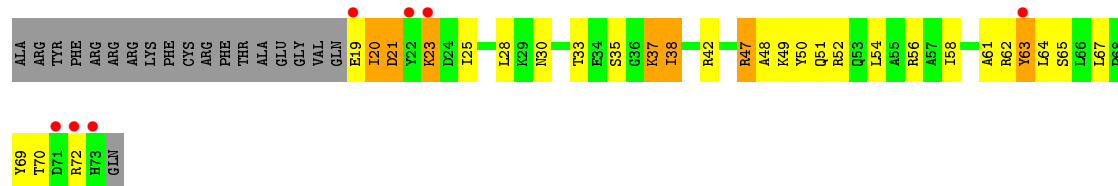
- Molecule 16: 30S ribosomal protein S17



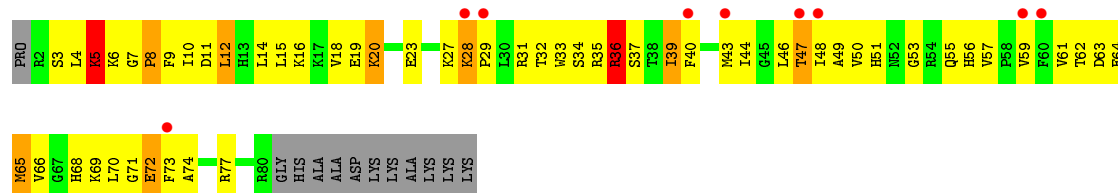
- Molecule 17: 30S ribosomal protein S18



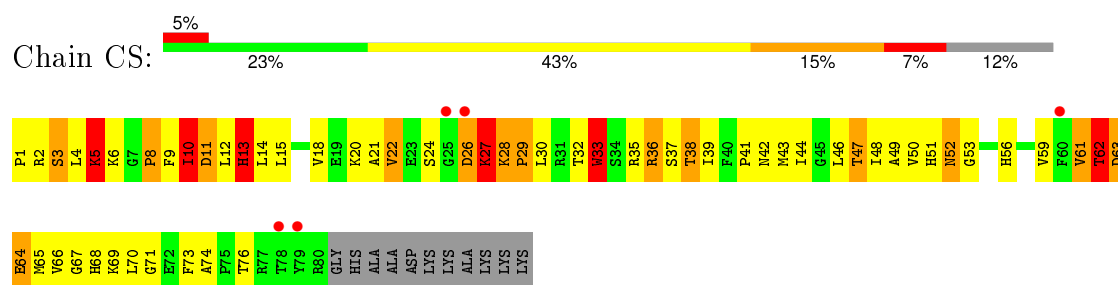
- Molecule 17: 30S ribosomal protein S18



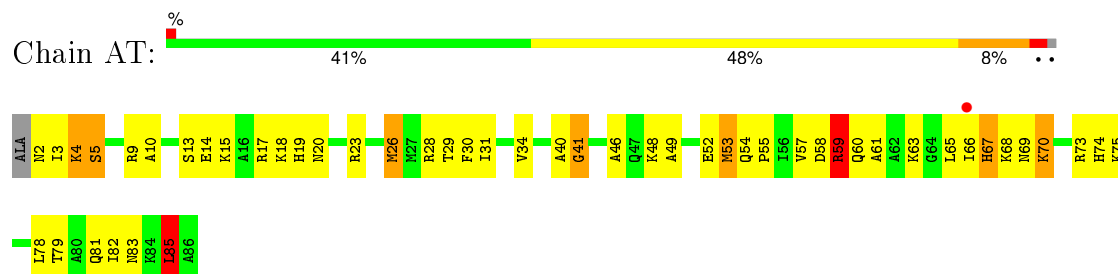
- Molecule 18: 30S ribosomal protein S19



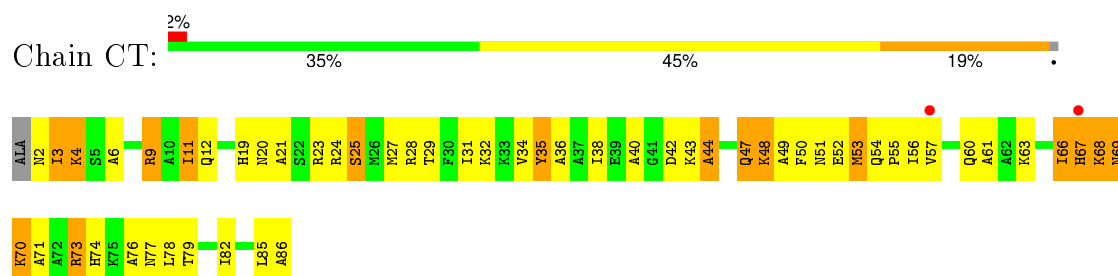
- Molecule 18: 30S ribosomal protein S19



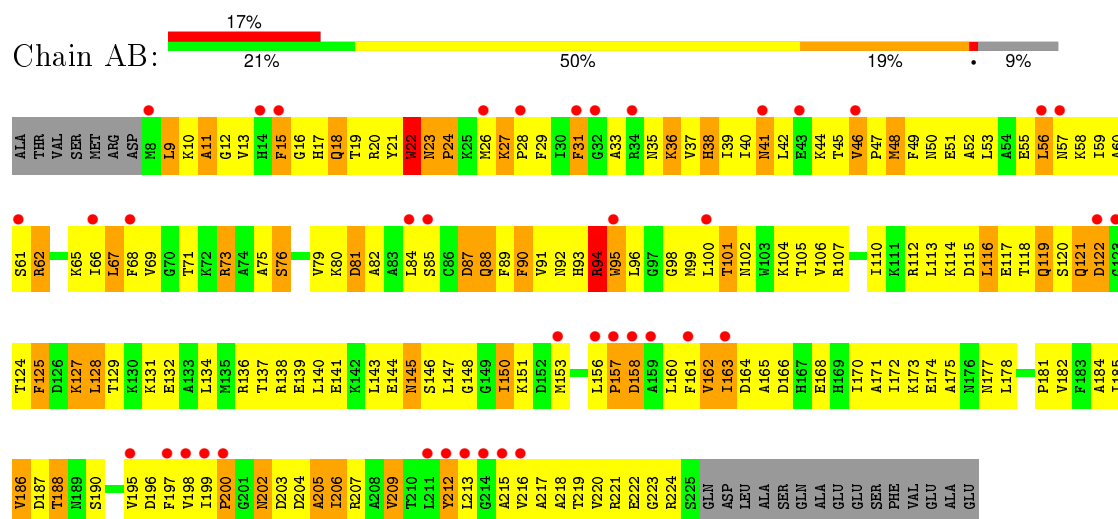
• Molecule 19: 30S ribosomal protein S20



• Molecule 19: 30S ribosomal protein S20

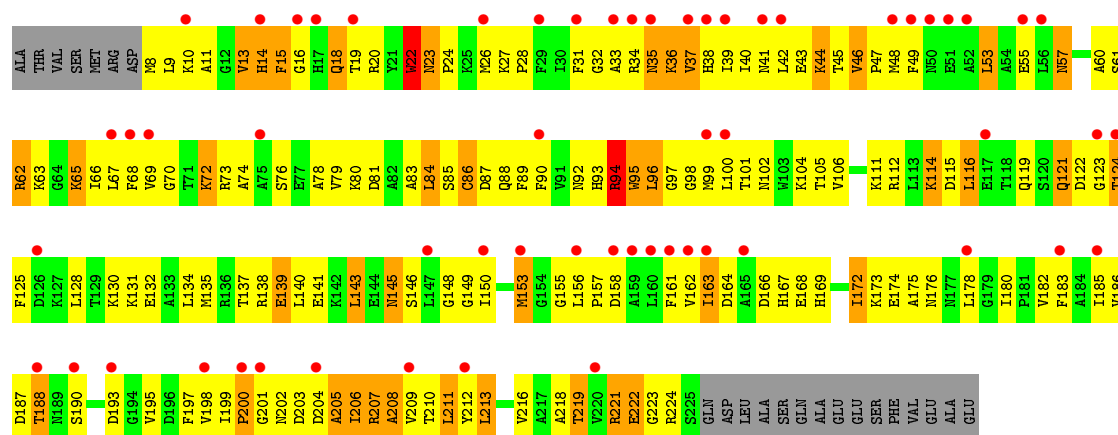


• Molecule 20: 30S ribosomal protein S2

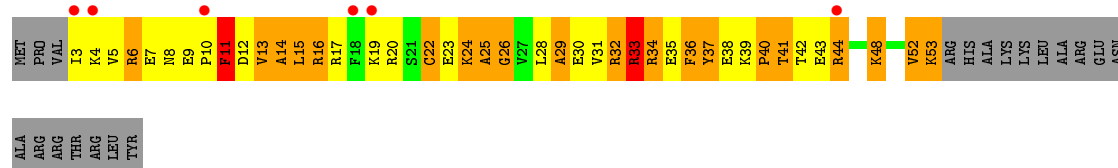


• Molecule 20: 30S ribosomal protein S2

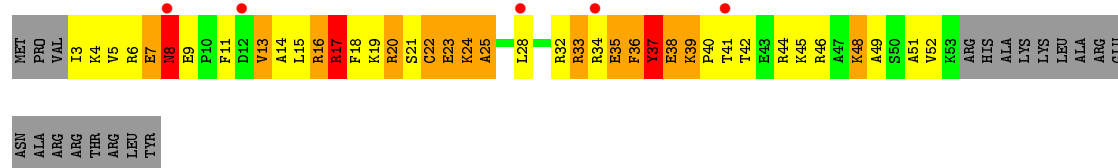




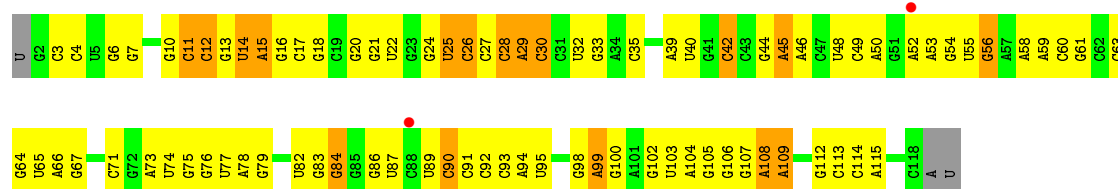
• Molecule 21: 30S ribosomal protein S21



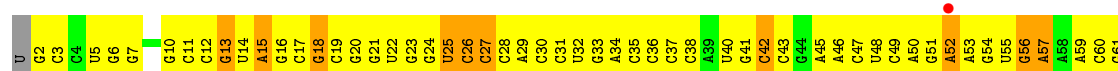
• Molecule 21: 30S ribosomal protein S21



• Molecule 22: 5S ribosomal RNA

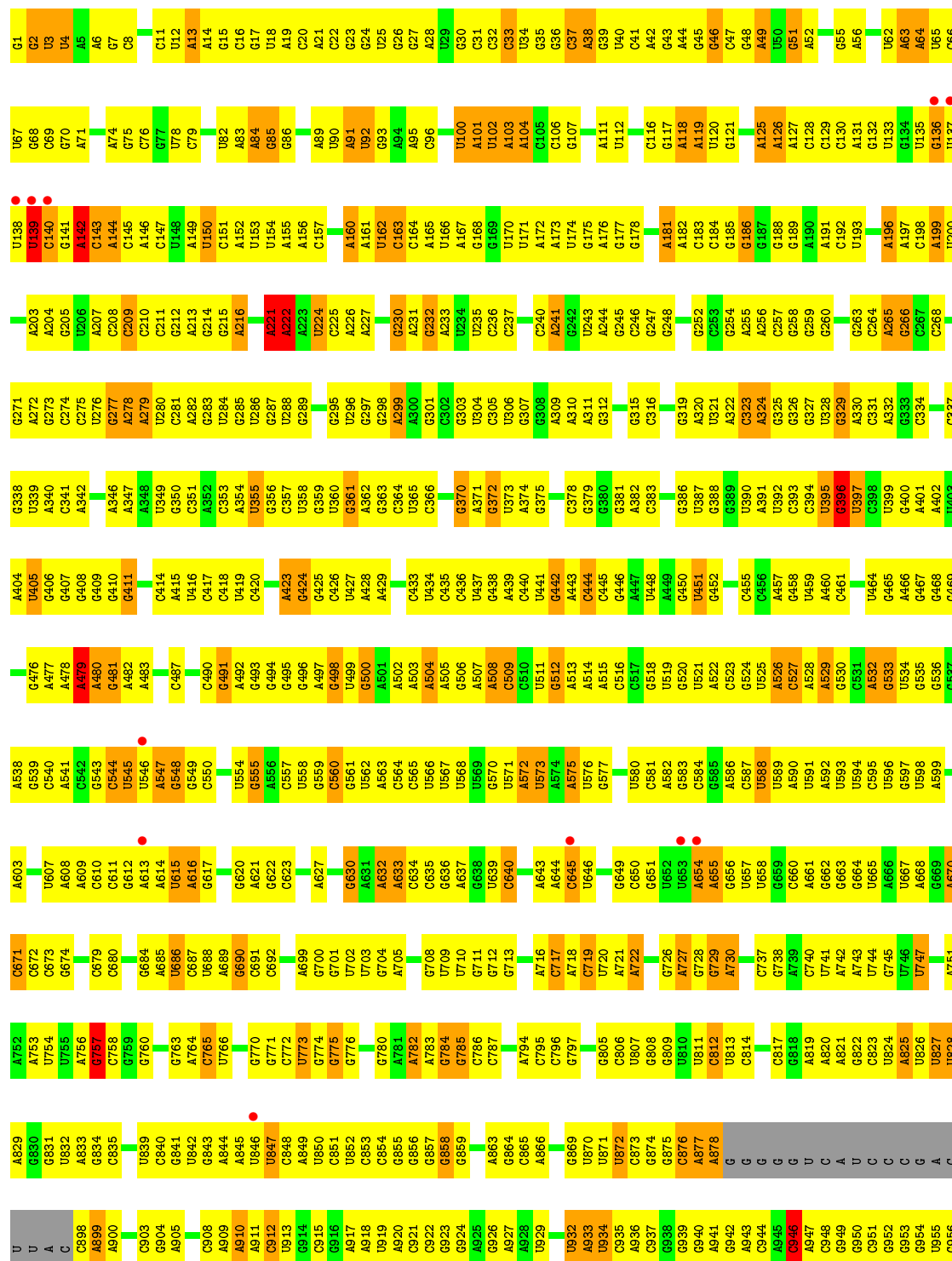


• Molecule 22: 5S ribosomal RNA

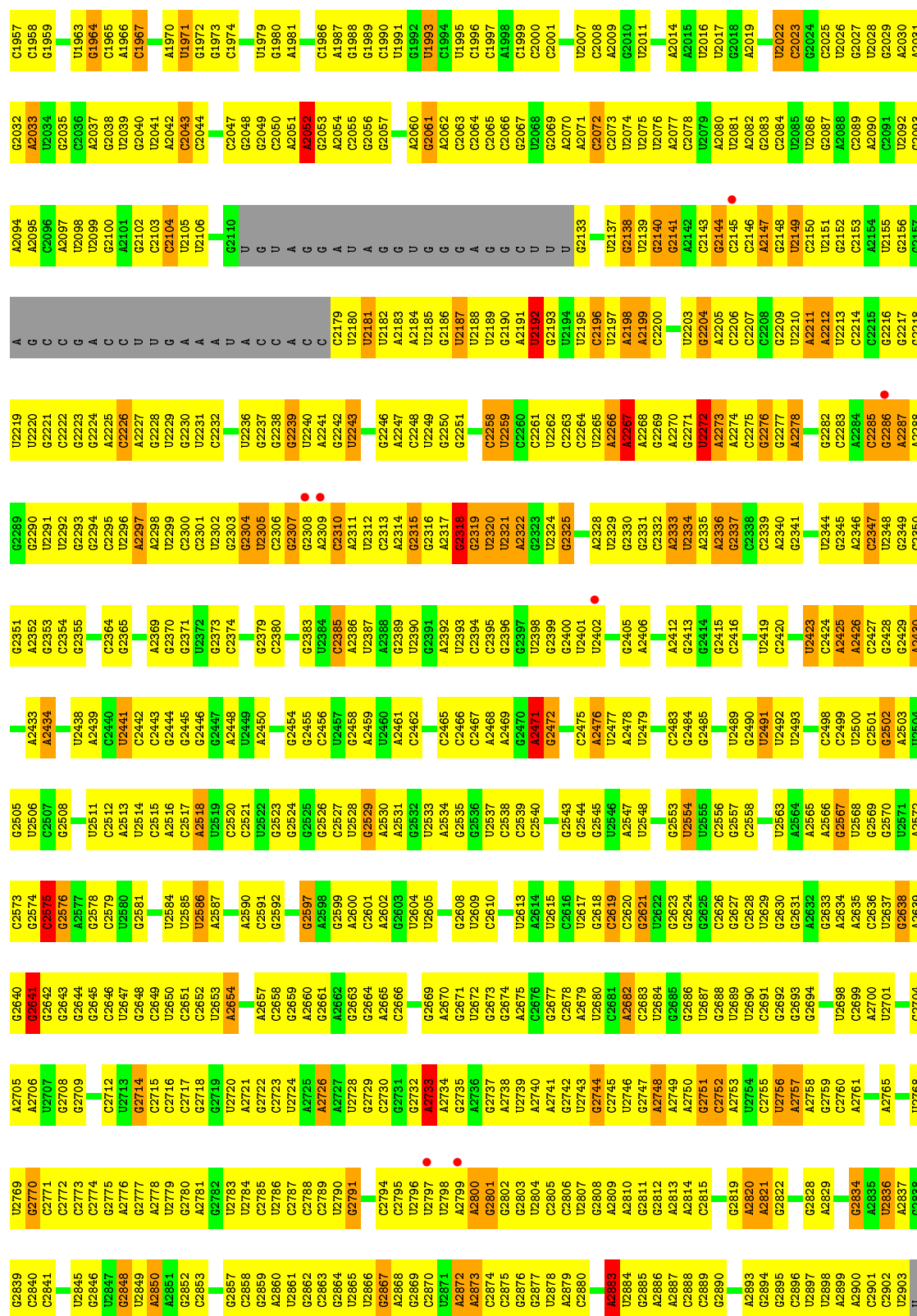




• Molecule 23: 23S ribosomal RNA



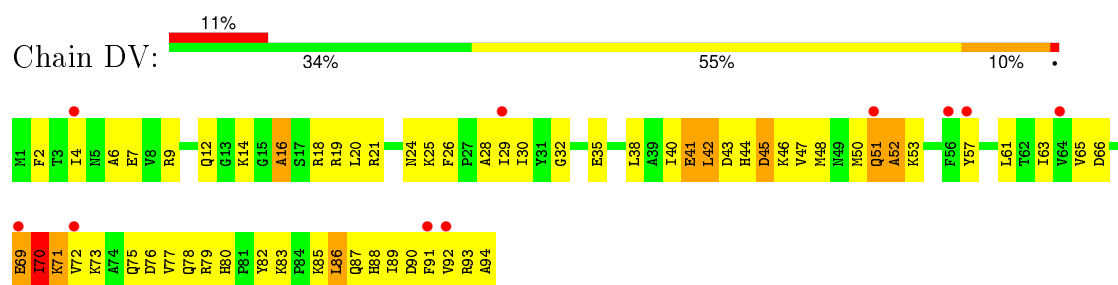
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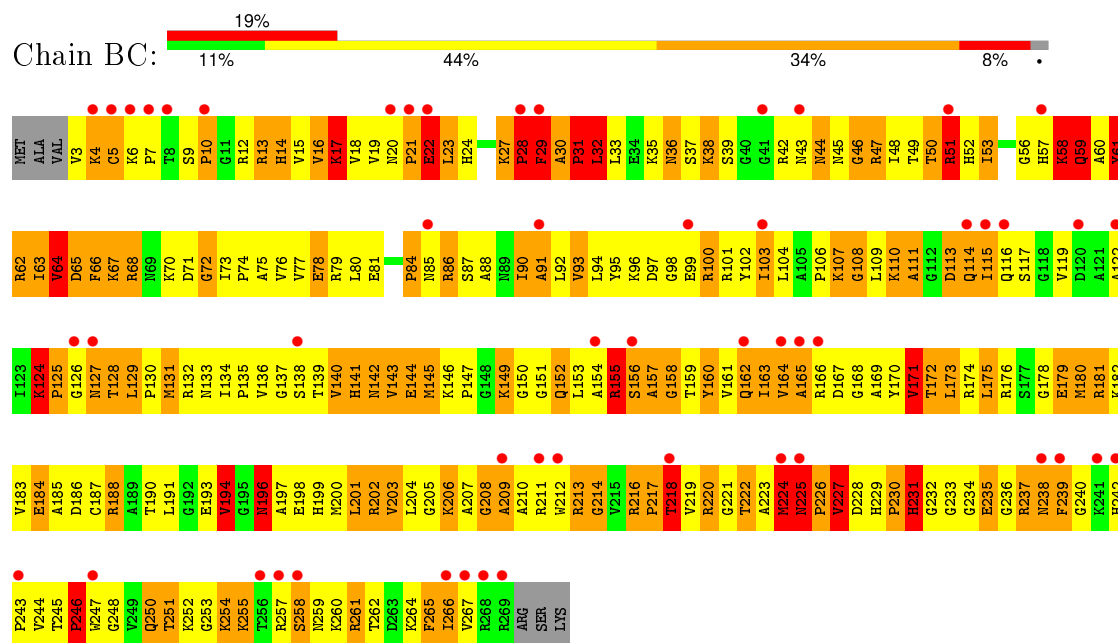
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		A925	A861	A794		C635	U572	U511	G438	U373	G307	C241	C170	U99	U29
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		A927	A863	C796	U714	A637	U573	A513	C440	G375	A309	G242	C172	A101	C31
		A928	G864	G797	A715	G638	A574	A514	U441	G376	A310	U243	C173	A102	G32
		A929	G865		A716	U639	A575	A515	G442	G377	A311	A244	C174	A103	G33
		A930	A866	G801	C717	C640	U576	C516	A443	C378	G312	G245	C175	A104	U34
		U929		A802	A718		U577	C517	C444	G379	G313	C246	C176	A105	G35
		G930		G805	C719	A643	U578	G518	C445	G380	G314	G247	C177	C106	G36
		U931		C806	U720	C645	U580	U519	U448	A382	C249	G248	C178	G107	C37
		U932			A721	A644	C581	U521	A449	C383	G319	C250	A181	A38	A38
		A933			A722	C645	A582	A522	A450	A384	A320	A251	A182	U40	U40
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		C935		C812	U725		G584	G524	G452	G386	A322	C253	C184	U112	U112
		U937		U813	G726	A654	U585	U525	A453	U387	C323	G254	G185	U113	A42
		C937		C814	G726	A655	A586	A526	A454	G388	A324	A255	C186		
		G938			A727	A656	A587	C527	C455	G389	G325		G188	G45	G45
		G939			G728	G656	C587	A528	C456	U390	G326		A118	G46	G46
		C940		G817	G729	U657	U588	A529	A457	A391	G327	G259	C189	C47	C47
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		G942	G	A819		G659	A590	G530	U459	C393	U329	G263	C193	A49	A49
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		C944	G		G738	A661	A592	A532	A460	U395	C331	G124	G51	G51	G51
		A945	U	C823		G662	U593	G533	C461	G396	A332	A265	A196	A52	A52
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		A947	A	A825	U741	G664	C595	G535	A467	C398	C334	C267	C198	C127	G55
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		G949	C	U827	A743	A666	G597	G537	G468	U400	C336	G271	C204	U62	U62
		C950	C	U828	U744	U667	U598	A538	G469	A401	G337	G132	G205	A63	A63
		C951	C	A829	G745	A668	A599	G539	U476	A402	C338	C274	U206	A64	A64
		G952	G	G830	U747	G669	G600	C540	A472	U403	U339	C275	A207	U135	U135
		A953	A			A670	C601	A541		A404	U340	U276	A207	G136	G136
		C956	C		A753	C671	A603	C542	C475	U405	C341	G277	C209	U137	U137
		G957	U	G834	U755	C673	A603	C543	G476	G406		A278	G209	G56	G56

A2054	G1983	U1915	C1844	G1776	A1711	A1641	C1565	G1501	C1437	G1368	G1299	G1238	G1171	G1107
C2055	C1986	A1916	G1845	U1779	U1712	G1642	A1566	A1502	U1438	G1368	G1300	G1239	C1172	U1108
G2056	A1987	U1917	A1846	U1780	A1713	G1645	G1567	A1503	A1939	U1372	A1302	U1240	U1173	C1109
A2060	A1988	A1918	A1847	U1781	A1714	G1645	A1568	A1504	U1440	U1372	A1302	A1241	U1174	G1110
G2061	G1989	A1919	A1848	U1781	A1715	G1646	A1569	A1505	G1441	A1373	G1303	U1242	U1175	A1111
A2062	G1990	G1920	U1851	A1784	U1716	U1647	A1571	C1507	U1442	A1374	A1304	G1243	U1176	G1112
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C2064	G1992	U1923	A1853	A1786	G1719	U1649	A1573	A1509	U1444	G1377	G1309	A1245	C1178	C1114
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G2069	A1998	G1928	A1857	A1789	A1722	A1654	U1578	C1512	G1448	G1380	U1312	U1249	G1182	C1118
A2070	C1999	G1929	A1858	A1791	G1723	A1655	A1579	U1513	G1449	G1381	U1313	G1250	U1183	U1119
A2071	C2000	G1930	C1856	U1792	G1724	C1856	A1580	G1514	G1450	G1382	G1314	C1251	U1184	G1120
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U2075	G1934	G1934	U1865	U1796	C1728	U1662	A1586	C1518	C1454	A1386	U1318	C1257	A1189	G1125
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U2017	U1941	U1941	A1872	A1803	U1736	U1671	A1593	G1530	C1462	C1398	U1326	A1264	G1198	A1133
G2018	U1942	U1942	G1873	C1804	G1737	A1672	U1594	C1531	C1463	C1399	A1327	A1265	U1199	A1134
U2086	A1945	A1945	G1874	A1805	G1738	G1673	C1595	A1532	A1464	U1400	A1328	G1266	U1200	G1135
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G2102	U1963	U1963	C1892	C1822	A1754	C1691	A1616	A1548	G1483	G1416	C1348	G1283	G1220	C1152
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G	A1912	A1912	A1912	U1841	A1773	C1708	C1638	U1562	C1499	A1434	G1364	C1298	A1237	C1170
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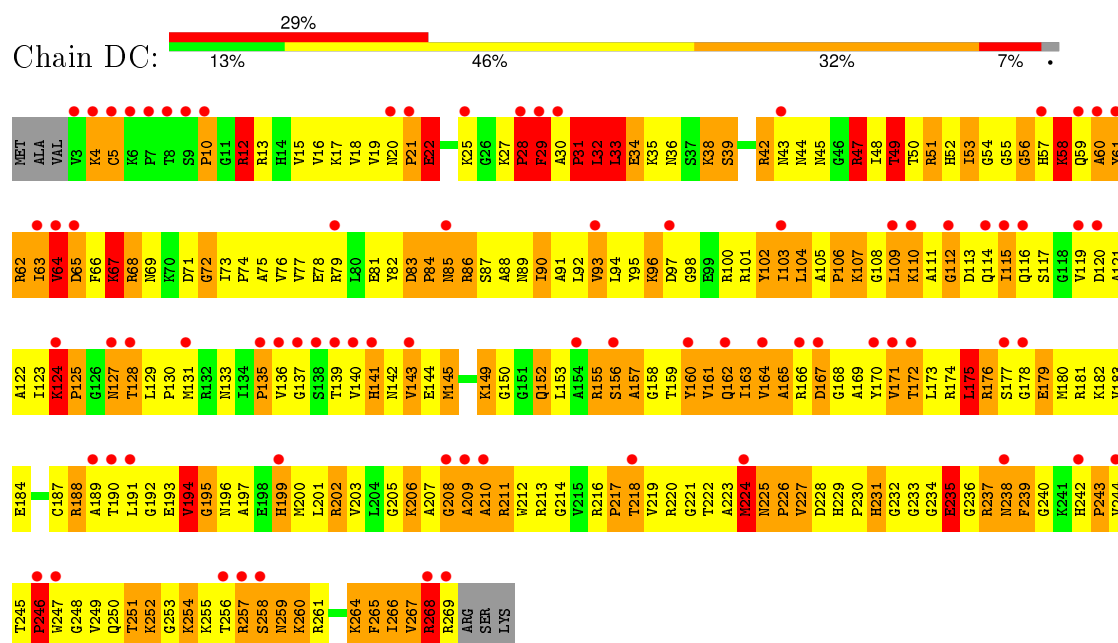




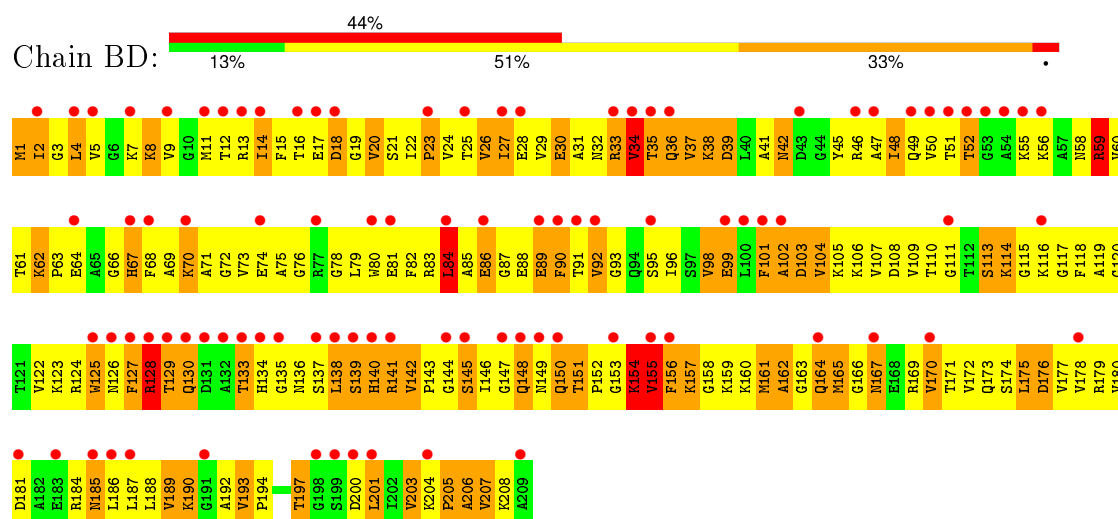
• Molecule 25: 50S ribosomal protein L2



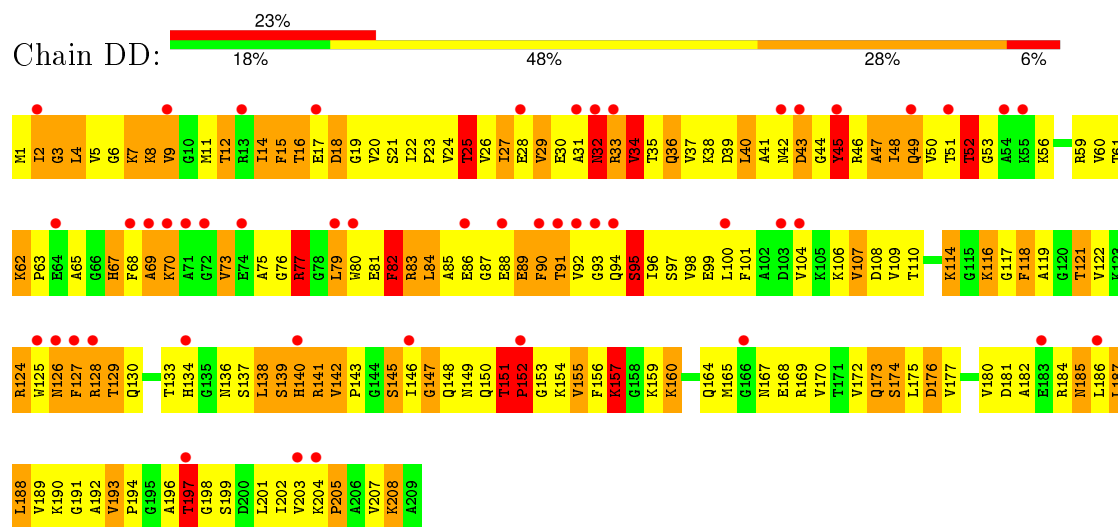
• Molecule 25: 50S ribosomal protein L2



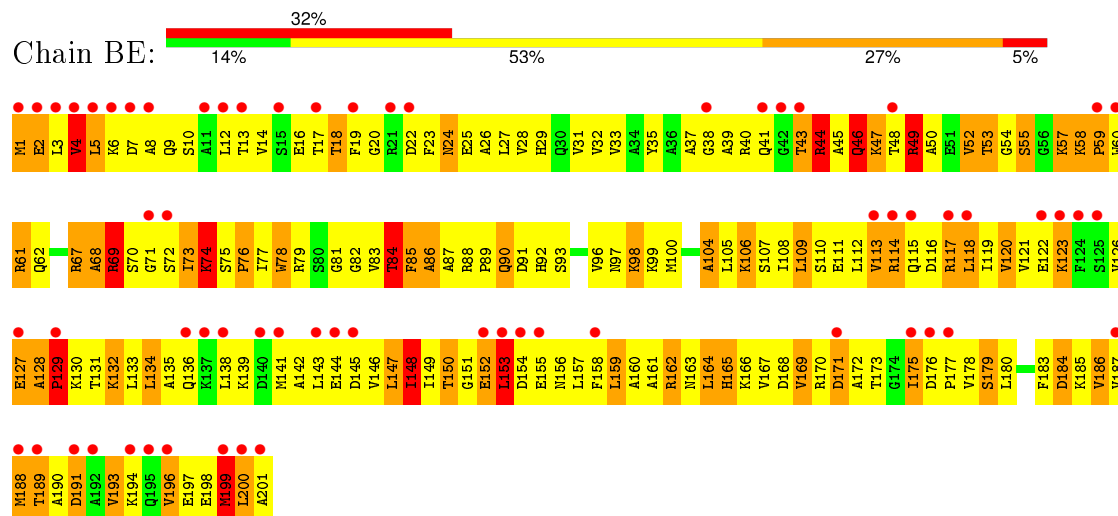
• Molecule 26: 50S ribosomal protein L3



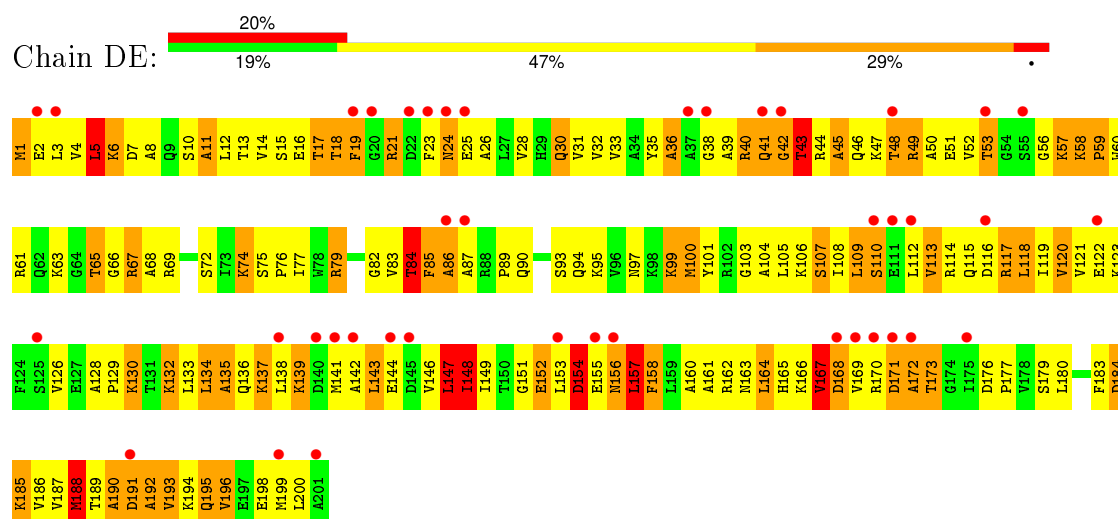
• Molecule 26: 50S ribosomal protein L3



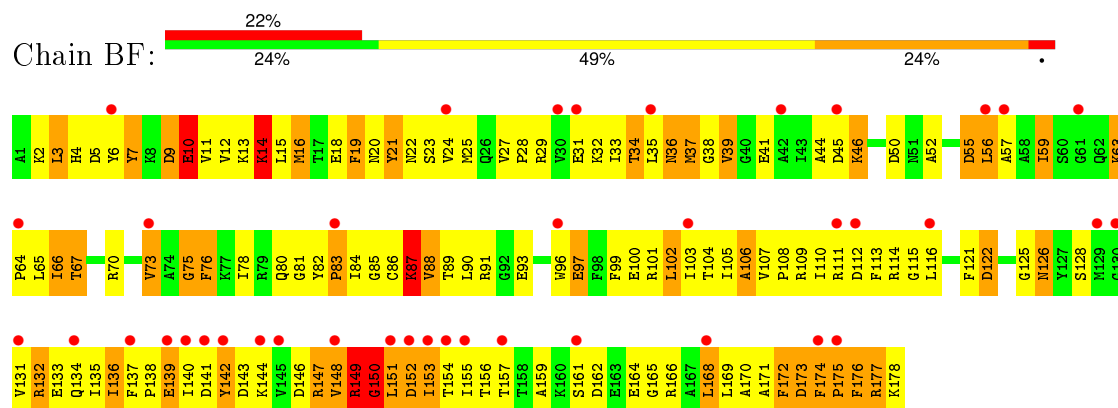
• Molecule 27: 50S ribosomal protein L4



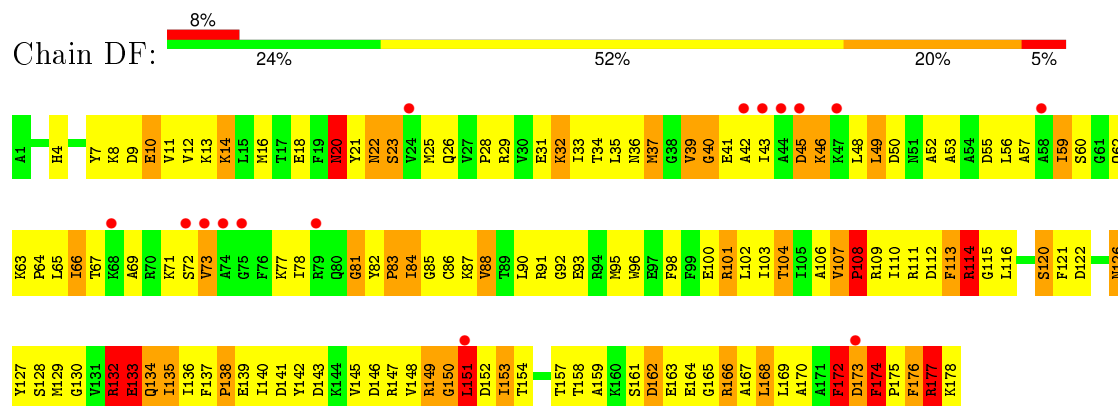
• Molecule 27: 50S ribosomal protein L4



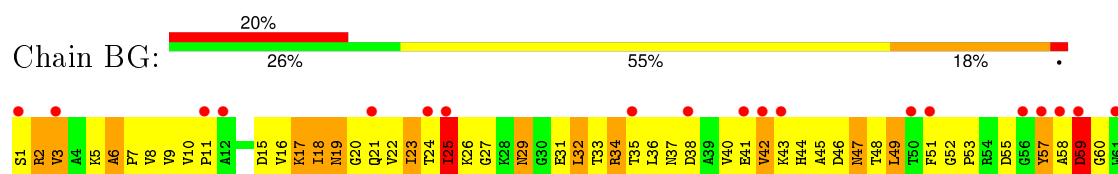
• Molecule 28: 50S ribosomal protein L5

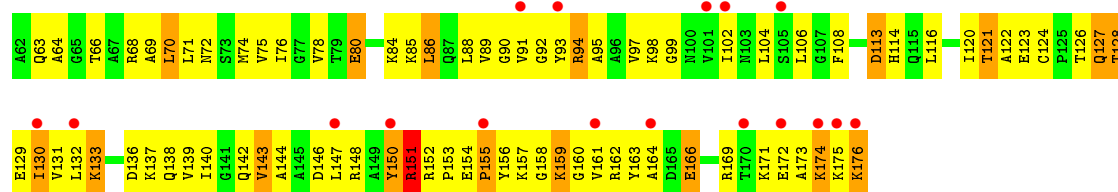


• Molecule 28: 50S ribosomal protein L5

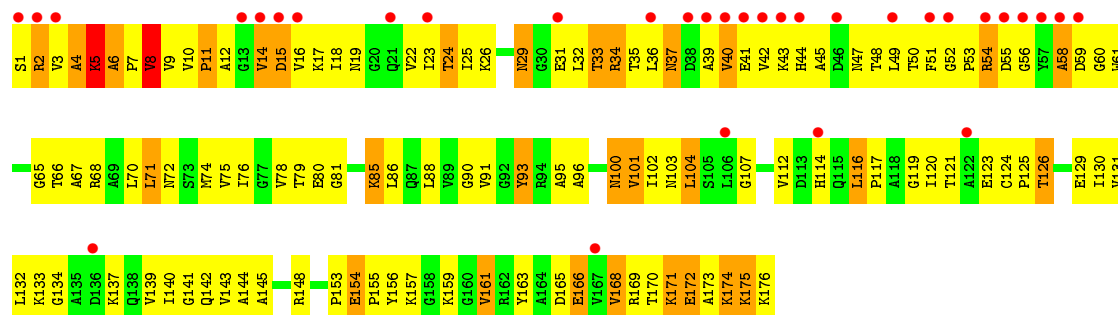


• Molecule 29: 50S ribosomal protein L6

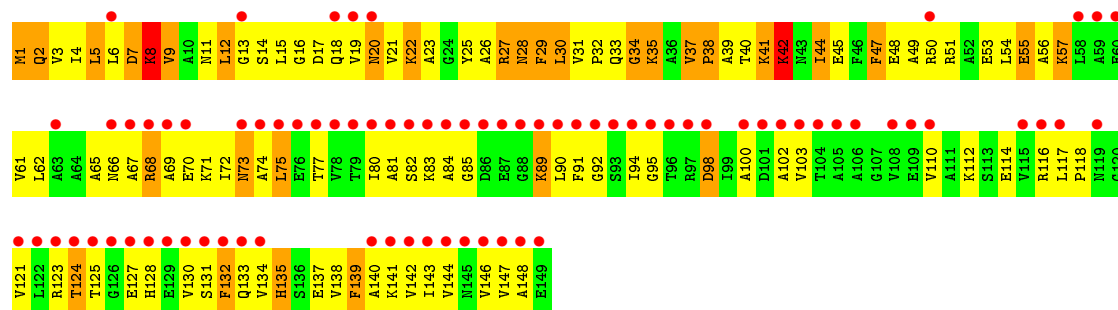




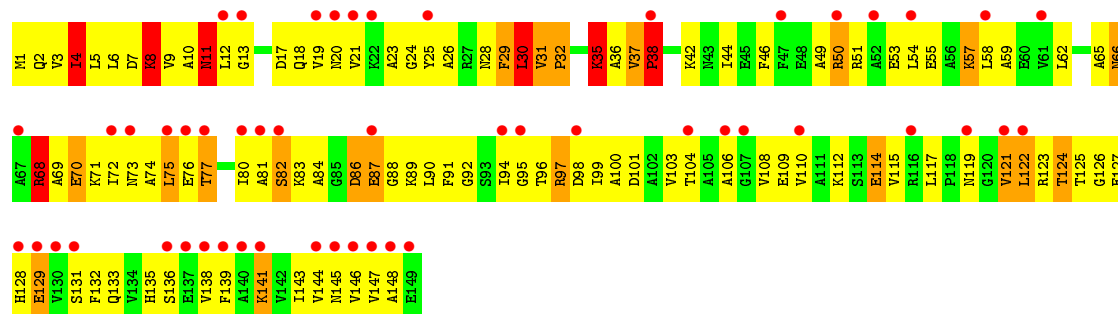
• Molecule 29: 50S ribosomal protein L6



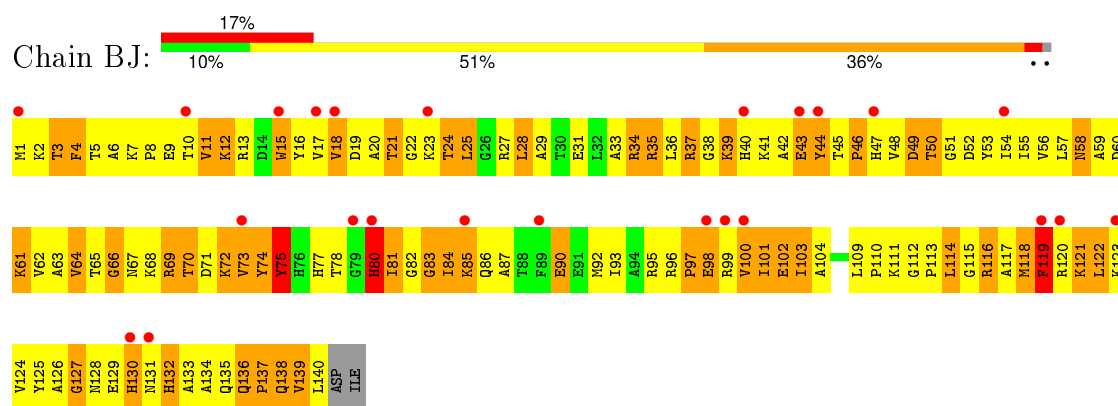
• Molecule 30: 50S ribosomal protein L9



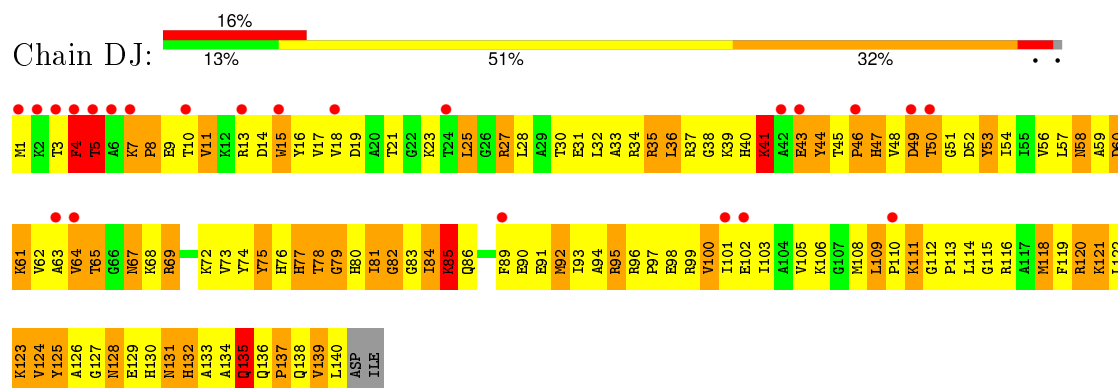
• Molecule 30: 50S ribosomal protein L9



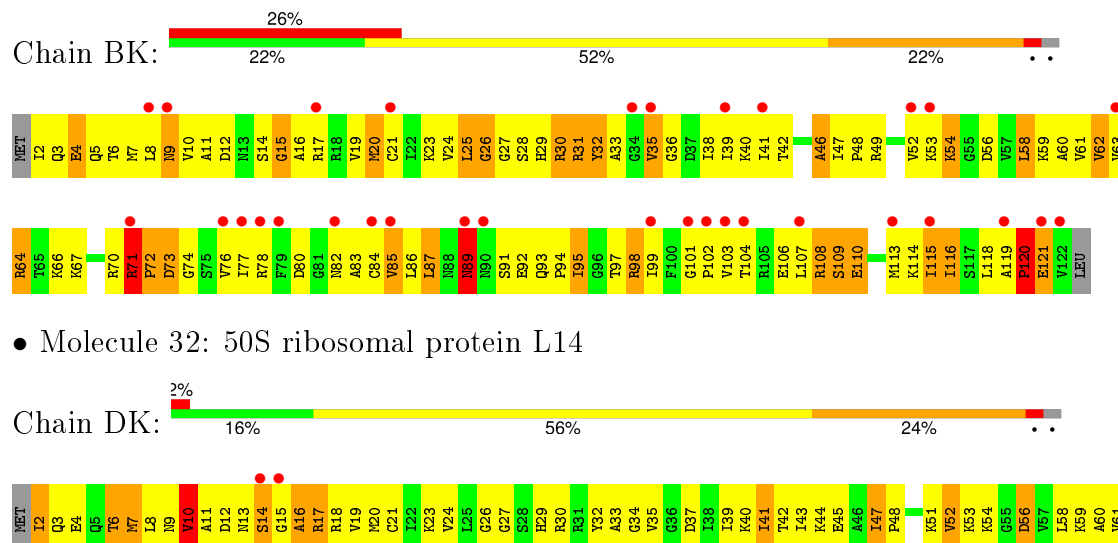
• Molecule 31: 50S ribosomal protein L13



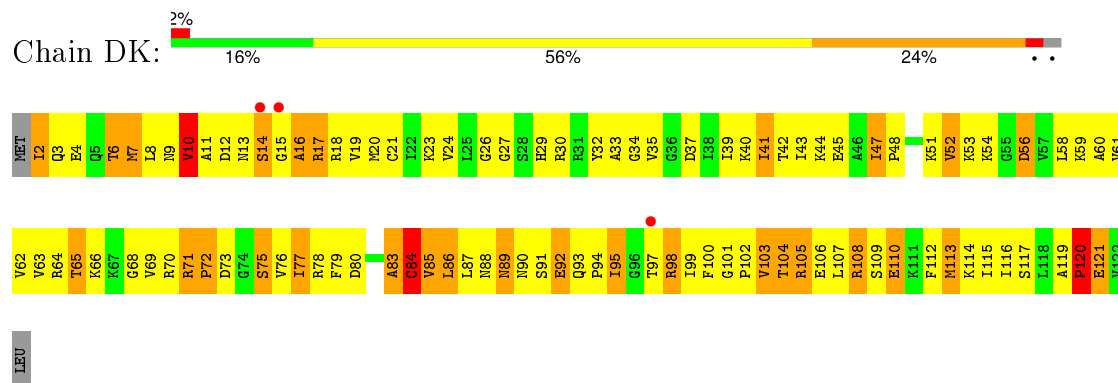
• Molecule 31: 50S ribosomal protein L13



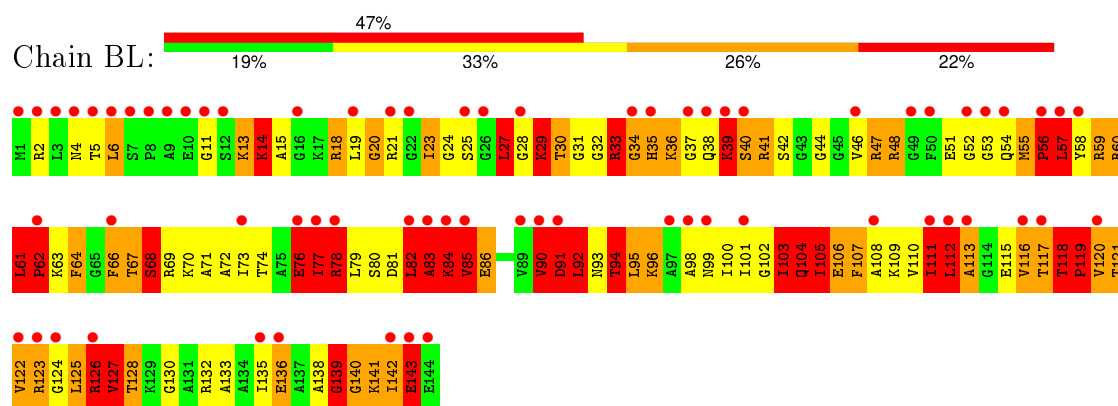
• Molecule 32: 50S ribosomal protein L14



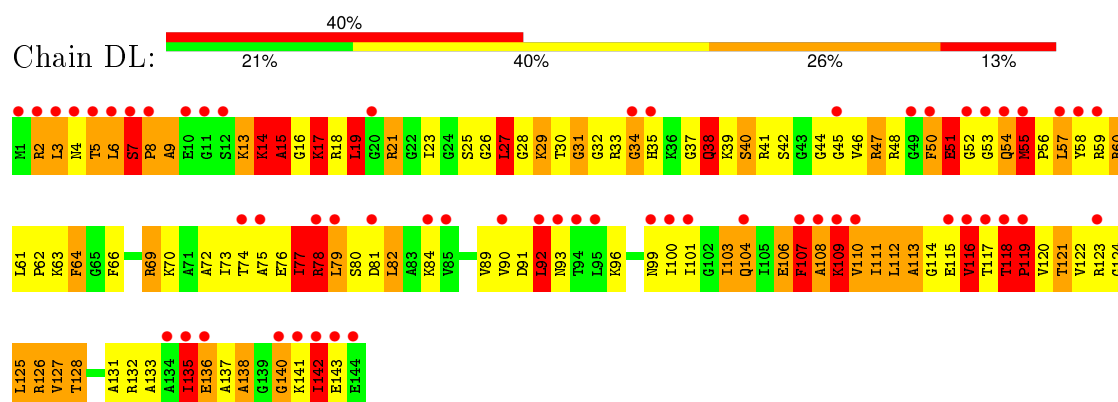
• Molecule 32: 50S ribosomal protein L14



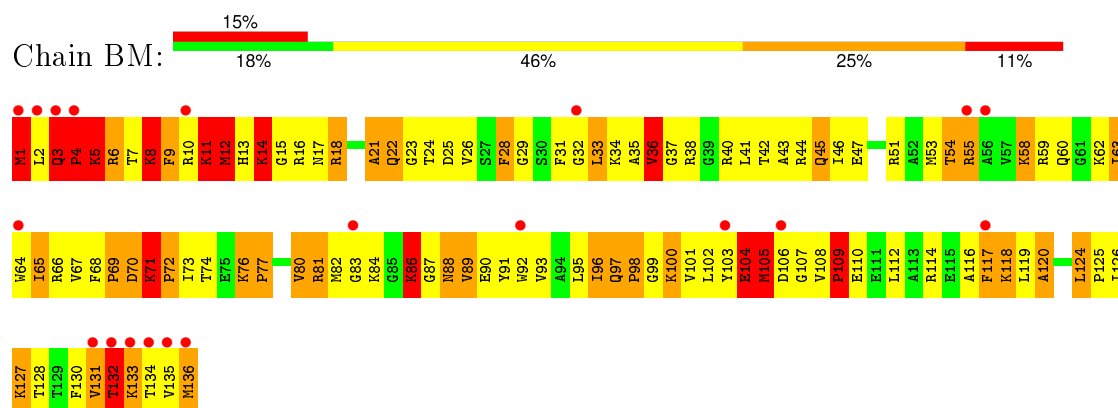
• Molecule 33: 50S ribosomal protein L15



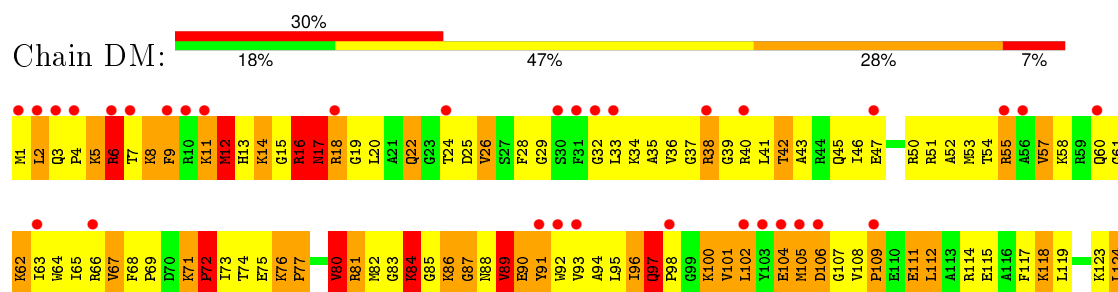
• Molecule 33: 50S ribosomal protein L15

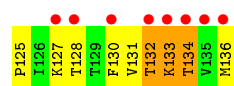


• Molecule 34: 50S ribosomal protein L16

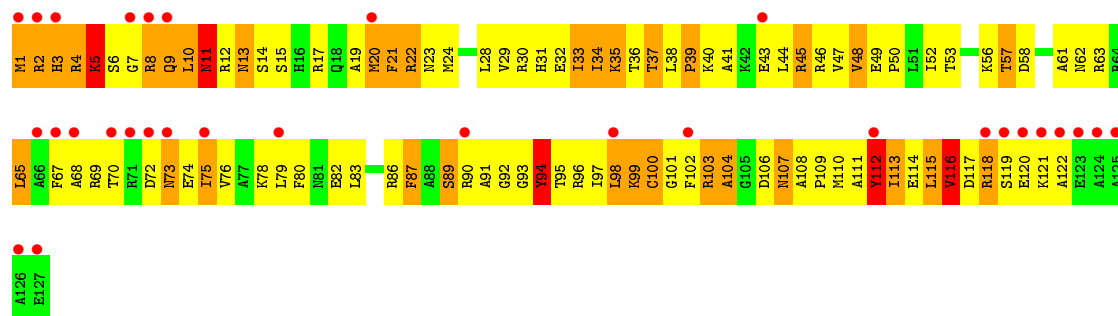


• Molecule 34: 50S ribosomal protein L16

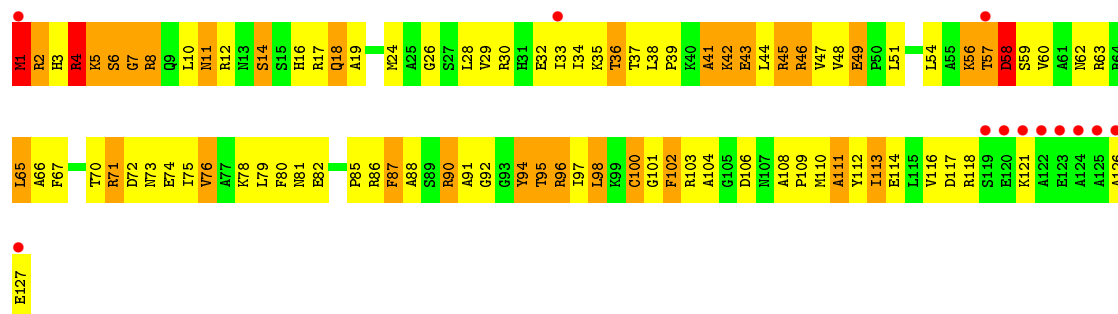




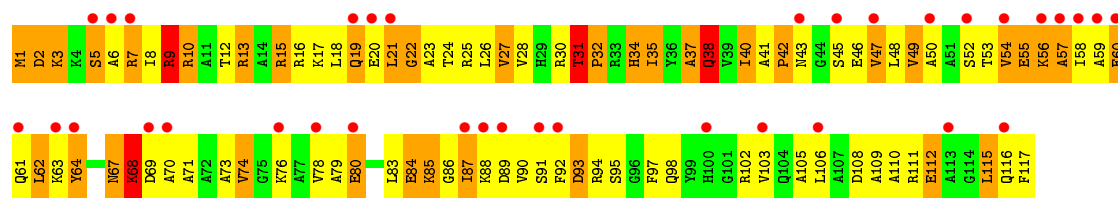
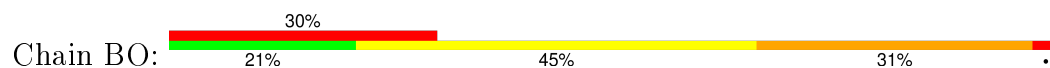
- Molecule 35: 50S ribosomal protein L17



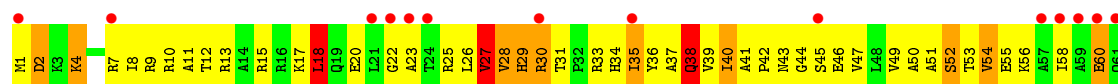
- Molecule 35: 50S ribosomal protein L17

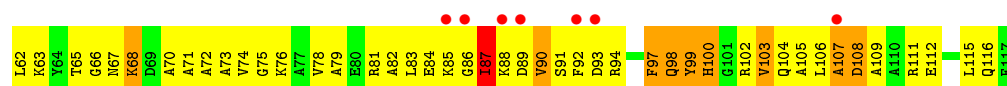


- Molecule 36: 50S ribosomal protein L18

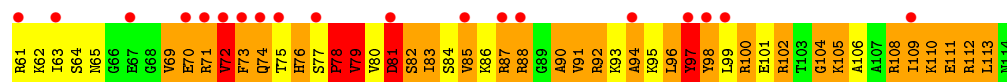
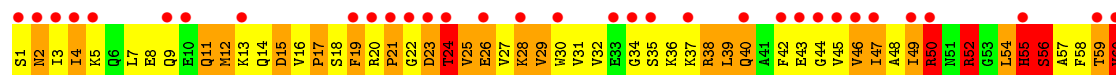


- Molecule 36: 50S ribosomal protein L18

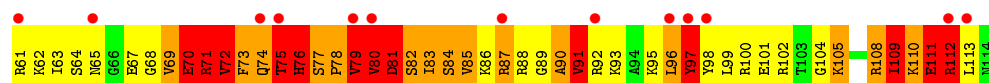
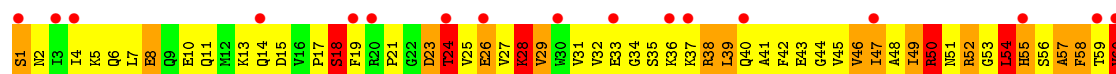




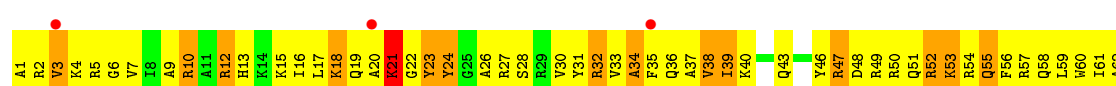
• Molecule 37: 50S ribosomal protein L19



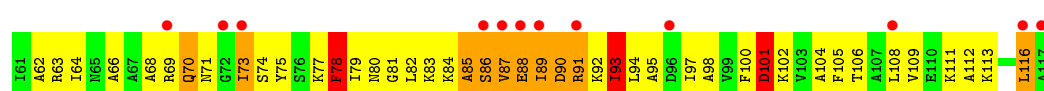
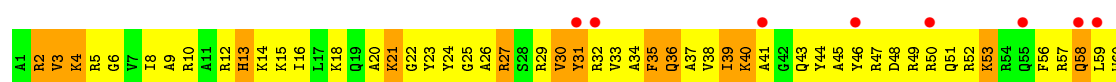
• Molecule 37: 50S ribosomal protein L19



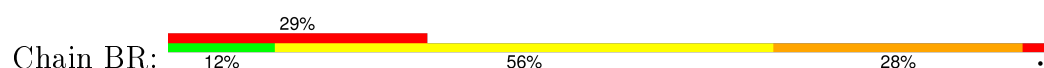
• Molecule 38: 50S ribosomal protein L20

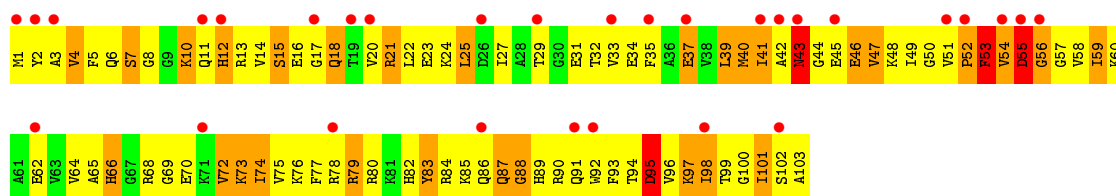


• Molecule 38: 50S ribosomal protein L20

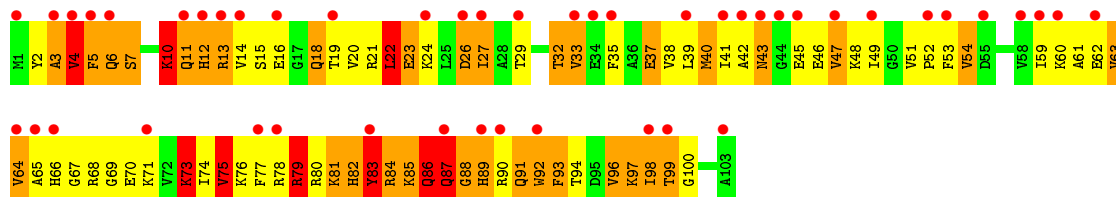
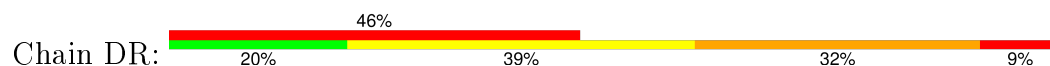


• Molecule 39: 50S ribosomal protein L21

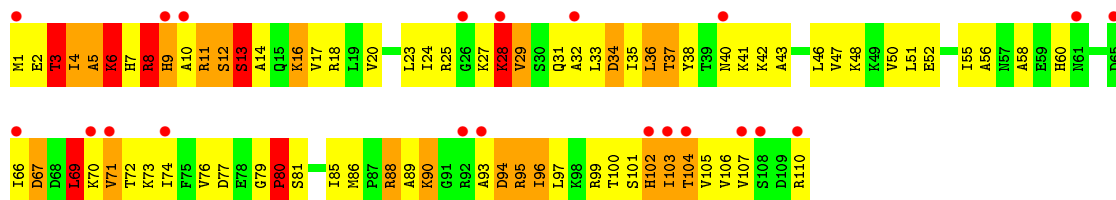




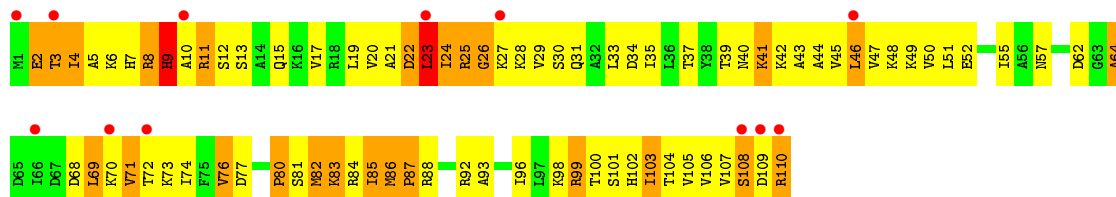
• Molecule 39: 50S ribosomal protein L21



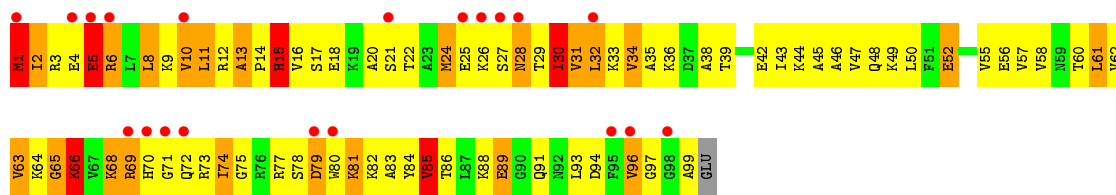
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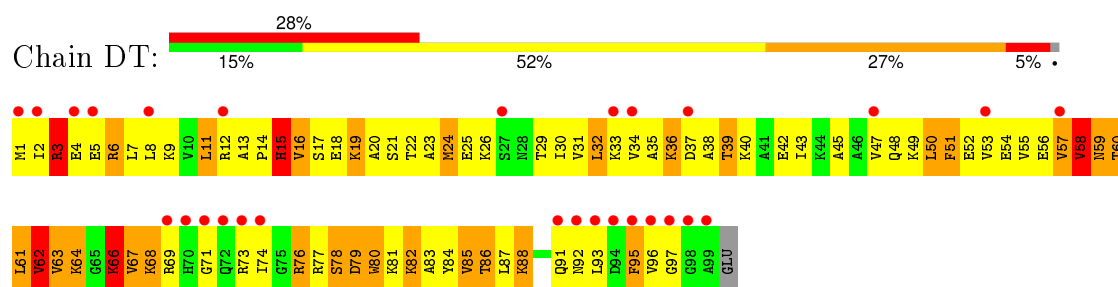
• Molecule 40: 50S ribosomal protein L22



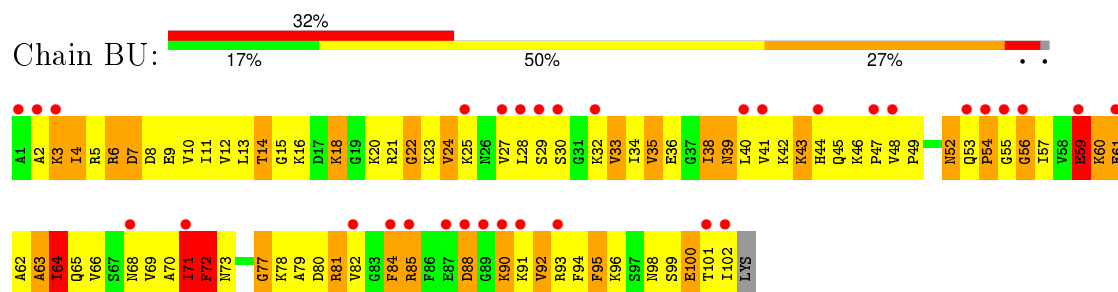
• Molecule 41: 50S ribosomal protein L23



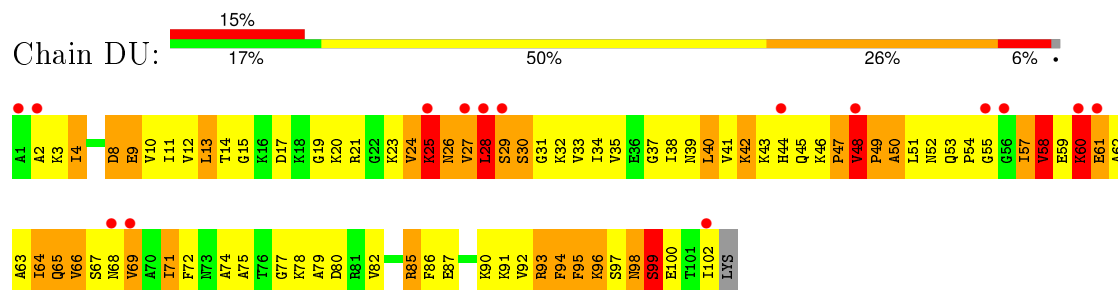
• Molecule 41: 50S ribosomal protein L23



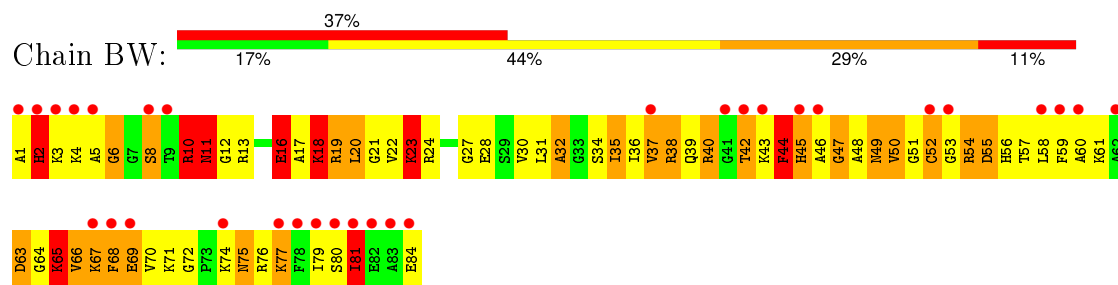
• Molecule 42: 50S ribosomal protein L24



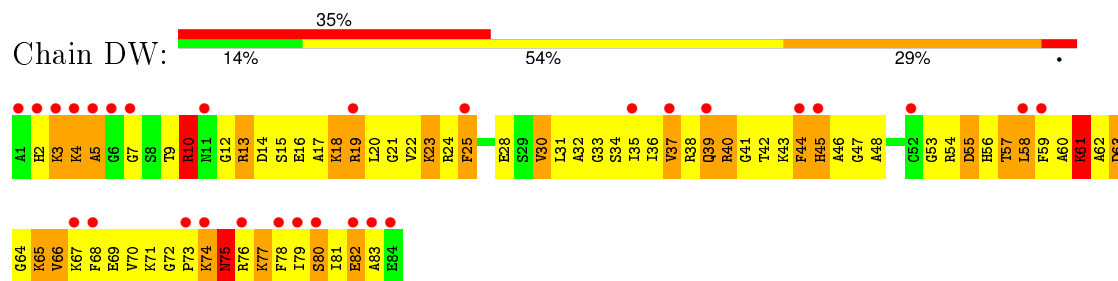
• Molecule 42: 50S ribosomal protein L24



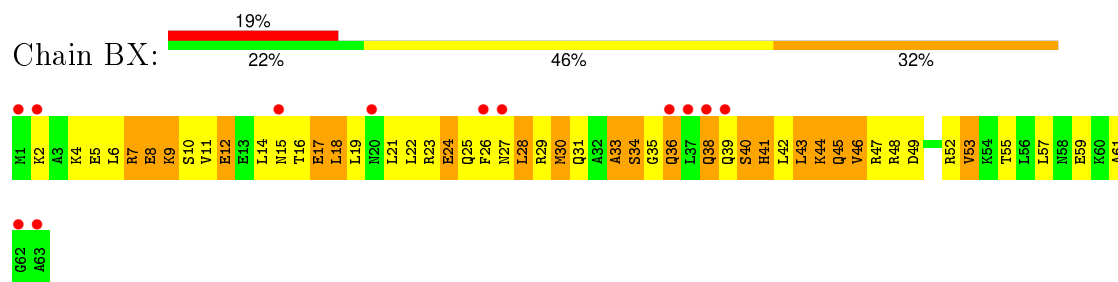
• Molecule 43: 50S ribosomal protein L27



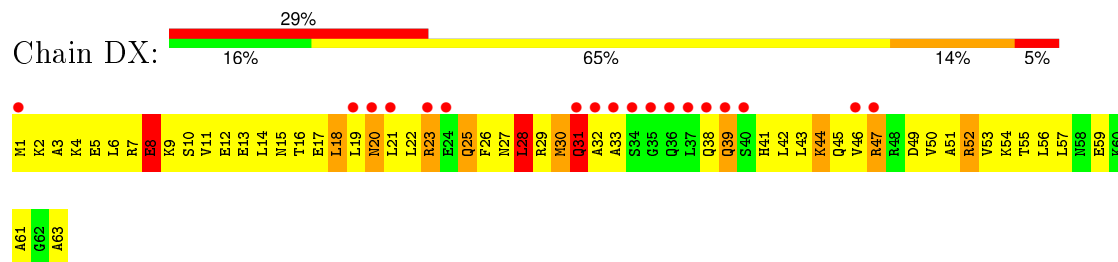
• Molecule 43: 50S ribosomal protein L27



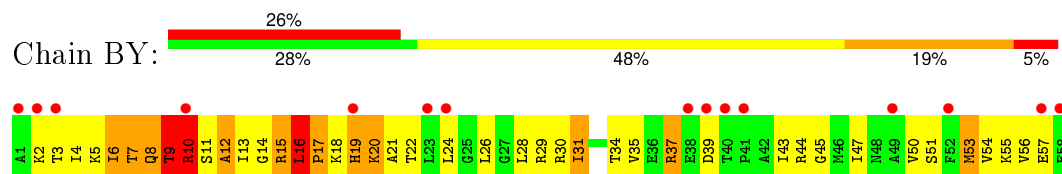
• Molecule 44: 50S ribosomal protein L29



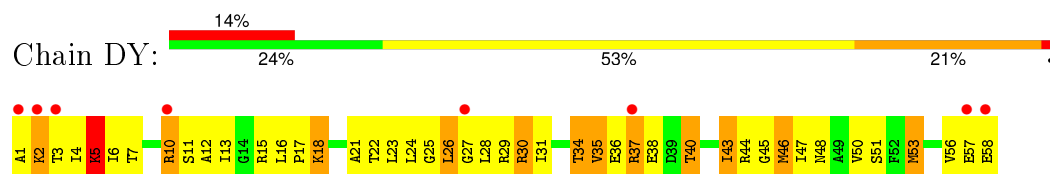
• Molecule 44: 50S ribosomal protein L29



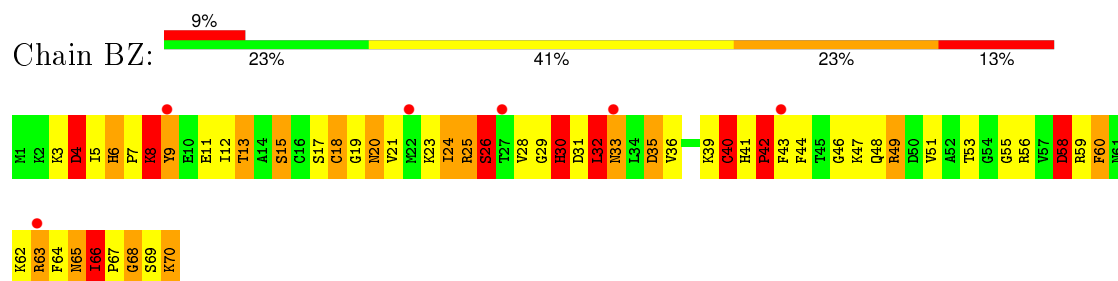
• Molecule 45: 50S ribosomal protein L30



• Molecule 45: 50S ribosomal protein L30

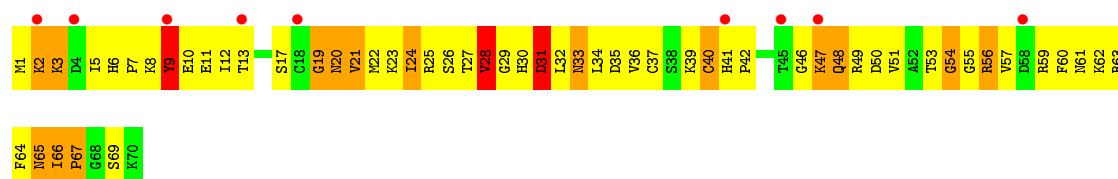


• Molecule 46: 50S ribosomal protein L31

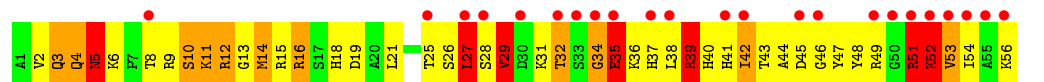
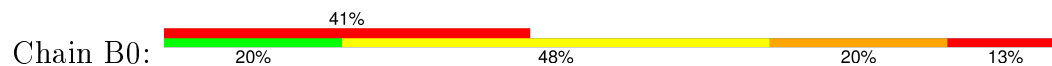


• Molecule 46: 50S ribosomal protein L31

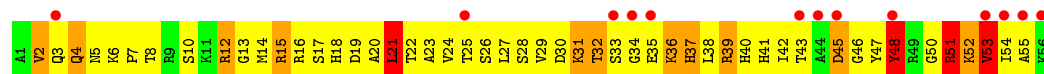
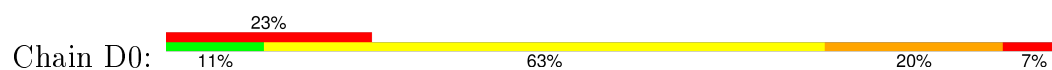




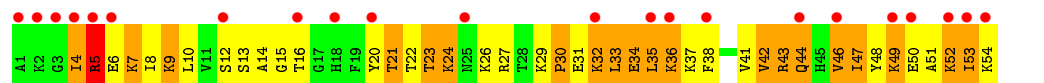
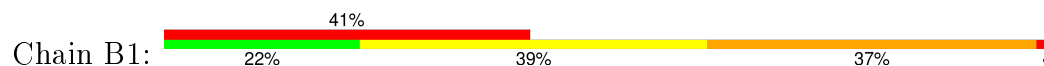
- Molecule 47: 50S ribosomal protein L32



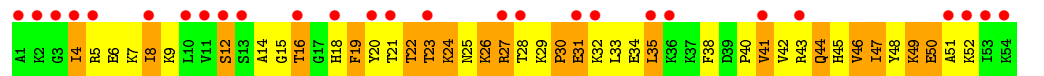
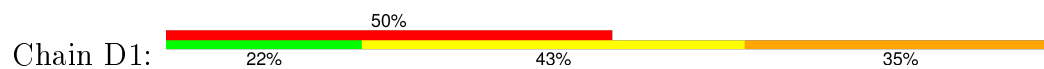
- Molecule 47: 50S ribosomal protein L32



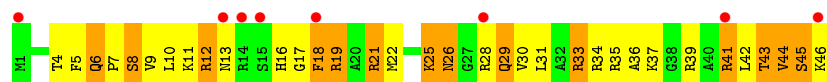
- Molecule 48: 50S ribosomal protein L33



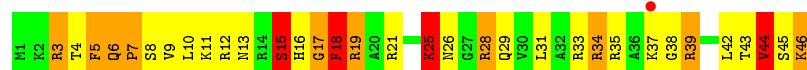
- Molecule 48: 50S ribosomal protein L33



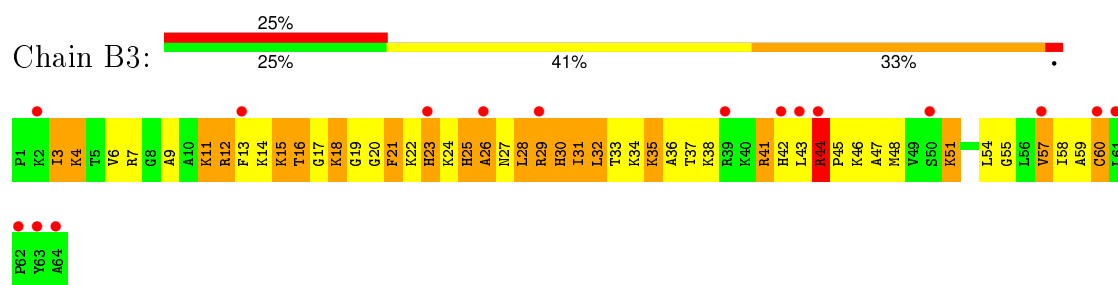
- Molecule 49: 50S ribosomal protein L34



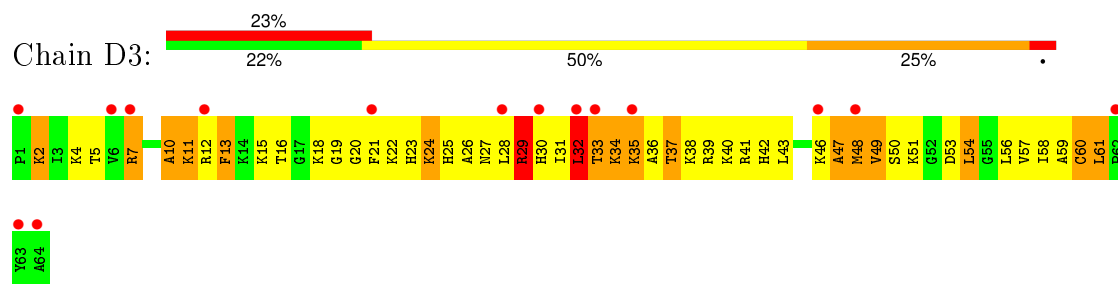
- Molecule 49: 50S ribosomal protein L34



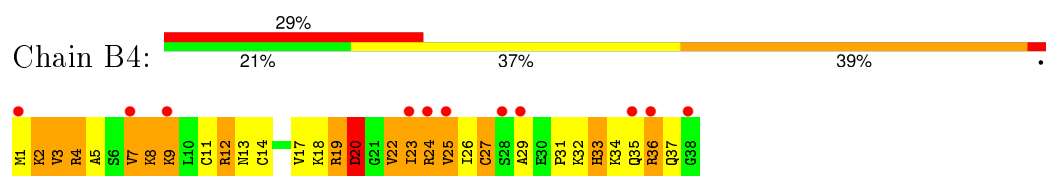
- Molecule 50: 50S ribosomal protein L35



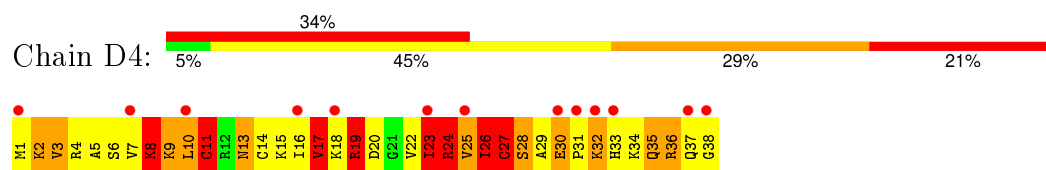
- Molecule 50: 50S ribosomal protein L35



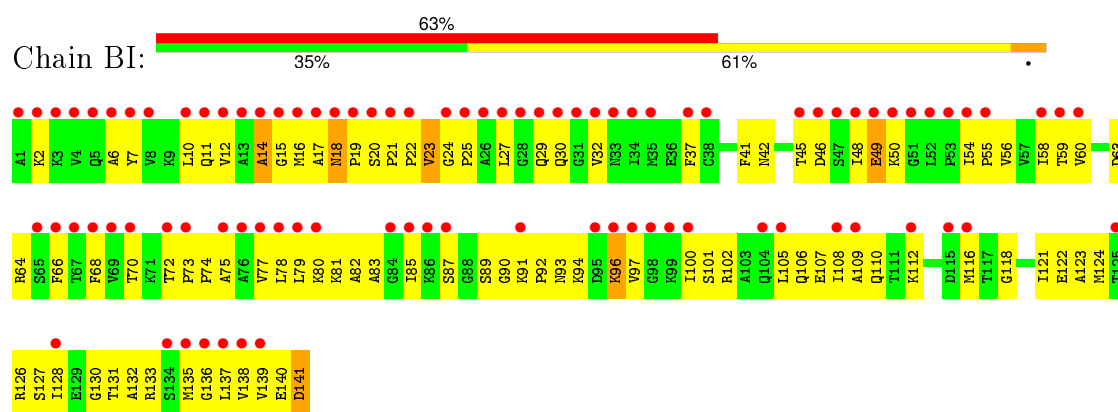
- Molecule 51: 50S ribosomal protein L36



- Molecule 51: 50S ribosomal protein L36

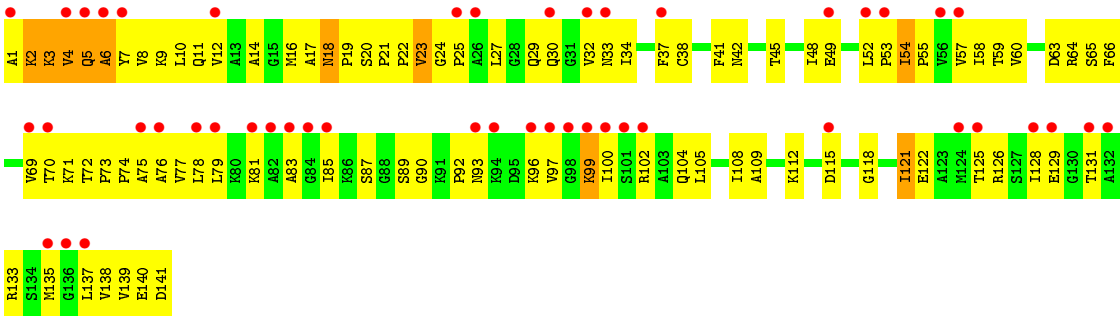


- Molecule 52: 50S ribosomal protein L11



- Molecule 52: 50S ribosomal protein L11





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 739.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.00 – 3.46 163.96 – 3.46	Depositor EDS
% Data completeness (in resolution range)	91.6 (70.00-3.46) 91.6 (163.96-3.46)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 3.49Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.279 , 0.331 0.262 , 0.308	Depositor DCC
R_{free} test set	35582 reflections (5.40%)	DCC
Wilson B-factor (Å ²)	77.0	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 65.0	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 720727 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	284107	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.43% 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: 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	0.26	1/36762 (0.0%)	0.75	7/57350 (0.0%)
1	CA	0.26	2/36762 (0.0%)	0.75	11/57350 (0.0%)
2	AC	0.23	0/1651	0.44	0/2225
2	CC	0.23	0/1651	0.47	0/2225
3	AD	0.23	0/1665	0.46	0/2227
3	CD	0.23	0/1665	0.45	0/2227
4	AE	0.23	0/1118	0.45	0/1504
4	CE	0.24	0/1118	0.45	0/1504
5	AF	0.25	0/835	0.47	0/1128
5	CF	0.24	0/835	0.49	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	0.45	0/1326
7	CH	0.23	0/989	0.46	0/1326
8	AI	0.24	0/1034	0.45	0/1375
8	CI	0.24	0/1034	0.46	0/1375
9	AJ	0.23	0/796	0.49	0/1077
9	CJ	0.22	0/796	0.49	0/1077
10	AK	0.24	0/893	0.46	0/1205
10	CK	0.24	0/893	0.47	0/1205
11	AL	0.22	0/969	0.47	0/1300
11	CL	0.22	0/969	0.48	0/1300
12	AM	0.21	0/892	0.48	0/1193
12	CM	0.21	0/884	0.46	0/1181
13	AN	0.24	0/785	0.46	0/1043
13	CN	0.24	0/785	0.45	0/1043
14	AO	0.23	0/724	0.45	0/966
14	CO	0.23	0/724	0.44	0/966
15	AP	0.26	0/659	0.44	0/884
15	CP	0.25	0/648	0.45	0/870
16	AQ	0.23	0/657	0.46	0/881
16	CQ	0.24	0/665	0.47	0/892

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AR	0.23	0/462	0.46	0/621
17	CR	0.23	0/462	0.45	0/621
18	AS	0.25	0/652	0.46	0/877
18	CS	0.25	0/660	0.47	0/888
19	AT	0.23	0/671	0.41	0/888
19	CT	0.24	0/671	0.42	0/888
20	AB	0.25	0/1735	0.47	0/2338
20	CB	0.25	0/1735	0.47	0/2338
21	AU	1.01	4/430 (0.9%)	0.74	2/570 (0.4%)
21	CU	0.98	3/430 (0.7%)	0.82	3/570 (0.5%)
22	BA	0.27	0/2803	0.74	0/4371
22	DA	0.28	0/2803	0.77	0/4371
23	BB	0.33	15/68314 (0.0%)	0.79	63/106569 (0.1%)
23	DB	0.34	18/68314 (0.0%)	0.79	75/106569 (0.1%)
24	BV	0.30	0/766	0.53	0/1025
24	DV	0.25	0/766	0.46	0/1025
25	BC	0.40	0/2092	0.88	7/2813 (0.2%)
25	DC	0.40	0/2092	0.90	8/2813 (0.3%)
26	BD	0.40	0/1586	0.80	2/2134 (0.1%)
26	DD	0.37	0/1586	0.82	4/2134 (0.2%)
27	BE	0.45	1/1571 (0.1%)	0.88	6/2113 (0.3%)
27	DE	0.70	4/1571 (0.3%)	0.83	5/2113 (0.2%)
28	BF	0.33	0/1444	0.87	5/1937 (0.3%)
28	DF	0.41	1/1444 (0.1%)	1.00	10/1937 (0.5%)
29	BG	0.31	0/1343	0.69	0/1816
29	DG	0.30	0/1343	0.67	1/1816 (0.1%)
30	BH	0.28	0/1122	0.60	0/1515
30	DH	0.34	0/1122	0.71	1/1515 (0.1%)
31	BJ	0.41	1/1135 (0.1%)	0.72	3/1529 (0.2%)
31	DJ	0.32	0/1135	0.76	3/1529 (0.2%)
32	BK	0.35	0/939	1.00	2/1258 (0.2%)
32	DK	0.35	0/939	0.99	4/1258 (0.3%)
33	BL	0.69	0/1062	1.60	31/1413 (2.2%)
33	DL	0.74	1/1062 (0.1%)	1.58	25/1413 (1.8%)
34	BM	0.48	0/1093	1.03	8/1460 (0.5%)
34	DM	0.39	0/1093	0.85	5/1460 (0.3%)
35	BN	0.37	0/1021	0.92	7/1364 (0.5%)
35	DN	0.37	0/1021	0.80	3/1364 (0.2%)
36	BO	0.30	0/910	0.67	0/1219
36	DO	0.31	0/910	0.64	0/1219
37	BP	0.55	0/929	1.40	16/1242 (1.3%)
37	DP	0.58	0/929	1.40	16/1242 (1.3%)
38	BQ	0.41	0/960	0.86	3/1278 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DQ	0.36	0/960	0.75	0/1278
39	BR	1.06	6/829 (0.7%)	1.42	13/1107 (1.2%)
39	DR	0.38	0/829	0.82	3/1107 (0.3%)
40	BS	0.27	0/864	0.68	1/1156 (0.1%)
40	DS	0.26	0/864	0.60	0/1156
41	BT	0.39	0/784	0.78	4/1048 (0.4%)
41	DT	0.45	1/784 (0.1%)	0.80	1/1048 (0.1%)
42	BU	0.33	0/787	0.74	0/1051
42	DU	0.37	0/787	0.94	7/1051 (0.7%)
43	BW	0.36	0/642	0.96	5/848 (0.6%)
43	DW	0.39	0/642	0.80	2/848 (0.2%)
44	BX	0.29	0/510	0.80	1/677 (0.1%)
44	DX	0.29	0/510	0.66	0/677
45	BY	0.31	0/453	0.64	0/605
45	DY	0.31	0/453	0.69	1/605 (0.2%)
46	BZ	0.48	0/559	1.04	5/745 (0.7%)
46	DZ	0.52	0/559	0.91	1/745 (0.1%)
47	B0	0.53	1/450 (0.2%)	1.15	7/599 (1.2%)
47	D0	0.41	0/450	0.97	3/599 (0.5%)
48	B1	0.36	0/448	0.71	0/594
48	D1	0.32	0/448	0.69	0/594
49	B2	0.33	0/380	0.64	0/498
49	D2	0.30	0/380	0.60	0/498
50	B3	0.47	0/513	0.95	1/676 (0.1%)
50	D3	0.39	0/513	0.80	1/676 (0.1%)
51	B4	0.40	0/303	0.73	0/397
51	D4	0.32	0/303	0.77	0/397
52	BI	0.26	0/1046	0.58	0/1410
52	DI	0.60	4/1046 (0.4%)	0.76	4/1410 (0.3%)
All	All	0.33	63/306469 (0.0%)	0.77	396/458101 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	16
1	CA	0	20
21	AU	0	1
22	DA	0	1
23	BB	0	60

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Mol	Chain	#Chirality outliers	#Planarity outliers
23	DB	1	65
25	BC	0	3
25	DC	0	2
31	BJ	0	2
33	BL	0	1
37	BP	0	1
37	DP	0	1
38	BQ	0	1
39	BR	0	1
39	DR	0	1
46	DZ	0	1
47	D0	0	1
All	All	1	178

The worst 5 of 63 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	DE	79	ARG	CD-NE	18.29	1.77	1.46
39	BR	53	PHE	CB-CG	17.86	1.81	1.51
23	DB	1086	A	C5-C6	-17.70	1.25	1.41
23	BB	1086	A	C5-C6	-17.70	1.25	1.41
21	CU	25	ALA	C-N	15.34	1.60	1.33

The worst 5 of 396 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	BB	2791	G	O5'-P-OP1	-28.71	76.25	110.70
23	DB	2791	G	O5'-P-OP2	-27.77	77.38	110.70
23	DB	2791	G	O5'-P-OP1	18.50	132.90	110.70
23	BB	2791	G	O5'-P-OP2	18.20	132.54	110.70
23	DB	448	U	N1-C1'-C2'	17.52	136.78	114.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	DB	2076	U	C3'

5 of 178 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	187	G	Sidechain
1	AA	281	G	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	437	U	Sidechain
1	AA	438	U	Sidechain
1	AA	58	C	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	1157	0
1	CA	32831	0	16521	1198	0
2	AC	1624	0	1699	159	0
2	CC	1624	0	1699	148	0
3	AD	1643	0	1710	172	0
3	CD	1643	0	1710	167	0
4	AE	1105	0	1148	109	0
4	CE	1105	0	1148	143	0
5	AF	817	0	808	78	0
5	CF	817	0	808	93	0
6	AG	1174	0	1230	100	0
6	CG	1196	0	1246	98	0
7	AH	979	0	1034	78	0
7	CH	979	0	1034	86	0
8	AI	1022	0	1070	144	0
8	CI	1022	0	1070	127	0
9	AJ	786	0	828	92	0
9	CJ	786	0	828	106	0
10	AK	877	0	887	111	0
10	CK	877	0	887	108	0
11	AL	955	0	1019	103	0
11	CL	955	0	1019	101	0
12	AM	883	0	944	88	0
12	CM	876	0	937	95	0
13	AN	774	0	827	93	0
13	CN	774	0	827	114	0
14	AO	716	0	742	53	0
14	CO	716	0	742	50	0
15	AP	649	0	666	77	0
15	CP	638	0	656	71	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	AQ	648	0	691	80	0
16	CQ	656	0	702	85	0
17	AR	455	0	478	39	0
17	CR	455	0	478	41	0
18	AS	637	0	665	75	0
18	CS	644	0	675	87	0
19	AT	665	0	714	52	0
19	CT	665	0	714	64	0
20	AB	1704	0	1732	195	0
20	CB	1704	0	1732	152	0
21	AU	425	0	447	104	0
21	CU	425	0	449	84	0
22	BA	2507	0	1270	87	0
22	DA	2507	0	1270	97	0
23	BB	60995	0	30678	2393	0
23	DB	60995	0	30677	2365	0
24	BV	753	0	780	107	0
24	DV	753	0	780	69	0
25	BC	2053	0	2122	436	0
25	DC	2053	0	2122	433	0
26	BD	1565	0	1616	372	0
26	DD	1565	0	1616	316	0
27	BE	1552	0	1619	261	0
27	DE	1552	0	1619	266	0
28	BF	1420	0	1460	169	0
28	DF	1420	0	1460	181	0
29	BG	1323	0	1374	175	0
29	DG	1323	0	1374	162	0
30	BH	1111	0	1148	160	0
30	DH	1111	0	1148	145	0
31	BJ	1112	0	1147	219	0
31	DJ	1112	0	1147	231	0
32	BK	930	0	1000	121	0
32	DK	930	0	1000	126	0
33	BL	1053	0	1129	284	0
33	DL	1053	0	1129	227	0
34	BM	1074	0	1157	237	0
34	DM	1074	0	1157	189	0
35	BN	1008	0	1045	157	0
35	DN	1008	0	1045	133	0
36	BO	900	0	935	128	0
36	DO	900	0	935	128	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	BP	917	0	965	206	0
37	DP	917	0	965	209	0
38	BQ	947	0	1022	178	0
38	DQ	947	0	1022	161	0
39	BR	816	0	838	165	0
39	DR	816	0	839	180	0
40	BS	857	0	922	122	0
40	DS	857	0	922	111	0
41	BT	777	0	840	139	0
41	DT	777	0	840	129	0
42	BU	779	0	834	152	0
42	DU	779	0	834	134	0
43	BW	634	0	656	155	0
43	DW	634	0	656	156	0
44	BX	509	0	543	73	0
44	DX	509	0	543	90	0
45	BY	449	0	491	57	0
45	DY	449	0	491	64	0
46	BZ	549	0	552	114	0
46	DZ	549	0	552	101	0
47	B0	444	0	461	75	0
47	D0	444	0	461	80	0
48	B1	441	0	485	63	0
48	D1	441	0	485	69	0
49	B2	377	0	418	55	0
49	D2	377	0	418	66	0
50	B3	504	0	574	111	0
50	D3	504	0	574	113	0
51	B4	302	0	343	44	0
51	D4	302	0	343	80	0
52	BI	1032	0	1088	129	0
52	DI	1032	0	1088	214	0
53	AA	59	0	0	0	0
53	AP	1	0	0	0	0
53	BB	110	0	0	0	0
53	CA	62	0	0	0	0
53	DB	110	0	0	0	0
53	DN	1	0	0	0	0
54	AA	290	0	0	0	0
54	AE	3	0	0	0	0
54	AK	2	0	0	0	0
54	AN	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	AP	1	0	0	0	0
54	BB	497	0	0	12	0
54	BC	1	0	0	0	0
54	BE	5	0	0	0	0
54	BH	1	0	0	0	0
54	BL	2	0	0	0	0
54	BN	1	0	0	0	0
54	CA	295	0	0	1	0
54	CE	3	0	0	0	0
54	CK	1	0	0	0	0
54	CL	4	0	0	0	0
54	CN	2	0	0	0	0
54	CP	1	0	0	0	0
54	CT	2	0	0	0	0
54	D2	2	0	0	0	0
54	DB	499	0	0	7	0
54	DC	1	0	0	0	0
54	DD	1	0	0	0	0
54	DE	3	0	0	0	0
54	DJ	2	0	0	1	0
54	DL	1	0	0	0	0
54	DN	2	0	0	0	0
54	DQ	1	0	0	0	0
All	All	284107	0	190766	18478	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 39.

The worst 5 of 18478 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)
52:DI:3:LYS:CE	52:DI:3:LYS:CD	1.74	1.64
39:BR:53:PHE:CG	39:BR:53:PHE:CB	1.81	1.61
39:BR:54:VAL:CA	39:BR:54:VAL:CB	1.78	1.57
27:DE:79:ARG:CG	27:DE:79:ARG:CD	1.78	1.57
52:DI:3:LYS:CG	52:DI:3:LYS:CD	1.81	1.56

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	135 (66%)	49 (24%)	20 (10%)	1	9
2	CC	204/232 (88%)	139 (68%)	45 (22%)	20 (10%)	1	9
3	AD	203/205 (99%)	131 (64%)	54 (27%)	18 (9%)	1	11
3	CD	203/205 (99%)	137 (68%)	49 (24%)	17 (8%)	1	12
4	AE	148/166 (89%)	107 (72%)	34 (23%)	7 (5%)	3	28
4	CE	148/166 (89%)	108 (73%)	31 (21%)	9 (6%)	2	19
5	AF	98/135 (73%)	69 (70%)	23 (24%)	6 (6%)	2	19
5	CF	98/135 (73%)	65 (66%)	23 (24%)	10 (10%)	1	9
6	AG	148/178 (83%)	103 (70%)	37 (25%)	8 (5%)	2	23
6	CG	150/178 (84%)	101 (67%)	36 (24%)	13 (9%)	1	11
7	AH	127/129 (98%)	105 (83%)	19 (15%)	3 (2%)	7	45
7	CH	127/129 (98%)	90 (71%)	31 (24%)	6 (5%)	3	28
8	AI	125/129 (97%)	87 (70%)	27 (22%)	11 (9%)	1	11
8	CI	125/129 (97%)	82 (66%)	33 (26%)	10 (8%)	1	13
9	AJ	96/103 (93%)	63 (66%)	21 (22%)	12 (12%)	0	5
9	CJ	96/103 (93%)	58 (60%)	21 (22%)	17 (18%)	0	2
10	AK	115/128 (90%)	75 (65%)	27 (24%)	13 (11%)	0	7
10	CK	115/128 (90%)	78 (68%)	27 (24%)	10 (9%)	1	11
11	AL	121/123 (98%)	74 (61%)	30 (25%)	17 (14%)	0	4
11	CL	121/123 (98%)	75 (62%)	28 (23%)	18 (15%)	0	3
12	AM	112/117 (96%)	87 (78%)	14 (12%)	11 (10%)	1	9
12	CM	111/117 (95%)	79 (71%)	17 (15%)	15 (14%)	0	4
13	AN	92/100 (92%)	59 (64%)	24 (26%)	9 (10%)	1	9
13	CN	92/100 (92%)	53 (58%)	24 (26%)	15 (16%)	0	2
14	AO	86/89 (97%)	66 (77%)	18 (21%)	2 (2%)	8	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	CO	86/89 (97%)	67 (78%)	16 (19%)	3 (4%)	4	36
15	AP	80/82 (98%)	59 (74%)	17 (21%)	4 (5%)	3	25
15	CP	78/82 (95%)	52 (67%)	19 (24%)	7 (9%)	1	10
16	AQ	78/83 (94%)	48 (62%)	26 (33%)	4 (5%)	2	25
16	CQ	79/83 (95%)	61 (77%)	13 (16%)	5 (6%)	2	19
17	AR	53/74 (72%)	27 (51%)	19 (36%)	7 (13%)	0	4
17	CR	53/74 (72%)	39 (74%)	11 (21%)	3 (6%)	2	22
18	AS	77/91 (85%)	57 (74%)	14 (18%)	6 (8%)	1	13
18	CS	78/91 (86%)	48 (62%)	17 (22%)	13 (17%)	0	2
19	AT	83/86 (96%)	69 (83%)	8 (10%)	6 (7%)	1	15
19	CT	83/86 (96%)	61 (74%)	16 (19%)	6 (7%)	1	15
20	AB	216/240 (90%)	145 (67%)	53 (24%)	18 (8%)	1	12
20	CB	216/240 (90%)	150 (69%)	36 (17%)	30 (14%)	0	4
21	AU	49/71 (69%)	22 (45%)	12 (24%)	15 (31%)	0	0
21	CU	49/71 (69%)	28 (57%)	15 (31%)	6 (12%)	0	6
24	BV	92/94 (98%)	62 (67%)	21 (23%)	9 (10%)	1	9
24	DV	92/94 (98%)	59 (64%)	27 (29%)	6 (6%)	1	18
25	BC	265/273 (97%)	103 (39%)	83 (31%)	79 (30%)	0	0
25	DC	265/273 (97%)	97 (37%)	93 (35%)	75 (28%)	0	0
26	BD	207/209 (99%)	90 (44%)	69 (33%)	48 (23%)	0	1
26	DD	207/209 (99%)	96 (46%)	67 (32%)	44 (21%)	0	1
27	BE	199/201 (99%)	98 (49%)	60 (30%)	41 (21%)	0	1
27	DE	199/201 (99%)	87 (44%)	63 (32%)	49 (25%)	0	1
28	BF	176/178 (99%)	95 (54%)	48 (27%)	33 (19%)	0	2
28	DF	176/178 (99%)	91 (52%)	53 (30%)	32 (18%)	0	2
29	BG	174/176 (99%)	118 (68%)	39 (22%)	17 (10%)	1	9
29	DG	174/176 (99%)	117 (67%)	39 (22%)	18 (10%)	1	8
30	BH	147/149 (99%)	87 (59%)	45 (31%)	15 (10%)	1	9
30	DH	147/149 (99%)	84 (57%)	44 (30%)	19 (13%)	0	5
31	BJ	138/142 (97%)	67 (49%)	42 (30%)	29 (21%)	0	1
31	DJ	138/142 (97%)	70 (51%)	36 (26%)	32 (23%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	BK	119/123 (97%)	71 (60%)	32 (27%)	16 (13%)	0	4
32	DK	119/123 (97%)	72 (60%)	25 (21%)	22 (18%)	0	2
33	BL	142/144 (99%)	60 (42%)	40 (28%)	42 (30%)	0	0
33	DL	142/144 (99%)	66 (46%)	37 (26%)	39 (28%)	0	0
34	BM	134/136 (98%)	69 (52%)	37 (28%)	28 (21%)	0	1
34	DM	134/136 (98%)	79 (59%)	31 (23%)	24 (18%)	0	2
35	BN	125/127 (98%)	73 (58%)	35 (28%)	17 (14%)	0	4
35	DN	125/127 (98%)	82 (66%)	32 (26%)	11 (9%)	1	11
36	BO	115/117 (98%)	64 (56%)	26 (23%)	25 (22%)	0	1
36	DO	115/117 (98%)	63 (55%)	33 (29%)	19 (16%)	0	2
37	BP	112/114 (98%)	39 (35%)	36 (32%)	37 (33%)	0	0
37	DP	112/114 (98%)	42 (38%)	38 (34%)	32 (29%)	0	0
38	BQ	115/117 (98%)	81 (70%)	22 (19%)	12 (10%)	1	8
38	DQ	115/117 (98%)	79 (69%)	22 (19%)	14 (12%)	0	6
39	BR	101/103 (98%)	44 (44%)	31 (31%)	26 (26%)	0	1
39	DR	101/103 (98%)	42 (42%)	31 (31%)	28 (28%)	0	0
40	BS	108/110 (98%)	63 (58%)	27 (25%)	18 (17%)	0	2
40	DS	108/110 (98%)	67 (62%)	20 (18%)	21 (19%)	0	2
41	BT	97/100 (97%)	42 (43%)	40 (41%)	15 (16%)	0	3
41	DT	97/100 (97%)	42 (43%)	32 (33%)	23 (24%)	0	1
42	BU	100/103 (97%)	33 (33%)	46 (46%)	21 (21%)	0	1
42	DU	100/103 (97%)	46 (46%)	41 (41%)	13 (13%)	0	4
43	BW	82/84 (98%)	29 (35%)	26 (32%)	27 (33%)	0	0
43	DW	82/84 (98%)	31 (38%)	30 (37%)	21 (26%)	0	1
44	BX	61/63 (97%)	28 (46%)	21 (34%)	12 (20%)	0	2
44	DX	61/63 (97%)	38 (62%)	15 (25%)	8 (13%)	0	4
45	BY	56/58 (97%)	29 (52%)	17 (30%)	10 (18%)	0	2
45	DY	56/58 (97%)	35 (62%)	17 (30%)	4 (7%)	1	16
46	BZ	68/70 (97%)	29 (43%)	26 (38%)	13 (19%)	0	2
46	DZ	68/70 (97%)	37 (54%)	22 (32%)	9 (13%)	0	4
47	B0	54/56 (96%)	30 (56%)	15 (28%)	9 (17%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	D0	54/56 (96%)	30 (56%)	15 (28%)	9 (17%)	0	2
48	B1	52/54 (96%)	19 (36%)	23 (44%)	10 (19%)	0	2
48	D1	52/54 (96%)	21 (40%)	22 (42%)	9 (17%)	0	2
49	B2	44/46 (96%)	23 (52%)	14 (32%)	7 (16%)	0	2
49	D2	44/46 (96%)	24 (54%)	12 (27%)	8 (18%)	0	2
50	B3	62/64 (97%)	30 (48%)	25 (40%)	7 (11%)	0	7
50	D3	62/64 (97%)	35 (56%)	17 (27%)	10 (16%)	0	2
51	B4	36/38 (95%)	18 (50%)	9 (25%)	9 (25%)	0	1
51	D4	36/38 (95%)	13 (36%)	11 (31%)	12 (33%)	0	0
52	BI	139/141 (99%)	124 (89%)	11 (8%)	4 (3%)	6	40
52	DI	139/141 (99%)	123 (88%)	11 (8%)	5 (4%)	4	35
All	All	11263/11902 (95%)	6645 (59%)	2936 (26%)	1682 (15%)	0	3

5 of 1682 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AC	2	GLN
2	AC	91	ALA
2	AC	153	SER
3	AD	18	LEU
3	AD	31	CYS

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%)	142 (84%)	28 (16%)	3	15
2	CC	170/189 (90%)	146 (86%)	24 (14%)	4	22
3	AD	172/172 (100%)	140 (81%)	32 (19%)	2	9
3	CD	172/172 (100%)	137 (80%)	35 (20%)	1	7
4	AE	113/125 (90%)	92 (81%)	21 (19%)	2	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	CE	113/125 (90%)	92 (81%)	21 (19%)	2	9
5	AF	87/116 (75%)	68 (78%)	19 (22%)	1	5
5	CF	87/116 (75%)	74 (85%)	13 (15%)	4	20
6	AG	123/146 (84%)	102 (83%)	21 (17%)	2	14
6	CG	125/146 (86%)	106 (85%)	19 (15%)	3	19
7	AH	104/104 (100%)	87 (84%)	17 (16%)	3	16
7	CH	104/104 (100%)	85 (82%)	19 (18%)	2	10
8	AI	105/106 (99%)	83 (79%)	22 (21%)	1	6
8	CI	105/106 (99%)	89 (85%)	16 (15%)	3	19
9	AJ	86/90 (96%)	66 (77%)	20 (23%)	1	4
9	CJ	86/90 (96%)	78 (91%)	8 (9%)	11	44
10	AK	90/98 (92%)	70 (78%)	20 (22%)	1	5
10	CK	90/98 (92%)	74 (82%)	16 (18%)	2	12
11	AL	103/103 (100%)	88 (85%)	15 (15%)	4	21
11	CL	103/103 (100%)	79 (77%)	24 (23%)	1	4
12	AM	92/95 (97%)	70 (76%)	22 (24%)	1	4
12	CM	91/95 (96%)	75 (82%)	16 (18%)	2	12
13	AN	79/83 (95%)	67 (85%)	12 (15%)	3	19
13	CN	79/83 (95%)	68 (86%)	11 (14%)	4	23
14	AO	76/77 (99%)	69 (91%)	7 (9%)	11	44
14	CO	76/77 (99%)	63 (83%)	13 (17%)	2	14
15	AP	65/65 (100%)	56 (86%)	9 (14%)	4	23
15	CP	65/65 (100%)	54 (83%)	11 (17%)	2	14
16	AQ	74/77 (96%)	60 (81%)	14 (19%)	2	9
16	CQ	75/77 (97%)	66 (88%)	9 (12%)	6	29
17	AR	48/64 (75%)	45 (94%)	3 (6%)	22	62
17	CR	48/64 (75%)	41 (85%)	7 (15%)	4	21
18	AS	70/78 (90%)	60 (86%)	10 (14%)	4	22
18	CS	71/78 (91%)	53 (75%)	18 (25%)	1	4
19	AT	65/65 (100%)	56 (86%)	9 (14%)	4	23
19	CT	65/65 (100%)	51 (78%)	14 (22%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	AB	180/198 (91%)	142 (79%)	38 (21%)	1	6
20	CB	180/198 (91%)	153 (85%)	27 (15%)	3	20
21	AU	44/61 (72%)	36 (82%)	8 (18%)	2	11
21	CU	44/61 (72%)	30 (68%)	14 (32%)	0	2
24	BV	78/78 (100%)	66 (85%)	12 (15%)	3	19
24	DV	78/78 (100%)	69 (88%)	9 (12%)	7	31
25	BC	213/218 (98%)	145 (68%)	68 (32%)	0	2
25	DC	213/218 (98%)	150 (70%)	63 (30%)	0	3
26	BD	164/164 (100%)	112 (68%)	52 (32%)	0	2
26	DD	164/164 (100%)	113 (69%)	51 (31%)	0	2
27	BE	165/165 (100%)	115 (70%)	50 (30%)	0	3
27	DE	165/165 (100%)	127 (77%)	38 (23%)	1	4
28	BF	149/149 (100%)	119 (80%)	30 (20%)	1	7
28	DF	149/149 (100%)	122 (82%)	27 (18%)	2	11
29	BG	137/137 (100%)	105 (77%)	32 (23%)	1	4
29	DG	137/137 (100%)	111 (81%)	26 (19%)	2	9
30	BH	114/114 (100%)	85 (75%)	29 (25%)	1	4
30	DH	114/114 (100%)	90 (79%)	24 (21%)	1	6
31	BJ	114/116 (98%)	84 (74%)	30 (26%)	0	3
31	DJ	114/116 (98%)	85 (75%)	29 (25%)	1	4
32	BK	102/104 (98%)	78 (76%)	24 (24%)	1	4
32	DK	102/104 (98%)	81 (79%)	21 (21%)	1	7
33	BL	103/103 (100%)	62 (60%)	41 (40%)	0	1
33	DL	103/103 (100%)	68 (66%)	35 (34%)	0	2
34	BM	109/109 (100%)	77 (71%)	32 (29%)	0	3
34	DM	109/109 (100%)	75 (69%)	34 (31%)	0	2
35	BN	103/103 (100%)	78 (76%)	25 (24%)	1	4
35	DN	103/103 (100%)	76 (74%)	27 (26%)	0	3
36	BO	87/87 (100%)	58 (67%)	29 (33%)	0	2
36	DO	87/87 (100%)	69 (79%)	18 (21%)	1	7
37	BP	99/99 (100%)	77 (78%)	22 (22%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	DP	99/99 (100%)	67 (68%)	32 (32%)	0	2
38	BQ	89/89 (100%)	66 (74%)	23 (26%)	0	3
38	DQ	89/89 (100%)	71 (80%)	18 (20%)	1	7
39	BR	84/84 (100%)	68 (81%)	16 (19%)	2	9
39	DR	84/84 (100%)	58 (69%)	26 (31%)	0	2
40	BS	93/93 (100%)	72 (77%)	21 (23%)	1	5
40	DS	93/93 (100%)	77 (83%)	16 (17%)	2	14
41	BT	83/84 (99%)	60 (72%)	23 (28%)	0	3
41	DT	83/84 (99%)	60 (72%)	23 (28%)	0	3
42	BU	83/84 (99%)	62 (75%)	21 (25%)	1	4
42	DU	83/84 (99%)	60 (72%)	23 (28%)	0	3
43	BW	62/62 (100%)	46 (74%)	16 (26%)	0	3
43	DW	62/62 (100%)	45 (73%)	17 (27%)	0	3
44	BX	55/55 (100%)	40 (73%)	15 (27%)	0	3
44	DX	55/55 (100%)	43 (78%)	12 (22%)	1	5
45	BY	48/48 (100%)	36 (75%)	12 (25%)	1	4
45	DY	48/48 (100%)	33 (69%)	15 (31%)	0	2
46	BZ	62/62 (100%)	43 (69%)	19 (31%)	0	2
46	DZ	62/62 (100%)	46 (74%)	16 (26%)	0	3
47	B0	47/47 (100%)	31 (66%)	16 (34%)	0	2
47	D0	47/47 (100%)	33 (70%)	14 (30%)	0	3
48	B1	48/48 (100%)	33 (69%)	15 (31%)	0	2
48	D1	48/48 (100%)	33 (69%)	15 (31%)	0	2
49	B2	38/38 (100%)	27 (71%)	11 (29%)	0	3
49	D2	38/38 (100%)	27 (71%)	11 (29%)	0	3
50	B3	51/51 (100%)	33 (65%)	18 (35%)	0	2
50	D3	51/51 (100%)	40 (78%)	11 (22%)	1	6
51	B4	34/34 (100%)	21 (62%)	13 (38%)	0	1
51	D4	34/34 (100%)	17 (50%)	17 (50%)	0	0
52	BI	109/109 (100%)	106 (97%)	3 (3%)	51	82
52	DI	109/109 (100%)	104 (95%)	5 (5%)	33	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9341/9692 (96%)	7268 (78%)	2073 (22%)	1 5

5 of 2073 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
43	BW	54	ARG
6	CG	10	LYS
41	DT	82	LYS
45	BY	19	HIS
51	B4	9	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 317 such sidechains are listed below:

Mol	Chain	Res	Type
40	BS	9	HIS
3	CD	53	GLN
39	DR	6	GLN
42	BU	65	GLN
46	BZ	41	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1529/1542 (99%)	277 (18%)	25 (1%)
1	CA	1529/1542 (99%)	249 (16%)	26 (1%)
22	BA	116/120 (96%)	23 (19%)	0
22	DA	116/120 (96%)	20 (17%)	1 (0%)
23	BB	2837/2904 (97%)	451 (15%)	18 (0%)
23	DB	2837/2904 (97%)	482 (16%)	22 (0%)
All	All	8964/9132 (98%)	1502 (16%)	92 (1%)

5 of 1502 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	7	A
1	AA	9	G
1	AA	14	U
1	AA	31	G
1	AA	32	A

5 of 92 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	BB	2425	A
1	CA	429	U
23	DB	2198	A
23	BB	2756	U
1	CA	279	A

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 343 ligands modelled in this entry, 343 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
21	AU	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AU	15:LEU	C	16:ARG	N	0.99

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%)	-0.26	11 (0%) 89 84	16, 66, 135, 180	0
1	CA	1530/1542 (99%)	-0.35	8 (0%) 91 89	11, 49, 119, 180	0
2	AC	206/232 (88%)	0.35	7 (3%) 49 42	8, 56, 116, 163	0
2	CC	206/232 (88%)	0.23	8 (3%) 43 37	13, 68, 122, 154	0
3	AD	205/205 (100%)	0.81	26 (12%) 5 6	16, 65, 125, 180	0
3	CD	205/205 (100%)	0.81	17 (8%) 14 14	5, 49, 103, 156	0
4	AE	150/166 (90%)	0.51	5 (3%) 50 43	5, 56, 104, 151	0
4	CE	150/166 (90%)	0.64	9 (6%) 25 22	5, 49, 101, 167	0
5	AF	100/135 (74%)	1.27	22 (22%) 1 1	19, 64, 113, 150	0
5	CF	100/135 (74%)	1.20	19 (19%) 2 2	10, 65, 113, 147	0
6	AG	150/178 (84%)	0.29	10 (6%) 21 19	23, 86, 133, 180	0
6	CG	152/178 (85%)	-0.05	4 (2%) 59 52	22, 83, 132, 166	0
7	AH	129/129 (100%)	0.86	17 (13%) 4 5	8, 63, 113, 155	0
7	CH	129/129 (100%)	0.77	15 (11%) 6 7	5, 49, 104, 154	0
8	AI	127/129 (98%)	0.28	11 (8%) 13 13	5, 83, 126, 169	0
8	CI	127/129 (98%)	-0.17	1 (0%) 87 81	23, 81, 135, 161	0
9	AJ	98/103 (95%)	0.39	5 (5%) 32 27	14, 76, 141, 160	0
9	CJ	98/103 (95%)	0.12	2 (2%) 68 62	27, 78, 122, 143	0
10	AK	117/128 (91%)	0.73	8 (6%) 20 19	6, 56, 99, 164	0
10	CK	117/128 (91%)	0.41	7 (5%) 25 22	5, 44, 95, 117	0
11	AL	123/123 (100%)	0.80	13 (10%) 8 8	18, 59, 115, 162	0
11	CL	123/123 (100%)	0.55	6 (4%) 33 28	5, 34, 109, 141	0
12	AM	114/117 (97%)	0.40	7 (6%) 25 22	37, 96, 137, 155	0
12	CM	113/117 (96%)	0.11	4 (3%) 48 40	19, 92, 143, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AN	96/100 (96%)	0.14	5 (5%) 31 27	11, 76, 133, 147	0
13	CN	96/100 (96%)	0.08	6 (6%) 23 21	32, 73, 130, 160	0
14	AO	88/89 (98%)	0.73	9 (10%) 9 9	15, 62, 104, 177	0
14	CO	88/89 (98%)	0.83	7 (7%) 15 14	5, 46, 113, 136	0
15	AP	82/82 (100%)	0.57	9 (10%) 7 8	20, 72, 132, 171	0
15	CP	80/82 (97%)	0.37	4 (5%) 32 27	5, 42, 126, 137	0
16	AQ	80/83 (96%)	1.34	23 (28%) 1 1	34, 77, 119, 158	0
16	CQ	81/83 (97%)	0.89	9 (11%) 7 8	11, 52, 113, 155	0
17	AR	55/74 (74%)	0.92	9 (16%) 2 3	16, 60, 124, 148	0
17	CR	55/74 (74%)	0.79	7 (12%) 5 6	17, 45, 118, 139	0
18	AS	79/91 (86%)	0.57	9 (11%) 7 7	44, 110, 140, 169	0
18	CS	80/91 (87%)	0.41	5 (6%) 23 21	47, 99, 151, 161	0
19	AT	85/86 (98%)	0.11	1 (1%) 81 74	37, 83, 123, 155	0
19	CT	85/86 (98%)	0.20	2 (2%) 62 55	9, 49, 103, 139	0
20	AB	218/240 (90%)	0.98	40 (18%) 2 2	17, 82, 131, 156	0
20	CB	218/240 (90%)	1.32	58 (26%) 1 1	13, 90, 135, 162	0
21	AU	51/71 (71%)	0.71	6 (11%) 6 7	29, 80, 131, 158	0
21	CU	51/71 (71%)	0.66	5 (9%) 10 11	34, 73, 112, 140	0
22	BA	117/120 (97%)	-0.22	2 (1%) 73 66	36, 62, 94, 157	0
22	DA	117/120 (97%)	-0.20	2 (1%) 73 66	27, 62, 113, 180	0
23	BB	2841/2904 (97%)	-0.07	31 (1%) 82 76	10, 49, 134, 180	0
23	DB	2841/2904 (97%)	-0.15	24 (0%) 87 81	5, 39, 133, 180	0
24	BV	94/94 (100%)	0.78	13 (13%) 4 5	20, 75, 130, 149	0
24	DV	94/94 (100%)	0.87	10 (10%) 8 8	17, 71, 119, 130	0
25	BC	267/273 (97%)	1.27	52 (19%) 1 2	5, 51, 136, 180	0
25	DC	267/273 (97%)	1.65	78 (29%) 1 1	5, 46, 139, 180	0
26	BD	209/209 (100%)	2.32	93 (44%) 0 0	21, 82, 174, 180	0
26	DD	209/209 (100%)	1.26	48 (22%) 1 1	5, 60, 139, 180	0
27	BE	201/201 (100%)	1.64	64 (31%) 1 1	8, 78, 147, 180	0
27	DE	201/201 (100%)	1.35	41 (20%) 1 2	5, 76, 164, 180	0
28	BF	178/178 (100%)	1.24	40 (22%) 1 1	43, 98, 152, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DF	178/178 (100%)	0.43	15 (8%) 14 14	29, 89, 138, 180	0
29	BG	176/176 (100%)	1.24	36 (20%) 1 2	23, 94, 154, 180	0
29	DG	176/176 (100%)	1.07	33 (18%) 2 2	20, 86, 154, 172	0
30	BH	149/149 (100%)	2.86	79 (53%) 0 0	23, 120, 170, 180	0
30	DH	149/149 (100%)	1.63	51 (34%) 0 0	31, 100, 153, 180	0
31	BJ	140/142 (98%)	1.07	24 (17%) 2 2	14, 79, 160, 180	0
31	DJ	140/142 (98%)	0.98	23 (16%) 2 3	14, 61, 136, 162	0
32	BK	121/123 (98%)	1.49	32 (26%) 1 1	13, 57, 106, 147	0
32	DK	121/123 (98%)	0.56	3 (2%) 61 54	5, 37, 84, 143	0
33	BL	144/144 (100%)	2.87	67 (46%) 0 0	19, 93, 160, 180	0
33	DL	144/144 (100%)	2.09	58 (40%) 0 0	7, 74, 150, 179	0
34	BM	136/136 (100%)	0.88	20 (14%) 3 4	16, 71, 168, 180	0
34	DM	136/136 (100%)	1.70	41 (30%) 1 1	10, 66, 152, 180	0
35	BN	127/127 (100%)	1.70	31 (24%) 1 1	19, 67, 149, 180	0
35	DN	127/127 (100%)	0.92	12 (9%) 11 11	5, 45, 143, 180	0
36	BO	117/117 (100%)	2.10	35 (29%) 1 1	20, 82, 150, 180	0
36	DO	117/117 (100%)	1.27	21 (17%) 2 2	20, 77, 150, 169	0
37	BP	114/114 (100%)	1.91	52 (45%) 0 0	21, 84, 177, 180	0
37	DP	114/114 (100%)	1.46	30 (26%) 1 1	8, 69, 148, 180	0
38	BQ	117/117 (100%)	0.49	9 (7%) 16 15	8, 63, 125, 174	0
38	DQ	117/117 (100%)	1.17	20 (17%) 2 2	11, 57, 127, 180	0
39	BR	103/103 (100%)	1.56	30 (29%) 1 1	33, 100, 153, 180	0
39	DR	103/103 (100%)	2.42	47 (45%) 0 0	26, 92, 154, 180	0
40	BS	110/110 (100%)	1.17	21 (19%) 2 2	14, 57, 132, 180	0
40	DS	110/110 (100%)	0.73	12 (10%) 7 8	5, 45, 137, 175	0
41	BT	99/100 (99%)	1.17	20 (20%) 1 2	25, 73, 150, 170	0
41	DT	99/100 (99%)	1.60	28 (28%) 1 1	16, 84, 160, 180	0
42	BU	102/103 (99%)	1.69	33 (32%) 1 0	18, 92, 158, 178	0
42	DU	102/103 (99%)	0.64	15 (14%) 3 4	11, 103, 161, 180	0
43	BW	84/84 (100%)	2.34	31 (36%) 0 0	22, 87, 153, 180	0
43	DW	84/84 (100%)	1.64	29 (34%) 0 0	20, 81, 149, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BX	63/63 (100%)	1.50	12 (19%) 2 2	28, 92, 148, 170	0
44	DX	63/63 (100%)	1.54	18 (28%) 1 1	47, 96, 162, 171	0
45	BY	58/58 (100%)	1.68	15 (25%) 1 1	29, 72, 150, 180	0
45	DY	58/58 (100%)	1.21	8 (13%) 4 5	5, 60, 129, 177	0
46	BZ	70/70 (100%)	0.74	6 (8%) 13 13	20, 68, 134, 168	0
46	DZ	70/70 (100%)	0.93	9 (12%) 5 5	16, 59, 132, 180	0
47	B0	56/56 (100%)	2.22	23 (41%) 0 0	23, 89, 163, 180	0
47	D0	56/56 (100%)	1.61	13 (23%) 1 1	12, 61, 148, 180	0
48	B1	54/54 (100%)	2.37	22 (40%) 0 0	18, 89, 142, 179	0
48	D1	54/54 (100%)	2.87	27 (50%) 0 0	22, 77, 153, 173	0
49	B2	46/46 (100%)	0.79	8 (17%) 2 2	11, 47, 152, 180	0
49	D2	46/46 (100%)	0.62	1 (2%) 65 59	13, 48, 112, 129	0
50	B3	64/64 (100%)	1.54	16 (25%) 1 1	15, 61, 149, 180	0
50	D3	64/64 (100%)	1.39	15 (23%) 1 1	8, 55, 125, 169	0
51	B4	38/38 (100%)	1.68	11 (28%) 1 1	36, 85, 161, 180	0
51	D4	38/38 (100%)	1.68	13 (34%) 0 0	20, 80, 168, 180	0
52	BI	141/141 (100%)	2.99	89 (63%) 0 0	61, 151, 180, 180	0
52	DI	141/141 (100%)	1.61	47 (33%) 0 0	84, 157, 180, 180	0
All	All	20439/21034 (97%)	0.55	2265 (11%) 7 8	5, 61, 145, 180	0

The worst 5 of 2265 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
36	BO	57	ALA	23.9
36	BO	58	ILE	22.0
33	BL	98	ALA	18.7
45	BY	3	THR	18.1
36	BO	59	ALA	16.8

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	AA	1656	1/1	0.93	0.26	8.42	66,66,66,66	0
53	MG	BB	3078	1/1	0.95	0.19	1.62	25,25,25,25	0
53	MG	DB	3110	1/1	0.90	0.18	0.55	54,54,54,54	0
53	MG	AA	1629	1/1	0.84	0.14	-0.49	138,138,138,138	0
53	MG	DB	3001	1/1	0.94	0.16	-0.52	7,7,7,7	0
53	MG	AA	1615	1/1	0.86	0.12	-0.59	43,43,43,43	0
53	MG	BB	3098	1/1	0.93	0.16	-0.62	45,45,45,45	0
53	MG	DB	3077	1/1	0.94	0.17	-0.79	57,57,57,57	0
53	MG	DB	3057	1/1	0.81	0.09	-0.85	28,28,28,28	0
53	MG	BB	3088	1/1	0.83	0.15	-0.86	34,34,34,34	0
53	MG	DN	201	1/1	0.92	0.19	-0.90	49,49,49,49	0
53	MG	BB	3110	1/1	0.86	0.13	-0.91	60,60,60,60	0
53	MG	BB	3005	1/1	0.90	0.12	-1.09	5,5,5,5	0
53	MG	DB	3083	1/1	0.93	0.17	-1.11	27,27,27,27	0
53	MG	CA	1634	1/1	0.93	0.14	-1.16	61,61,61,61	0
53	MG	DB	3024	1/1	0.80	0.11	-1.19	36,36,36,36	0
53	MG	AA	1634	1/1	0.93	0.10	-1.25	85,85,85,85	0
53	MG	DB	3095	1/1	0.97	0.16	-1.30	55,55,55,55	0
53	MG	DB	3063	1/1	0.91	0.08	-1.33	13,13,13,13	0
53	MG	DB	3055	1/1	0.93	0.09	-1.36	19,19,19,19	0
53	MG	BB	3021	1/1	0.86	0.14	-1.37	55,55,55,55	0
53	MG	DB	3062	1/1	0.93	0.13	-1.45	43,43,43,43	0
53	MG	DB	3010	1/1	0.97	0.09	-1.46	12,12,12,12	0
53	MG	BB	3034	1/1	0.86	0.12	-1.48	25,25,25,25	0
53	MG	DB	3025	1/1	0.92	0.15	-1.52	21,21,21,21	0
53	MG	DB	3003	1/1	0.98	0.07	-1.56	14,14,14,14	0
53	MG	CA	1614	1/1	0.91	0.09	-1.59	47,47,47,47	0
53	MG	DB	3068	1/1	0.98	0.12	-1.61	14,14,14,14	0
53	MG	CA	1616	1/1	0.91	0.08	-1.70	68,68,68,68	0
53	MG	AA	1637	1/1	0.93	0.11	-1.76	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	DB	3030	1/1	0.80	0.15	-1.81	23,23,23,23	0
53	MG	CA	1641	1/1	0.97	0.11	-1.84	92,92,92,92	0
53	MG	BB	3051	1/1	0.84	0.09	-1.86	71,71,71,71	0
53	MG	BB	3012	1/1	0.99	0.08	-1.90	41,41,41,41	0
53	MG	BB	3081	1/1	0.83	0.16	-1.90	46,46,46,46	0
53	MG	DB	3026	1/1	0.95	0.14	-1.92	18,18,18,18	0
53	MG	AA	1653	1/1	0.85	0.10	-2.09	65,65,65,65	0
53	MG	BB	3049	1/1	0.85	0.10	-2.09	11,11,11,11	0
53	MG	BB	3087	1/1	0.94	0.13	-2.27	45,45,45,45	0
53	MG	CA	1639	1/1	0.89	0.08	-2.28	117,117,117,117	0
53	MG	DB	3109	1/1	0.97	0.07	-2.31	24,24,24,24	0
53	MG	CA	1612	1/1	0.95	0.08	-2.48	29,29,29,29	0
53	MG	CA	1656	1/1	0.94	0.11	-2.49	48,48,48,48	0
53	MG	DB	3073	1/1	0.96	0.11	-2.54	16,16,16,16	0
53	MG	BB	3029	1/1	0.97	0.08	-2.63	13,13,13,13	0
53	MG	DB	3047	1/1	0.98	0.13	-2.81	17,17,17,17	0
53	MG	BB	3056	1/1	0.97	0.10	-2.85	19,19,19,19	0
53	MG	BB	3096	1/1	0.91	0.14	-2.86	43,43,43,43	0
53	MG	BB	3016	1/1	0.95	0.13	-2.87	15,15,15,15	0
53	MG	CA	1646	1/1	0.92	0.08	-2.99	42,42,42,42	0
53	MG	AA	1603	1/1	0.94	0.11	-3.00	43,43,43,43	0
53	MG	BB	3086	1/1	0.99	0.15	-3.05	37,37,37,37	0
53	MG	BB	3011	1/1	0.97	0.13	-3.06	7,7,7,7	0
53	MG	CA	1618	1/1	0.96	0.10	-3.08	5,5,5,5	0
53	MG	AA	1607	1/1	0.86	0.09	-3.22	27,27,27,27	0
53	MG	DB	3088	1/1	0.95	0.14	-3.25	35,35,35,35	0
53	MG	DB	3051	1/1	0.96	0.13	-3.26	53,53,53,53	0
53	MG	AA	1652	1/1	0.95	0.08	-3.29	25,25,25,25	0
53	MG	AA	1601	1/1	0.95	0.06	-3.29	26,26,26,26	0
53	MG	AA	1610	1/1	0.96	0.09	-3.33	34,34,34,34	0
53	MG	BB	3090	1/1	0.75	0.08	-3.35	74,74,74,74	0
53	MG	AA	1632	1/1	0.93	0.05	-3.38	53,53,53,53	0
53	MG	DB	3086	1/1	0.97	0.14	-3.44	69,69,69,69	0
53	MG	DB	3036	1/1	0.96	0.09	-3.45	16,16,16,16	0
53	MG	DB	3091	1/1	0.96	0.08	-3.45	96,96,96,96	0
53	MG	DB	3035	1/1	0.97	0.10	-3.51	30,30,30,30	0
53	MG	DB	3014	1/1	0.88	0.07	-3.68	5,5,5,5	0
53	MG	AA	1609	1/1	0.98	0.14	-3.69	8,8,8,8	0
53	MG	CA	1657	1/1	0.91	0.07	-3.79	37,37,37,37	0
53	MG	BB	3073	1/1	0.97	0.09	-3.81	28,28,28,28	0
53	MG	DB	3098	1/1	0.95	0.12	-4.07	18,18,18,18	0
53	MG	BB	3040	1/1	0.92	0.10	-4.12	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	BB	3079	1/1	0.91	0.10	-4.13	38,38,38,38	0
53	MG	BB	3077	1/1	0.96	0.08	-4.14	44,44,44,44	0
53	MG	BB	3018	1/1	0.87	0.09	-4.15	27,27,27,27	0
53	MG	DB	3097	1/1	0.99	0.11	-4.21	15,15,15,15	0
53	MG	BB	3052	1/1	0.93	0.10	-4.24	19,19,19,19	0
53	MG	DB	3087	1/1	0.97	0.12	-4.25	6,6,6,6	0
53	MG	DB	3012	1/1	0.98	0.12	-4.27	6,6,6,6	0
53	MG	BB	3026	1/1	0.97	0.10	-4.35	5,5,5,5	0
53	MG	CA	1617	1/1	0.98	0.10	-4.63	9,9,9,9	0
53	MG	CA	1605	1/1	0.95	0.07	-4.85	18,18,18,18	0
53	MG	BB	3019	1/1	0.95	0.08	-4.88	27,27,27,27	0
53	MG	DB	3107	1/1	0.94	0.09	-4.95	19,19,19,19	0
53	MG	BB	3013	1/1	0.96	0.09	-5.04	31,31,31,31	0
53	MG	BB	3061	1/1	0.97	0.06	-5.06	42,42,42,42	0
53	MG	BB	3108	1/1	0.96	0.08	-5.10	19,19,19,19	0
53	MG	CA	1601	1/1	0.98	0.06	-5.13	5,5,5,5	0
53	MG	BB	3037	1/1	0.96	0.08	-5.16	24,24,24,24	0
53	MG	BB	3083	1/1	0.94	0.09	-5.22	20,20,20,20	0
53	MG	DB	3069	1/1	0.98	0.09	-5.28	44,44,44,44	0
53	MG	BB	3094	1/1	0.82	0.09	-5.38	35,35,35,35	0
53	MG	BB	3065	1/1	0.93	0.13	-5.46	47,47,47,47	0
53	MG	CA	1647	1/1	0.99	0.06	-5.59	32,32,32,32	0
53	MG	DB	3007	1/1	0.91	0.10	-5.95	12,12,12,12	0
53	MG	BB	3066	1/1	0.97	0.09	-6.04	59,59,59,59	0
53	MG	DB	3084	1/1	0.98	0.07	-6.08	8,8,8,8	0
53	MG	DB	3027	1/1	0.95	0.08	-6.14	10,10,10,10	0
53	MG	DB	3009	1/1	0.98	0.08	-6.34	7,7,7,7	0
53	MG	BB	3069	1/1	0.97	0.07	-6.50	9,9,9,9	0
53	MG	AA	1642	1/1	0.94	0.08	-6.65	70,70,70,70	0
53	MG	BB	3103	1/1	0.98	0.07	-6.86	7,7,7,7	0
53	MG	DB	3002	1/1	0.95	0.12	-7.09	37,37,37,37	0
53	MG	BB	3035	1/1	0.93	0.08	-7.33	12,12,12,12	0
53	MG	BB	3002	1/1	0.98	0.10	-7.69	10,10,10,10	0
53	MG	DB	3078	1/1	0.98	0.08	-8.04	18,18,18,18	0
53	MG	BB	3023	1/1	0.98	0.07	-8.15	22,22,22,22	0
53	MG	CA	1633	1/1	0.97	0.09	-8.28	47,47,47,47	0
53	MG	DB	3102	1/1	0.94	0.10	-8.54	26,26,26,26	0
53	MG	BB	3085	1/1	0.97	0.07	-9.40	22,22,22,22	0
53	MG	DB	3079	1/1	0.98	0.10	-10.18	5,5,5,5	0
53	MG	DB	3006	1/1	0.98	0.07	-10.25	5,5,5,5	0
53	MG	CA	1644	1/1	0.96	0.06	-10.32	29,29,29,29	0
53	MG	DB	3056	1/1	0.98	0.09	-10.43	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	BB	3001	1/1	0.97	0.06	-10.68	10,10,10,10	0
53	MG	DB	3019	1/1	0.98	0.04	-11.05	5,5,5,5	0
53	MG	BB	3062	1/1	0.98	0.09	-15.28	22,22,22,22	0
53	MG	DB	3103	1/1	0.96	0.12	-	50,50,50,50	0
53	MG	BB	3045	1/1	0.97	0.05	-	31,31,31,31	0
53	MG	AA	1643	1/1	0.93	0.09	-	73,73,73,73	0
53	MG	AA	1635	1/1	0.92	0.06	-	85,85,85,85	0
53	MG	BB	3053	1/1	0.93	0.07	-	6,6,6,6	0
53	MG	BB	3033	1/1	0.78	0.29	-	93,93,93,93	0
53	MG	CA	1645	1/1	0.90	0.12	-	82,82,82,82	0
53	MG	AA	1646	1/1	0.95	0.30	-	60,60,60,60	0
53	MG	DB	3082	1/1	0.69	0.16	-	73,73,73,73	0
53	MG	AA	1636	1/1	0.77	0.60	-	127,127,127,127	0
53	MG	DB	3050	1/1	0.84	0.11	-	74,74,74,74	0
53	MG	DB	3101	1/1	0.98	0.11	-	27,27,27,27	0
53	MG	AA	1626	1/1	0.96	0.06	-	35,35,35,35	0
53	MG	CA	1630	1/1	0.87	0.09	-	5,5,5,5	1
53	MG	CA	1615	1/1	0.96	0.09	-	101,101,101,101	0
53	MG	DB	3099	1/1	0.95	0.07	-	9,9,9,9	0
53	MG	CA	1620	1/1	0.95	0.07	-	35,35,35,35	0
53	MG	AA	1654	1/1	0.81	0.10	-	59,59,59,59	0
53	MG	DB	3058	1/1	0.78	0.31	-	30,30,30,30	1
53	MG	DB	3064	1/1	0.98	0.07	-	28,28,28,28	0
53	MG	BB	3054	1/1	0.83	0.13	-	72,72,72,72	0
53	MG	DB	3096	1/1	0.94	0.08	-	20,20,20,20	0
53	MG	AA	1627	1/1	0.95	0.14	-	72,72,72,72	0
53	MG	AA	1658	1/1	0.94	0.21	-	167,167,167,167	0
53	MG	BB	3102	1/1	0.97	0.13	-	19,19,19,19	0
53	MG	CA	1623	1/1	0.53	0.16	-	151,151,151,151	0
53	MG	CA	1653	1/1	0.93	0.26	-	45,45,45,45	0
53	MG	DB	3049	1/1	0.98	0.06	-	5,5,5,5	0
53	MG	DB	3034	1/1	0.84	0.16	-	66,66,66,66	0
53	MG	AA	1633	1/1	0.95	0.05	-	75,75,75,75	0
53	MG	BB	3030	1/1	0.95	0.05	-	53,53,53,53	0
53	MG	BB	3015	1/1	0.97	0.08	-	24,24,24,24	0
53	MG	DB	3076	1/1	0.94	0.07	-	17,17,17,17	0
53	MG	DB	3054	1/1	0.87	0.07	-	15,15,15,15	0
53	MG	BB	3048	1/1	0.96	0.06	-	20,20,20,20	0
53	MG	BB	3080	1/1	0.92	0.08	-	31,31,31,31	0
53	MG	BB	3067	1/1	0.87	0.18	-	78,78,78,78	0
53	MG	BB	3038	1/1	0.96	0.04	-	58,58,58,58	0
53	MG	DB	3059	1/1	0.72	0.09	-	127,127,127,127	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	AA	1630	1/1	0.94	0.08	-	30,30,30,30	0
53	MG	AP	101	1/1	0.41	0.38	-	53,53,53,53	1
53	MG	CA	1613	1/1	0.93	0.14	-	78,78,78,78	0
53	MG	CA	1638	1/1	0.93	0.04	-	37,37,37,37	0
53	MG	DB	3031	1/1	0.92	0.12	-	18,18,18,18	0
53	MG	DB	3041	1/1	0.97	0.07	-	18,18,18,18	0
53	MG	DB	3044	1/1	0.97	0.07	-	7,7,7,7	0
53	MG	BB	3046	1/1	0.88	0.07	-	51,51,51,51	0
53	MG	BB	3027	1/1	0.95	0.09	-	23,23,23,23	0
53	MG	AA	1647	1/1	0.93	0.10	-	23,23,23,23	0
53	MG	CA	1627	1/1	0.88	0.14	-	29,29,29,29	1
53	MG	AA	1623	1/1	0.82	0.17	-	32,32,32,32	1
53	MG	DB	3020	1/1	0.95	0.12	-	20,20,20,20	0
53	MG	BB	3042	1/1	0.49	0.09	-	95,95,95,95	0
53	MG	DB	3022	1/1	0.96	0.07	-	15,15,15,15	0
53	MG	DB	3018	1/1	0.93	0.09	-	29,29,29,29	0
53	MG	BB	3097	1/1	0.92	0.16	-	74,74,74,74	0
53	MG	AA	1657	1/1	0.91	0.06	-	81,81,81,81	0
53	MG	CA	1631	1/1	0.91	0.08	-	36,36,36,36	0
53	MG	BB	3025	1/1	0.97	0.16	-	53,53,53,53	0
53	MG	CA	1602	1/1	0.98	0.15	-	32,32,32,32	0
53	MG	BB	3055	1/1	0.96	0.13	-	27,27,27,27	0
53	MG	BB	3072	1/1	0.94	0.09	-	24,24,24,24	0
53	MG	DB	3094	1/1	0.90	0.24	-	5,5,5,5	1
53	MG	DB	3080	1/1	0.98	0.09	-	12,12,12,12	0
53	MG	DB	3060	1/1	0.79	0.11	-	77,77,77,77	0
53	MG	DB	3005	1/1	0.96	0.07	-	9,9,9,9	0
53	MG	CA	1629	1/1	0.92	0.06	-	45,45,45,45	0
53	MG	BB	3064	1/1	0.95	0.06	-	39,39,39,39	0
53	MG	DB	3071	1/1	0.93	0.08	-	39,39,39,39	0
53	MG	AA	1613	1/1	0.94	0.06	-	42,42,42,42	0
53	MG	BB	3004	1/1	0.96	0.04	-	21,21,21,21	0
53	MG	CA	1625	1/1	0.95	0.09	-	26,26,26,26	0
53	MG	DB	3013	1/1	0.84	0.15	-	34,34,34,34	0
53	MG	DB	3105	1/1	0.95	0.10	-	23,23,23,23	0
53	MG	DB	3061	1/1	0.91	0.07	-	78,78,78,78	0
53	MG	DB	3052	1/1	0.89	0.17	-	60,60,60,60	0
53	MG	DB	3090	1/1	0.96	0.15	-	28,28,28,28	0
53	MG	BB	3017	1/1	0.82	0.10	-	72,72,72,72	0
53	MG	BB	3043	1/1	0.90	0.09	-	75,75,75,75	0
53	MG	DB	3017	1/1	0.93	0.12	-	5,5,5,5	0
53	MG	DB	3040	1/1	0.95	0.12	-	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	DB	3042	1/1	0.96	0.10	-	27,27,27,27	0
53	MG	CA	1606	1/1	0.95	0.09	-	74,74,74,74	0
53	MG	AA	1617	1/1	0.91	0.12	-	78,78,78,78	0
53	MG	AA	1648	1/1	0.95	0.05	-	94,94,94,94	0
53	MG	DB	3053	1/1	0.88	0.12	-	27,27,27,27	0
53	MG	DB	3066	1/1	0.95	0.08	-	5,5,5,5	0
53	MG	BB	3060	1/1	0.91	0.08	-	69,69,69,69	0
53	MG	BB	3076	1/1	0.96	0.05	-	24,24,24,24	0
53	MG	CA	1648	1/1	0.95	0.08	-	56,56,56,56	0
53	MG	BB	3082	1/1	0.68	0.16	-	19,19,19,19	0
53	MG	AA	1631	1/1	0.90	0.08	-	61,61,61,61	0
53	MG	DB	3081	1/1	0.99	0.06	-	25,25,25,25	0
53	MG	BB	3028	1/1	0.84	0.20	-	40,40,40,40	0
53	MG	CA	1650	1/1	0.92	0.12	-	82,82,82,82	0
53	MG	BB	3036	1/1	0.95	0.14	-	37,37,37,37	0
53	MG	BB	3101	1/1	0.95	0.05	-	12,12,12,12	0
53	MG	BB	3109	1/1	0.92	0.14	-	15,15,15,15	0
53	MG	BB	3058	1/1	0.95	0.10	-	28,28,28,28	0
53	MG	AA	1604	1/1	0.93	0.14	-	45,45,45,45	0
53	MG	AA	1612	1/1	0.58	0.16	-	104,104,104,104	0
53	MG	CA	1632	1/1	0.92	0.12	-	61,61,61,61	0
53	MG	DB	3067	1/1	0.92	0.11	-	17,17,17,17	0
53	MG	CA	1654	1/1	0.94	0.05	-	40,40,40,40	0
53	MG	DB	3039	1/1	0.96	0.07	-	19,19,19,19	0
53	MG	DB	3065	1/1	0.84	0.16	-	47,47,47,47	1
53	MG	AA	1622	1/1	0.75	0.21	-	116,116,116,116	0
53	MG	DB	3043	1/1	0.94	0.14	-	9,9,9,9	0
53	MG	DB	3075	1/1	0.98	0.04	-	5,5,5,5	0
53	MG	BB	3059	1/1	0.92	0.08	-	10,10,10,10	0
53	MG	BB	3006	1/1	0.98	0.07	-	10,10,10,10	0
53	MG	AA	1650	1/1	0.90	0.05	-	72,72,72,72	0
53	MG	AA	1625	1/1	0.80	0.19	-	5,5,5,5	1
53	MG	BB	3068	1/1	0.98	0.09	-	24,24,24,24	0
53	MG	BB	3095	1/1	0.98	0.09	-	34,34,34,34	0
53	MG	AA	1645	1/1	0.94	0.11	-	27,27,27,27	0
53	MG	CA	1642	1/1	0.94	0.09	-	45,45,45,45	0
53	MG	AA	1620	1/1	0.90	0.12	-	62,62,62,62	0
53	MG	AA	1616	1/1	0.95	0.07	-	46,46,46,46	0
53	MG	CA	1624	1/1	0.90	0.13	-	48,48,48,48	0
53	MG	BB	3107	1/1	0.97	0.07	-	27,27,27,27	0
53	MG	BB	3093	1/1	0.94	0.23	-	5,5,5,5	1
53	MG	CA	1611	1/1	0.91	0.12	-	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	BB	3104	1/1	0.89	0.12	-	18,18,18,18	0
53	MG	DB	3016	1/1	0.91	0.11	-	23,23,23,23	0
53	MG	BB	3031	1/1	0.94	0.19	-	45,45,45,45	0
53	MG	BB	3010	1/1	0.85	0.11	-	39,39,39,39	0
53	MG	DB	3015	1/1	0.95	0.09	-	49,49,49,49	0
53	MG	DB	3093	1/1	0.98	0.06	-	10,10,10,10	0
53	MG	BB	3024	1/1	0.98	0.09	-	22,22,22,22	0
53	MG	AA	1606	1/1	0.93	0.06	-	59,59,59,59	0
53	MG	BB	3044	1/1	0.99	0.07	-	32,32,32,32	0
53	MG	DB	3070	1/1	0.96	0.08	-	46,46,46,46	0
53	MG	CA	1603	1/1	0.95	0.13	-	69,69,69,69	0
53	MG	AA	1651	1/1	0.97	0.07	-	84,84,84,84	0
53	MG	AA	1619	1/1	0.73	0.13	-	100,100,100,100	0
53	MG	DB	3048	1/1	0.99	0.05	-	20,20,20,20	0
53	MG	CA	1652	1/1	0.94	0.07	-	44,44,44,44	0
53	MG	BB	3063	1/1	0.96	0.14	-	27,27,27,27	0
53	MG	DB	3072	1/1	0.94	0.07	-	30,30,30,30	0
53	MG	BB	3039	1/1	0.95	0.18	-	45,45,45,45	0
53	MG	CA	1609	1/1	0.91	0.18	-	45,45,45,45	0
53	MG	CA	1661	1/1	0.98	0.04	-	62,62,62,62	0
53	MG	CA	1604	1/1	0.98	0.09	-	18,18,18,18	0
53	MG	BB	3014	1/1	0.97	0.04	-	29,29,29,29	0
53	MG	DB	3046	1/1	0.96	0.08	-	33,33,33,33	0
53	MG	DB	3028	1/1	0.97	0.12	-	28,28,28,28	0
53	MG	DB	3037	1/1	0.98	0.09	-	13,13,13,13	0
53	MG	AA	1640	1/1	0.97	0.08	-	44,44,44,44	0
53	MG	AA	1659	1/1	0.85	0.12	-	105,105,105,105	0
53	MG	CA	1651	1/1	0.97	0.09	-	14,14,14,14	0
53	MG	BB	3003	1/1	0.97	0.06	-	13,13,13,13	0
53	MG	CA	1607	1/1	0.92	0.06	-	18,18,18,18	0
53	MG	CA	1643	1/1	0.90	0.08	-	41,41,41,41	0
53	MG	CA	1655	1/1	0.97	0.14	-	48,48,48,48	0
53	MG	CA	1635	1/1	0.91	0.11	-	20,20,20,20	0
53	MG	CA	1619	1/1	0.97	0.09	-	26,26,26,26	0
53	MG	BB	3020	1/1	0.97	0.06	-	23,23,23,23	0
53	MG	CA	1636	1/1	0.83	0.10	-	51,51,51,51	0
53	MG	DB	3104	1/1	0.85	0.12	-	50,50,50,50	0
53	MG	CA	1621	1/1	0.96	0.24	-	113,113,113,113	0
53	MG	AA	1628	1/1	0.95	0.10	-	26,26,26,26	0
53	MG	AA	1602	1/1	0.91	0.08	-	62,62,62,62	0
53	MG	CA	1659	1/1	0.96	0.17	-	48,48,48,48	0
53	MG	BB	3100	1/1	0.87	0.20	-	11,11,11,11	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	DB	3038	1/1	0.98	0.09	-	16,16,16,16	0
53	MG	CA	1640	1/1	0.94	0.07	-	11,11,11,11	0
53	MG	BB	3070	1/1	0.99	0.09	-	32,32,32,32	0
53	MG	CA	1608	1/1	0.90	0.06	-	110,110,110,110	0
53	MG	AA	1621	1/1	0.96	0.09	-	23,23,23,23	0
53	MG	DB	3045	1/1	0.92	0.07	-	61,61,61,61	0
53	MG	BB	3099	1/1	0.94	0.11	-	30,30,30,30	0
53	MG	DB	3074	1/1	0.98	0.09	-	25,25,25,25	0
53	MG	BB	3106	1/1	0.98	0.11	-	46,46,46,46	0
53	MG	DB	3092	1/1	0.98	0.08	-	23,23,23,23	0
53	MG	BB	3041	1/1	0.95	0.05	-	30,30,30,30	0
53	MG	AA	1614	1/1	0.72	0.11	-	62,62,62,62	0
53	MG	DB	3021	1/1	0.92	0.10	-	16,16,16,16	0
53	MG	DB	3033	1/1	0.96	0.09	-	11,11,11,11	0
53	MG	BB	3091	1/1	0.92	0.07	-	19,19,19,19	0
53	MG	BB	3105	1/1	0.90	0.22	-	64,64,64,64	0
53	MG	BB	3057	1/1	0.90	0.17	-	27,27,27,27	0
53	MG	AA	1649	1/1	0.77	0.18	-	114,114,114,114	0
53	MG	BB	3089	1/1	0.92	0.09	-	45,45,45,45	0
53	MG	BB	3009	1/1	0.92	0.07	-	35,35,35,35	0
53	MG	BB	3075	1/1	0.94	0.18	-	31,31,31,31	0
53	MG	AA	1644	1/1	0.70	0.10	-	96,96,96,96	0
53	MG	AA	1611	1/1	0.94	0.06	-	40,40,40,40	0
53	MG	DB	3004	1/1	0.95	0.13	-	19,19,19,19	0
53	MG	CA	1660	1/1	0.81	0.15	-	65,65,65,65	0
53	MG	CA	1626	1/1	0.91	0.10	-	73,73,73,73	0
53	MG	DB	3085	1/1	0.97	0.09	-	17,17,17,17	0
53	MG	CA	1628	1/1	0.92	0.06	-	55,55,55,55	1
53	MG	BB	3047	1/1	0.96	0.06	-	114,114,114,114	0
53	MG	BB	3008	1/1	0.97	0.06	-	58,58,58,58	0
53	MG	DB	3008	1/1	0.96	0.13	-	24,24,24,24	0
53	MG	BB	3007	1/1	0.87	0.15	-	28,28,28,28	0
53	MG	BB	3032	1/1	0.96	0.12	-	9,9,9,9	0
53	MG	AA	1655	1/1	0.66	0.18	-	75,75,75,75	0
53	MG	DB	3106	1/1	0.95	0.06	-	21,21,21,21	0
53	MG	BB	3084	1/1	0.93	0.11	-	5,5,5,5	0
53	MG	AA	1638	1/1	0.82	0.20	-	98,98,98,98	0
53	MG	BB	3074	1/1	0.87	0.11	-	13,13,13,13	0
53	MG	CA	1658	1/1	0.97	0.07	-	38,38,38,38	0
53	MG	BB	3022	1/1	0.97	0.09	-	38,38,38,38	0
53	MG	CA	1610	1/1	0.98	0.03	-	34,34,34,34	0
53	MG	AA	1605	1/1	0.93	0.09	-	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	DB	3108	1/1	0.93	0.07	-	5,5,5,5	0
53	MG	CA	1637	1/1	0.90	0.09	-	68,68,68,68	0
53	MG	CA	1649	1/1	0.90	0.18	-	88,88,88,88	0
53	MG	BB	3092	1/1	0.98	0.07	-	11,11,11,11	0
53	MG	DB	3011	1/1	0.99	0.09	-	8,8,8,8	0
53	MG	AA	1639	1/1	0.89	0.06	-	47,47,47,47	0
53	MG	DB	3032	1/1	0.94	0.10	-	46,46,46,46	0
53	MG	CA	1662	1/1	0.85	0.14	-	26,26,26,26	0
53	MG	AA	1641	1/1	0.86	0.11	-	49,49,49,49	0
53	MG	BB	3071	1/1	0.93	0.11	-	24,24,24,24	0
53	MG	BB	3050	1/1	0.98	0.10	-	35,35,35,35	0
53	MG	AA	1618	1/1	0.92	0.06	-	46,46,46,46	0
53	MG	DB	3023	1/1	0.92	0.06	-	34,34,34,34	0
53	MG	AA	1608	1/1	0.81	0.08	-	121,121,121,121	0
53	MG	AA	1624	1/1	0.92	0.17	-	79,79,79,79	0
53	MG	DB	3089	1/1	0.94	0.06	-	65,65,65,65	0
53	MG	CA	1622	1/1	0.92	0.09	-	67,67,67,67	0
53	MG	DB	3100	1/1	0.97	0.09	-	11,11,11,11	0
53	MG	DB	3029	1/1	0.91	0.29	-	41,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.