



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:47 PM GMT

PDB ID : 4V64
Title : Crystal structure of the bacterial ribosome from Escherichia coli in complex with hygromycin B.
Authors : Borovinskaya, M.A.; Shoji, S.; Fredrick, K.; Cate, J.H.D.
Deposited on : 2008-06-11
Resolution : 3.50 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

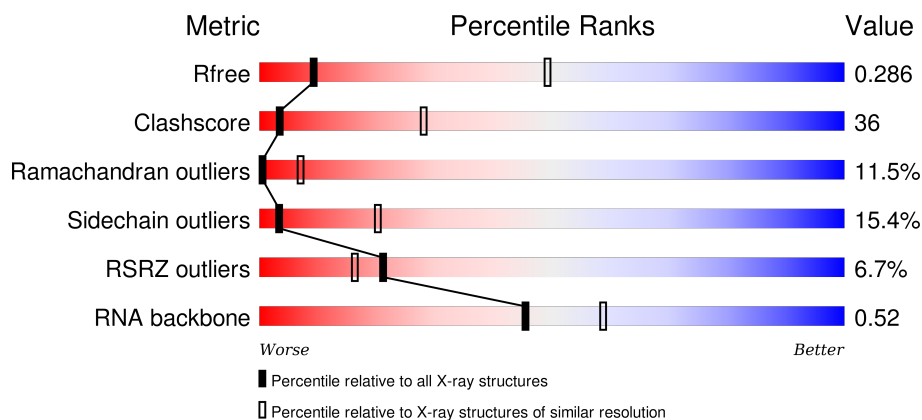
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

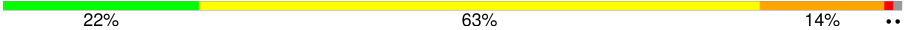
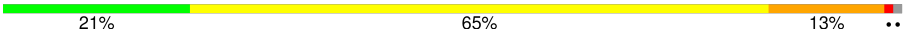
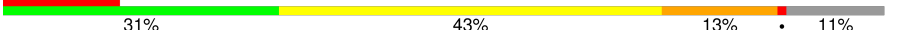
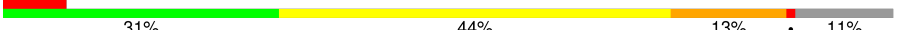
The reported resolution of this entry is 3.50 Å.

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	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)
RNA backbone	2183	1050 (4.20-2.80)

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	
1	CA	1542	
2	AC	232	
2	CC	232	

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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	78	
46	DZ	78	
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	2023	-	-	-	X
53	MG	BB	3086	-	-	-	X
53	MG	BB	3097	-	-	-	X
53	MG	CA	2020	-	-	-	X
53	MG	CA	2045	-	-	-	X
54	HYG	CA	2062	-	-	-	X

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 284077 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
			715	440	146	128	1			
14	CO	88	Total	C	N	O	S	0	0	0
			715	440	146	128	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	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			
25	DC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			

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

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

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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	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			
31	DJ	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	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	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			
33	DL	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			

- 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	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			
35	DN	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			

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

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

- 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	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			
41	DT	93	Total	C	N	O	S	0	0	0
			738	466	139	131	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	79	Total	C	N	O	S		
			596	367	120	108	1	0	0
43	DW	79	Total	C	N	O	S		
			596	367	120	108	1	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
44	DX	63	Total	C	N	O	S		
			509	313	99	95	2	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
45	DY	58	Total	C	N	O	S		
			449	281	87	79	2	0	0

- Molecule 46 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
46	BZ	77	Total	C	N	O	S		
			625	388	129	106	2	0	0
46	DZ	77	Total	C	N	O	S		
			625	388	129	106	2	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
47	D0	56	Total	C	N	O	S		
			444	269	94	80	1	0	0

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

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

- 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			

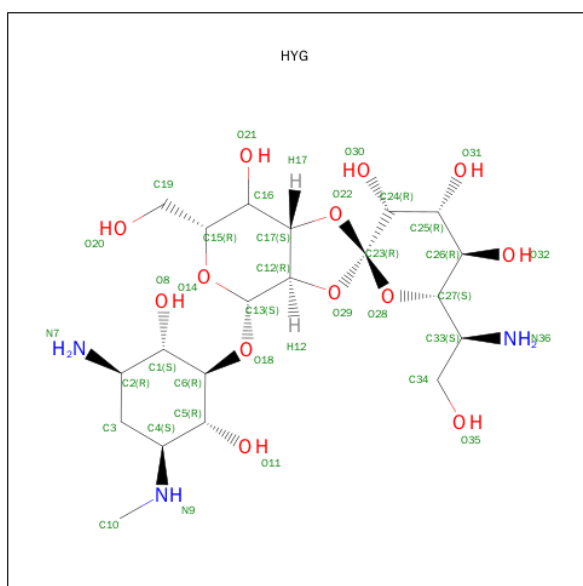
- Molecule 52 is a protein called 50S ribosomal protein L11.

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	BB	110	Total	Mg	0	0
			110	110		
53	CA	61	Total	Mg	0	0
			61	61		
53	AE	1	Total	Mg	0	0
			1	1		
53	AA	58	Total	Mg	0	0
			58	58		
53	AN	1	Total	Mg	0	0
			1	1		
53	CE	1	Total	Mg	0	0
			1	1		
53	DB	111	Total	Mg	0	0
			111	111		

- Molecule 54 is HYGROMYCIN B (three-letter code: HYG) (formula: $C_{20}H_{37}N_3O_{13}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
54	AA	1	Total	C	N	O	0	0
			36	20	3	13		
54	CA	1	Total	C	N	O	0	0
			36	20	3	13		

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

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

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

- Molecule 56 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AA	282	Total	O	0	0
			282	282		
56	AE	4	Total	O	0	0
			4	4		
56	AK	2	Total	O	0	0
			2	2		
56	AL	5	Total	O	0	0
			5	5		
56	AN	4	Total	O	0	0
			4	4		
56	AT	3	Total	O	0	0
			3	3		
56	BB	492	Total	O	0	0
			492	492		
56	BC	8	Total	O	0	0
			8	8		
56	BD	1	Total	O	0	0
			1	1		
56	BE	2	Total	O	0	0
			2	2		
56	BH	1	Total	O	0	0
			1	1		
56	BL	2	Total	O	0	0
			2	2		
56	B2	1	Total	O	0	0
			1	1		
56	CA	294	Total	O	0	0
			294	294		
56	CE	4	Total	O	0	0
			4	4		
56	CI	1	Total	O	0	0
			1	1		
56	CK	1	Total	O	0	0
			1	1		
56	CL	3	Total	O	0	0
			3	3		

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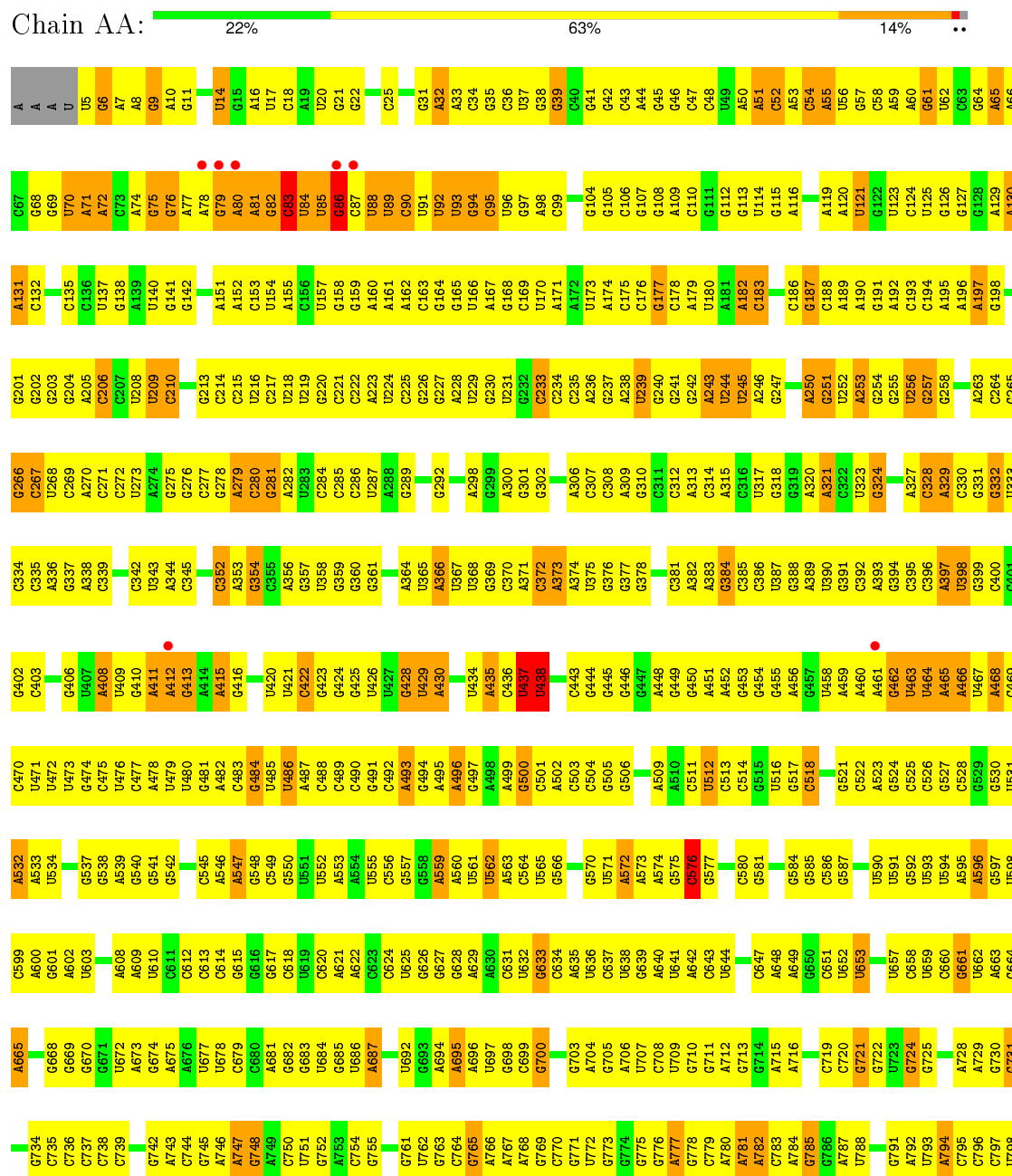
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	CN	3	Total O 3 3	0	0
56	CT	1	Total O 1 1	0	0
56	DB	499	Total O 499 499	0	0
56	DC	5	Total O 5 5	0	0
56	DD	1	Total O 1 1	0	0
56	DE	1	Total O 1 1	0	0
56	DL	5	Total O 5 5	0	0
56	DP	1	Total O 1 1	0	0
56	D2	1	Total O 1 1	0	0

3 Residue-property plots

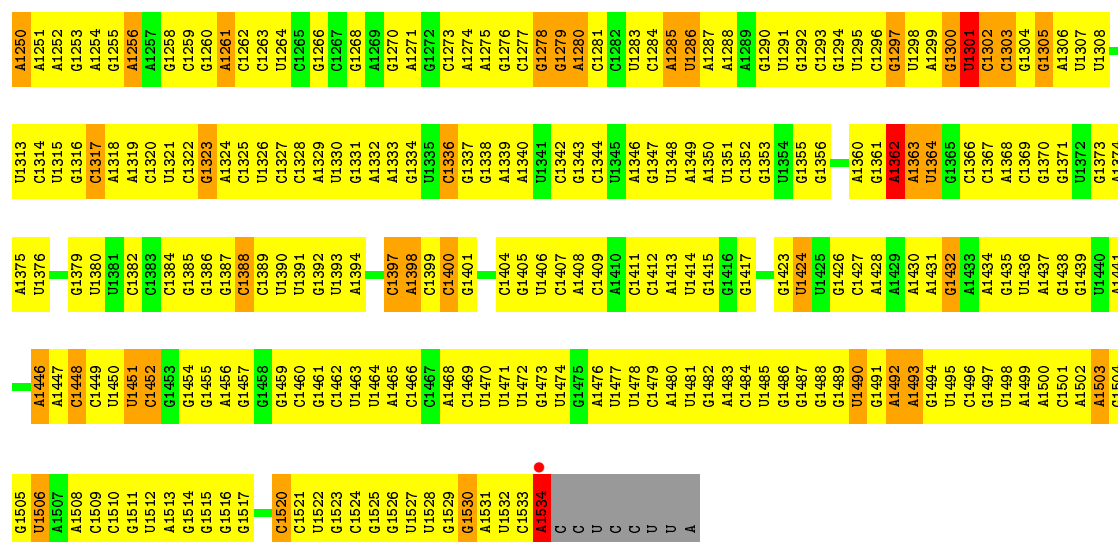
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

- Molecule 1: 16S ribosomal RNA

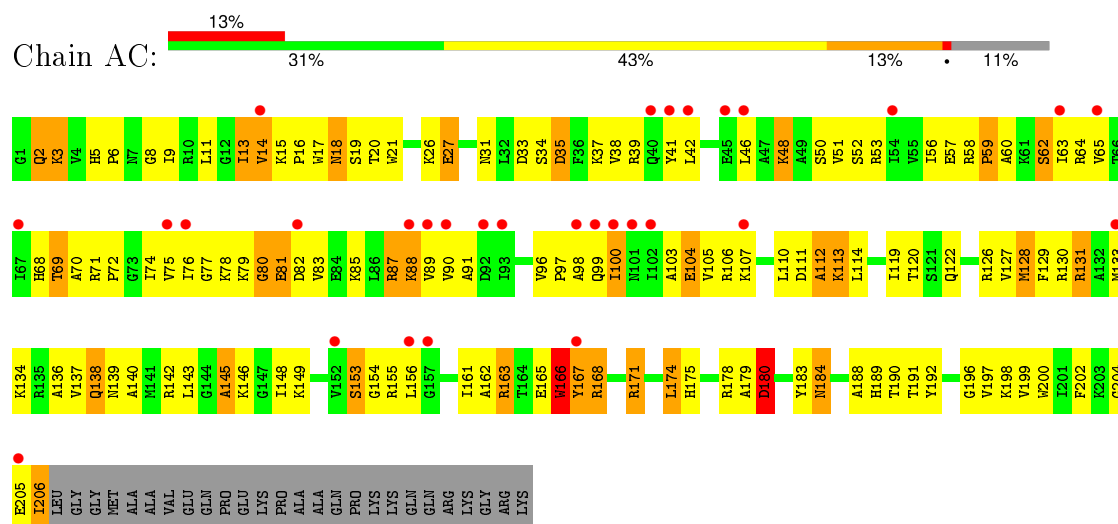


C135	C136	U137	G138	G141	G142	A143	G144	G145	A149	G150	C151	A152	C153	U154	A155	G156	U157	G158	G159	A161	A162	C163	G164	G165	U166	A167	G168	G169	U170	A171	A174	C175	G176	G177	C178	A179	U180	A181	A182	C183	C186	G187	C188	U189	G190	G191	C192	G193	A194	G195	A196	A197	G198	G199	C200	C201	A202	C203	G206	G207	C208	C209	G210	C211	U212	U213	A214	A215	C216	C217	G218	C219	A220	C221	C222	A223	C224	C225	C226	C227	C228	C229	C230	C231	C232	C233	C234	C235	A236	C237	C238	C239	C240	C241	C242	C243	C244	C245	C246	C247	C248	C249	A250	A251	C252	C253	C254	C255	C256	C257	C258	C259	A260	C261	C262	C263	C264	C265	C266	C267	C268	C269	C270	C271	C272	C273	C274	C275	C276	C277	C278	C279	C280	C281	C282	C283	C284	C285	C286	C287	C288	C289	C290	C291	C292	C293	C294	C295	C296	C297	C298	C299	C300	C301	C302	C303	C304	C305	C306	C307	C308	C309	C310	C311	C312	C313	C314	C315	C316	C317	C318	C319	C320	C321	C322	C323	C324	C325	C326	C327	C328	C329	C330	C331	C332	C333	C334	C335	C336	C337	C338	C339	C340	C341	C342	C343	C344	C345	C346	C347	C348	C349	C350	C351	C352	C353	C354	C355	C356	C357	C358	C359	C360	C361	C362	C363	C364	C365	C366	C367	C368	C369	C370	C371	C372	C373	C374	C375	C376	C377	C378	C379	C380	C381	C382	C383	C384	C385	C386	C387	C388	C389	C390	C391	C392	C393	C394	C395	C396	C397	C398	C399	C400	C401	C402	C403	C404	C405	C406	C407	C408	C409	C410	C411	C412	C413	C414	C415	C416	C417	C418	C419	C420	C421	C422	C423	C424	C425	C426	C427	C428	C429	C430	C431	C432	C433	C434	C435	C436	C437	C438	C439	C440	C441	C442	C443	C444	C445	C446	C447	C448	C449	C450	C451	C452	C453	C454	C455	C456	C457	C458	C459	C460	C461	C462	C463	C464	C465	C466	C467	C468	C469	C470	C471	C472	C473	C474	C475	C476	C477	C478	C479	C480	C481	C482	C483	C484	C485	C486	C487	C488	C489	C490	C491	C492	C493	C494	C495	C496	C497	C498	C499	C500	C501	C502	C503	C504	C505	C506	C507	C508	C509	C510	C511	C512	C513	C514	C515	C516	C517	C518	C519	C520	C521	C522	C523	C524	C525	C526	C527	C528	C529	C530	C531	C532	C533	C534	C535	C536	C537	C538	C539	C540	C541	C542	C543	C544	C545	C546	C547	C548	C549	C550	C551	C552	C553	C554	C555	C556	C557	C558	C559	C560	C561	C562	C563	C564	C565	C566	C567	C568	C569	C570	C571	C572	C573	C574	C575	C576	C577	C578	C579	C580	C581	C582	C583	C584	C585	C586	C587	C588	C589	C590	C591	C592	C593	C594	C595	C596	C597	C598	C599	C600	C601	C602	C603	C604	C605	C606	C607	C608	C609	C610	C611	C612	C613	C614	C615	C616	C617	C618	C619	C620	C621	C622	C623	C624	C625	C626	C627	C628	C629	C630	C631	C632	C633	C634	C635	C636	C637	C638	C639	C640	C641	C642	C643	C644	C645	C646	C647	C648	C649	C650	C651	C652	C653	C654	C655	C656	C657	C658	C659	C660	C661	C662	C663	C664	C665	C666	C667	C668	C669	C670	C671	C672	C673	C674	C675	C676	C677	C678	C679	C680	C681	C682	C683	C684	C685	C686	C687	C688	C689	C690	C691	C692	C693	C694	C695	C696	C697	C698	C699	C700	C701	C702	C703	C704	C705	C706	C707	C708	C709	C710	C711	C712	C713	C714	C715	C716	C717	C718	C719	C720	C721	C722	C723	C724	C725	C726	C727	C728	C729	C730	C731	C732	C733	C734	C735	C736	C737	C738	C739	C740	C741	C742	C743	C744	C745	C746	C747	C748	C749	C750	C751	C752	C753	C754	C755	C756	C757	C758	C759	C760	C761	C762	C763	C764	C765	C766	C767	C768	C769	C770	C771	C772	C773	C774	C775	C776	C777	C778	C779	C780	C781	C782	C783	C784	C785	C786	C787	C788	C789	C790	C791	C792	C793	C794	C795	C796	C797	C798	C799	C800	C801	C802	C803	C804	C805	C806	C807	C808	C809	C810	C811	C812	C813	C814	C815	C816	C817	C818	C819	C820	C821	C822	C823	C824	C825	C826	C827	C828	C829	C830	C831	C832	C833	C834	C835	C836	C837	C838	C839	C840	C841	C842	C843	C844	C845	C846	C847	C848	C849	C850	C851	C852	C853	C854	C855	C856	C857	C858	C859	C860	C861	C862	C863	C864	C865	C866	C867	C868	C869	C870	C871	C872	C873	C874	C875	C876	C877	C878	C879	C880	C881	C882	C883	C884	C885	C886	C887	C888	C889	C890	C891	C892	C893	C894	C895	C896	C897	C898	C899	C900	C901	C902	C903	C904	C905	C906	C907	C908	C909	C910	C911	C912	C913	C914	C915	C916	C917	C918	C919	C920	C921	C922	C923	C924	C925	C926	C927	C928	C929	C930	C931	C932	C933	C934	C935	C936	C937	C938	C939	C940	C941	C942	C943	C944	C945	C946	C947	C948	C949	C950	C951	C952	C953	C954	C955	C956	C957	C958	C959	C960	C961	C962	C963	C964	C965	C966	C967	C968	C969	C970	C971	C972	C973	C974	C975	C976	C977	C978	C979	C980	C981	C982	C983	C984	C985	C986	C987	C988	C989	C990	C991	C992	C993	C994	C995	C996	C997	C998	C999	C1000	C1001	C1002	C1003	C1004	C1005	C1006	C1007	C1008	C1009	C1010	C1011	C1012	C1013	C1014	C1015	C1016	C1017	C1018	C1019	C1020	C1021	C1022	C1023	C1024	C1025	C1026	C1027	C1028	C1029	C1030	C1031	C1032	C1033	C1034	C1035	C1036	C1037	C1038	C1039	C1040	C1041	C1042	C1043	C1044	C1045	C1046	C1047	C1048	C1049	C1050	C1051	C1052	C1053	C1054	C1055	C1056	C1057	C1058	C1059	C1060	C1061	C1062	C1063	C1064	C1065	C1066	C1067	C1068	C1069	C1070	C1071	C1072	C1073	C1074	C1075	C1076	C1077	C1078	C1079	C1080	C1081	C1082	C1083	C1084	C1085	C1086	C1087	C1088	C1089	C1090	C1091	C1092	C1093	C1094	C1095	C1096	C1097	C1098	C1099	C1100	C1101	C1102	C1103	C1104	C1105	C1106	C1107	C1108	C1109	C1110	C1111	C1112	C1113	C1114	C1115	C1116	C1117	C1118	C1119	C1120	C1121	C11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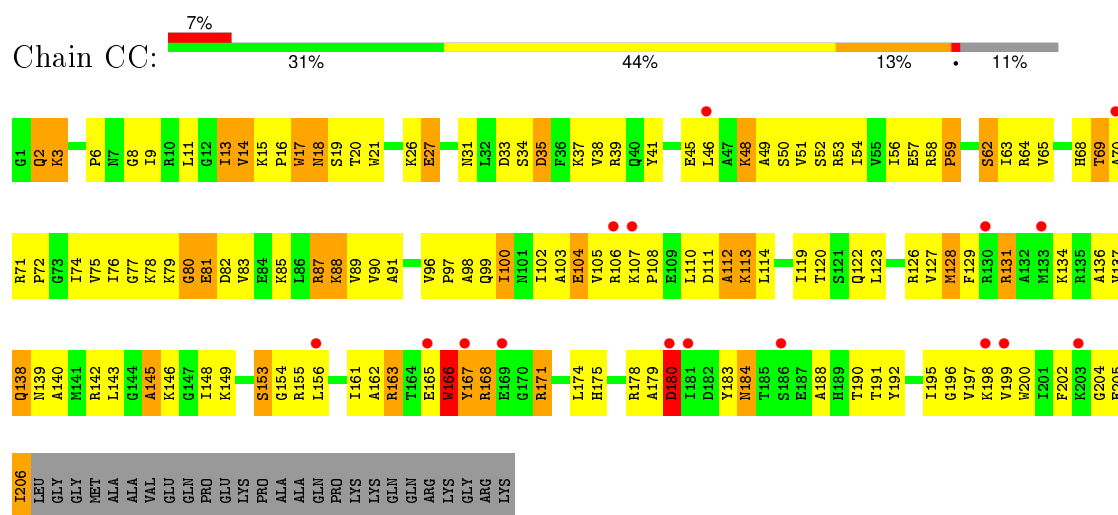
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G1187	C1059	G1123	U1060	C998	G862	U62	C795		U62	G597	U531	A466	C399	G334	G265	G203
A1191	G1061	G1124	U1061	C999	G863	A63	A728		A63	U598	A532	U467	C400	C335	G266	G204
U1194	U1062	U1125	G1062	A1000	A864	A729	C797		C664	C599	C401	A468	A336	A336	C267	A205
C1195	C1063	G1126	C1063	G1002	A938	G730	G731		A665	A600	U534	C469	G402	G337	U268	C206
C1196	G1064	G1127	G1064	G1003	A939	G866	G731		G668	G601	G537	C470	C403	A338	C269	C207
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G1198	A1005	G1130	C1066	A1005	G869	G670	C735		G670	U603	A539	U472	U407	C271	C271	U209
U1199	G1069	G1131		U1007	U875	G671	C736		A607		A540	U473	U408	C272	U273	
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A1201	C1071	G1133	C1071	U1009	G877	U673	C738		A609		G542	U476	G410	U344	G275	G214
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C1210	G1142	C1141	U1080	U1017	A815	C883	A746		G816		C549	C483		A356	A282	C221
U1211	G1143	G1143	U1081	G1018	G884	A747			G817		G550	C484	U420	U283	G283	C222
U1212	A1081	G1144	A1081	U1019	G885	A748			C818		U551	U485	U421	U358	A223	A223
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G1215	U1085	A1146	U1085	A1022	C893	C754			U555		U555	C488	G424	C361	U287	G226
A1216	G1086	C1147	G1086	U1023	G894	G755			C556		C556	C489	G425	C362	A288	G227
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C1233	C1103	U1168	C1103	G1039	A915	A777			U641		C578	C512	G449	C381	C314	A246
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U1236	A1105	U1170	A1105	G1041	G917	C779			C643		C580	C514	C443	A383	U317	A250
G1237	G1106	C1171	G1106	U1043	A918	U780			U644		G581	C515	G451	G384	G318	G251
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C1239	A1110	G1174	A1110	C1045	U920	A782			A648		G585	C517	G453	C386	A320	A253
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G1241	C1112	U1176	C1112	G1047	G922	A784			G650		C587	C519	G455	G388	A322	G255
C1242	U1113	G1177	U1113	U1048	A923	G785			U651		G587	C520	G456	U389	U323	U256
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A1245	U1116	U1180	U1116	G1051	C926	U788			C719		U592	C523	G459	C392	G258	G258
C1246	A1117	G1181	A1117	G1053	G927	U789			C720		U593	C524	A460	A393	C328	G259
U1247	C1118	U1182	C1118	A1054	G928	A790			G721		U594	C525	A461	G394	A329	G260
A1248	U1183	G1183	U1183	C1055	G929	G791			G722		C588	C526	G462	C395	C330	U261
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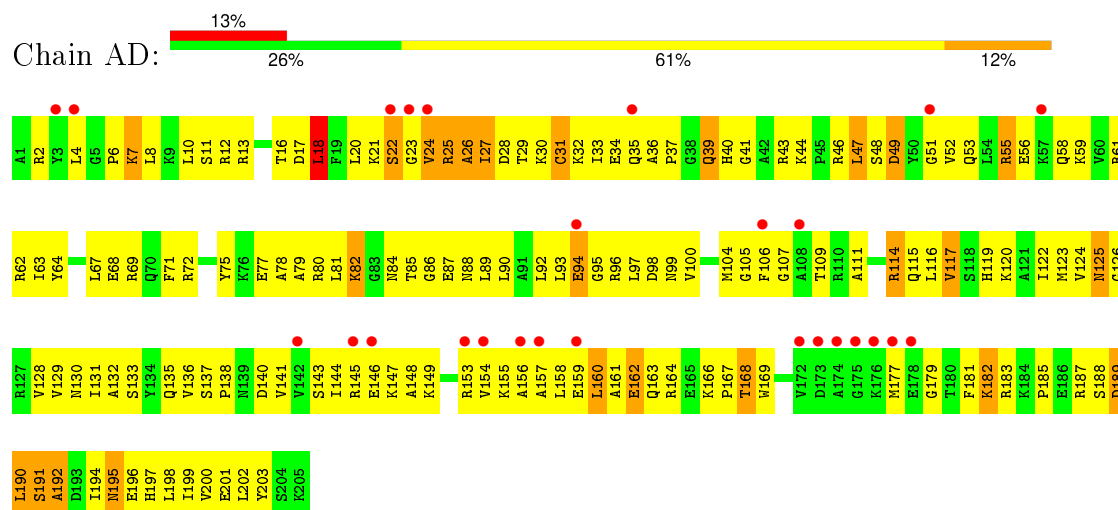
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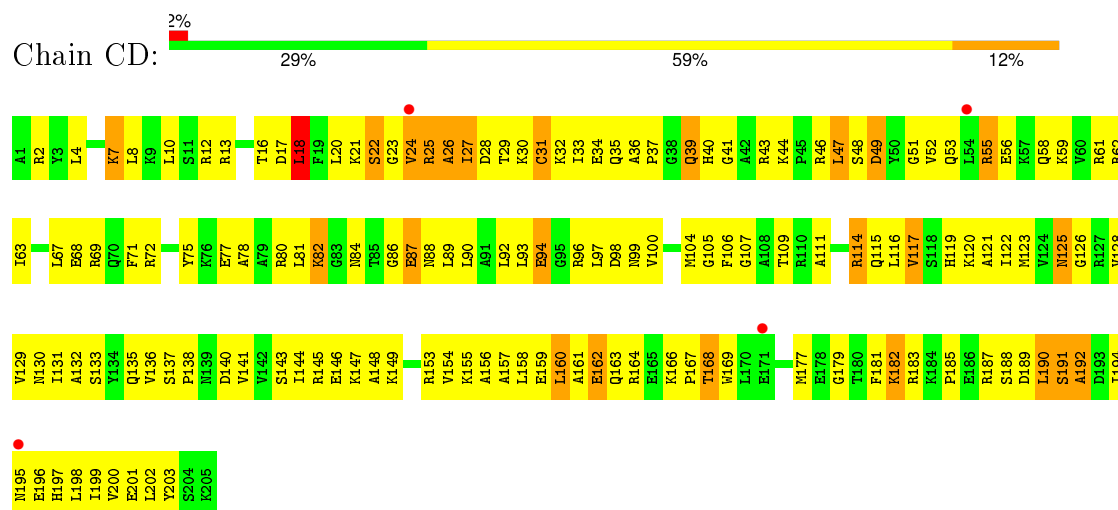
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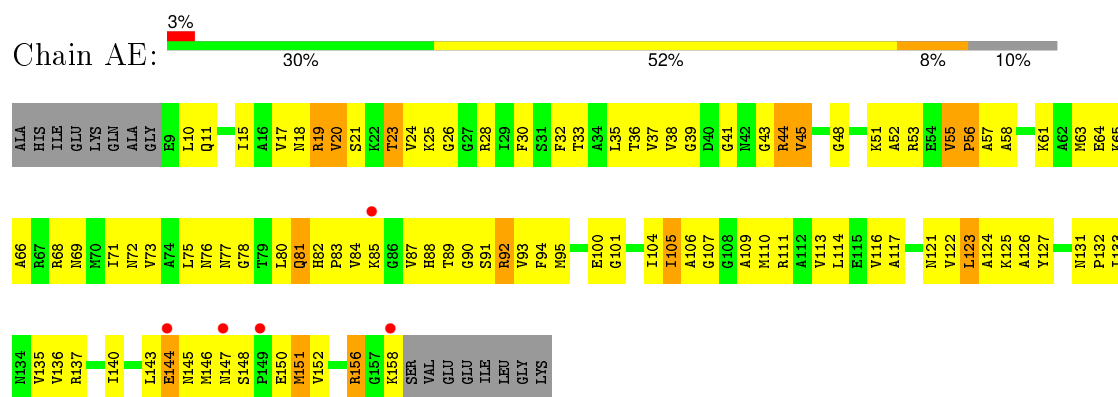
- Molecule 3: 30S ribosomal protein S4



- Molecule 3: 30S ribosomal protein S4

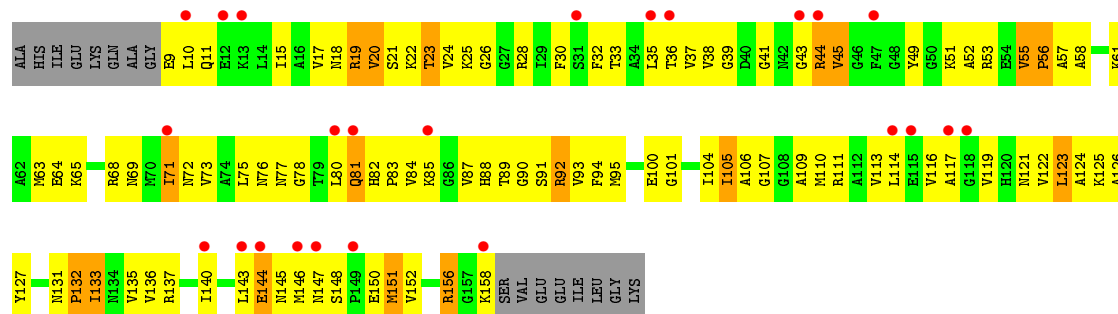


- Molecule 4: 30S ribosomal protein S5

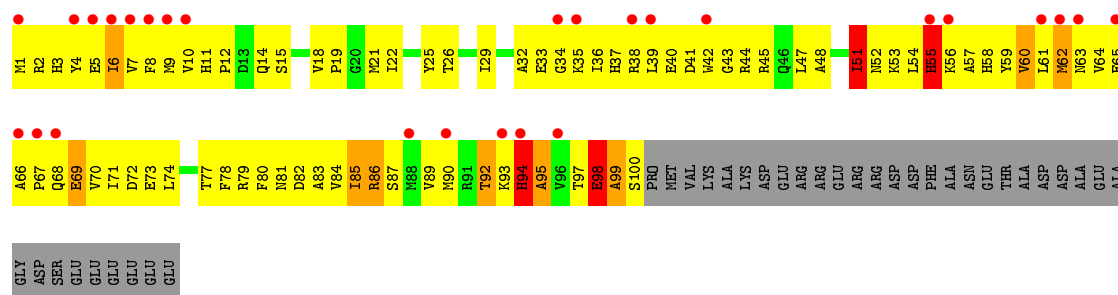
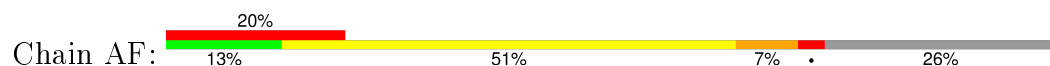


- Molecule 4: 30S ribosomal protein S5

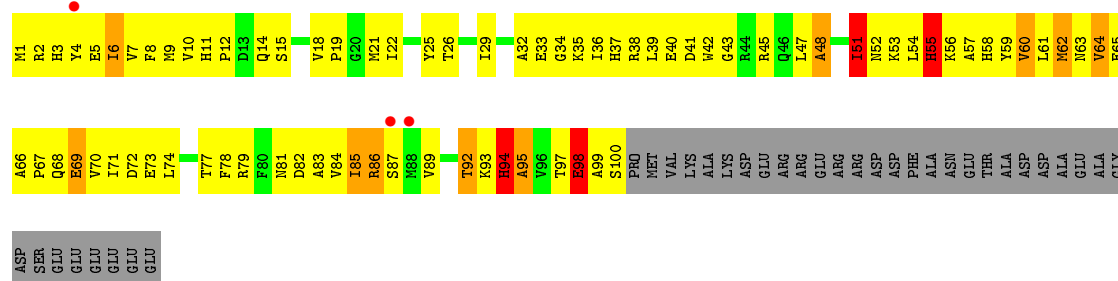
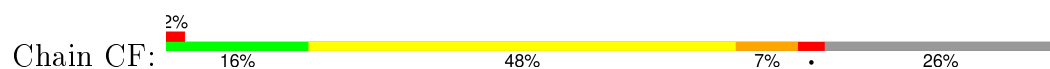




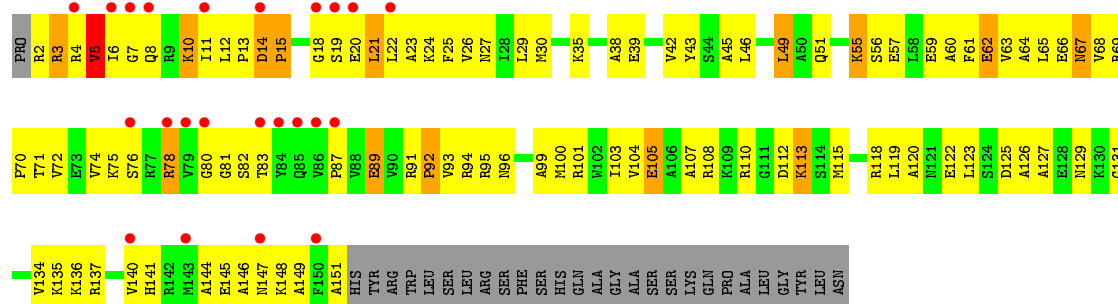
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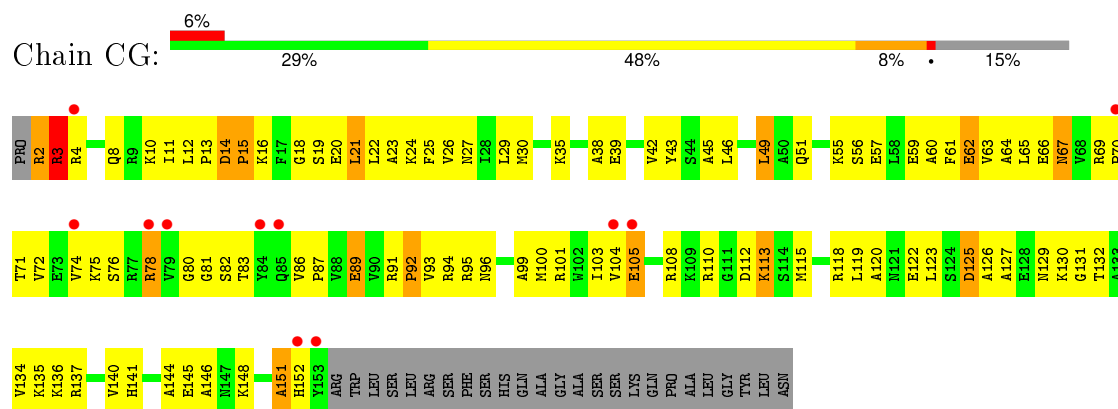
• Molecule 5: 30S ribosomal protein S6



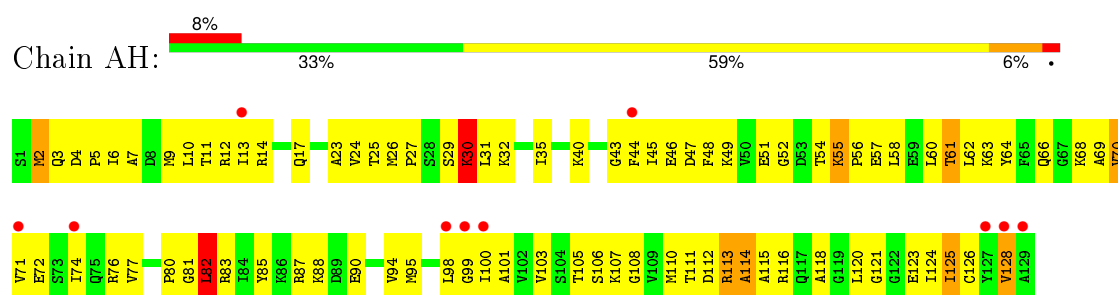
• Molecule 6: 30S ribosomal protein S7



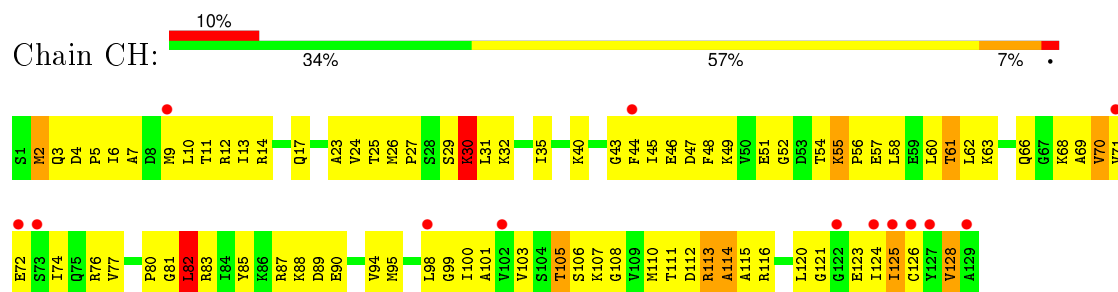
- Molecule 6: 30S ribosomal protein S7



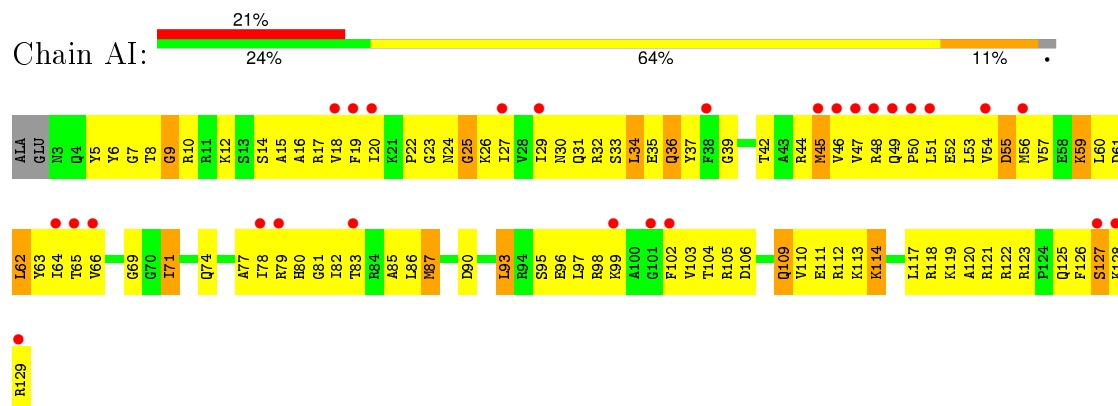
- Molecule 7: 30S ribosomal protein S8



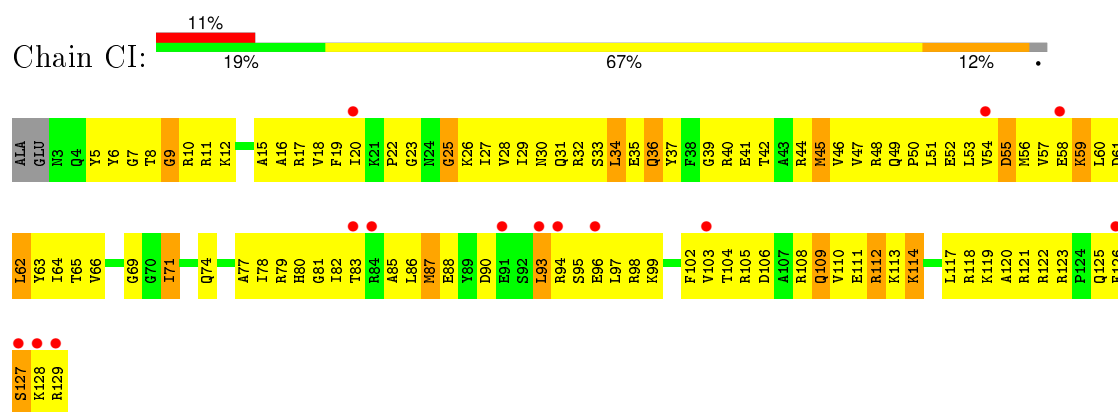
- Molecule 7: 30S ribosomal protein S8



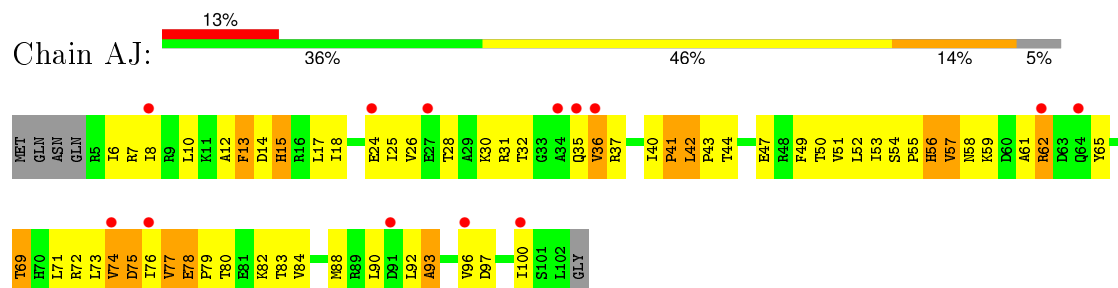
- Molecule 8: 30S ribosomal protein S9



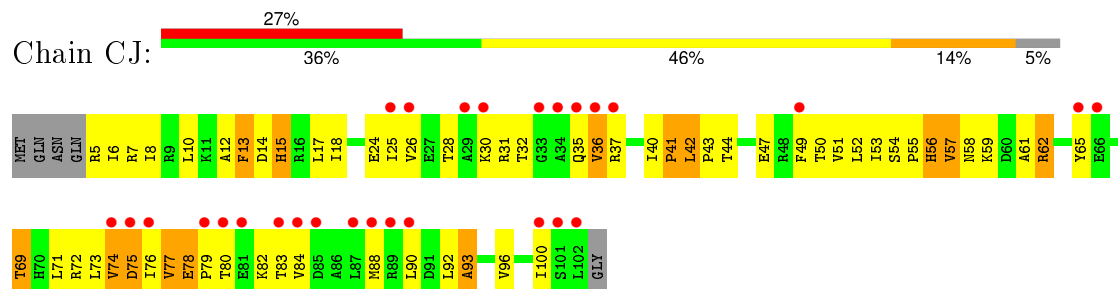
- Molecule 8: 30S ribosomal protein S9



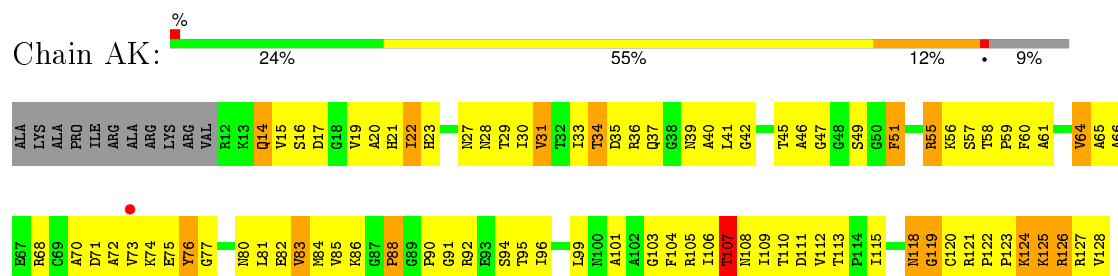
• Molecule 9: 30S ribosomal protein S10



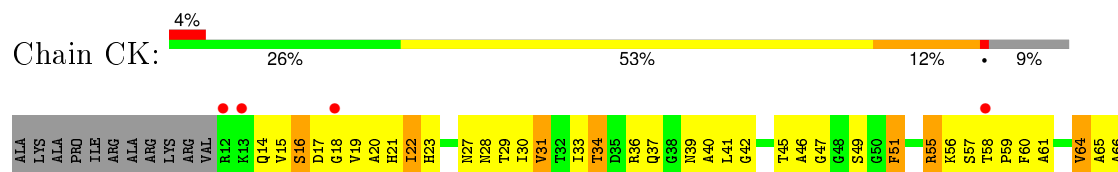
• Molecule 9: 30S ribosomal protein S10

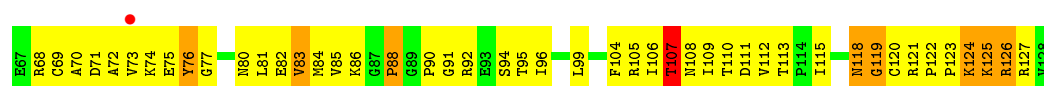


• Molecule 10: 30S ribosomal protein S11

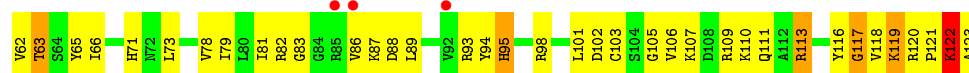
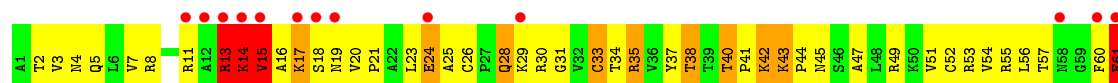


• Molecule 10: 30S ribosomal protein S11

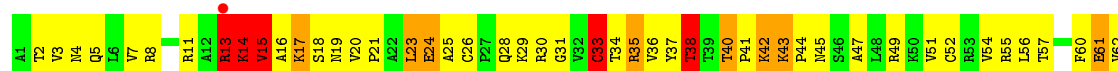




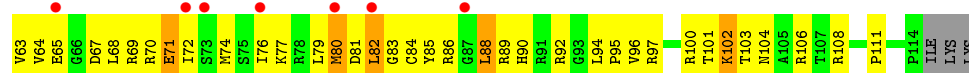
- Molecule 11: 30S ribosomal protein S12



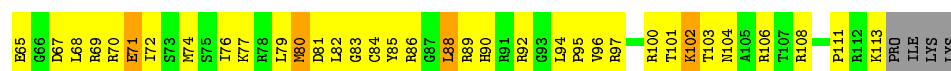
- Molecule 11: 30S ribosomal protein S12



- Molecule 12: 30S ribosomal protein S13

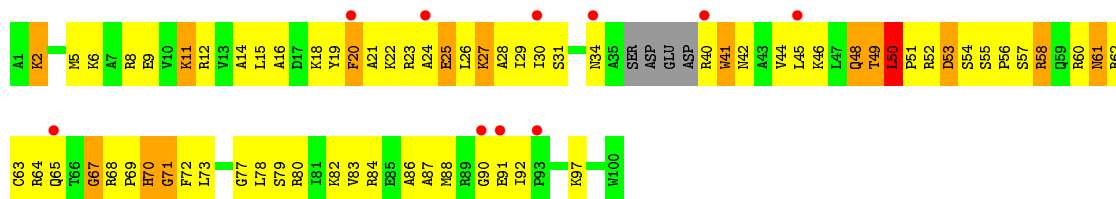


- Molecule 12: 30S ribosomal protein S13

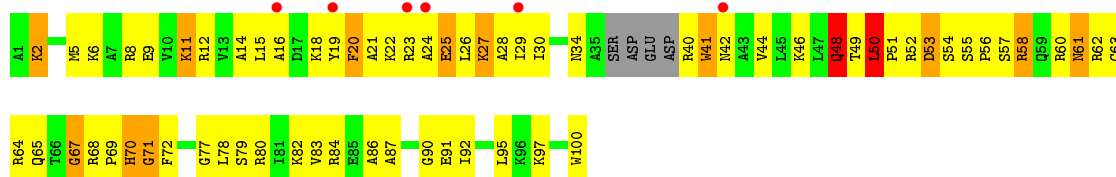


- Molecule 13: 30S ribosomal protein S14

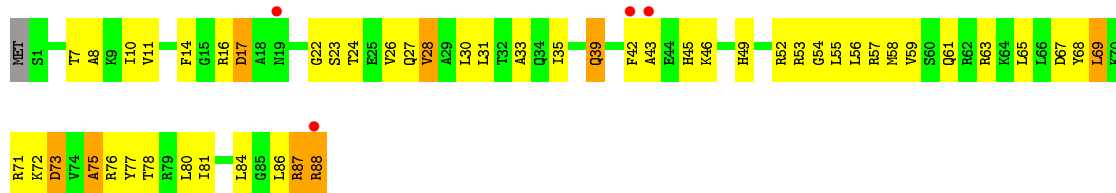
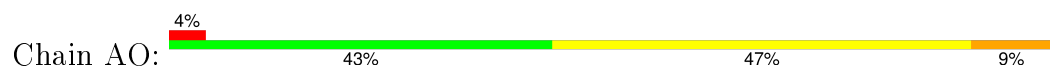




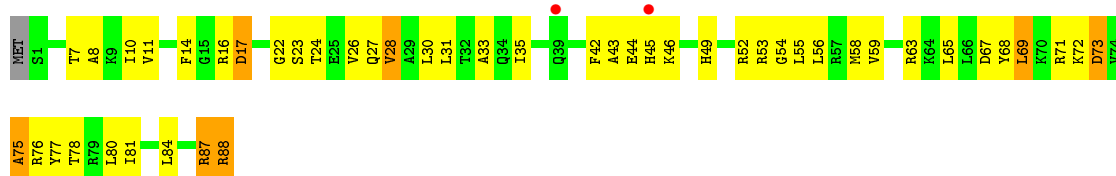
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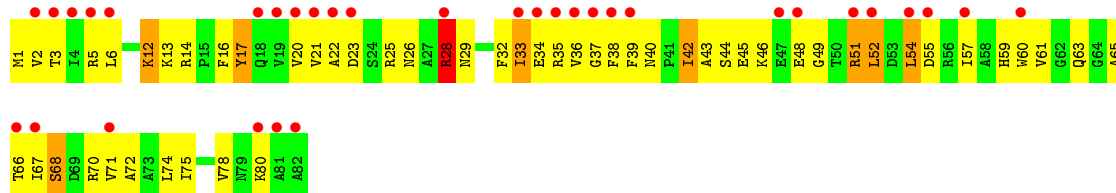
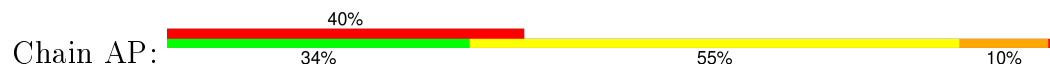
• Molecule 14: 30S ribosomal protein S15



• Molecule 14: 30S ribosomal protein S15

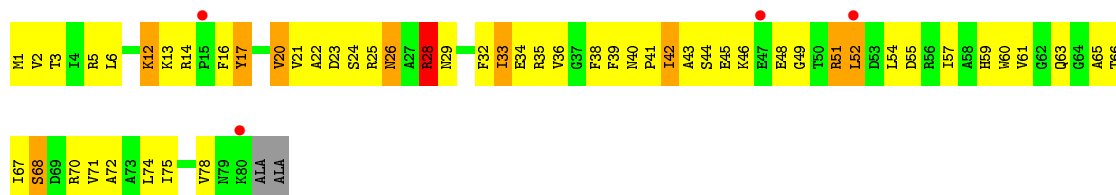


• Molecule 15: 30S ribosomal protein S16

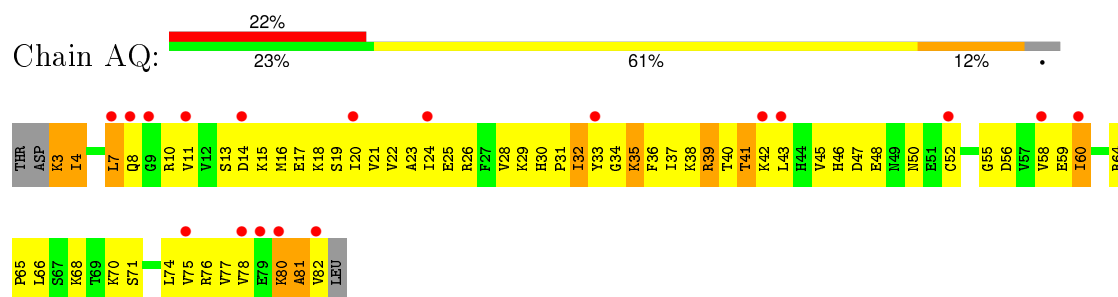


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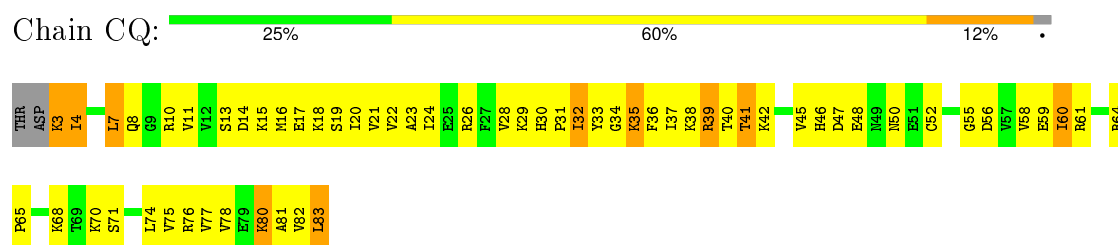




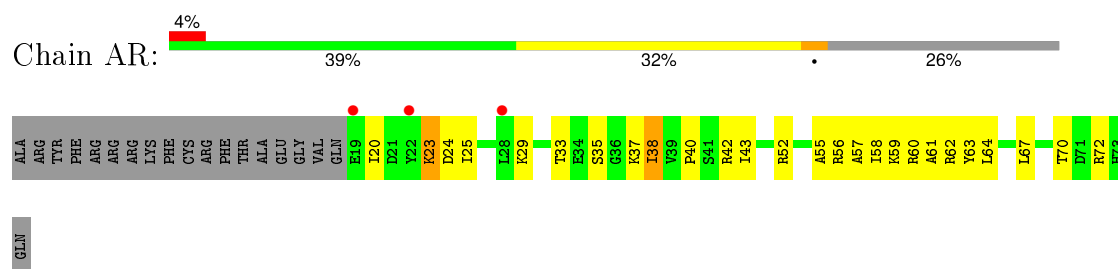
- Molecule 16: 30S ribosomal protein S17



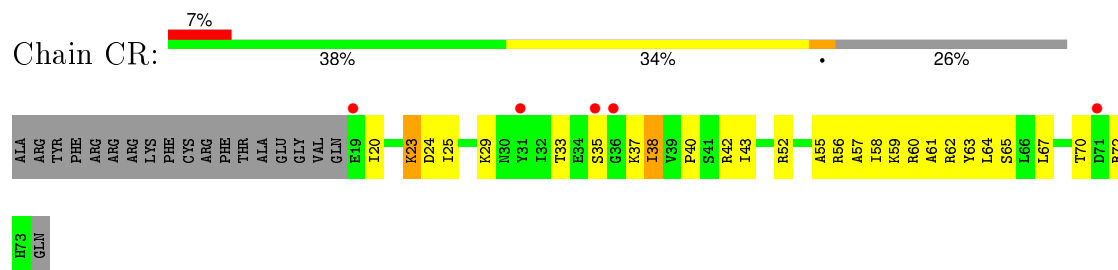
- Molecule 16: 30S ribosomal protein S17



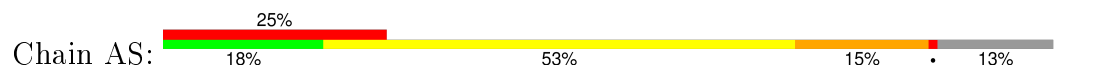
- Molecule 17: 30S ribosomal protein S18

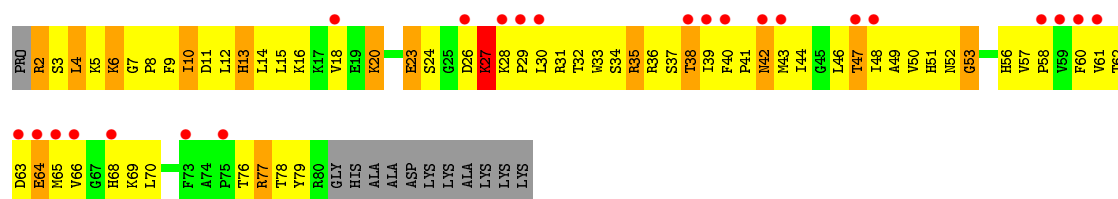


- Molecule 17: 30S ribosomal protein S18

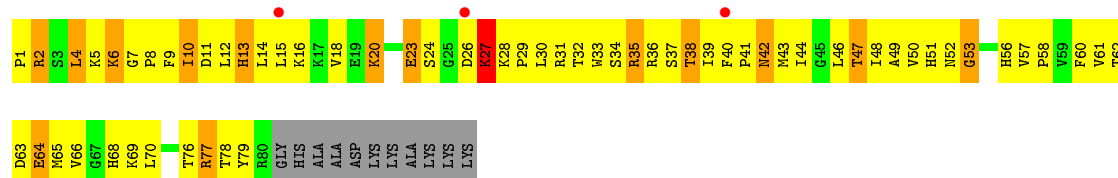


- Molecule 18: 30S ribosomal protein S19

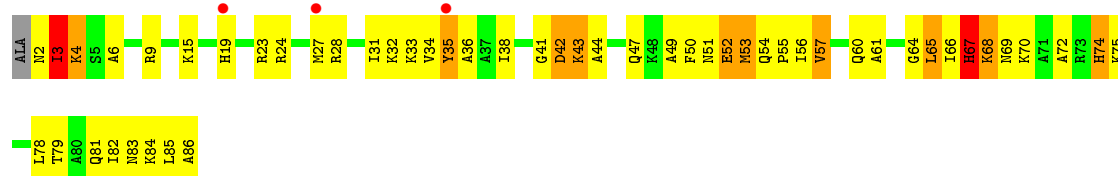
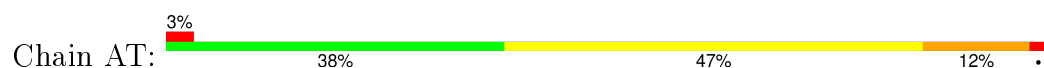




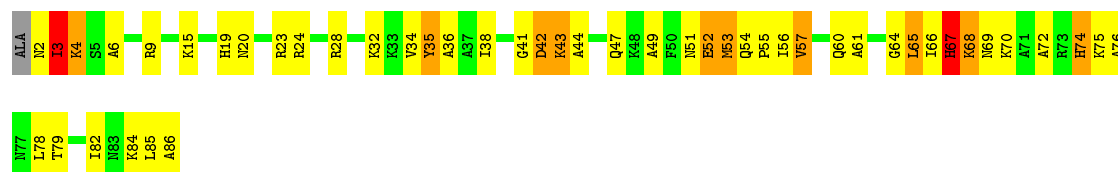
- Molecule 18: 30S ribosomal protein S19



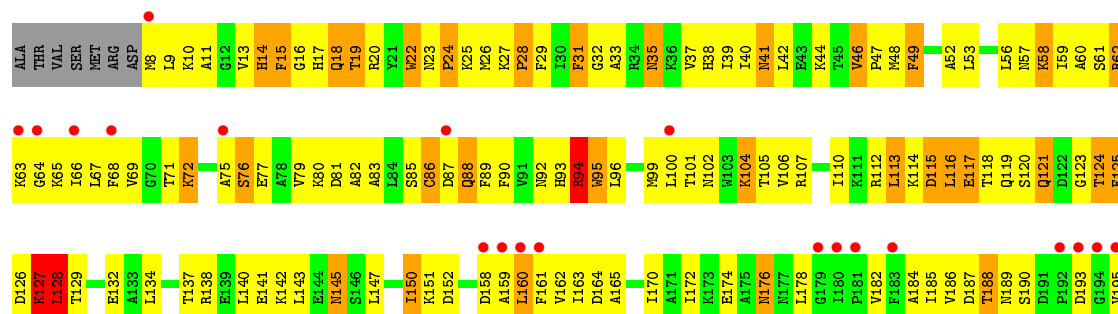
- Molecule 19: 30S ribosomal protein S20

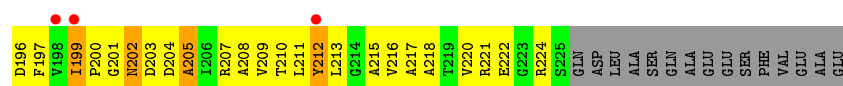


- Molecule 20: 30S ribosomal protein S2

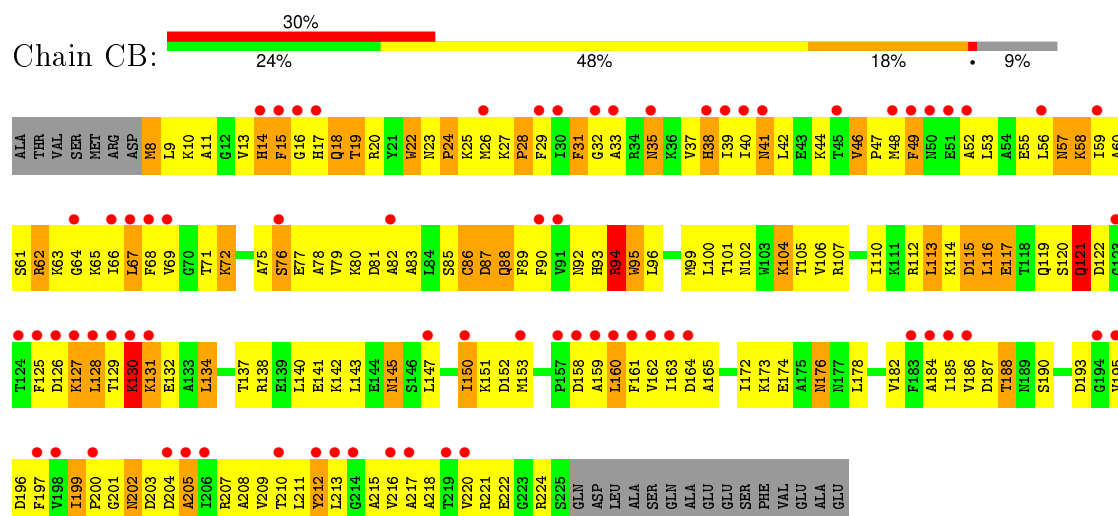


- Molecule 20: 30S ribosomal protein S2

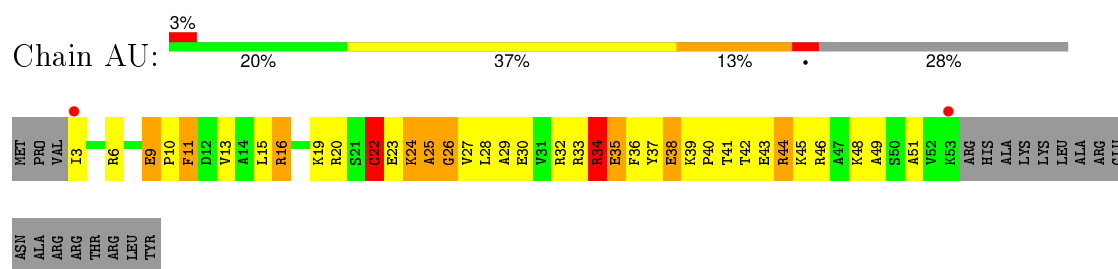




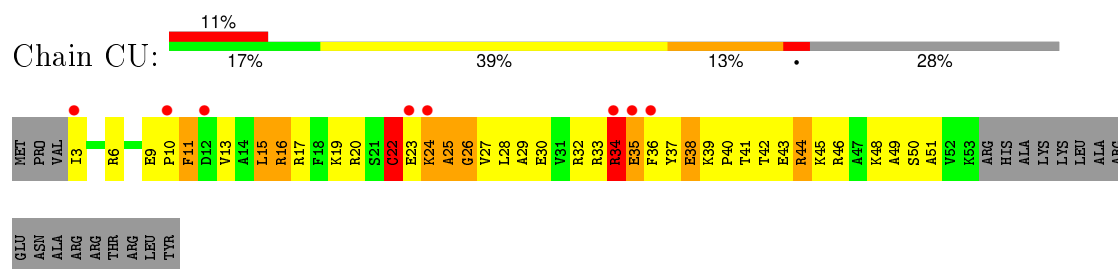
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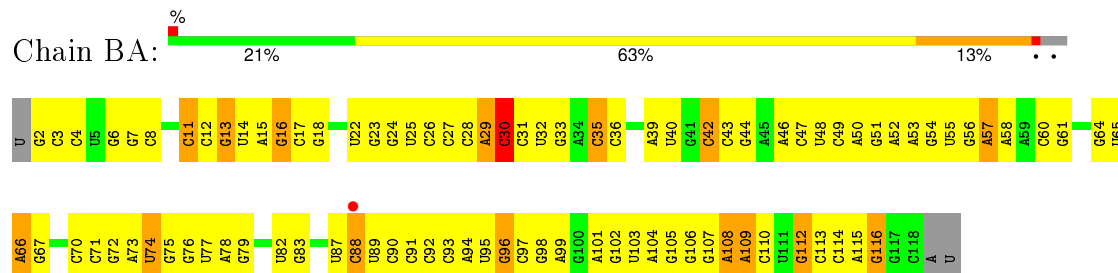
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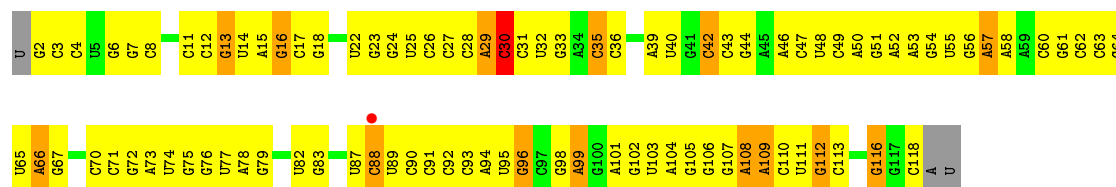
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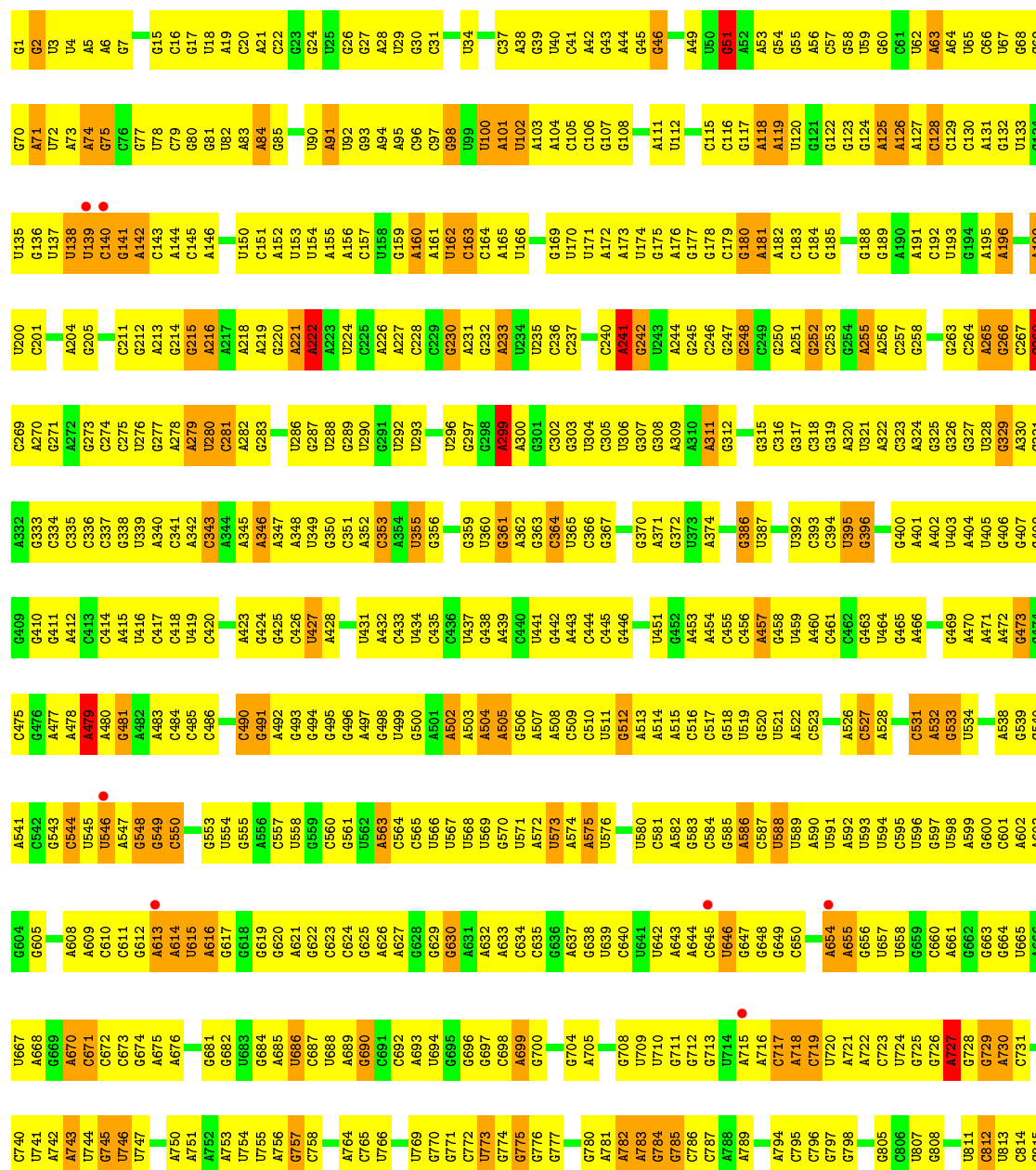
• Molecule 22: 5S ribosomal RNA



• Molecule 22: 5S ribosomal RNA



• Molecule 23: 23S ribosomal RNA




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U2885
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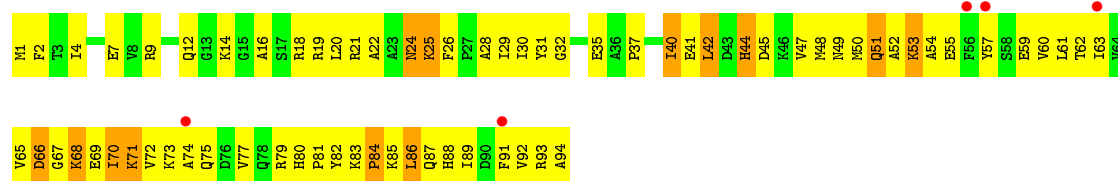
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Chain DB:  23% 63% 12% ..

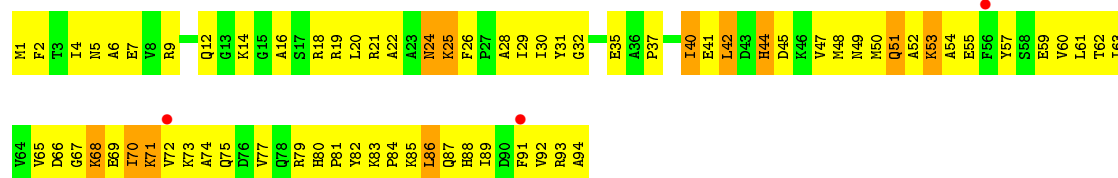
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U871	U810	U667		U667	A603	C540	G474	C335	G409	C335	G274		U137	G70	G3
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C873	C812	U741	U741	G669	G605		G476	C337	G411	C337	U276	G205	U139	U72	A5
C874	U813	A742	A742	A670		C544	A477	G338	A412	G338	G277		C140	A73	A6
G875	C814	A743		C671	A608	U545		U339	C413	U339	A278	C211	G141	A74	G7
C876	C815	U744	A744	C672	A609	U546	A478	U340	G414	A340	A279	G212	A142	G75	
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A878	C817	U746	G746	G674	C611	A548	G480	C342	U416	A342	C281	G214	A144	G77	C16
G	G818	U747	U747	A675	G612	U549	A482	C343	C417	C343	A282	G215	C145	U78	G17
A819	A819				A613	C550	A483	A344	C418	A344	G283	A216	A146	C79	U18
G	A820	C678	A750	C678	A614	G551	C484	A345	U419	A345	U284	A217		G80	A19
G	A751	C679	A751	C679	U615	U552	C485	A346	C420		U285	A218	U150	G81	C20
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C	U824	A684		A684	G619	G555	C490	U349	G424	U349	U289	A222	U154	A84	G23
A	A825	A685	U755	A685	G620	A556	G491	G350	G425	G350	G289	A223		G85	G24
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C	G836	C696		C696	A831	U567	A502	G361	U437	G361	A300	A233	A165	U99	
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C901	C940	G700	C772	G700	C635	U571	G506	U365	U441	U365	U304		U170		U40
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G904		G775	G775	A705	G638	A574	C509	C444	C444	C444	G307	U243	G108		C43
A905	A945	G776	C776	U706	U639	A575	C510	G370	C445	G370	G308	A244	U174	C109	C44
U909	U846	G777	G777	C707	C640	U576	G511	C371	G446	A371	A309	G245	G175	G45	C45
A909	U847				U841		G512	U373		U373	A310	C246	A176	G46	C46
A910	C848	U709	G780	U709	U642	U580	A513	A374	U451	A374	A311	G247	G177	U113	C47
A911	A849	U710	A781	U710	A643	C581	A514		G452		G312	G248	G178	C115	C48
C912	U850	G711	A782	G711	A644	A582	A515	G379	A453			C249	C179	C116	A49
U913	C851	G712	A783	G712	C645	U583		G379	A454	G379	G315	G250	G180	G117	U50
G916	U852	G713	A784	G713	U646	C584	G518		A455		G316	A251	A181	A118	G51
A917	C853	U714	G785	U714	C646	G585	U519	G386	C456	G386	G317	G252	A182	A119	A52
A918	C854	A715	C786	G648	G648	A586	G520	U387	A457	U387	C318		C183	U120	A53
G919	G855	U716		C587	G649	C587	U521		G458		G319	A255	C184	G121	G54
U919	G856	C717	A789	C717	C650	U588	A522	U392	U459	U392	A320	A256	G185	G122	G55
A920	G857	A718		U718		U589	C523	U392	A460	U392	U321	C257	G188	G123	A56
C921	G858	C719	A794	C719	A654	A590	G524	C394	C461	C394	A322	G258	G189	G124	A57
C922	G859	U720	C795	U720	A655	U591	U525	U395	C462	U395	C323		A125	G125	C57
G923	U860	A721	C796	A721	C645	A592	A526	G396	G463	G396	A324	G263	A190	A126	U59
G924	A861	G722	G797	G722	U657	U593	C527		U464		G325	C264	A191	A127	G60
A925	G862	C723	G798	C723	U658	U594	A528		G465		G326	A265	C192	G128	C81
G926	G863	U724		C595	G659	C595		G400	A466		G327	G266	A193	G129	U62
A927	G864	G725	U803	G659	C660	U596	C531	A401	G467	A401	U328	C267	G194	C130	A63
C928	C865	A726	A904	G661	A661	G597	A532	G329	G468	U403	G329	C268	A195	A131	A64
A929	A866	G727	G805	G662	G662	U598	G533	G330	G469	A404	A330	C269	A196	G132	U65
C930	C867	G728	C906	G663	G663	A599	U534	U405	A470	U405	A331	C270	A196	U133	C66
G931	U868	G729	C907	G664	C664	C600		C406	A471		G332	C271	A197	C134	U67

G1944	C1879	A1745	A1679	U1599	G1536	G1473	G1410	G1341	U1273	C1207	C1145	A1077	A1000	U932
G1945	U1800	A1746	G1682	C1600	G1537	U1474	U1411	G1344	A1274	C1208	C1146	U1080	A1001	A933
G1946	C1881	U1747	U1683	G1601	U1538	G1475	U1412	U1344	A1275	U1209	C1147	U1081	G1002	U934
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G1950	A1885	U1821	C1686	C1607	G1543	C1480	G1418	C1348	G1282	A1213	C1151	A1085	U1012	C938
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G1954	A1889	A1756	A1690	G1547	G1546	U1484	G1422	C1353	A1286	U1219	A1155	A1090	G1016	G942
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U1956	G1891	A1759	A1698	A1616	A1548	U1486	G1424	C1354	A1288	U1221	U1159	U1092	U1019	C946
C1958	C1892	C1760	A1699	A1617	C1550	U1487	G1425	G1355	G1289	U1222	G1160	C1093	A1020	A947
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U1960	A1894	U1700	U1700	G1619	A1552	C1489	A1427	U1365	C1290	U1224	G1162	U1097	G1023	G949
G1961	G1897	A1701	G1702	G1622	A1553	A1490	G1428	A1366	G1291	U1225	G1163	U1098	G1024	G950
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A1970	C1902	G1708	G1708	A1635	G1560	A1495	A1433	G1371	C1297	G1233	G1168	U1101	A1029	A959
G1971	G1903	A1772	U1709	U1636	U1571	U1496	A1434	U1372	G1298	U1234	A1169	C1102	C1030	A960
G1972	C1904	A1773	G1710	A1637	U1572	U1497	G1435	A1373	G1300	G1235	A1172	A1103	G1031	C961
C1973	C1905	C1774	G1710	A1637	U1573	C1498	G1436	G1374	G1301	G1236	U1173	G1106	A1032	G962
C1974	U1906	U1775	A1711	C1638	C1564	U1501	C1437	U1375	A1302	A1237	U1174	G1107	U1033	G963
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A1981	C1913	U1778	G1715	A1641	G1567	A1504	U1441	G1380	A1307	U1242	C1177	G1110	G1042	C968
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C1985	U1915	A1780	U1717	C1644	U1569	U1506	U1443	G1382	G1309	A1244	G1179	G1112	C1043	C970
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A1918	A1918	A1785	U1720	U1647	G1573	A1509	C1446	A1385	G1317	A1247	U1183	C1117	A1048	A973
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A1932	C1933	C1800	G1734	A1668	G1588	A1525	C1462	C1399	G1331	C1261	U1197	A1134	G1063	C991
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C1940	A1876	A1676	U1742	A1676	A1596	A1533	A1470	G1408	G1339	A1272	G1206			
A2019	U1812	G1743	U1742	A1677	U1597	U1534	C1471	G1408	U1340					
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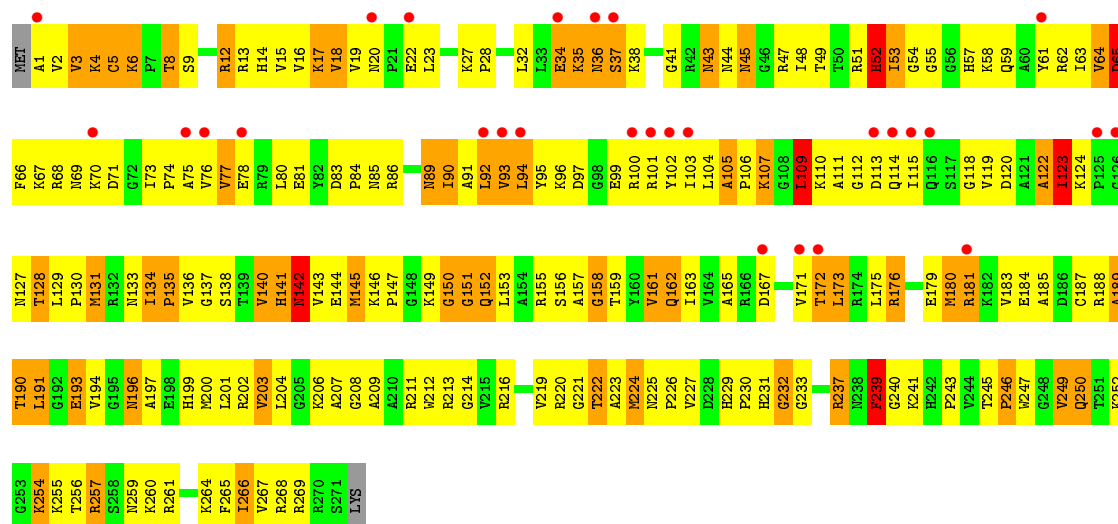




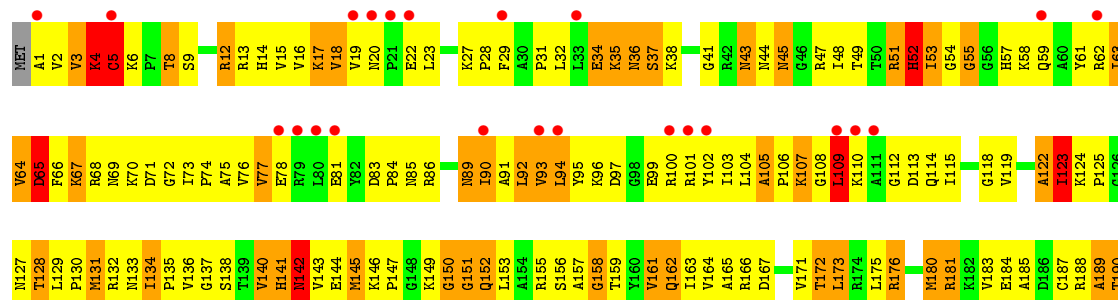
• Molecule 24: 50S ribosomal protein L25

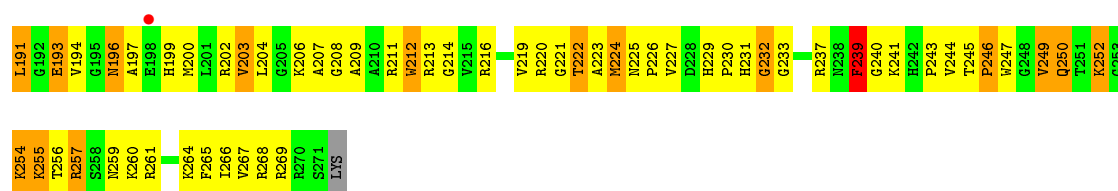


• Molecule 25: 50S ribosomal protein L2

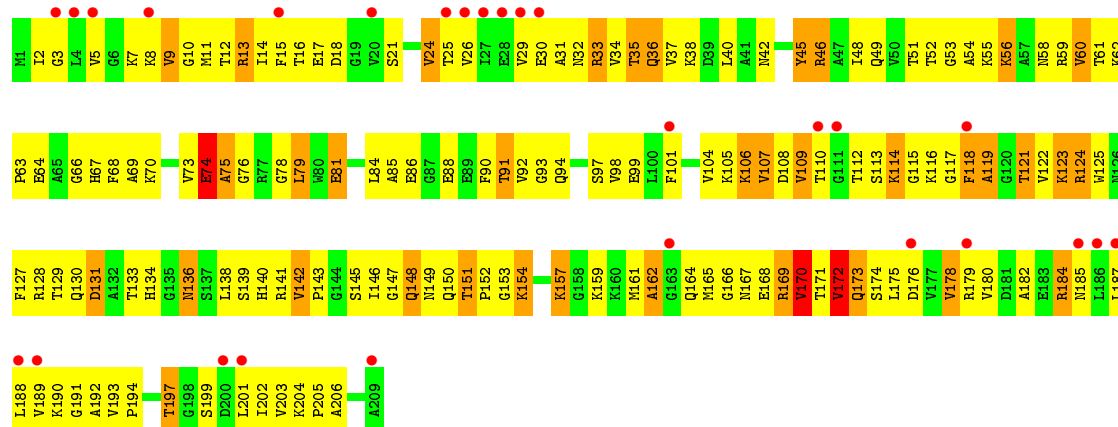


• Molecule 25: 50S ribosomal protein L2

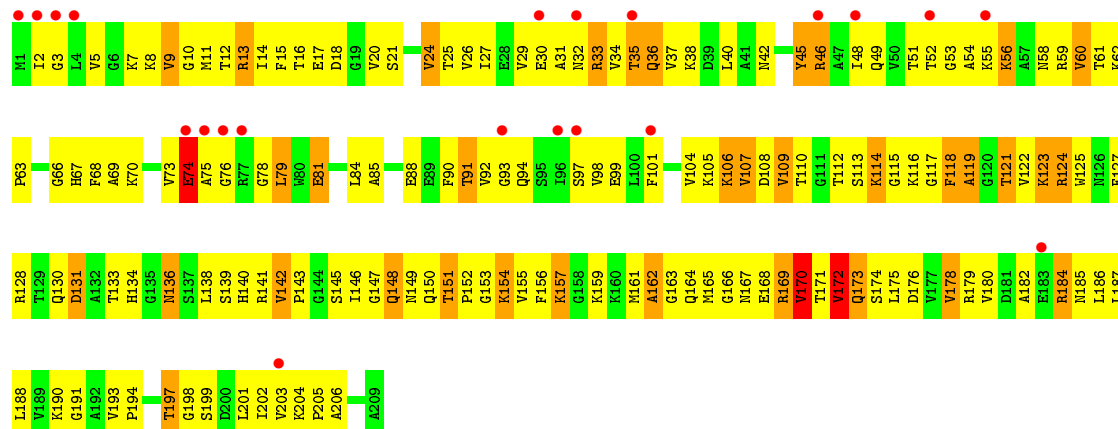




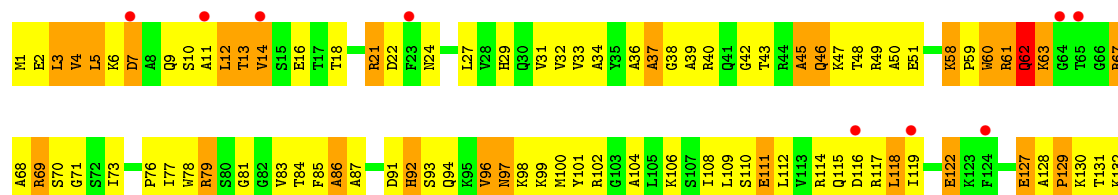
● Molecule 26: 50S ribosomal protein L3

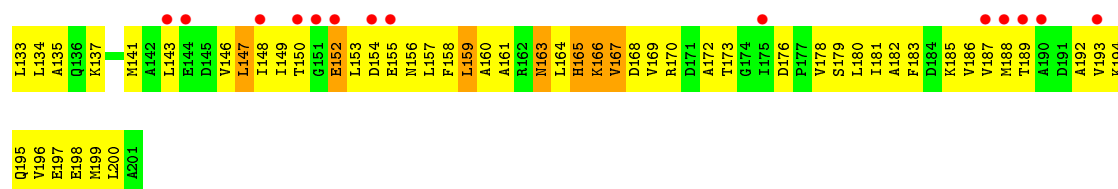


● Molecule 26: 50S ribosomal protein L3

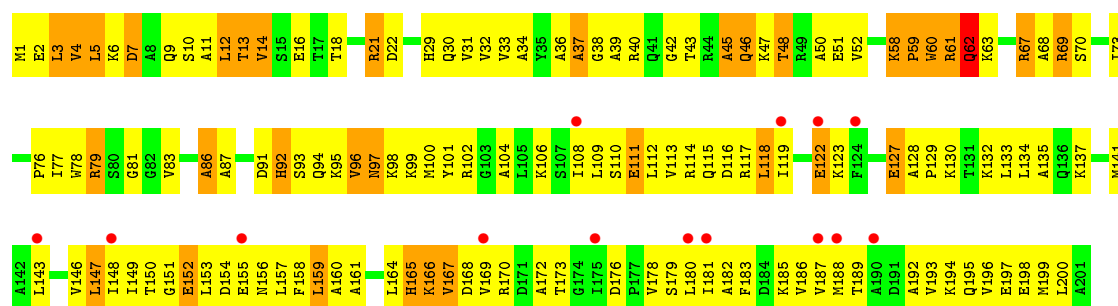


● Molecule 27: 50S ribosomal protein L4

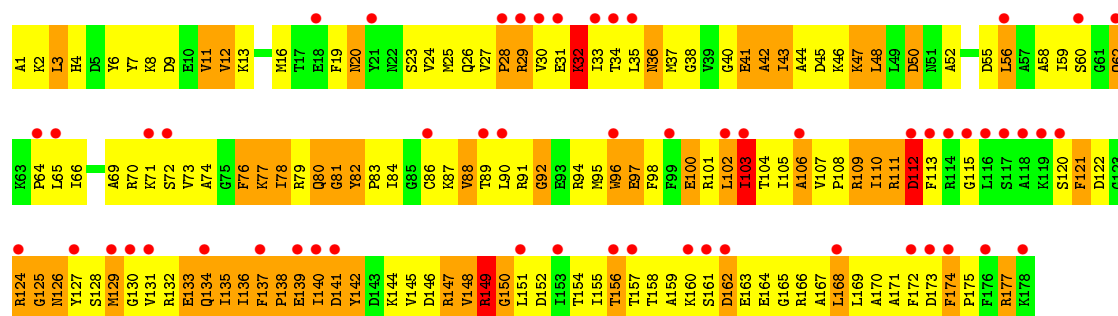
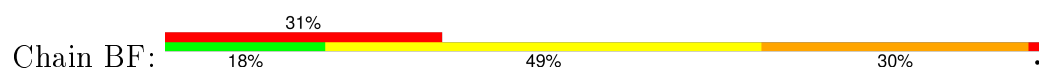




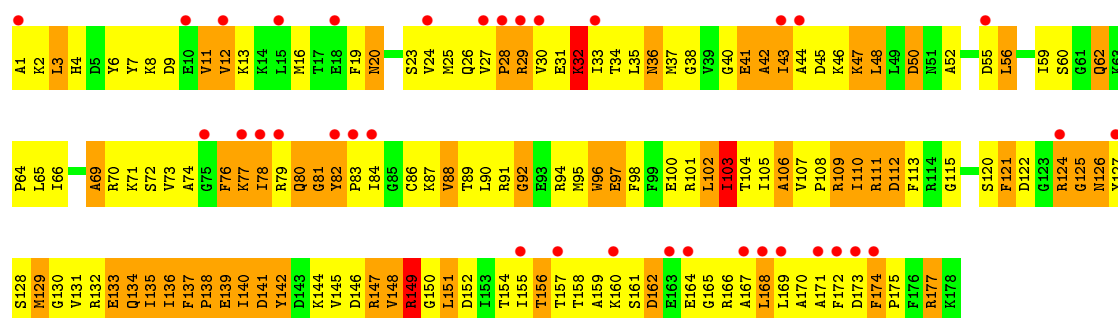
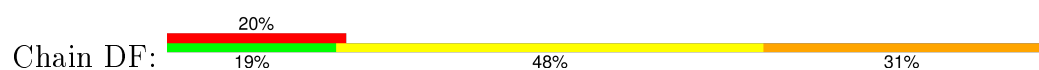
• Molecule 27: 50S ribosomal protein L4



• Molecule 28: 50S ribosomal protein L5

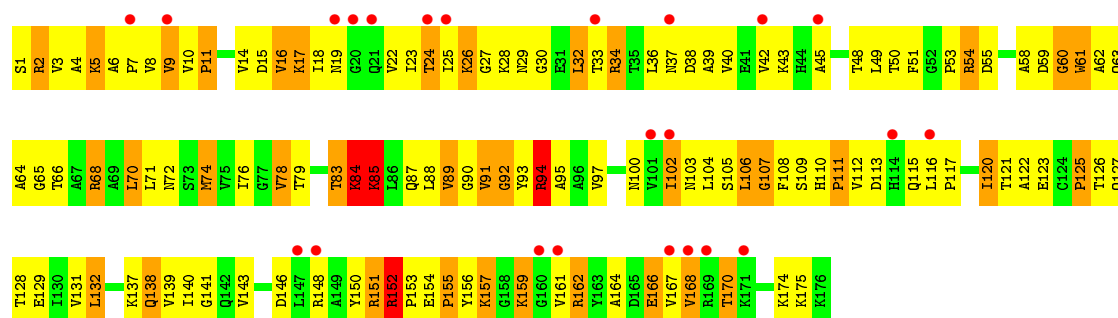


• Molecule 28: 50S ribosomal protein L5

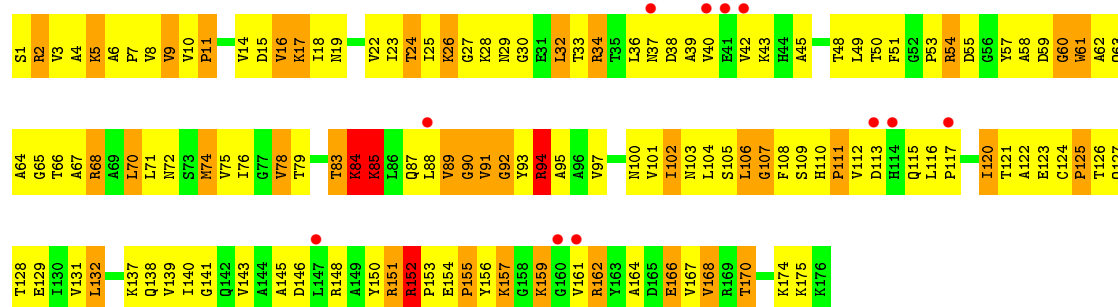


• Molecule 29: 50S ribosomal protein L6

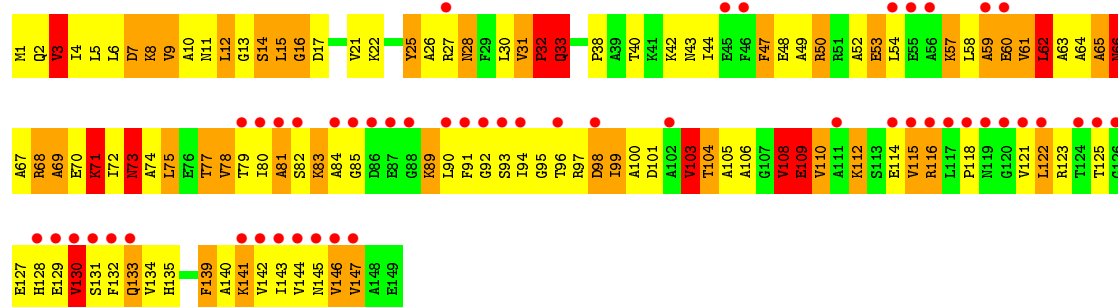




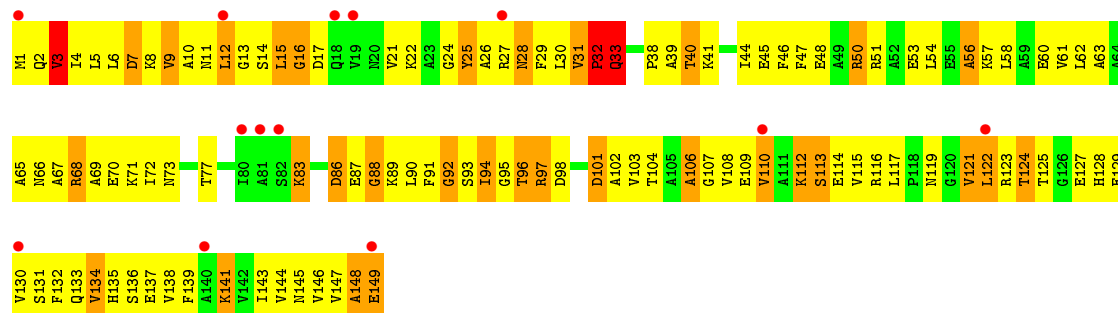
• Molecule 29: 50S ribosomal protein L6



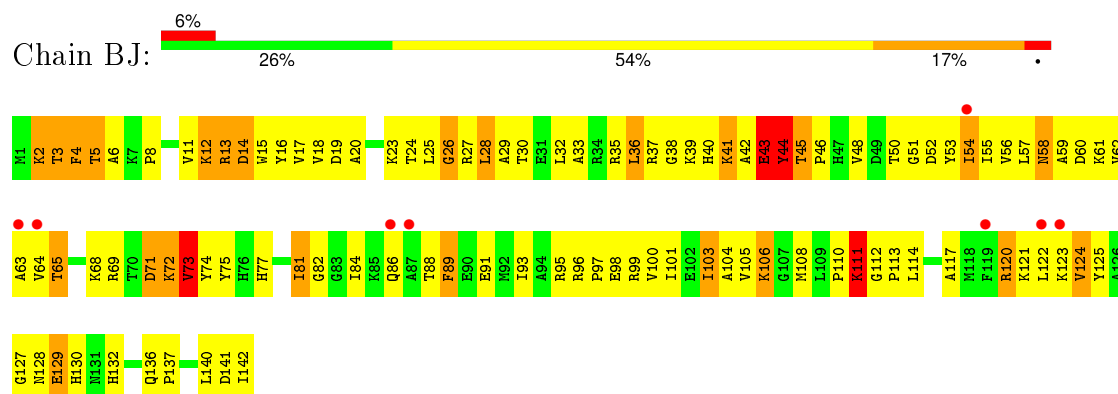
• Molecule 30: 50S ribosomal protein L9

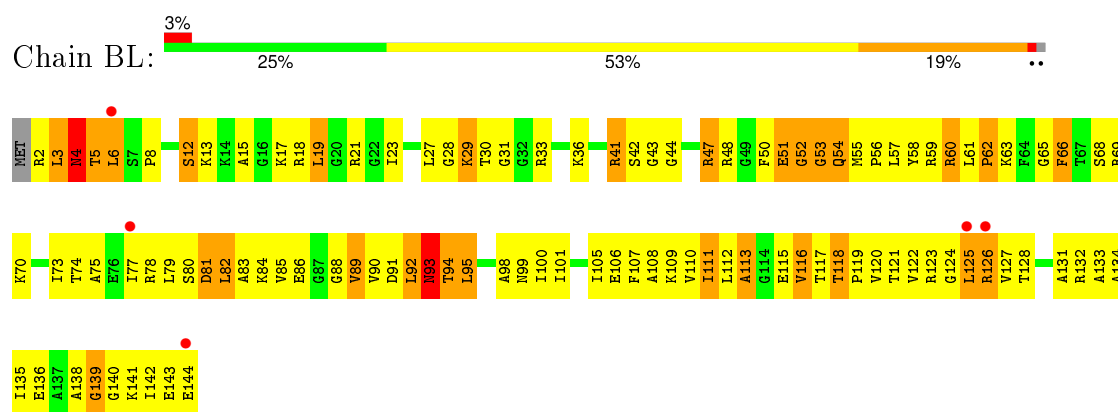


• Molecule 30: 50S ribosomal protein L9

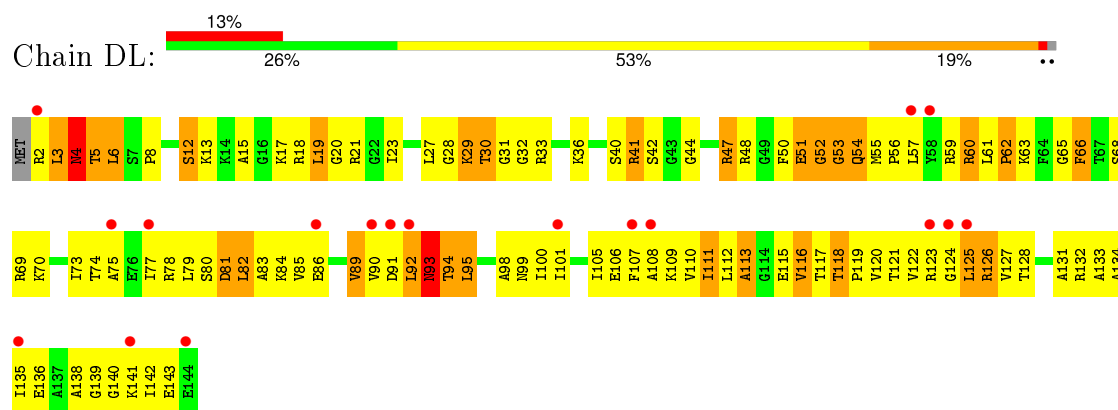


- Molecule 31: 50S ribosomal protein L13

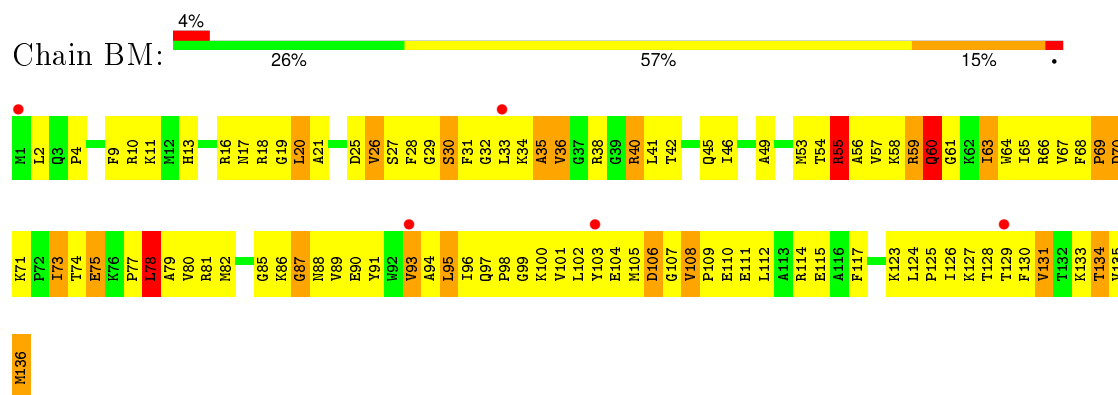




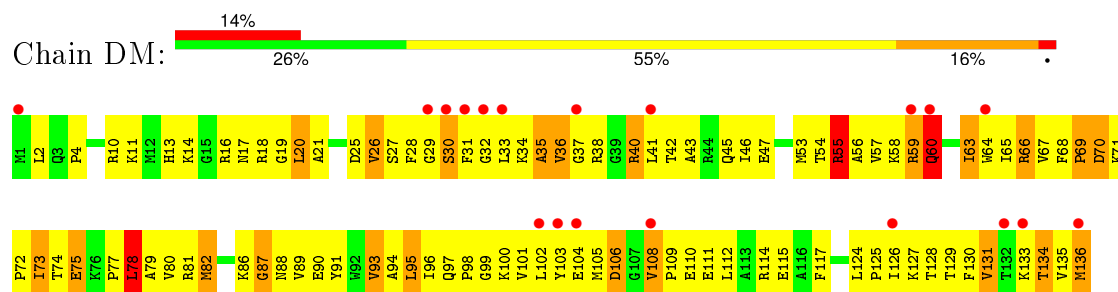
• Molecule 33: 50S ribosomal protein L15



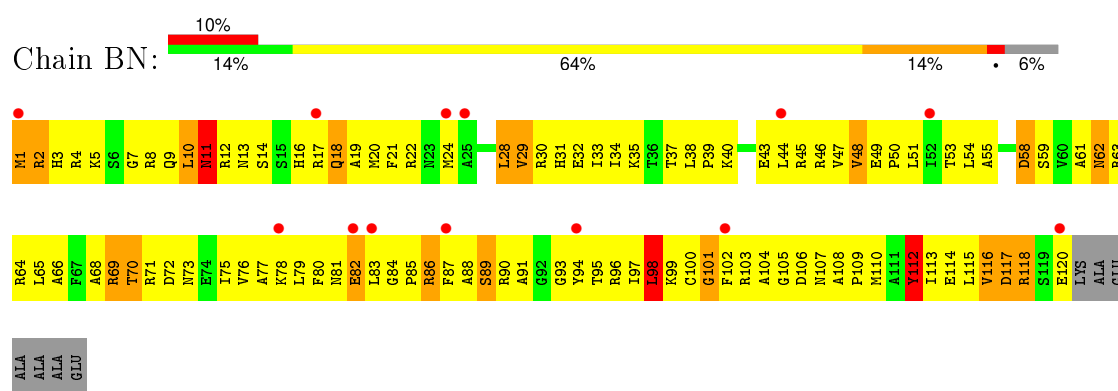
• Molecule 34: 50S ribosomal protein L16



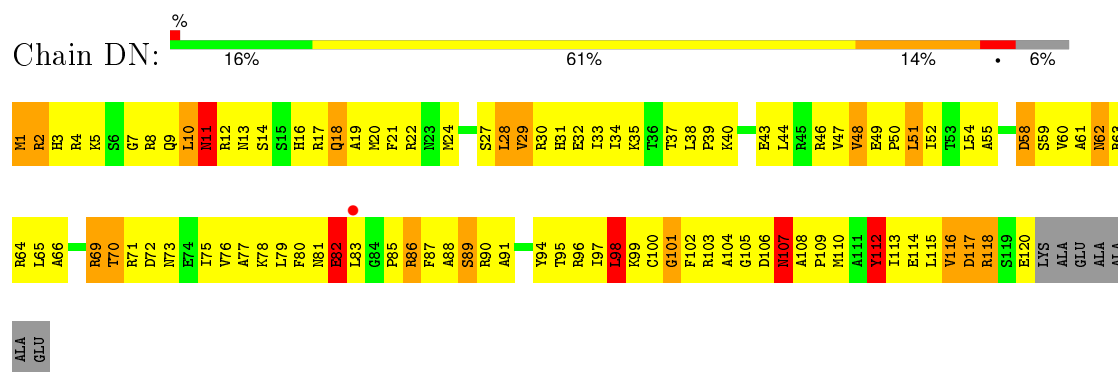
• Molecule 34: 50S ribosomal protein L16



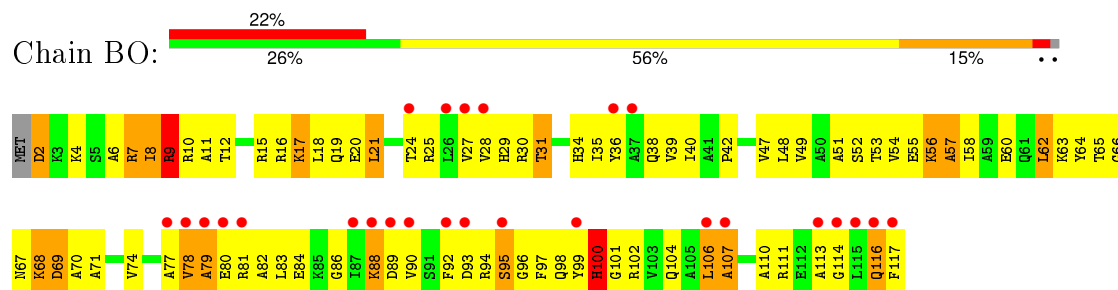
• Molecule 35: 50S ribosomal protein L17



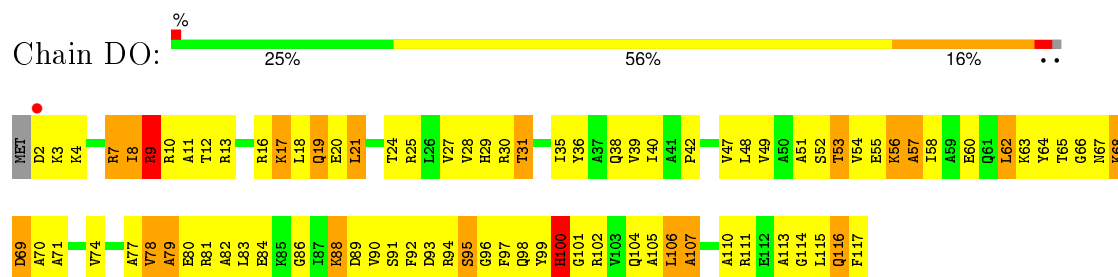
- Molecule 35: 50S ribosomal protein L17



- Molecule 36: 50S ribosomal protein L18

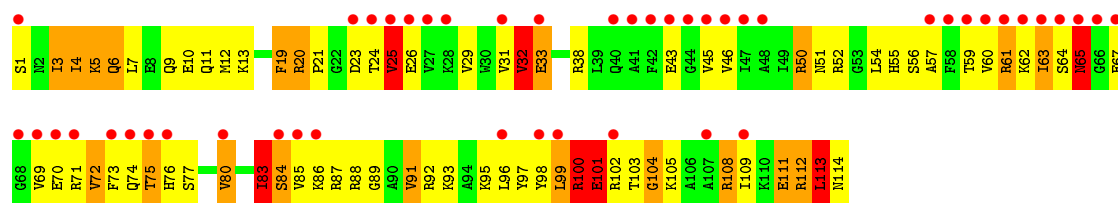


- Molecule 36: 50S ribosomal protein L18

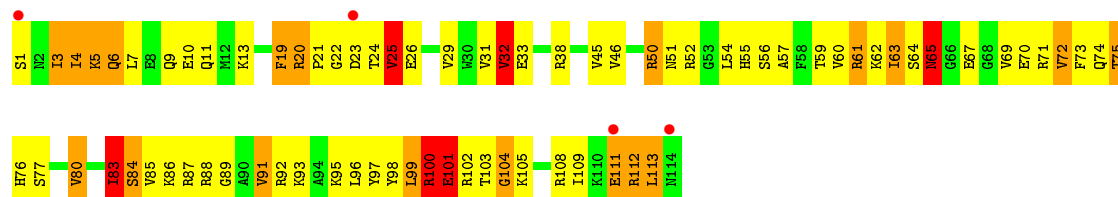


- Molecule 37: 50S ribosomal protein L19

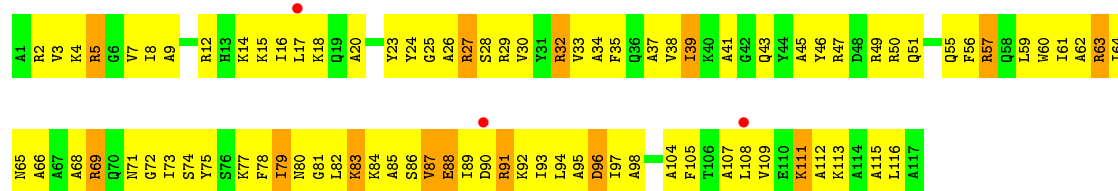




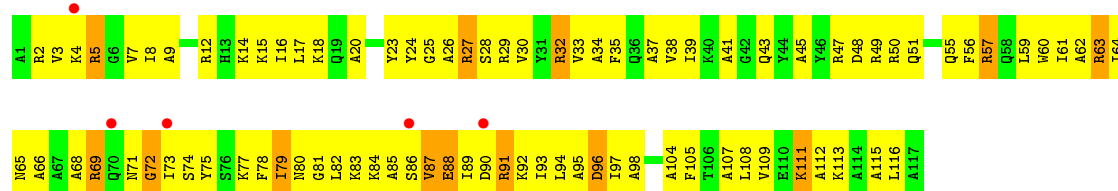
• Molecule 37: 50S ribosomal protein L19



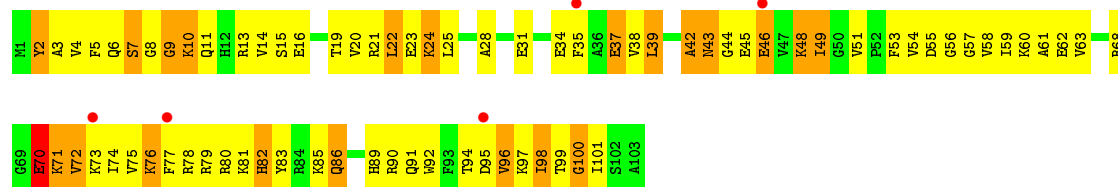
• Molecule 38: 50S ribosomal protein L20



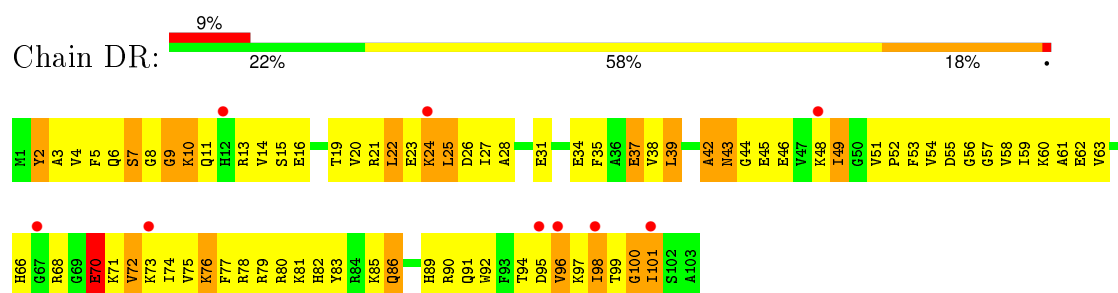
• Molecule 38: 50S ribosomal protein L20



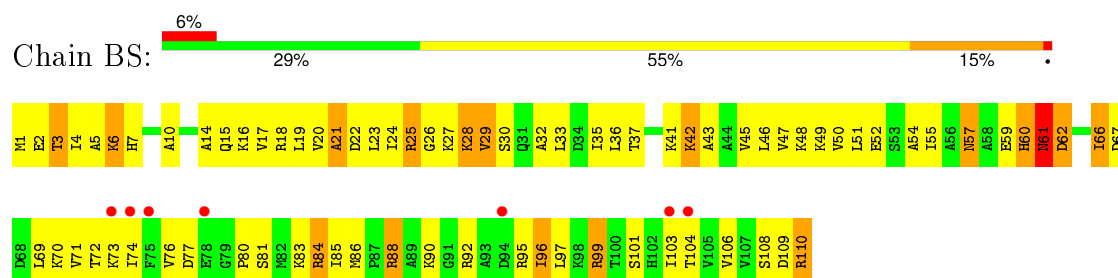
• Molecule 39: 50S ribosomal protein L21



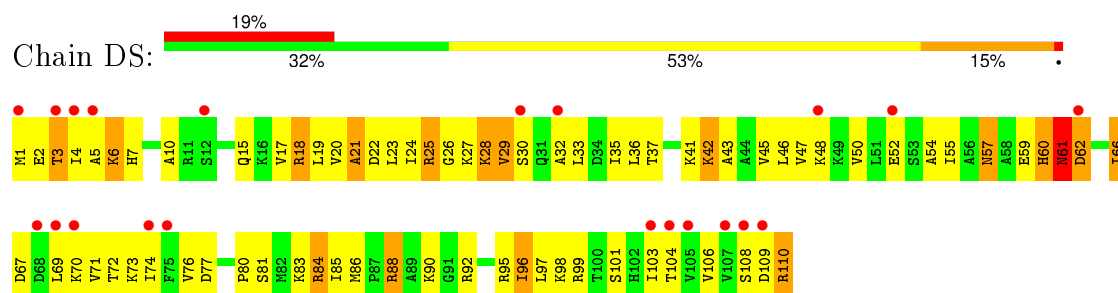
• Molecule 39: 50S ribosomal protein L21



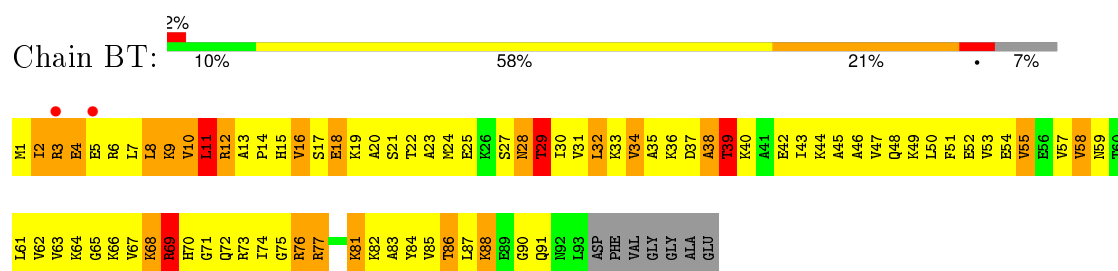
• Molecule 40: 50S ribosomal protein L22



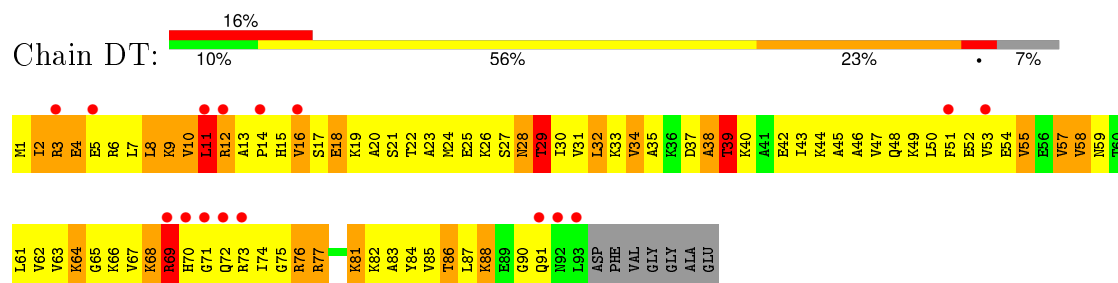
• Molecule 40: 50S ribosomal protein L22



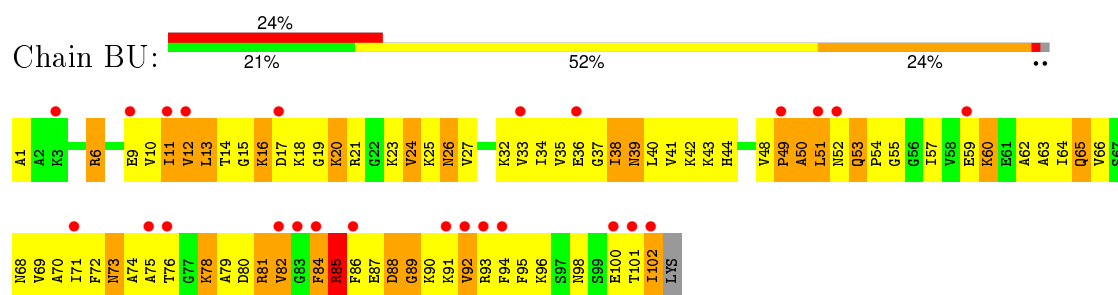
• Molecule 41: 50S ribosomal protein L23



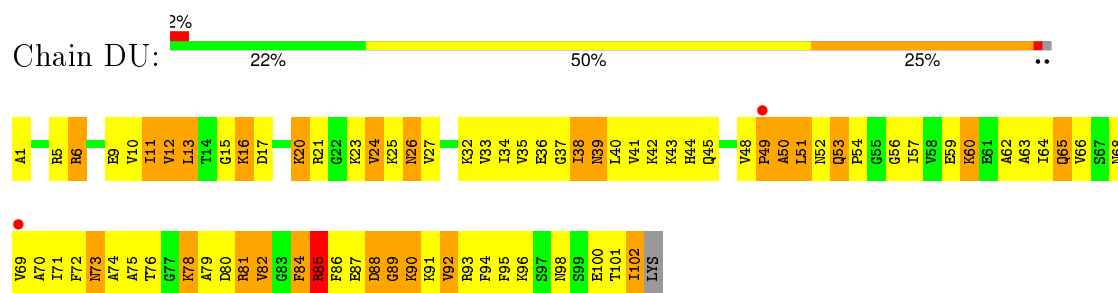
• Molecule 41: 50S ribosomal protein L23



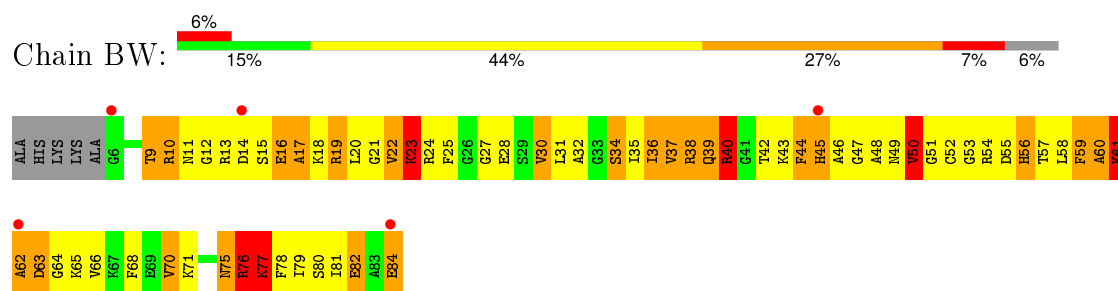
• Molecule 42: 50S ribosomal protein L24



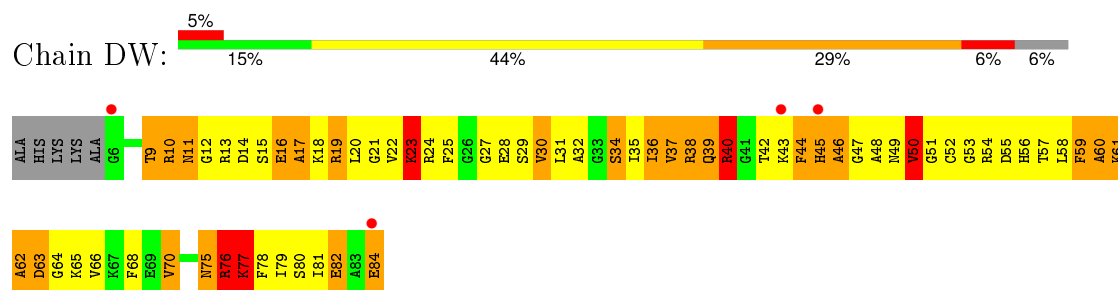
- Molecule 42: 50S ribosomal protein L24



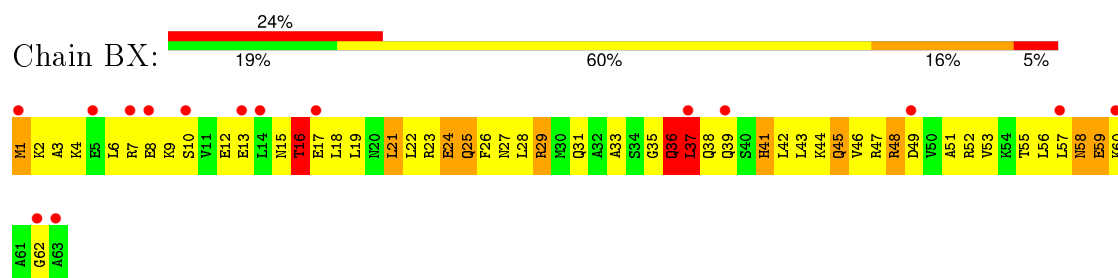
- Molecule 43: 50S ribosomal protein L27



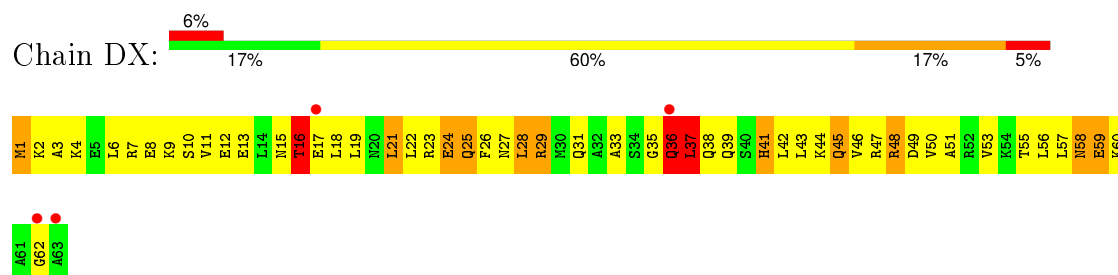
- Molecule 43: 50S ribosomal protein L27



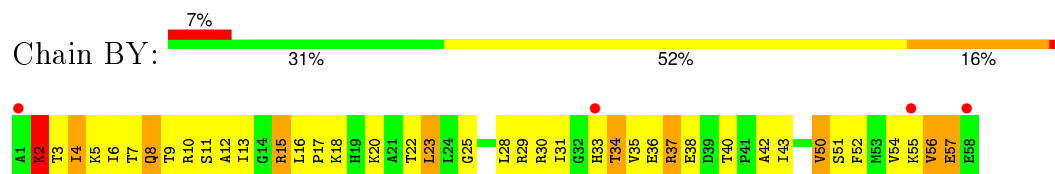
- Molecule 44: 50S ribosomal protein L29



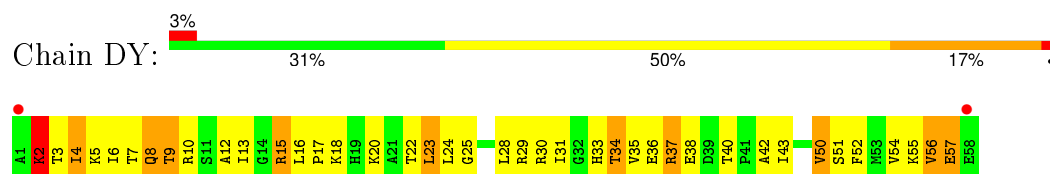
- Molecule 44: 50S ribosomal protein L29



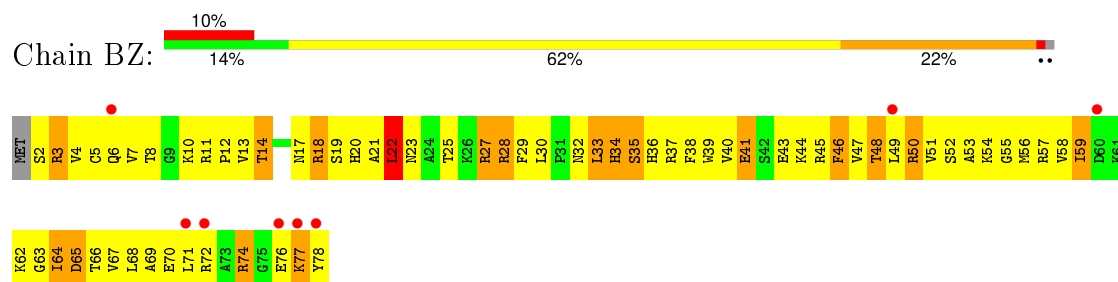
- Molecule 45: 50S ribosomal protein L30



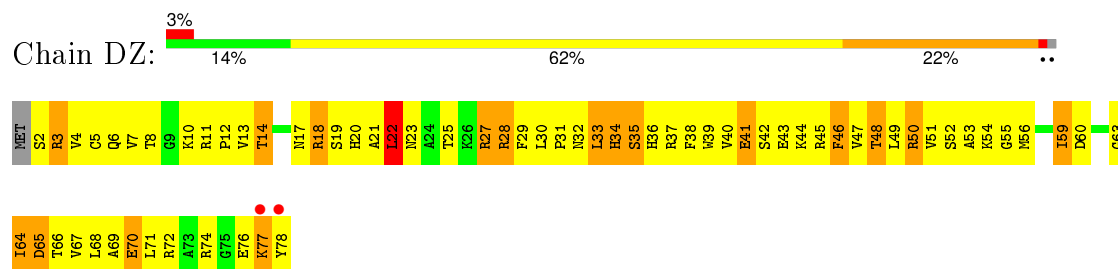
- Molecule 45: 50S ribosomal protein L30



- Molecule 46: 50S ribosomal protein L28



- Molecule 46: 50S ribosomal protein L28

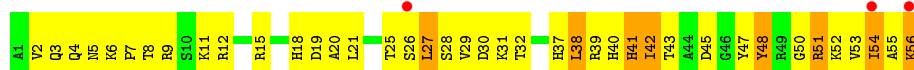


- Molecule 47: 50S ribosomal protein L32





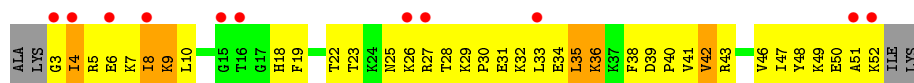
- Molecule 47: 50S ribosomal protein L32



- Molecule 48: 50S ribosomal protein L33



- Molecule 48: 50S ribosomal protein L33



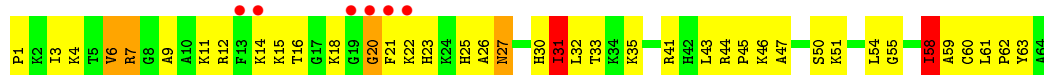
- Molecule 49: 50S ribosomal protein L34



- Molecule 49: 50S ribosomal protein L34

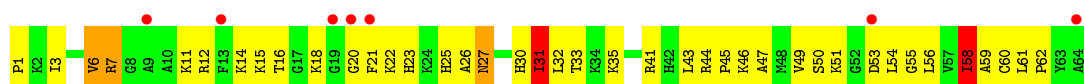


- Molecule 50: 50S ribosomal protein L35



- Molecule 50: 50S ribosomal protein L35





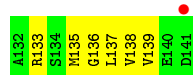
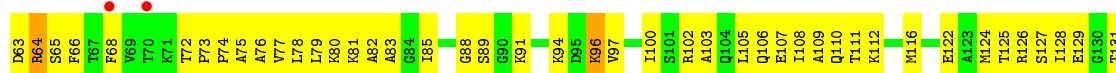
- Molecule 51: 50S ribosomal protein L36



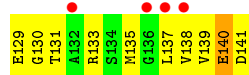
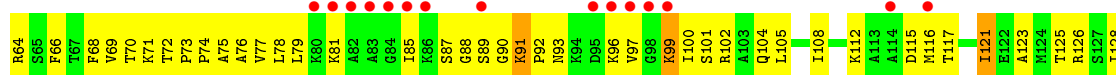
- Molecule 51: 50S ribosomal protein L36



- 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	208.70 Å 379.50 Å 739.30 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.00 – 3.50 137.77 – 3.50	Depositor EDS
% Data completeness (in resolution range)	62.1 (70.00-3.50) 62.3 (137.77-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 3.49 Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.269 , 0.318 0.241 , 0.286	Depositor DCC
R_{free} test set	22227 reflections (5.14%)	DCC
Wilson B-factor (Å ²)	117.9	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 67.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 454411 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	284077	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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%)	0.77	13/57350 (0.0%)
1	CA	0.26	1/36762 (0.0%)	0.77	17/57350 (0.0%)
2	AC	0.23	0/1651	0.44	0/2225
2	CC	0.23	0/1651	0.44	0/2225
3	AD	0.23	0/1665	0.43	0/2227
3	CD	0.23	0/1665	0.43	0/2227
4	AE	0.23	0/1118	0.45	0/1504
4	CE	0.23	0/1118	0.45	0/1504
5	AF	0.24	0/835	0.44	0/1128
5	CF	0.24	0/835	0.44	0/1128
6	AG	0.23	0/1187	0.45	0/1591
6	CG	0.23	0/1211	0.44	0/1624
7	AH	0.23	0/989	0.45	0/1326
7	CH	0.23	0/989	0.45	0/1326
8	AI	0.24	0/1034	0.44	0/1375
8	CI	0.24	0/1034	0.44	0/1375
9	AJ	0.22	0/796	0.47	0/1077
9	CJ	0.22	0/796	0.47	0/1077
10	AK	0.24	0/893	0.46	0/1205
10	CK	0.24	0/893	0.46	0/1205
11	AL	0.22	0/969	0.47	0/1300
11	CL	0.22	0/969	0.47	0/1300
12	AM	0.21	0/892	0.45	0/1193
12	CM	0.21	0/884	0.45	0/1181
13	AN	0.24	0/785	0.43	0/1043
13	CN	0.24	0/785	0.43	0/1043
14	AO	0.22	0/723	0.44	0/966
14	CO	0.22	0/723	0.44	0/966
15	AP	0.25	0/659	0.45	0/884
15	CP	0.25	0/648	0.44	0/870
16	AQ	0.24	0/657	0.46	0/881
16	CQ	0.24	0/665	0.48	0/892

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AR	0.23	0/462	0.44	0/621
17	CR	0.23	0/462	0.44	0/621
18	AS	0.25	0/652	0.45	0/877
18	CS	0.25	0/660	0.46	0/888
19	AT	0.23	0/671	0.41	0/888
19	CT	0.24	0/671	0.41	0/888
20	AB	0.25	0/1735	0.44	0/2338
20	CB	0.25	0/1735	0.44	0/2338
21	AU	0.26	0/430	0.46	0/570
21	CU	0.26	0/430	0.46	0/570
22	BA	0.24	0/2803	0.75	2/4371 (0.0%)
22	DA	0.25	0/2803	0.75	1/4371 (0.0%)
23	BB	0.27	7/68314 (0.0%)	0.78	41/106569 (0.0%)
23	DB	0.28	7/68314 (0.0%)	0.78	49/106569 (0.0%)
24	BV	0.25	0/766	0.43	0/1025
24	DV	0.25	0/766	0.43	0/1025
25	BC	0.22	0/2121	0.47	0/2852
25	DC	0.22	0/2121	0.47	0/2852
26	BD	0.24	0/1586	0.46	0/2134
26	DD	0.24	0/1586	0.47	0/2134
27	BE	0.23	0/1571	0.49	0/2113
27	DE	0.24	0/1571	0.49	0/2113
28	BF	0.26	0/1444	0.51	0/1937
28	DF	0.26	0/1444	0.51	0/1937
29	BG	0.23	0/1343	0.46	0/1816
29	DG	0.23	0/1343	0.46	0/1816
30	BH	0.25	0/1122	0.46	0/1515
30	DH	0.25	0/1122	0.46	0/1515
31	BJ	0.23	0/1152	0.47	0/1551
31	DJ	0.23	0/1152	0.47	0/1551
32	BK	0.24	0/939	0.52	0/1258
32	DK	0.23	0/939	0.52	0/1258
33	BL	0.23	0/1054	0.47	0/1403
33	DL	0.23	0/1054	0.47	0/1403
34	BM	0.25	0/1093	0.47	0/1460
34	DM	0.25	0/1093	0.47	0/1460
35	BN	0.24	0/973	0.51	0/1301
35	DN	0.24	0/973	0.51	0/1301
36	BO	0.23	0/902	0.47	0/1209
36	DO	0.23	0/902	0.48	0/1209
37	BP	0.24	0/929	0.48	0/1242
37	DP	0.24	0/929	0.48	0/1242
38	BQ	0.25	0/960	0.46	0/1278

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DQ	0.25	0/960	0.46	0/1278
39	BR	0.25	0/829	0.48	0/1107
39	DR	0.25	0/829	0.48	0/1107
40	BS	0.22	0/864	0.49	0/1156
40	DS	0.22	0/864	0.49	0/1156
41	BT	0.23	0/744	0.52	0/994
41	DT	0.23	0/744	0.52	0/994
42	BU	0.25	0/787	0.45	0/1051
42	DU	0.25	0/787	0.45	0/1051
43	BW	0.28	0/603	0.48	0/797
43	DW	0.27	0/603	0.48	0/797
44	BX	0.23	0/510	0.51	0/677
44	DX	0.23	0/510	0.51	0/677
45	BY	0.23	0/453	0.49	0/605
45	DY	0.23	0/453	0.49	0/605
46	BZ	0.25	0/635	0.51	0/848
46	DZ	0.25	0/635	0.51	0/848
47	B0	0.22	0/450	0.52	0/599
47	D0	0.22	0/450	0.52	0/599
48	B1	0.27	0/416	0.47	0/554
48	D1	0.27	0/416	0.47	0/554
49	B2	0.25	0/380	0.49	0/498
49	D2	0.26	0/380	0.49	0/498
50	B3	0.24	0/513	0.46	0/676
50	D3	0.24	0/513	0.46	0/676
51	B4	0.22	0/303	0.46	0/397
51	D4	0.22	0/303	0.46	0/397
52	BI	0.24	0/1046	0.46	0/1410
52	DI	0.25	0/1046	0.47	0/1410
All	All	0.26	16/306361 (0.0%)	0.70	123/457973 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	13
1	CA	0	13
23	BB	0	36
23	DB	0	38
All	All	0	100

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	DB	1086	A	C5-C6	-16.14	1.26	1.41
23	BB	1086	A	C5-C6	-16.11	1.26	1.41
23	BB	1088	A	C6-N1	-10.49	1.28	1.35
23	DB	1088	A	C6-N1	-10.45	1.28	1.35
23	DB	1060	U	C2-N3	7.89	1.43	1.37

The worst 5 of 123 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	BB	2791	G	O5'-P-OP1	-31.87	72.45	110.70
23	DB	2791	G	O5'-P-OP2	-31.41	73.01	110.70
23	DB	2204	G	O5'-P-OP1	-29.65	75.12	110.70
1	AA	1213	A	O5'-P-OP2	-29.58	75.21	110.70
23	BB	2204	G	O5'-P-OP2	-28.34	76.69	110.70

There are no chirality outliers.

5 of 100 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	187	G	Sidechain
1	AA	281	G	Sidechain
1	AA	324	G	Sidechain
1	AA	437	U	Sidechain
1	AA	83	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	1355	0
1	CA	32831	0	16521	1385	0
2	AC	1624	0	1699	137	0
2	CC	1624	0	1699	145	0
3	AD	1643	0	1710	166	0
3	CD	1643	0	1710	156	0
4	AE	1105	0	1148	105	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	CE	1105	0	1148	115	0
5	AF	817	0	808	98	0
5	CF	817	0	808	88	0
6	AG	1174	0	1230	118	0
6	CG	1196	0	1246	110	0
7	AH	979	0	1034	93	0
7	CH	979	0	1034	93	0
8	AI	1022	0	1070	153	0
8	CI	1022	0	1070	151	0
9	AJ	786	0	828	78	0
9	CJ	786	0	828	84	0
10	AK	877	0	887	100	0
10	CK	877	0	887	101	0
11	AL	955	0	1019	90	0
11	CL	955	0	1019	94	0
12	AM	883	0	944	110	0
12	CM	876	0	937	109	0
13	AN	774	0	827	96	0
13	CN	774	0	827	90	0
14	AO	715	0	742	48	0
14	CO	715	0	742	41	0
15	AP	649	0	666	53	0
15	CP	638	0	656	55	0
16	AQ	648	0	691	73	0
16	CQ	656	0	702	73	0
17	AR	455	0	478	34	0
17	CR	455	0	478	34	0
18	AS	637	0	665	101	0
18	CS	644	0	675	98	0
19	AT	665	0	714	49	0
19	CT	665	0	714	49	0
20	AB	1704	0	1732	205	0
20	CB	1704	0	1732	208	0
21	AU	425	0	449	75	0
21	CU	425	0	449	68	0
22	BA	2507	0	1270	109	0
22	DA	2507	0	1270	111	0
23	BB	60995	0	30678	2412	0
23	DB	60995	0	30677	2498	0
24	BV	753	0	780	89	0
24	DV	753	0	780	90	0
25	BC	2082	0	2157	261	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	DC	2082	0	2157	274	0
26	BD	1565	0	1616	216	0
26	DD	1565	0	1616	220	0
27	BE	1552	0	1619	180	0
27	DE	1552	0	1619	170	0
28	BF	1420	0	1460	236	0
28	DF	1420	0	1460	238	0
29	BG	1323	0	1374	163	0
29	DG	1323	0	1374	161	0
30	BH	1111	0	1148	176	0
30	DH	1111	0	1148	146	0
31	BJ	1129	0	1162	150	0
31	DJ	1129	0	1162	154	0
32	BK	930	0	1000	122	0
32	DK	930	0	1000	134	0
33	BL	1045	0	1117	150	0
33	DL	1045	0	1117	155	0
34	BM	1074	0	1157	114	0
34	DM	1074	0	1157	112	0
35	BN	960	0	1000	135	0
35	DN	960	0	1000	129	0
36	BO	892	0	923	97	0
36	DO	892	0	923	104	0
37	BP	917	0	965	112	0
37	DP	917	0	965	113	0
38	BQ	947	0	1022	156	0
38	DQ	947	0	1022	167	0
39	BR	816	0	839	123	0
39	DR	816	0	839	138	0
40	BS	857	0	922	93	0
40	DS	857	0	922	93	0
41	BT	738	0	807	127	0
41	DT	738	0	807	122	0
42	BU	779	0	834	132	0
42	DU	779	0	834	121	0
43	BW	596	0	610	128	0
43	DW	596	0	610	137	0
44	BX	509	0	543	54	0
44	DX	509	0	543	50	0
45	BY	449	0	491	48	0
45	DY	449	0	491	50	0
46	BZ	625	0	652	89	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	DZ	625	0	652	92	0
47	B0	444	0	461	40	0
47	D0	444	0	461	42	0
48	B1	409	0	440	57	0
48	D1	409	0	440	44	0
49	B2	377	0	418	43	0
49	D2	377	0	418	43	0
50	B3	504	0	574	40	0
50	D3	504	0	574	40	0
51	B4	302	0	340	40	0
51	D4	302	0	340	35	0
52	BI	1032	0	1088	111	0
52	DI	1032	0	1088	182	0
53	AA	58	0	0	0	0
53	AE	1	0	0	0	0
53	AN	1	0	0	0	0
53	BB	110	0	0	0	0
53	CA	61	0	0	0	0
53	CE	1	0	0	0	0
53	DB	111	0	0	0	0
54	AA	36	0	37	2	0
54	CA	36	0	37	1	0
55	B4	1	0	0	0	0
55	D4	1	0	0	0	0
56	AA	282	0	0	4	0
56	AE	4	0	0	0	0
56	AK	2	0	0	0	0
56	AL	5	0	0	0	0
56	AN	4	0	0	0	0
56	AT	3	0	0	0	0
56	B2	1	0	0	0	0
56	BB	492	0	0	5	0
56	BC	8	0	0	0	0
56	BD	1	0	0	0	0
56	BE	2	0	0	0	0
56	BH	1	0	0	0	0
56	BL	2	0	0	0	0
56	CA	294	0	0	0	0
56	CE	4	0	0	0	0
56	CI	1	0	0	0	0
56	CK	1	0	0	0	0
56	CL	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	CN	3	0	0	0	0
56	CT	1	0	0	0	0
56	D2	1	0	0	0	0
56	DB	499	0	0	8	0
56	DC	5	0	0	0	0
56	DD	1	0	0	0	0
56	DE	1	0	0	0	0
56	DL	5	0	0	1	0
56	DP	1	0	0	0	0
All	All	284077	0	190751	17232	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 36.

The worst 5 of 17232 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:DB:1099:G:H8	52:DI:3:LYS:N	1.38	1.20
23:BB:855:G:H21	43:BW:23:LYS:HG2	1.08	1.15
42:DU:85:ARG:HD3	42:DU:86:PHE:H	1.13	1.14
41:DT:5:GLU:HA	41:DT:8:LEU:HB2	1.25	1.13
42:BU:85:ARG:HD3	42:BU:86:PHE:H	1.11	1.12

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	AC	204/232 (88%)	147 (72%)	40 (20%)	17 (8%)	1 13
2	CC	204/232 (88%)	148 (72%)	40 (20%)	16 (8%)	1 14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AD	203/205 (99%)	136 (67%)	52 (26%)	15 (7%)	1	16
3	CD	203/205 (99%)	134 (66%)	54 (27%)	15 (7%)	1	16
4	AE	148/166 (89%)	117 (79%)	27 (18%)	4 (3%)	6	44
4	CE	148/166 (89%)	117 (79%)	25 (17%)	6 (4%)	3	33
5	AF	98/135 (73%)	66 (67%)	21 (21%)	11 (11%)	0	7
5	CF	98/135 (73%)	67 (68%)	21 (21%)	10 (10%)	1	9
6	AG	148/178 (83%)	122 (82%)	18 (12%)	8 (5%)	2	25
6	CG	150/178 (84%)	124 (83%)	20 (13%)	6 (4%)	4	33
7	AH	127/129 (98%)	92 (72%)	26 (20%)	9 (7%)	1	17
7	CH	127/129 (98%)	90 (71%)	28 (22%)	9 (7%)	1	17
8	AI	125/129 (97%)	88 (70%)	29 (23%)	8 (6%)	2	20
8	CI	125/129 (97%)	88 (70%)	29 (23%)	8 (6%)	2	20
9	AJ	96/103 (93%)	69 (72%)	17 (18%)	10 (10%)	1	8
9	CJ	96/103 (93%)	68 (71%)	18 (19%)	10 (10%)	1	8
10	AK	115/128 (90%)	81 (70%)	26 (23%)	8 (7%)	1	18
10	CK	115/128 (90%)	80 (70%)	27 (24%)	8 (7%)	1	18
11	AL	121/123 (98%)	78 (64%)	29 (24%)	14 (12%)	0	7
11	CL	121/123 (98%)	79 (65%)	28 (23%)	14 (12%)	0	7
12	AM	112/117 (96%)	72 (64%)	36 (32%)	4 (4%)	4	37
12	CM	111/117 (95%)	69 (62%)	38 (34%)	4 (4%)	4	37
13	AN	92/100 (92%)	57 (62%)	25 (27%)	10 (11%)	0	8
13	CN	92/100 (92%)	56 (61%)	26 (28%)	10 (11%)	0	8
14	AO	86/89 (97%)	65 (76%)	16 (19%)	5 (6%)	2	23
14	CO	86/89 (97%)	65 (76%)	16 (19%)	5 (6%)	2	23
15	AP	80/82 (98%)	56 (70%)	15 (19%)	9 (11%)	0	7
15	CP	78/82 (95%)	53 (68%)	15 (19%)	10 (13%)	0	5
16	AQ	78/83 (94%)	56 (72%)	17 (22%)	5 (6%)	2	20
16	CQ	79/83 (95%)	56 (71%)	17 (22%)	6 (8%)	1	15
17	AR	53/74 (72%)	41 (77%)	10 (19%)	2 (4%)	4	35
17	CR	53/74 (72%)	41 (77%)	10 (19%)	2 (4%)	4	35
18	AS	77/91 (85%)	58 (75%)	17 (22%)	2 (3%)	7	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	CS	78/91 (86%)	58 (74%)	18 (23%)	2 (3%)	7	45
19	AT	83/86 (96%)	59 (71%)	19 (23%)	5 (6%)	2	21
19	CT	83/86 (96%)	59 (71%)	19 (23%)	5 (6%)	2	21
20	AB	216/240 (90%)	143 (66%)	53 (24%)	20 (9%)	1	11
20	CB	216/240 (90%)	148 (68%)	46 (21%)	22 (10%)	1	9
21	AU	49/71 (69%)	28 (57%)	14 (29%)	7 (14%)	0	4
21	CU	49/71 (69%)	28 (57%)	14 (29%)	7 (14%)	0	4
24	BV	92/94 (98%)	63 (68%)	23 (25%)	6 (6%)	1	20
24	DV	92/94 (98%)	62 (67%)	24 (26%)	6 (6%)	1	20
25	BC	269/273 (98%)	158 (59%)	65 (24%)	46 (17%)	0	3
25	DC	269/273 (98%)	158 (59%)	65 (24%)	46 (17%)	0	3
26	BD	207/209 (99%)	121 (58%)	56 (27%)	30 (14%)	0	4
26	DD	207/209 (99%)	123 (59%)	52 (25%)	32 (16%)	0	3
27	BE	199/201 (99%)	120 (60%)	56 (28%)	23 (12%)	0	7
27	DE	199/201 (99%)	120 (60%)	56 (28%)	23 (12%)	0	7
28	BF	176/178 (99%)	103 (58%)	39 (22%)	34 (19%)	0	2
28	DF	176/178 (99%)	101 (57%)	41 (23%)	34 (19%)	0	2
29	BG	174/176 (99%)	105 (60%)	37 (21%)	32 (18%)	0	2
29	DG	174/176 (99%)	105 (60%)	36 (21%)	33 (19%)	0	2
30	BH	147/149 (99%)	68 (46%)	43 (29%)	36 (24%)	0	1
30	DH	147/149 (99%)	88 (60%)	32 (22%)	27 (18%)	0	2
31	BJ	140/142 (99%)	85 (61%)	39 (28%)	16 (11%)	0	7
31	DJ	140/142 (99%)	83 (59%)	40 (29%)	17 (12%)	0	6
32	BK	119/123 (97%)	70 (59%)	28 (24%)	21 (18%)	0	2
32	DK	119/123 (97%)	69 (58%)	27 (23%)	23 (19%)	0	2
33	BL	141/144 (98%)	75 (53%)	40 (28%)	26 (18%)	0	2
33	DL	141/144 (98%)	75 (53%)	40 (28%)	26 (18%)	0	2
34	BM	134/136 (98%)	77 (58%)	38 (28%)	19 (14%)	0	4
34	DM	134/136 (98%)	78 (58%)	35 (26%)	21 (16%)	0	3
35	BN	118/127 (93%)	73 (62%)	33 (28%)	12 (10%)	1	9
35	DN	118/127 (93%)	73 (62%)	32 (27%)	13 (11%)	0	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	BO	114/117 (97%)	83 (73%)	21 (18%)	10 (9%)	1	12
36	DO	114/117 (97%)	83 (73%)	20 (18%)	11 (10%)	1	10
37	BP	112/114 (98%)	59 (53%)	35 (31%)	18 (16%)	0	3
37	DP	112/114 (98%)	58 (52%)	36 (32%)	18 (16%)	0	3
38	BQ	115/117 (98%)	79 (69%)	27 (24%)	9 (8%)	1	14
38	DQ	115/117 (98%)	75 (65%)	32 (28%)	8 (7%)	1	18
39	BR	101/103 (98%)	60 (59%)	31 (31%)	10 (10%)	1	10
39	DR	101/103 (98%)	61 (60%)	29 (29%)	11 (11%)	0	8
40	BS	108/110 (98%)	75 (69%)	21 (19%)	12 (11%)	0	7
40	DS	108/110 (98%)	75 (69%)	20 (18%)	13 (12%)	0	6
41	BT	91/100 (91%)	47 (52%)	25 (28%)	19 (21%)	0	1
41	DT	91/100 (91%)	47 (52%)	23 (25%)	21 (23%)	0	1
42	BU	100/103 (97%)	53 (53%)	35 (35%)	12 (12%)	0	6
42	DU	100/103 (97%)	51 (51%)	35 (35%)	14 (14%)	0	4
43	BW	77/84 (92%)	29 (38%)	23 (30%)	25 (32%)	0	0
43	DW	77/84 (92%)	29 (38%)	22 (29%)	26 (34%)	0	0
44	BX	61/63 (97%)	37 (61%)	14 (23%)	10 (16%)	0	3
44	DX	61/63 (97%)	37 (61%)	14 (23%)	10 (16%)	0	3
45	BY	56/58 (97%)	40 (71%)	11 (20%)	5 (9%)	1	11
45	DY	56/58 (97%)	40 (71%)	11 (20%)	5 (9%)	1	11
46	BZ	75/78 (96%)	47 (63%)	20 (27%)	8 (11%)	0	8
46	DZ	75/78 (96%)	48 (64%)	19 (25%)	8 (11%)	0	8
47	B0	54/56 (96%)	33 (61%)	16 (30%)	5 (9%)	1	11
47	D0	54/56 (96%)	33 (61%)	16 (30%)	5 (9%)	1	11
48	B1	48/54 (89%)	34 (71%)	12 (25%)	2 (4%)	3	32
48	D1	48/54 (89%)	34 (71%)	12 (25%)	2 (4%)	3	32
49	B2	44/46 (96%)	31 (70%)	9 (20%)	4 (9%)	1	11
49	D2	44/46 (96%)	30 (68%)	8 (18%)	6 (14%)	0	4
50	B3	62/64 (97%)	41 (66%)	15 (24%)	6 (10%)	1	10
50	D3	62/64 (97%)	42 (68%)	14 (23%)	6 (10%)	1	10
51	B4	36/38 (95%)	21 (58%)	10 (28%)	5 (14%)	0	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	D4	36/38 (95%)	21 (58%)	9 (25%)	6 (17%)	0	3
52	BI	139/141 (99%)	119 (86%)	16 (12%)	4 (3%)	6	42
52	DI	139/141 (99%)	115 (83%)	19 (14%)	5 (4%)	4	37
All	All	11241/11918 (94%)	7279 (65%)	2673 (24%)	1289 (12%)	0	7

5 of 1289 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AC	112	ALA
2	AC	180	ASP
2	AC	205	GLU
4	AE	20	VAL
5	AF	98	GLU

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%)	144 (85%)	26 (15%)	3	21
2	CC	170/189 (90%)	145 (85%)	25 (15%)	4	22
3	AD	172/172 (100%)	148 (86%)	24 (14%)	4	24
3	CD	172/172 (100%)	149 (87%)	23 (13%)	5	26
4	AE	113/125 (90%)	100 (88%)	13 (12%)	7	33
4	CE	113/125 (90%)	98 (87%)	15 (13%)	5	26
5	AF	87/116 (75%)	76 (87%)	11 (13%)	5	28
5	CF	87/116 (75%)	75 (86%)	12 (14%)	4	25
6	AG	123/146 (84%)	108 (88%)	15 (12%)	6	29
6	CG	125/146 (86%)	108 (86%)	17 (14%)	5	26
7	AH	104/104 (100%)	96 (92%)	8 (8%)	16	54
7	CH	104/104 (100%)	96 (92%)	8 (8%)	16	54
8	AI	105/106 (99%)	94 (90%)	11 (10%)	8	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	CI	105/106 (99%)	93 (89%)	12 (11%)	7	33
9	AJ	86/90 (96%)	79 (92%)	7 (8%)	15	52
9	CJ	86/90 (96%)	80 (93%)	6 (7%)	19	59
10	AK	90/98 (92%)	77 (86%)	13 (14%)	4	23
10	CK	90/98 (92%)	77 (86%)	13 (14%)	4	23
11	AL	103/103 (100%)	85 (82%)	18 (18%)	2	14
11	CL	103/103 (100%)	84 (82%)	19 (18%)	2	11
12	AM	92/95 (97%)	82 (89%)	10 (11%)	8	37
12	CM	91/95 (96%)	82 (90%)	9 (10%)	10	41
13	AN	79/83 (95%)	67 (85%)	12 (15%)	3	21
13	CN	79/83 (95%)	67 (85%)	12 (15%)	3	21
14	AO	76/77 (99%)	69 (91%)	7 (9%)	11	45
14	CO	76/77 (99%)	70 (92%)	6 (8%)	15	53
15	AP	65/65 (100%)	57 (88%)	8 (12%)	6	29
15	CP	65/65 (100%)	57 (88%)	8 (12%)	6	29
16	AQ	74/77 (96%)	65 (88%)	9 (12%)	6	29
16	CQ	75/77 (97%)	65 (87%)	10 (13%)	5	26
17	AR	48/64 (75%)	46 (96%)	2 (4%)	36	74
17	CR	48/64 (75%)	46 (96%)	2 (4%)	36	74
18	AS	70/78 (90%)	52 (74%)	18 (26%)	0	4
18	CS	71/78 (91%)	53 (75%)	18 (25%)	1	4
19	AT	65/65 (100%)	53 (82%)	12 (18%)	2	11
19	CT	65/65 (100%)	53 (82%)	12 (18%)	2	11
20	AB	180/198 (91%)	152 (84%)	28 (16%)	3	20
20	CB	180/198 (91%)	150 (83%)	30 (17%)	3	16
21	AU	44/61 (72%)	35 (80%)	9 (20%)	1	8
21	CU	44/61 (72%)	35 (80%)	9 (20%)	1	8
24	BV	78/78 (100%)	68 (87%)	10 (13%)	5	28
24	DV	78/78 (100%)	69 (88%)	9 (12%)	7	33
25	BC	216/218 (99%)	178 (82%)	38 (18%)	2	13
25	DC	216/218 (99%)	175 (81%)	41 (19%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	BD	164/164 (100%)	140 (85%)	24 (15%)	4	22
26	DD	164/164 (100%)	140 (85%)	24 (15%)	4	22
27	BE	165/165 (100%)	146 (88%)	19 (12%)	7	33
27	DE	165/165 (100%)	146 (88%)	19 (12%)	7	33
28	BF	149/149 (100%)	114 (76%)	35 (24%)	1	5
28	DF	149/149 (100%)	115 (77%)	34 (23%)	1	6
29	BG	137/137 (100%)	116 (85%)	21 (15%)	3	21
29	DG	137/137 (100%)	116 (85%)	21 (15%)	3	21
30	BH	114/114 (100%)	77 (68%)	37 (32%)	0	2
30	DH	114/114 (100%)	93 (82%)	21 (18%)	2	11
31	BJ	116/116 (100%)	98 (84%)	18 (16%)	3	20
31	DJ	116/116 (100%)	98 (84%)	18 (16%)	3	20
32	BK	102/104 (98%)	79 (78%)	23 (22%)	1	6
32	DK	102/104 (98%)	79 (78%)	23 (22%)	1	6
33	BL	102/103 (99%)	89 (87%)	13 (13%)	5	28
33	DL	102/103 (99%)	90 (88%)	12 (12%)	6	31
34	BM	109/109 (100%)	88 (81%)	21 (19%)	2	10
34	DM	109/109 (100%)	88 (81%)	21 (19%)	2	10
35	BN	100/103 (97%)	82 (82%)	18 (18%)	2	12
35	DN	100/103 (97%)	81 (81%)	19 (19%)	2	10
36	BO	86/87 (99%)	69 (80%)	17 (20%)	1	9
36	DO	86/87 (99%)	69 (80%)	17 (20%)	1	9
37	BP	99/99 (100%)	80 (81%)	19 (19%)	2	10
37	DP	99/99 (100%)	81 (82%)	18 (18%)	2	12
38	BQ	89/89 (100%)	79 (89%)	10 (11%)	7	35
38	DQ	89/89 (100%)	79 (89%)	10 (11%)	7	35
39	BR	84/84 (100%)	68 (81%)	16 (19%)	2	10
39	DR	84/84 (100%)	70 (83%)	14 (17%)	3	16
40	BS	93/93 (100%)	81 (87%)	12 (13%)	5	27
40	DS	93/93 (100%)	82 (88%)	11 (12%)	6	31
41	BT	80/84 (95%)	62 (78%)	18 (22%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	DT	80/84 (95%)	62 (78%)	18 (22%)	1	6
42	BU	83/84 (99%)	67 (81%)	16 (19%)	2	10
42	DU	83/84 (99%)	67 (81%)	16 (19%)	2	10
43	BW	59/62 (95%)	42 (71%)	17 (29%)	0	3
43	DW	59/62 (95%)	42 (71%)	17 (29%)	0	3
44	BX	55/55 (100%)	42 (76%)	13 (24%)	1	5
44	DX	55/55 (100%)	42 (76%)	13 (24%)	1	5
45	BY	48/48 (100%)	40 (83%)	8 (17%)	3	16
45	DY	48/48 (100%)	40 (83%)	8 (17%)	3	16
46	BZ	67/68 (98%)	54 (81%)	13 (19%)	2	10
46	DZ	67/68 (98%)	53 (79%)	14 (21%)	1	8
47	B0	47/47 (100%)	39 (83%)	8 (17%)	2	15
47	D0	47/47 (100%)	40 (85%)	7 (15%)	4	22
48	B1	45/48 (94%)	40 (89%)	5 (11%)	8	35
48	D1	45/48 (94%)	41 (91%)	4 (9%)	12	47
49	B2	38/38 (100%)	32 (84%)	6 (16%)	3	19
49	D2	38/38 (100%)	32 (84%)	6 (16%)	3	19
50	B3	51/51 (100%)	46 (90%)	5 (10%)	10	42
50	D3	51/51 (100%)	46 (90%)	5 (10%)	10	42
51	B4	34/34 (100%)	32 (94%)	2 (6%)	24	65
51	D4	34/34 (100%)	32 (94%)	2 (6%)	24	65
52	BI	109/109 (100%)	108 (99%)	1 (1%)	84	94
52	DI	109/109 (100%)	103 (94%)	6 (6%)	27	67
All	All	9333/9704 (96%)	7895 (85%)	1438 (15%)	3	20

5 of 1438 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
43	BW	38	ARG
6	CG	49	LEU
41	DT	24	MET
44	BX	28	LEU
2	CC	35	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 346 such sidechains are listed below:

Mol	Chain	Res	Type
44	BX	25	GLN
6	CG	129	ASN
42	DU	26	ASN
45	BY	48	ASN
2	CC	7	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1529/1542 (99%)	257 (16%)	27 (1%)
1	CA	1529/1542 (99%)	240 (15%)	27 (1%)
22	BA	116/120 (96%)	22 (18%)	0
22	DA	116/120 (96%)	22 (18%)	0
23	BB	2837/2904 (97%)	460 (16%)	17 (0%)
23	DB	2837/2904 (97%)	460 (16%)	21 (0%)
All	All	8964/9132 (98%)	1461 (16%)	92 (1%)

5 of 1461 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	9	G
1	AA	14	U
1	AA	32	A
1	AA	39	G

5 of 92 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	BB	2756	U
1	CA	372	C
23	DB	2282	G
23	BB	2808	G
1	CA	243	A

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 347 ligands modelled in this entry, 345 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
54	HYG	AA	2059	-	35,39,39	1.30	3 (8%)	41,60,60	1.49	5 (12%)
54	HYG	CA	2062	-	35,39,39	1.33	4 (11%)	41,60,60	1.49	5 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	HYG	AA	2059	-	-	0/12/87/87	0/4/4/4
54	HYG	CA	2062	-	-	0/12/87/87	0/4/4/4

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	CA	2062	HYG	O22-C17	-2.35	1.38	1.43
54	AA	2059	HYG	C16-C15	2.10	1.57	1.53
54	CA	2062	HYG	C16-C15	2.15	1.57	1.53
54	CA	2062	HYG	C27-C33	2.60	1.56	1.52
54	AA	2059	HYG	C27-C33	2.62	1.56	1.52

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	CA	2062	HYG	O8-C1-C2	-4.36	101.78	109.87
54	AA	2059	HYG	O8-C1-C2	-4.34	101.81	109.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	CA	2062	HYG	O35-C34-C33	-3.60	103.94	111.53
54	AA	2059	HYG	O35-C34-C33	-3.59	103.97	111.53
54	AA	2059	HYG	C26-C25-C24	-2.20	108.22	111.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	AA	2059	HYG	2	0
54	CA	2062	HYG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1530/1542 (99%)	-0.65	7 (0%) 91 88	16, 85, 158, 180	0
1	CA	1530/1542 (99%)	-0.67	5 (0%) 94 91	8, 57, 142, 180	0
2	AC	206/232 (88%)	0.86	30 (14%) 3 3	8, 89, 145, 180	0
2	CC	206/232 (88%)	0.33	16 (7%) 16 13	15, 81, 138, 180	0
3	AD	205/205 (100%)	0.65	26 (12%) 5 5	19, 97, 160, 180	0
3	CD	205/205 (100%)	-0.01	4 (1%) 68 59	5, 63, 135, 180	0
4	AE	150/166 (90%)	0.18	5 (3%) 50 41	5, 76, 136, 167	0
4	CE	150/166 (90%)	0.87	24 (16%) 3 3	5, 62, 135, 175	0
5	AF	100/135 (74%)	1.20	27 (27%) 1 1	13, 81, 137, 180	0
5	CF	100/135 (74%)	0.37	3 (3%) 54 43	14, 78, 126, 166	0
6	AG	150/178 (84%)	0.41	23 (15%) 3 3	41, 110, 166, 180	0
6	CG	152/178 (85%)	0.19	11 (7%) 18 15	27, 98, 156, 177	0
7	AH	129/129 (100%)	0.26	10 (7%) 16 13	26, 91, 148, 180	0
7	CH	129/129 (100%)	0.30	13 (10%) 9 9	5, 53, 117, 153	0
8	AI	127/129 (98%)	0.87	27 (21%) 1 1	32, 103, 160, 180	0
8	CI	127/129 (98%)	0.67	14 (11%) 7 7	32, 103, 162, 180	0
9	AJ	98/103 (95%)	0.86	13 (13%) 4 5	34, 106, 162, 180	0
9	CJ	98/103 (95%)	1.24	28 (28%) 1 1	42, 107, 156, 180	0
10	AK	117/128 (91%)	-0.04	1 (0%) 85 78	5, 71, 122, 174	0
10	CK	117/128 (91%)	0.14	5 (4%) 39 30	5, 57, 112, 179	0
11	AL	123/123 (100%)	0.54	16 (13%) 5 5	15, 82, 132, 153	0
11	CL	123/123 (100%)	-0.02	3 (2%) 62 52	5, 44, 109, 165	0
12	AM	114/117 (97%)	0.70	17 (14%) 3 3	68, 130, 178, 180	0
12	CM	113/117 (96%)	0.05	4 (3%) 48 38	32, 108, 156, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AN	96/100 (96%)	0.58	10 (10%) 8 8	32, 103, 161, 180	0
13	CN	96/100 (96%)	0.20	6 (6%) 23 18	38, 99, 137, 171	0
14	AO	88/89 (98%)	0.42	4 (4%) 37 29	35, 83, 132, 180	0
14	CO	88/89 (98%)	-0.01	2 (2%) 64 54	8, 54, 111, 165	0
15	AP	82/82 (100%)	1.82	33 (40%) 0 0	43, 99, 163, 180	0
15	CP	80/82 (97%)	0.10	4 (5%) 32 25	5, 51, 143, 164	0
16	AQ	80/83 (96%)	1.12	18 (22%) 1 1	49, 106, 156, 177	0
16	CQ	81/83 (97%)	-0.06	0 100 100	5, 51, 121, 157	0
17	AR	55/74 (74%)	0.32	3 (5%) 29 22	16, 78, 142, 152	0
17	CR	55/74 (74%)	0.74	5 (9%) 11 10	13, 69, 132, 149	0
18	AS	79/91 (86%)	1.09	23 (29%) 1 1	67, 128, 175, 180	0
18	CS	80/91 (87%)	-0.09	3 (3%) 44 36	49, 113, 171, 180	0
19	AT	85/86 (98%)	0.05	3 (3%) 48 38	43, 100, 153, 175	0
19	CT	85/86 (98%)	-0.15	0 100 100	14, 58, 121, 177	0
20	AB	218/240 (90%)	0.30	23 (10%) 8 7	30, 102, 152, 180	0
20	CB	218/240 (90%)	1.42	71 (32%) 1 0	26, 106, 160, 180	0
21	AU	51/71 (71%)	0.39	2 (3%) 43 35	26, 102, 172, 180	0
21	CU	51/71 (71%)	0.79	8 (15%) 3 3	19, 85, 151, 180	0
22	BA	117/120 (97%)	-0.71	1 (0%) 85 78	43, 83, 131, 173	0
22	DA	117/120 (97%)	-0.75	1 (0%) 85 78	32, 75, 118, 180	0
23	BB	2841/2904 (97%)	-0.43	15 (0%) 91 88	6, 56, 146, 180	0
23	DB	2841/2904 (97%)	-0.47	7 (0%) 95 93	5, 40, 139, 180	0
24	BV	94/94 (100%)	0.11	5 (5%) 30 23	11, 96, 146, 176	0
24	DV	94/94 (100%)	-0.08	3 (3%) 51 42	14, 86, 143, 180	0
25	BC	271/273 (99%)	0.68	28 (10%) 9 8	7, 48, 104, 170	0
25	DC	271/273 (99%)	0.48	24 (8%) 12 10	5, 28, 81, 120	0
26	BD	209/209 (100%)	0.54	27 (12%) 5 5	5, 73, 138, 180	0
26	DD	209/209 (100%)	0.45	21 (10%) 9 9	5, 42, 118, 180	0
27	BE	201/201 (100%)	0.82	23 (11%) 7 7	5, 65, 142, 180	0
27	DE	201/201 (100%)	0.38	14 (6%) 19 15	5, 67, 135, 180	0
28	BF	178/178 (100%)	1.41	56 (31%) 1 1	50, 116, 175, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DF	178/178 (100%)	1.10	35 (19%) 1 2	7, 101, 172, 180	0
29	BG	176/176 (100%)	0.66	23 (13%) 5 5	23, 102, 155, 180	0
29	DG	176/176 (100%)	0.21	11 (6%) 23 18	24, 90, 161, 180	0
30	BH	149/149 (100%)	1.73	51 (34%) 0 0	14, 117, 177, 180	0
30	DH	149/149 (100%)	0.55	13 (8%) 13 12	11, 100, 156, 180	0
31	BJ	142/142 (100%)	0.37	8 (5%) 28 22	6, 80, 141, 171	0
31	DJ	142/142 (100%)	0.33	9 (6%) 23 18	5, 60, 119, 165	0
32	BK	121/123 (98%)	1.76	46 (38%) 0 0	5, 73, 135, 180	0
32	DK	121/123 (98%)	0.58	11 (9%) 11 10	5, 35, 102, 145	0
33	BL	143/144 (99%)	0.05	5 (3%) 48 38	10, 64, 128, 180	0
33	DL	143/144 (99%)	0.56	18 (12%) 5 6	5, 54, 118, 162	0
34	BM	136/136 (100%)	0.10	5 (3%) 45 36	8, 70, 129, 172	0
34	DM	136/136 (100%)	0.76	19 (13%) 4 4	5, 51, 114, 168	0
35	BN	120/127 (94%)	0.51	13 (10%) 8 7	7, 67, 132, 163	0
35	DN	120/127 (94%)	-0.07	1 (0%) 87 80	5, 42, 86, 145	0
36	BO	116/117 (99%)	0.79	26 (22%) 1 1	27, 87, 135, 156	0
36	DO	116/117 (99%)	-0.02	1 (0%) 85 78	17, 78, 142, 180	0
37	BP	114/114 (100%)	1.72	47 (41%) 0 0	20, 85, 149, 178	0
37	DP	114/114 (100%)	0.17	4 (3%) 48 38	5, 48, 107, 159	0
38	BQ	117/117 (100%)	-0.15	3 (2%) 59 49	5, 63, 127, 180	0
38	DQ	117/117 (100%)	0.43	5 (4%) 39 30	5, 48, 116, 150	0
39	BR	103/103 (100%)	0.01	5 (4%) 33 25	16, 82, 145, 158	0
39	DR	103/103 (100%)	0.56	9 (8%) 13 12	5, 73, 136, 180	0
40	BS	110/110 (100%)	0.42	7 (6%) 23 17	5, 53, 116, 142	0
40	DS	110/110 (100%)	1.00	21 (19%) 2 2	5, 42, 116, 146	0
41	BT	93/100 (93%)	0.03	2 (2%) 65 55	6, 72, 139, 179	0
41	DT	93/100 (93%)	0.81	16 (17%) 2 2	11, 64, 156, 180	0
42	BU	102/103 (99%)	1.24	25 (24%) 1 1	5, 78, 144, 178	0
42	DU	102/103 (99%)	0.11	2 (1%) 68 59	10, 90, 154, 180	0
43	BW	79/84 (94%)	0.38	5 (6%) 23 18	10, 79, 157, 163	0
43	DW	79/84 (94%)	0.18	4 (5%) 32 24	5, 75, 131, 174	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BX	63/63 (100%)	0.91	15 (23%) 1 1	9, 74, 146, 179	0
44	DX	63/63 (100%)	0.54	4 (6%) 23 18	17, 96, 147, 180	0
45	BY	58/58 (100%)	0.34	4 (6%) 20 16	14, 78, 135, 170	0
45	DY	58/58 (100%)	-0.05	2 (3%) 49 40	10, 73, 129, 160	0
46	BZ	77/78 (98%)	0.62	8 (10%) 8 8	5, 49, 121, 160	0
46	DZ	77/78 (98%)	0.00	2 (2%) 59 49	5, 42, 107, 141	0
47	B0	56/56 (100%)	0.45	5 (8%) 12 10	5, 77, 144, 166	0
47	D0	56/56 (100%)	0.29	3 (5%) 29 23	8, 52, 128, 160	0
48	B1	50/54 (92%)	2.28	28 (56%) 0 0	51, 99, 149, 165	0
48	D1	50/54 (92%)	1.44	11 (22%) 1 1	43, 93, 138, 171	0
49	B2	46/46 (100%)	0.44	2 (4%) 39 30	7, 49, 103, 135	0
49	D2	46/46 (100%)	0.20	1 (2%) 65 55	5, 28, 99, 180	0
50	B3	64/64 (100%)	0.62	6 (9%) 11 10	16, 56, 110, 137	0
50	D3	64/64 (100%)	0.37	7 (10%) 7 7	5, 43, 112, 152	0
51	B4	38/38 (100%)	0.17	1 (2%) 59 49	33, 92, 143, 146	0
51	D4	38/38 (100%)	-0.39	0 100 100	5, 68, 112, 150	0
52	BI	141/141 (100%)	1.01	27 (19%) 2 2	67, 169, 180, 180	0
52	DI	141/141 (100%)	0.85	23 (16%) 2 3	91, 160, 180, 180	0
All	All	20417/21050 (96%)	0.07	1374 (6%) 21 16	5, 70, 153, 180	0

The worst 5 of 1374 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
30	BH	84	ALA	9.6
15	AP	81	ALA	9.4
15	AP	80	LYS	9.4
48	D1	52	LYS	9.4
30	BH	45	GLU	9.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	AA	2023	1/1	0.54	0.35	9.31	66,66,66,66	1
53	MG	BB	3097	1/1	0.88	0.18	4.08	114,114,114,114	0
53	MG	CA	2045	1/1	0.98	0.16	2.97	48,48,48,48	0
53	MG	CA	2020	1/1	0.96	0.21	2.72	73,73,73,73	0
54	HYG	CA	2062	36/36	0.91	0.22	2.29	45,45,45,45	0
53	MG	BB	3086	1/1	0.98	0.25	2.05	42,42,42,42	0
53	MG	CA	2038	1/1	0.83	0.12	1.73	128,128,128,128	0
53	MG	BB	3083	1/1	0.95	0.22	1.40	12,12,12,12	0
53	MG	DB	3099	1/1	0.98	0.19	1.37	7,7,7,7	0
54	HYG	AA	2059	36/36	0.90	0.24	1.10	52,52,52,52	0
53	MG	AA	2033	1/1	0.79	0.11	0.90	99,99,99,99	0
53	MG	BB	3040	1/1	0.98	0.18	0.90	26,26,26,26	0
53	MG	AA	2028	1/1	0.95	0.17	0.47	100,100,100,100	0
53	MG	BB	3081	1/1	0.86	0.22	0.43	46,46,46,46	0
53	MG	CA	2036	1/1	0.94	0.17	0.34	101,101,101,101	0
53	MG	CA	2033	1/1	0.94	0.15	0.34	56,56,56,56	0
53	MG	DB	3003	1/1	0.96	0.19	0.27	63,63,63,63	0
53	MG	AA	2014	1/1	0.68	0.22	0.22	112,112,112,112	0
53	MG	DB	3051	1/1	0.98	0.19	-0.02	23,23,23,23	0
53	MG	DB	3089	1/1	0.98	0.17	-0.32	7,7,7,7	0
53	MG	BB	3011	1/1	0.98	0.19	-0.37	5,5,5,5	0
53	MG	BB	3087	1/1	0.96	0.16	-0.40	57,57,57,57	0
53	MG	AA	2031	1/1	0.75	0.09	-0.46	58,58,58,58	0
53	MG	BB	3062	1/1	0.97	0.17	-0.52	14,14,14,14	0
53	MG	AN	201	1/1	0.72	0.12	-0.53	69,69,69,69	0
53	MG	DB	3110	1/1	0.95	0.14	-0.57	21,21,21,21	0
53	MG	DB	3087	1/1	0.97	0.15	-0.61	53,53,53,53	0
53	MG	BB	3005	1/1	0.97	0.19	-0.75	5,5,5,5	0
53	MG	BB	3085	1/1	0.93	0.17	-0.78	103,103,103,103	0
53	MG	CA	2039	1/1	0.98	0.12	-0.82	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	BB	3099	1/1	0.85	0.17	-0.90	40,40,40,40	0
53	MG	DB	3030	1/1	0.97	0.17	-0.97	6,6,6,6	0
53	MG	DB	3007	1/1	0.97	0.14	-1.02	18,18,18,18	0
53	MG	BB	3098	1/1	0.96	0.15	-1.03	35,35,35,35	0
53	MG	DB	3100	1/1	0.97	0.16	-1.15	13,13,13,13	0
53	MG	BB	3090	1/1	0.97	0.12	-1.16	112,112,112,112	0
53	MG	BB	3018	1/1	0.99	0.14	-1.25	32,32,32,32	0
53	MG	DB	3084	1/1	0.98	0.17	-1.25	5,5,5,5	0
53	MG	DB	3092	1/1	0.91	0.13	-1.26	66,66,66,66	0
53	MG	AA	2049	1/1	0.91	0.06	-1.26	75,75,75,75	0
53	MG	DB	3088	1/1	0.97	0.14	-1.41	25,25,25,25	0
53	MG	CA	2053	1/1	0.99	0.06	-1.42	30,30,30,30	0
53	MG	CA	2016	1/1	0.95	0.04	-1.50	53,53,53,53	0
53	MG	AA	2034	1/1	0.97	0.06	-1.54	68,68,68,68	0
53	MG	BB	3037	1/1	0.86	0.11	-1.54	23,23,23,23	0
53	MG	DB	3078	1/1	0.97	0.08	-1.54	27,27,27,27	0
53	MG	DB	3047	1/1	0.96	0.17	-1.57	14,14,14,14	0
53	MG	CA	2012	1/1	0.99	0.08	-1.62	93,93,93,93	0
53	MG	CA	2014	1/1	0.90	0.07	-1.66	47,47,47,47	0
53	MG	CA	2017	1/1	0.98	0.11	-1.74	5,5,5,5	0
53	MG	DB	3096	1/1	0.98	0.12	-1.76	6,6,6,6	0
53	MG	AA	2040	1/1	0.97	0.09	-1.80	83,83,83,83	0
53	MG	BB	3013	1/1	0.97	0.10	-1.86	43,43,43,43	0
55	ZN	B4	101	1/1	0.97	0.04	-1.91	80,80,80,80	0
53	MG	AA	2007	1/1	0.95	0.06	-1.92	31,31,31,31	0
53	MG	BB	3082	1/1	0.96	0.16	-1.94	46,46,46,46	0
53	MG	DB	3069	1/1	0.98	0.18	-2.02	11,11,11,11	0
53	MG	BB	3059	1/1	0.98	0.12	-2.05	26,26,26,26	0
53	MG	BB	3023	1/1	0.97	0.14	-2.15	5,5,5,5	0
55	ZN	D4	101	1/1	0.98	0.06	-2.18	46,46,46,46	0
53	MG	BB	3012	1/1	0.98	0.09	-2.39	32,32,32,32	0
53	MG	BB	3048	1/1	0.92	0.11	-2.45	44,44,44,44	0
53	MG	BB	3021	1/1	0.95	0.08	-2.46	30,30,30,30	0
53	MG	AA	2009	1/1	0.96	0.10	-2.51	7,7,7,7	0
53	MG	CA	2005	1/1	0.97	0.09	-2.78	24,24,24,24	0
53	MG	BB	3103	1/1	0.98	0.08	-2.82	5,5,5,5	0
53	MG	DB	3006	1/1	0.98	0.10	-2.87	5,5,5,5	0
53	MG	DB	3022	1/1	0.97	0.08	-2.93	25,25,25,25	0
53	MG	CA	2056	1/1	0.98	0.05	-2.98	5,5,5,5	0
53	MG	DB	3070	1/1	0.97	0.08	-3.00	45,45,45,45	0
53	MG	DB	3074	1/1	0.95	0.09	-3.00	12,12,12,12	0
53	MG	AA	2001	1/1	0.93	0.07	-3.01	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	CA	2040	1/1	0.96	0.09	-3.01	48,48,48,48	0
53	MG	BB	3032	1/1	0.93	0.10	-3.05	56,56,56,56	0
53	MG	BB	3066	1/1	0.97	0.12	-3.10	23,23,23,23	0
53	MG	DB	3103	1/1	0.97	0.13	-3.11	27,27,27,27	0
53	MG	AA	2051	1/1	0.91	0.10	-3.12	41,41,41,41	0
53	MG	DB	3111	1/1	0.96	0.09	-3.18	38,38,38,38	0
53	MG	AA	2036	1/1	0.97	0.04	-3.39	31,31,31,31	0
53	MG	CA	2004	1/1	0.97	0.09	-3.42	8,8,8,8	0
53	MG	DB	3044	1/1	0.93	0.11	-3.49	24,24,24,24	0
53	MG	DB	3035	1/1	0.96	0.06	-3.58	55,55,55,55	0
53	MG	DB	3019	1/1	0.99	0.09	-3.58	5,5,5,5	0
53	MG	BB	3001	1/1	0.94	0.10	-3.64	51,51,51,51	0
53	MG	BB	3108	1/1	0.98	0.10	-3.71	47,47,47,47	0
53	MG	DB	3085	1/1	0.99	0.12	-3.76	5,5,5,5	0
53	MG	DB	3080	1/1	0.95	0.10	-3.83	10,10,10,10	0
53	MG	BB	3069	1/1	0.97	0.11	-3.86	17,17,17,17	0
53	MG	DB	3014	1/1	0.99	0.05	-3.87	5,5,5,5	0
53	MG	BB	3088	1/1	0.95	0.06	-3.95	28,28,28,28	0
53	MG	BB	3065	1/1	0.97	0.06	-3.99	29,29,29,29	0
53	MG	AA	2052	1/1	0.91	0.07	-4.00	78,78,78,78	0
53	MG	DB	3090	1/1	0.88	0.08	-4.02	37,37,37,37	0
53	MG	BB	3056	1/1	0.96	0.08	-4.09	26,26,26,26	0
53	MG	DB	3055	1/1	0.97	0.11	-4.13	26,26,26,26	0
53	MG	DB	3001	1/1	0.99	0.10	-4.81	5,5,5,5	0
53	MG	DB	3068	1/1	0.98	0.10	-4.96	5,5,5,5	0
53	MG	DB	3056	1/1	0.97	0.09	-5.10	5,5,5,5	0
53	MG	BB	3029	1/1	0.97	0.07	-5.19	14,14,14,14	0
53	MG	BB	3052	1/1	0.90	0.08	-5.71	38,38,38,38	0
53	MG	CA	2044	1/1	0.96	0.07	-5.89	59,59,59,59	0
53	MG	BB	3019	1/1	0.98	0.05	-6.02	22,22,22,22	0
53	MG	CA	2018	1/1	0.99	0.03	-6.04	6,6,6,6	0
53	MG	AA	2010	1/1	0.97	0.04	-6.26	60,60,60,60	0
53	MG	CA	2001	1/1	0.98	0.05	-7.01	5,5,5,5	0
53	MG	AA	2041	1/1	0.96	0.07	-7.04	83,83,83,83	0
53	MG	DB	3002	1/1	0.98	0.07	-8.03	12,12,12,12	0
53	MG	BB	3035	1/1	0.97	0.07	-8.14	15,15,15,15	0
53	MG	BB	3002	1/1	0.99	0.07	-8.43	5,5,5,5	0
53	MG	DB	3010	1/1	0.97	0.08	-9.61	8,8,8,8	0
53	MG	CA	2055	1/1	0.98	0.07	-9.77	11,11,11,11	0
53	MG	BB	3094	1/1	0.98	0.07	-10.47	28,28,28,28	0
53	MG	DB	3009	1/1	0.97	0.07	-14.19	29,29,29,29	0
53	MG	AA	2035	1/1	0.83	0.34	-	137,137,137,137	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	AA	2037	1/1	0.58	0.33	-	138,138,138,138	0
53	MG	DB	3095	1/1	0.86	0.15	-	89,89,89,89	0
53	MG	CA	2050	1/1	0.99	0.11	-	8,8,8,8	0
53	MG	BB	3067	1/1	0.98	0.09	-	44,44,44,44	0
53	MG	DB	3036	1/1	0.91	0.09	-	30,30,30,30	0
53	MG	AA	2056	1/1	0.79	0.12	-	124,124,124,124	0
53	MG	AE	201	1/1	0.79	0.07	-	144,144,144,144	0
53	MG	BB	3079	1/1	0.98	0.04	-	19,19,19,19	0
53	MG	CA	2031	1/1	0.99	0.06	-	28,28,28,28	0
53	MG	DB	3033	1/1	0.97	0.08	-	9,9,9,9	0
53	MG	DB	3058	1/1	0.93	0.33	-	151,151,151,151	0
53	MG	BB	3101	1/1	0.98	0.09	-	24,24,24,24	0
53	MG	DB	3102	1/1	0.98	0.09	-	12,12,12,12	0
53	MG	BB	3063	1/1	0.95	0.09	-	11,11,11,11	0
53	MG	CA	2037	1/1	0.93	0.09	-	94,94,94,94	0
53	MG	AA	2022	1/1	0.95	0.07	-	82,82,82,82	0
53	MG	DB	3104	1/1	0.98	0.08	-	33,33,33,33	0
53	MG	BB	3096	1/1	0.97	0.11	-	34,34,34,34	0
53	MG	AA	2047	1/1	0.74	0.04	-	100,100,100,100	0
53	MG	BB	3046	1/1	0.93	0.11	-	22,22,22,22	0
53	MG	CA	2051	1/1	0.98	0.05	-	39,39,39,39	0
53	MG	DB	3057	1/1	0.96	0.06	-	71,71,71,71	0
53	MG	DB	3017	1/1	0.98	0.10	-	13,13,13,13	0
53	MG	AA	2042	1/1	0.96	0.09	-	69,69,69,69	0
53	MG	DB	3023	1/1	0.90	0.08	-	32,32,32,32	0
53	MG	DB	3091	1/1	0.99	0.18	-	13,13,13,13	0
53	MG	DB	3105	1/1	0.97	0.14	-	23,23,23,23	0
53	MG	BB	3084	1/1	0.98	0.16	-	24,24,24,24	0
53	MG	BB	3030	1/1	0.99	0.03	-	35,35,35,35	0
53	MG	DB	3052	1/1	0.94	0.12	-	100,100,100,100	0
53	MG	DB	3076	1/1	0.99	0.10	-	5,5,5,5	0
53	MG	CA	2013	1/1	0.97	0.08	-	73,73,73,73	0
53	MG	BB	3055	1/1	0.94	0.15	-	17,17,17,17	0
53	MG	CA	2035	1/1	0.90	0.08	-	89,89,89,89	0
53	MG	DB	3081	1/1	0.99	0.13	-	18,18,18,18	0
53	MG	CA	2027	1/1	0.69	0.13	-	50,50,50,50	1
53	MG	DB	3106	1/1	0.98	0.13	-	23,23,23,23	0
53	MG	DB	3005	1/1	0.95	0.12	-	10,10,10,10	0
53	MG	BB	3071	1/1	0.90	0.09	-	26,26,26,26	0
53	MG	CA	2003	1/1	0.99	0.04	-	35,35,35,35	0
53	MG	BB	3014	1/1	0.91	0.05	-	50,50,50,50	0
53	MG	BB	3042	1/1	0.13	0.10	-	168,168,168,168	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	CA	2022	1/1	0.97	0.10	-	63,63,63,63	0
53	MG	BB	3045	1/1	0.95	0.10	-	31,31,31,31	0
53	MG	DB	3073	1/1	0.95	0.10	-	14,14,14,14	0
53	MG	CA	2060	1/1	0.81	0.05	-	80,80,80,80	0
53	MG	BB	3102	1/1	0.95	0.12	-	20,20,20,20	0
53	MG	AA	2046	1/1	0.93	0.07	-	5,5,5,5	0
53	MG	BB	3061	1/1	0.95	0.04	-	48,48,48,48	0
53	MG	DB	3071	1/1	0.96	0.06	-	16,16,16,16	0
53	MG	DB	3098	1/1	0.99	0.22	-	44,44,44,44	0
53	MG	BB	3073	1/1	0.98	0.09	-	39,39,39,39	0
53	MG	BB	3036	1/1	0.95	0.11	-	42,42,42,42	0
53	MG	AA	2018	1/1	0.82	0.09	-	131,131,131,131	0
53	MG	BB	3058	1/1	0.97	0.10	-	22,22,22,22	0
53	MG	BB	3041	1/1	0.99	0.08	-	7,7,7,7	0
53	MG	AA	2025	1/1	0.95	0.17	-	58,58,58,58	0
53	MG	DB	3011	1/1	0.96	0.16	-	17,17,17,17	0
53	MG	BB	3003	1/1	0.96	0.07	-	32,32,32,32	0
53	MG	DB	3093	1/1	0.96	0.22	-	11,11,11,11	0
53	MG	BB	3109	1/1	0.96	0.09	-	54,54,54,54	0
53	MG	AA	2050	1/1	0.87	0.14	-	105,105,105,105	0
53	MG	DB	3094	1/1	0.97	0.03	-	29,29,29,29	0
53	MG	CA	2021	1/1	0.79	0.36	-	125,125,125,125	0
53	MG	DB	3079	1/1	0.98	0.14	-	28,28,28,28	0
53	MG	AA	2039	1/1	0.96	0.12	-	64,64,64,64	0
53	MG	BB	3039	1/1	0.94	0.18	-	7,7,7,7	0
53	MG	BB	3092	1/1	0.99	0.06	-	54,54,54,54	0
53	MG	CA	2054	1/1	0.91	0.08	-	104,104,104,104	0
53	MG	BB	3095	1/1	0.98	0.07	-	33,33,33,33	0
53	MG	BB	3054	1/1	0.93	0.06	-	77,77,77,77	0
53	MG	DB	3061	1/1	0.97	0.09	-	69,69,69,69	0
53	MG	AA	2044	1/1	0.88	0.12	-	112,112,112,112	0
53	MG	BB	3049	1/1	0.93	0.10	-	10,10,10,10	0
53	MG	DB	3107	1/1	0.98	0.07	-	10,10,10,10	0
53	MG	BB	3076	1/1	0.99	0.05	-	38,38,38,38	0
53	MG	BB	3106	1/1	0.99	0.12	-	62,62,62,62	0
53	MG	BB	3074	1/1	0.97	0.07	-	28,28,28,28	0
53	MG	DB	3043	1/1	0.98	0.11	-	5,5,5,5	0
53	MG	DB	3031	1/1	0.98	0.18	-	8,8,8,8	0
53	MG	CA	2008	1/1	0.83	0.09	-	93,93,93,93	0
53	MG	DB	3086	1/1	0.97	0.14	-	11,11,11,11	0
53	MG	CA	2007	1/1	0.91	0.05	-	46,46,46,46	0
53	MG	DB	3062	1/1	0.98	0.04	-	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	AA	2027	1/1	0.97	0.09	-	36,36,36,36	0
53	MG	CA	2042	1/1	0.87	0.08	-	58,58,58,58	0
53	MG	AA	2003	1/1	0.99	0.17	-	39,39,39,39	0
53	MG	BB	3044	1/1	0.98	0.15	-	53,53,53,53	0
53	MG	AA	2020	1/1	0.98	0.07	-	5,5,5,5	0
53	MG	AA	2011	1/1	0.97	0.07	-	85,85,85,85	0
53	MG	BB	3038	1/1	0.96	0.03	-	71,71,71,71	0
53	MG	BB	3047	1/1	0.95	0.06	-	75,75,75,75	0
53	MG	DB	3013	1/1	0.88	0.17	-	51,51,51,51	0
53	MG	DB	3046	1/1	0.95	0.09	-	24,24,24,24	0
53	MG	DB	3075	1/1	0.98	0.10	-	57,57,57,57	0
53	MG	DB	3038	1/1	0.97	0.12	-	5,5,5,5	0
53	MG	CA	2015	1/1	0.68	0.10	-	149,149,149,149	0
53	MG	BB	3072	1/1	0.98	0.12	-	17,17,17,17	0
53	MG	CA	2048	1/1	0.96	0.11	-	58,58,58,58	0
53	MG	DB	3063	1/1	0.98	0.12	-	43,43,43,43	0
53	MG	CA	2025	1/1	0.96	0.12	-	50,50,50,50	0
53	MG	BB	3051	1/1	0.92	0.14	-	35,35,35,35	0
53	MG	AA	2053	1/1	0.98	0.07	-	79,79,79,79	0
53	MG	AA	2048	1/1	0.96	0.03	-	99,99,99,99	0
53	MG	BB	3105	1/1	0.98	0.08	-	20,20,20,20	0
53	MG	CE	201	1/1	0.86	0.15	-	127,127,127,127	0
53	MG	BB	3025	1/1	0.98	0.13	-	30,30,30,30	0
53	MG	AA	2021	1/1	0.92	0.31	-	5,5,5,5	1
53	MG	BB	3075	1/1	0.97	0.21	-	40,40,40,40	0
53	MG	DB	3034	1/1	0.96	0.16	-	52,52,52,52	0
53	MG	BB	3064	1/1	0.95	0.07	-	35,35,35,35	0
53	MG	DB	3027	1/1	0.98	0.15	-	6,6,6,6	0
53	MG	AA	2006	1/1	0.95	0.03	-	60,60,60,60	0
53	MG	DB	3020	1/1	0.99	0.15	-	5,5,5,5	0
53	MG	DB	3083	1/1	0.98	0.16	-	85,85,85,85	0
53	MG	AA	2029	1/1	0.95	0.07	-	39,39,39,39	0
53	MG	DB	3077	1/1	0.98	0.21	-	54,54,54,54	0
53	MG	BB	3010	1/1	0.82	0.10	-	44,44,44,44	0
53	MG	CA	2049	1/1	0.95	0.06	-	74,74,74,74	0
53	MG	AA	2026	1/1	0.89	0.08	-	65,65,65,65	0
53	MG	DB	3108	1/1	0.96	0.09	-	37,37,37,37	0
53	MG	BB	3104	1/1	0.91	0.18	-	36,36,36,36	0
53	MG	DB	3015	1/1	0.94	0.07	-	33,33,33,33	0
53	MG	AA	2054	1/1	0.93	0.08	-	110,110,110,110	0
53	MG	AA	2019	1/1	0.79	0.05	-	107,107,107,107	0
53	MG	BB	3020	1/1	0.94	0.10	-	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	CA	2058	1/1	0.94	0.11	-	106,106,106,106	0
53	MG	DB	3072	1/1	0.96	0.12	-	18,18,18,18	0
53	MG	BB	3017	1/1	0.90	0.14	-	34,34,34,34	0
53	MG	BB	3078	1/1	0.96	0.15	-	70,70,70,70	0
53	MG	DB	3109	1/1	0.97	0.10	-	9,9,9,9	0
53	MG	CA	2009	1/1	0.95	0.06	-	67,67,67,67	0
53	MG	BB	3026	1/1	0.97	0.08	-	39,39,39,39	0
53	MG	BB	3068	1/1	0.96	0.12	-	53,53,53,53	0
53	MG	DB	3064	1/1	0.98	0.05	-	20,20,20,20	0
53	MG	DB	3018	1/1	0.99	0.07	-	22,22,22,22	0
53	MG	AA	2017	1/1	0.91	0.12	-	87,87,87,87	0
53	MG	DB	3021	1/1	0.96	0.23	-	11,11,11,11	0
53	MG	AA	2045	1/1	0.92	0.64	-	92,92,92,92	0
53	MG	AA	2057	1/1	0.62	0.18	-	141,141,141,141	0
53	MG	DB	3039	1/1	0.97	0.04	-	22,22,22,22	0
53	MG	CA	2047	1/1	0.95	0.06	-	121,121,121,121	0
53	MG	CA	2061	1/1	0.97	0.08	-	23,23,23,23	0
53	MG	DB	3041	1/1	0.95	0.11	-	29,29,29,29	0
53	MG	CA	2057	1/1	0.79	0.10	-	99,99,99,99	0
53	MG	CA	2010	1/1	0.94	0.07	-	33,33,33,33	0
53	MG	DB	3016	1/1	0.98	0.05	-	15,15,15,15	0
53	MG	DB	3048	1/1	0.98	0.12	-	28,28,28,28	0
53	MG	BB	3091	1/1	0.97	0.09	-	16,16,16,16	0
53	MG	DB	3045	1/1	0.87	0.06	-	57,57,57,57	0
53	MG	AA	2013	1/1	0.87	0.12	-	122,122,122,122	0
53	MG	CA	2023	1/1	0.78	0.20	-	137,137,137,137	0
53	MG	CA	2024	1/1	0.95	0.06	-	29,29,29,29	0
53	MG	DB	3042	1/1	0.98	0.10	-	6,6,6,6	0
53	MG	CA	2019	1/1	0.94	0.10	-	73,73,73,73	0
53	MG	AA	2012	1/1	0.81	0.09	-	84,84,84,84	0
53	MG	DB	3050	1/1	0.92	0.08	-	90,90,90,90	0
53	MG	BB	3107	1/1	0.99	0.11	-	6,6,6,6	0
53	MG	BB	3100	1/1	0.72	0.20	-	129,129,129,129	0
53	MG	CA	2034	1/1	0.97	0.11	-	6,6,6,6	0
53	MG	AA	2038	1/1	0.96	0.11	-	71,71,71,71	0
53	MG	BB	3004	1/1	0.97	0.06	-	32,32,32,32	0
53	MG	BB	3028	1/1	0.98	0.20	-	86,86,86,86	0
53	MG	DB	3029	1/1	0.90	0.15	-	88,88,88,88	0
53	MG	BB	3007	1/1	0.99	0.14	-	82,82,82,82	0
53	MG	DB	3101	1/1	0.99	0.20	-	5,5,5,5	0
53	MG	BB	3057	1/1	0.94	0.20	-	28,28,28,28	0
53	MG	DB	3066	1/1	0.81	0.08	-	146,146,146,146	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	BB	3016	1/1	0.96	0.07	-	38,38,38,38	0
53	MG	DB	3049	1/1	0.98	0.09	-	36,36,36,36	0
53	MG	DB	3097	1/1	0.95	0.14	-	38,38,38,38	0
53	MG	AA	2004	1/1	0.92	0.13	-	56,56,56,56	0
53	MG	BB	3043	1/1	0.97	0.05	-	104,104,104,104	0
53	MG	BB	3031	1/1	0.93	0.14	-	41,41,41,41	0
53	MG	BB	3070	1/1	0.99	0.14	-	37,37,37,37	0
53	MG	BB	3009	1/1	0.97	0.04	-	46,46,46,46	0
53	MG	DB	3040	1/1	0.98	0.16	-	5,5,5,5	0
53	MG	AA	2032	1/1	0.93	0.08	-	62,62,62,62	0
53	MG	BB	3015	1/1	0.99	0.09	-	13,13,13,13	0
53	MG	AA	2055	1/1	0.83	0.20	-	102,102,102,102	0
53	MG	CA	2032	1/1	0.98	0.17	-	33,33,33,33	0
53	MG	CA	2028	1/1	0.93	0.07	-	75,75,75,75	0
53	MG	DB	3053	1/1	0.99	0.07	-	35,35,35,35	0
53	MG	DB	3082	1/1	0.97	0.10	-	30,30,30,30	0
53	MG	BB	3077	1/1	0.88	0.09	-	36,36,36,36	0
53	MG	BB	3006	1/1	0.98	0.07	-	5,5,5,5	0
53	MG	BB	3027	1/1	0.94	0.08	-	33,33,33,33	0
53	MG	BB	3093	1/1	0.93	0.23	-	71,71,71,71	0
53	MG	CA	2059	1/1	0.78	0.12	-	94,94,94,94	0
53	MG	DB	3004	1/1	0.98	0.11	-	6,6,6,6	0
53	MG	DB	3065	1/1	0.98	0.05	-	37,37,37,37	0
53	MG	DB	3026	1/1	0.96	0.08	-	34,34,34,34	0
53	MG	AA	2002	1/1	0.94	0.06	-	99,99,99,99	0
53	MG	AA	2043	1/1	0.97	0.08	-	96,96,96,96	0
53	MG	DB	3032	1/1	0.96	0.09	-	63,63,63,63	0
53	MG	CA	2011	1/1	0.66	0.28	-	132,132,132,132	0
53	MG	BB	3024	1/1	0.93	0.12	-	15,15,15,15	0
53	MG	AA	2005	1/1	0.82	0.08	-	69,69,69,69	0
53	MG	BB	3060	1/1	0.97	0.13	-	19,19,19,19	0
53	MG	AA	2016	1/1	0.93	0.09	-	89,89,89,89	0
53	MG	AA	2058	1/1	0.96	0.14	-	86,86,86,86	0
53	MG	BB	3053	1/1	0.93	0.06	-	28,28,28,28	0
53	MG	CA	2026	1/1	0.83	0.19	-	26,26,26,26	1
53	MG	CA	2046	1/1	0.97	0.10	-	57,57,57,57	0
53	MG	DB	3008	1/1	0.98	0.18	-	6,6,6,6	0
53	MG	DB	3025	1/1	0.97	0.15	-	5,5,5,5	0
53	MG	BB	3089	1/1	0.98	0.15	-	56,56,56,56	0
53	MG	DB	3024	1/1	0.98	0.13	-	63,63,63,63	0
53	MG	CA	2006	1/1	0.98	0.05	-	95,95,95,95	0
53	MG	CA	2052	1/1	0.90	0.09	-	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	BB	3050	1/1	0.99	0.12	-	28,28,28,28	0
53	MG	DB	3059	1/1	0.80	0.12	-	180,180,180,180	0
53	MG	DB	3060	1/1	0.71	0.20	-	112,112,112,112	0
53	MG	BB	3110	1/1	0.99	0.15	-	23,23,23,23	0
53	MG	BB	3008	1/1	0.95	0.10	-	89,89,89,89	0
53	MG	BB	3033	1/1	0.93	0.34	-	125,125,125,125	0
53	MG	AA	2008	1/1	0.76	0.08	-	125,125,125,125	0
53	MG	AA	2024	1/1	0.87	0.08	-	5,5,5,5	1
53	MG	DB	3028	1/1	0.97	0.06	-	24,24,24,24	0
53	MG	CA	2043	1/1	0.95	0.04	-	19,19,19,19	0
53	MG	AA	2015	1/1	0.93	0.06	-	24,24,24,24	0
53	MG	CA	2029	1/1	0.90	0.05	-	23,23,23,23	1
53	MG	CA	2041	1/1	0.96	0.05	-	46,46,46,46	0
53	MG	DB	3054	1/1	0.96	0.04	-	19,19,19,19	0
53	MG	DB	3012	1/1	0.99	0.20	-	9,9,9,9	0
53	MG	BB	3022	1/1	0.98	0.26	-	34,34,34,34	0
53	MG	CA	2030	1/1	0.98	0.12	-	7,7,7,7	0
53	MG	BB	3080	1/1	0.81	0.18	-	39,39,39,39	0
53	MG	BB	3034	1/1	0.96	0.10	-	35,35,35,35	0
53	MG	AA	2030	1/1	0.90	0.09	-	99,99,99,99	0
53	MG	DB	3037	1/1	0.98	0.16	-	28,28,28,28	0
53	MG	DB	3067	1/1	0.98	0.07	-	5,5,5,5	0
53	MG	CA	2002	1/1	1.00	0.11	-	5,5,5,5	0

6.5 Other polymers [i](#)

There are no such residues in this entry.