



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 11:49 PM UTC

PDB ID : 4V6D / pdb_00004v6d
Title : Crystal structure of the E. coli 70S ribosome in an intermediate state of ratcheting
Authors : Zhang, W.; Dunkle, J.A.; Cate, J.H.D.
Deposited on : 2009-06-27
Resolution : 3.81 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

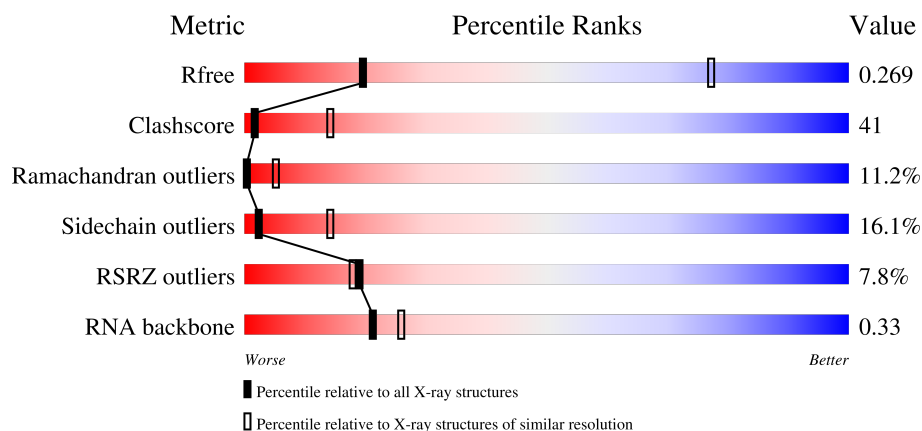
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.81 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}	180053	1043 (3.98-3.66)
Clashscore	190562	1075 (3.98-3.66)
Ramachandran outliers	187476	1029 (3.98-3.66)
Sidechain outliers	187428	1024 (3.98-3.66)
RSRZ outliers	180081	1042 (3.98-3.66)
RNA backbone	3983	1009 (4.52-3.10)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	AB	241	26% 17% 54% 17% • 10%
1	CB	241	9% 19% 58% 13% • 10%
2	AC	233	32% 43% 11% • 12%
2	CC	233	% 30% 46% 12% 12%

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Mol	Chain	Length	Quality of chain
3	AD	206	
3	CD	206	
4	AE	167	
4	CE	167	
5	AF	135	
5	CF	135	
6	AG	179	
6	CG	179	
7	AH	130	
7	CH	130	
8	AI	130	
8	CI	130	
9	AJ	103	
9	CJ	103	
10	AK	129	
10	CK	129	
11	AL	124	
11	CL	124	
12	AM	118	
12	CM	118	
13	AN	101	
13	CN	101	
14	AO	89	
14	CO	89	
15	AP	82	

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Mol	Chain	Length	Quality of chain
15	CP	82	
16	AQ	84	
16	CQ	84	
17	AR	75	
17	CR	75	
18	AS	92	
18	CS	92	
19	AT	87	
19	CT	87	
20	AU	71	
20	CU	71	
21	AA	1533	
22	AV	17	
22	CV	17	
23	AW	6	
23	CW	6	
24	BA	2903	
24	DA	2903	
25	BB	118	
26	BC	273	
26	DC	273	
27	BD	209	
27	DD	209	
28	BE	201	
28	DE	201	

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Mol	Chain	Length	Quality of chain
29	BF	179	
29	DF	179	
30	BG	177	
30	DG	177	
31	BH	149	
31	DH	149	
32	BI	142	
32	DI	142	
33	BJ	142	
33	DJ	142	
34	BK	123	
34	DK	123	
35	BL	144	
35	DL	144	
36	BM	136	
36	DM	136	
37	BN	127	
37	DN	127	
38	BO	117	
38	DO	117	
39	BP	115	
39	DP	115	
40	BQ	118	
40	DQ	118	
41	BR	103	

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Mol	Chain	Length	Quality of chain
41	DR	103	
42	BS	110	
42	DS	110	
43	BT	100	
43	DT	100	
44	BU	104	
44	DU	104	
45	BV	94	
45	DV	94	
46	BW	85	
46	DW	85	
47	BX	78	
47	DX	78	
48	BY	63	
48	DY	63	
49	BZ	59	
49	DZ	59	
50	B0	57	
50	D0	57	
51	B1	55	
51	D1	55	
52	B2	46	
52	D2	46	
53	B3	65	
53	D3	65	

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Mol	Chain	Length	Quality of chain
54	B4	38	
54	D4	38	
55	CA	1530	
56	DB	117	

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
57	MG	BA	3015	-	-	-	X
57	MG	BA	3131	-	-	-	X
57	MG	BA	3132	-	-	-	X
57	MG	BA	3133	-	-	-	X
57	MG	CA	1624	-	-	-	X
57	MG	DA	3004	-	-	-	X
57	MG	DA	3016	-	-	-	X
57	MG	DA	3062	-	-	-	X
57	MG	DA	3065	-	-	-	X
57	MG	DA	3076	-	-	-	X
57	MG	DA	3110	-	-	-	X
57	MG	DA	3131	-	-	-	X
57	MG	DA	3134	-	-	-	X

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 285420 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 30S ribosomal protein S2.

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

- 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	151	Total	C	N	O	S	0	0	0
			1181	735	227	215	4			
6	CG	150	Total	C	N	O	S	0	0	0
			1174	730	226	214	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	95	Total	C	N	O	S	0	0	0
			769	480	159	127	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
			714	439	144	130	1			
14	CO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	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	80	Total	C	N	O	S	0	0	0
			648	411	121	113	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	79	Total	C	N	O	S	0	0	0
			637	408	120	107	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 S21.

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

- Molecule 21 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AA	1533	Total	C	N	O	P	0	0	0
			32895	14671	6036	10655	1533			

- Molecule 22 is a RNA chain called P-site tRNA ASL fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	17	Total	C	N	O	P	0	0	0
			360	161	64	118	17			
22	CV	17	Total	C	N	O	P	0	0	0
			360	161	64	118	17			

- Molecule 23 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	6	Total	C	N	O	P	0	0	0
			125	56	18	45	6			
23	CW	6	Total	C	N	O	P	0	0	0
			125	56	18	45	6			

- Molecule 24 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	BA	2854	Total	C	N	O	P	0	0	0
			61274	27334	11279	19807	2854			
24	DA	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			

- Molecule 25 is a RNA chain called 5S rRNA.

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

- Molecule 26 is a protein called 50S ribosomal protein L2.

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

- Molecule 27 is a protein called 50S ribosomal protein L3.

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

- Molecule 28 is a protein called 50S ribosomal protein L4.

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

- Molecule 29 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BF	177	Total	C	N	O	S	0	0	0
			1410	899	249	256	6			
29	DF	178	Total	C	N	O	S	0	0	0
			1420	905	251	258	6			

- Molecule 30 is a protein called 50S ribosomal protein L6.

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

- Molecule 31 is a protein called 50S ribosomal protein L9.

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

- Molecule 32 is a protein called 50S ribosomal protein L11.

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

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

- Molecule 33 is a protein called 50S ribosomal protein L13.

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

- Molecule 34 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BK	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			
34	DK	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			

- Molecule 35 is a protein called 50S ribosomal protein L15.

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

- Molecule 36 is a protein called 50S ribosomal protein L16.

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

- Molecule 37 is a protein called 50S ribosomal protein L17.

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

- Molecule 38 is a protein called 50S ribosomal protein L18.

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

- Molecule 39 is a protein called 50S ribosomal protein L19.

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

- Molecule 40 is a protein called 50S ribosomal protein L20.

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

- Molecule 41 is a protein called 50S ribosomal protein L21.

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

- Molecule 42 is a protein called 50S ribosomal protein L22.

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

- Molecule 43 is a protein called 50S ribosomal protein L23.

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

- Molecule 44 is a protein called 50S ribosomal protein L24.

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

- Molecule 45 is a protein called 50S ribosomal protein L25.

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

- Molecule 46 is a protein called 50S ribosomal protein L27.

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

- Molecule 47 is a protein called 50S ribosomal protein L28.

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

- Molecule 48 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BY	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			

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

- Molecule 49 is a protein called 50S ribosomal protein L30.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L33.

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

- Molecule 52 is a protein called 50S ribosomal protein L34.

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

- Molecule 53 is a protein called 50S ribosomal protein L35.

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

- Molecule 54 is a protein called 50S ribosomal protein L36.

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

- Molecule 55 is a RNA chain called 16S rRNA.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	DB	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	AA	43	Total	Mg	0	0
			43	43		
57	BA	136	Total	Mg	0	0
			136	136		
57	BB	4	Total	Mg	0	0
			4	4		
57	BD	1	Total	Mg	0	0
			1	1		
57	CA	42	Total	Mg	0	0
			42	42		
57	DC	1	Total	Mg	0	0
			1	1		
57	DJ	1	Total	Mg	0	0
			1	1		
57	DA	134	Total	Mg	0	0
			134	134		
57	DB	1	Total	Mg	0	0
			1	1		

- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 59 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	AE	1	Total O 1 1	0	0
59	AL	3	Total O 3 3	0	0
59	AN	5	Total O 5 5	0	0
59	AT	3	Total O 3 3	0	0
59	AU	1	Total O 1 1	0	0
59	AA	195	Total O 195 195	0	0
59	BA	615	Total O 615 615	0	0
59	BB	19	Total O 19 19	0	0
59	BC	7	Total O 7 7	0	0
59	BD	2	Total O 2 2	0	0
59	BE	1	Total O 1 1	0	0
59	BL	4	Total O 4 4	0	0
59	BN	2	Total O 2 2	0	0
59	BQ	1	Total O 1 1	0	0
59	BT	1	Total O 1 1	0	0
59	BV	1	Total O 1 1	0	0
59	B2	2	Total O 2 2	0	0
59	B3	3	Total O 3 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	B4	2	Total 2	O 2	0	0
59	CE	3	Total 3	O 3	0	0
59	CI	1	Total 1	O 1	0	0
59	CL	1	Total 1	O 1	0	0
59	CN	2	Total 2	O 2	0	0
59	CT	2	Total 2	O 2	0	0
59	CU	2	Total 2	O 2	0	0
59	CA	196	Total 196	O 196	0	0
59	DC	14	Total 14	O 14	0	0
59	DD	4	Total 4	O 4	0	0
59	DE	2	Total 2	O 2	0	0
59	DJ	3	Total 3	O 3	0	0
59	DL	5	Total 5	O 5	0	0
59	DN	2	Total 2	O 2	0	0
59	DT	2	Total 2	O 2	0	0
59	DU	1	Total 1	O 1	0	0
59	DV	1	Total 1	O 1	0	0
59	D2	1	Total 1	O 1	0	0
59	D3	1	Total 1	O 1	0	0
59	D4	5	Total 5	O 5	0	0
59	DA	598	Total 598	O 598	0	0

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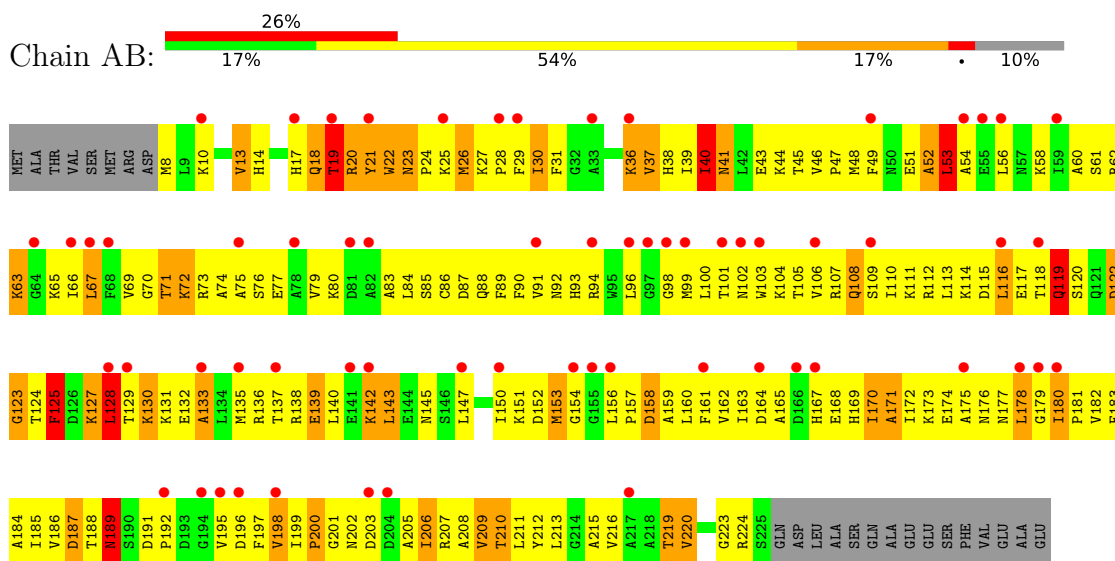
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	DB	4	Total	O	0	0
			4	4		

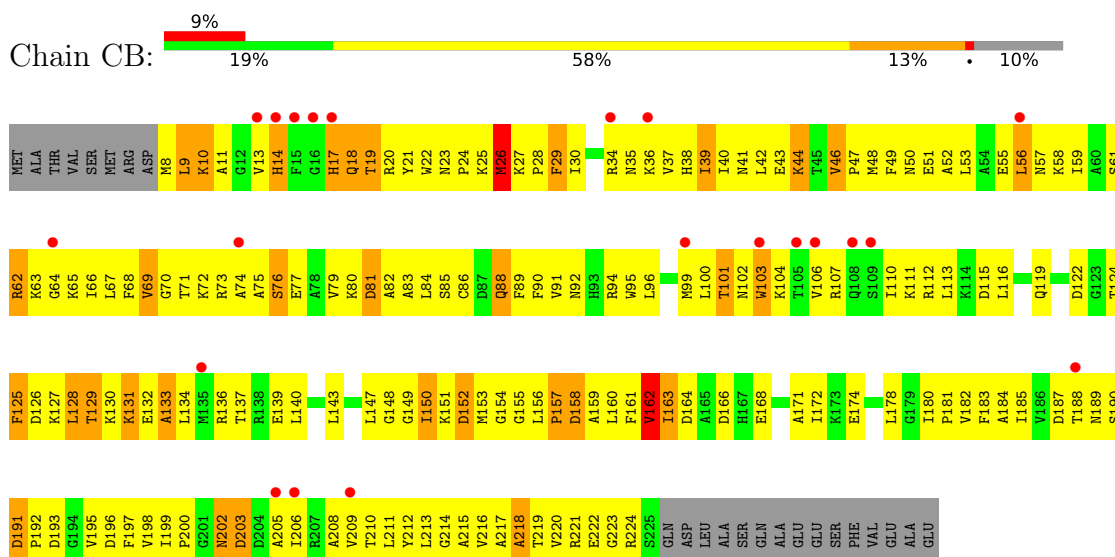
3 Residue-property plots [i](#)

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

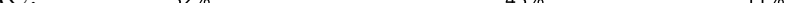
• Molecule 1: 30S ribosomal protein S2

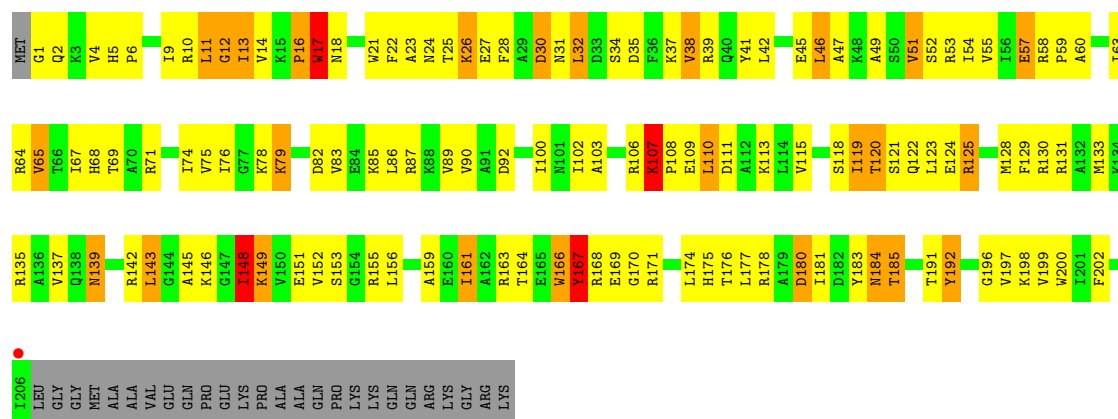


• Molecule 1: 30S ribosomal protein S2

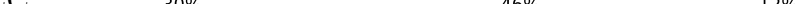


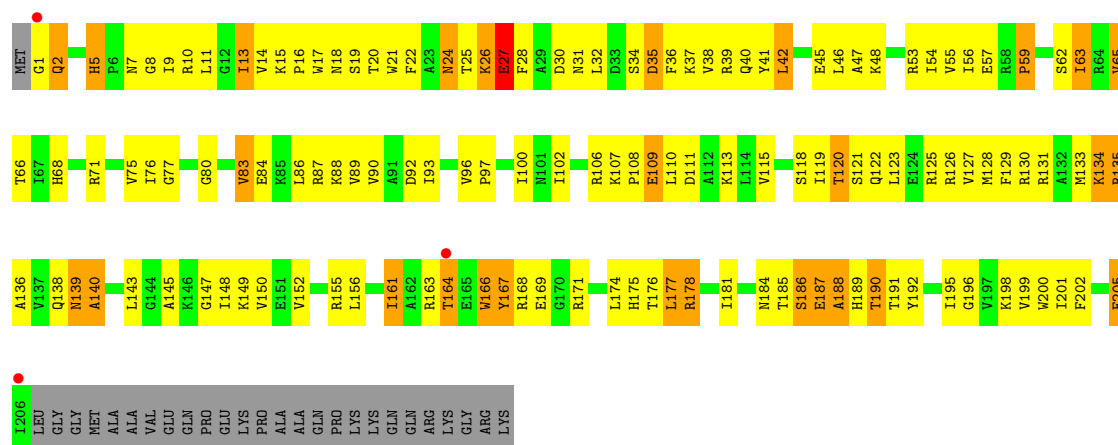
• Molecule 2: 30S ribosomal protein S3

Chain AC: 

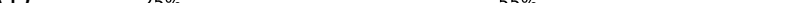


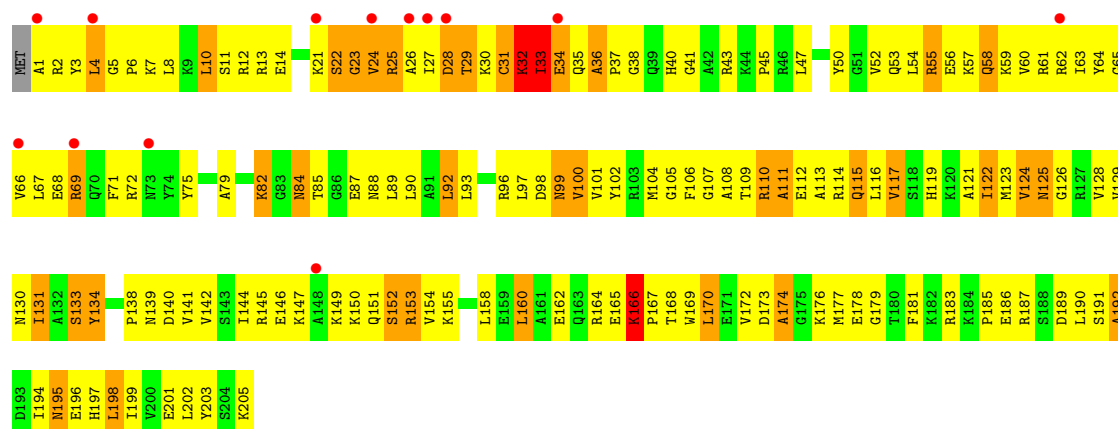
- Molecule 2: 30S ribosomal protein S3

Chain CC:  %

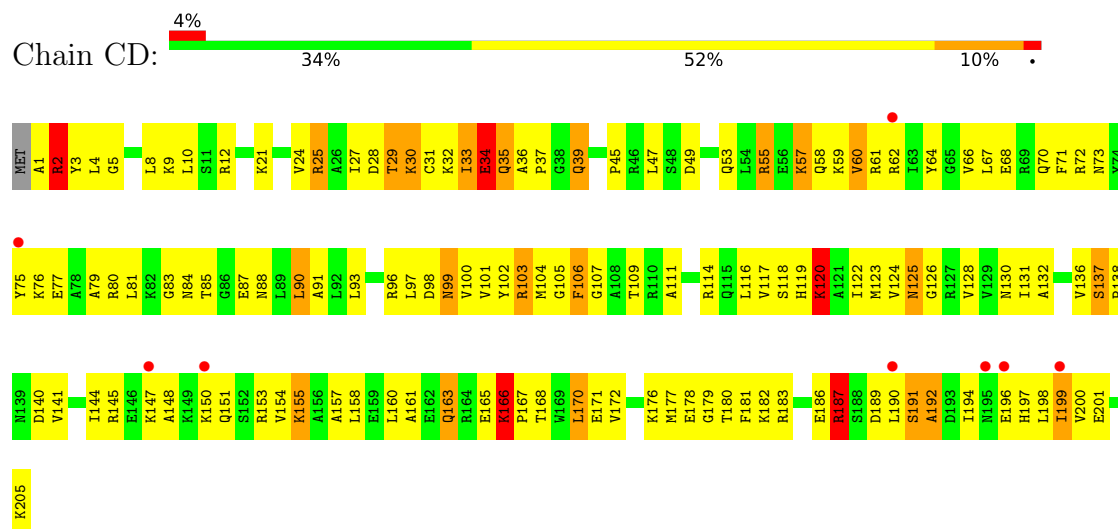


- Molecule 3: 30S ribosomal protein S4

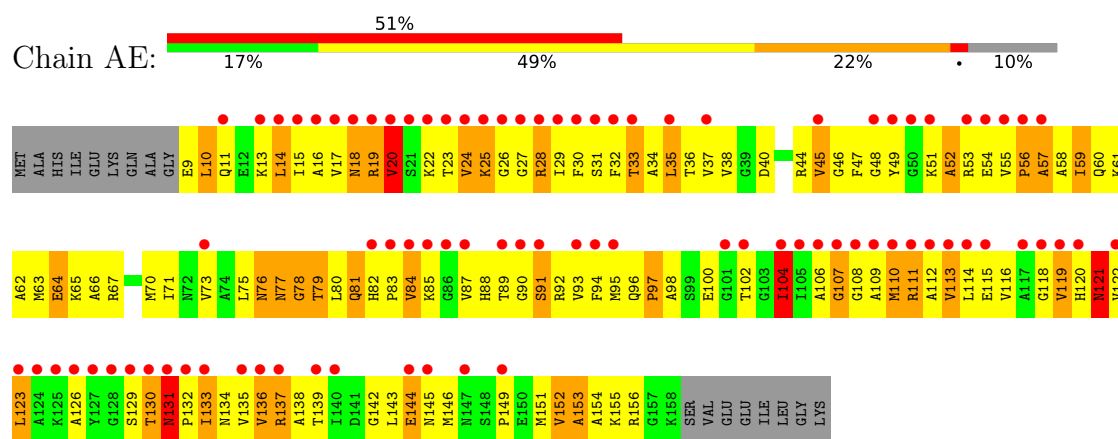
Chain AD: 



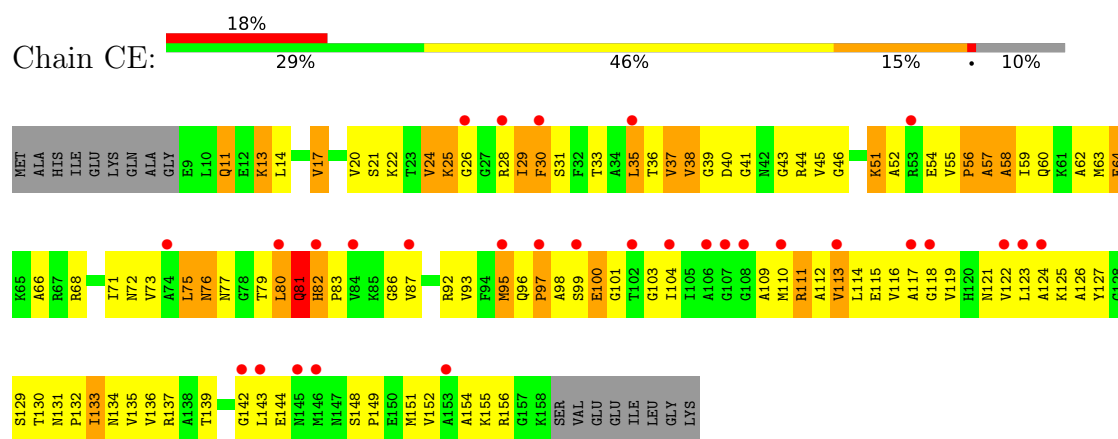
- Molecule 3: 30S ribosomal protein S4



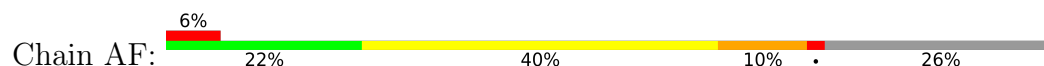
- Molecule 4: 30S ribosomal protein S5

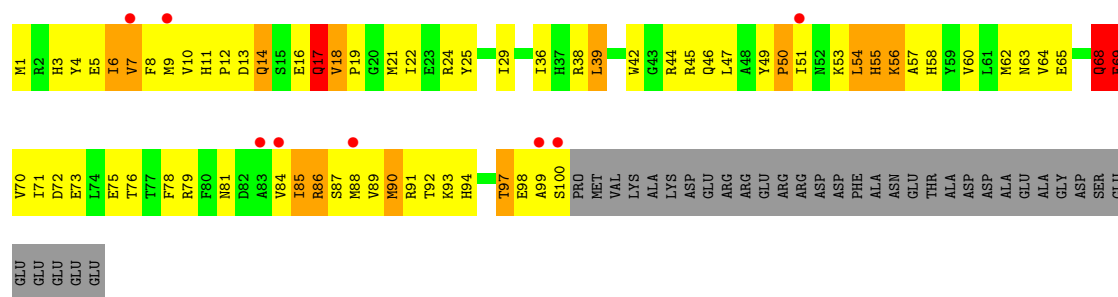


- Molecule 4: 30S ribosomal protein S5

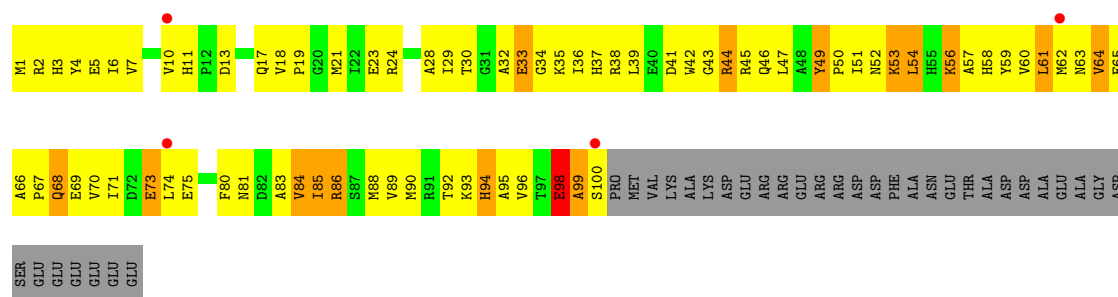
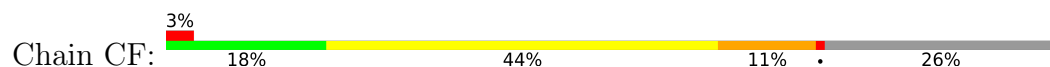


- Molecule 5: 30S ribosomal protein S6

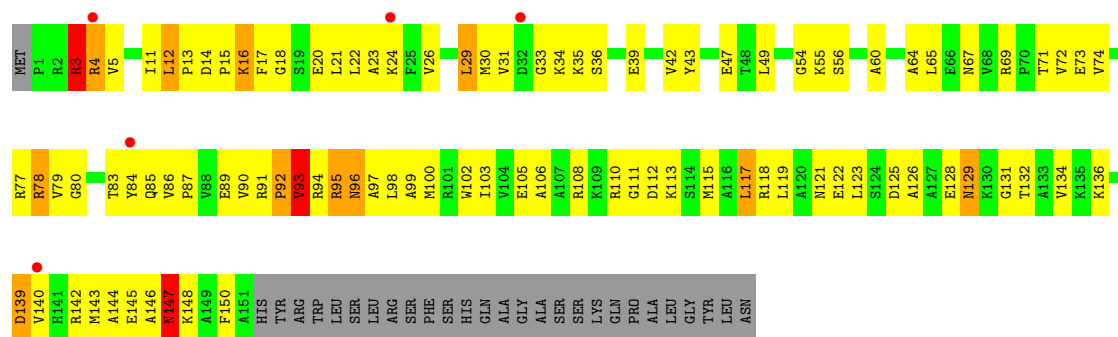




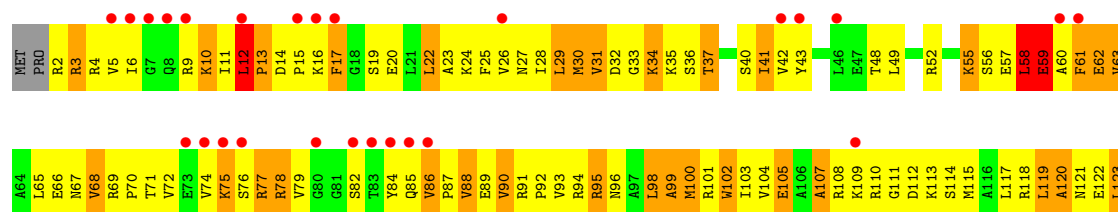
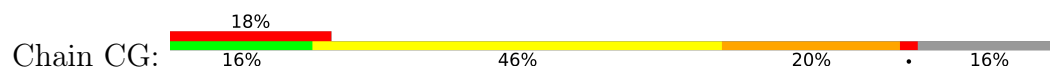
• Molecule 5: 30S ribosomal protein S6

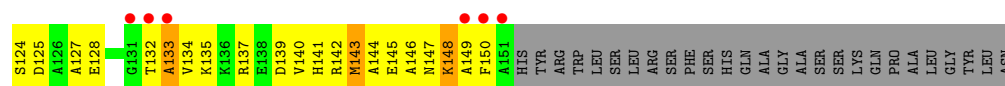


• Molecule 6: 30S ribosomal protein S7

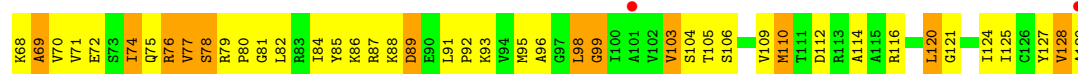


• Molecule 6: 30S ribosomal protein S7

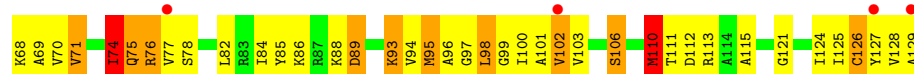
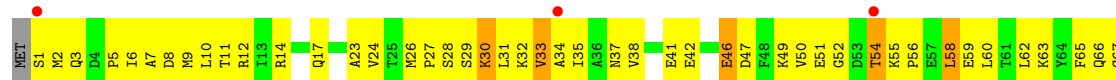




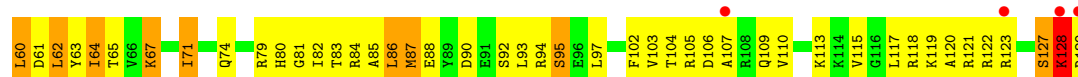
• Molecule 7: 30S ribosomal protein S8



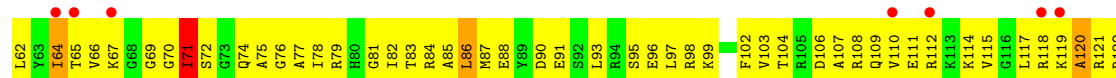
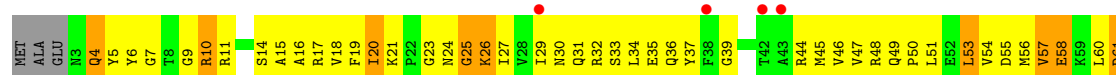
• Molecule 7: 30S ribosomal protein S8



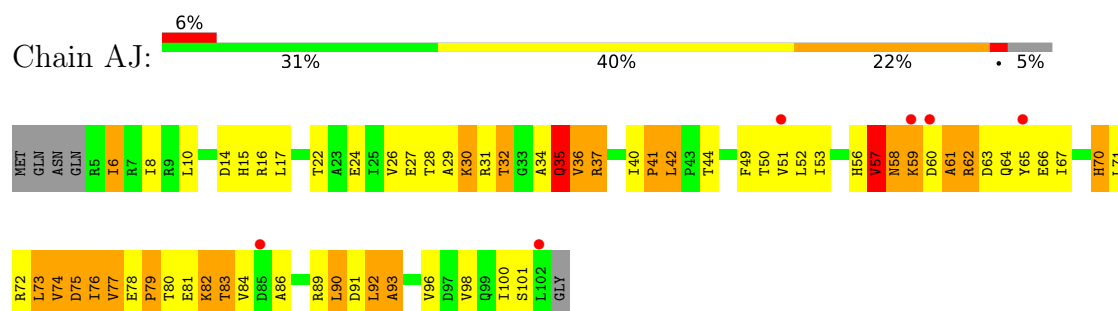
• Molecule 8: 30S ribosomal protein S9



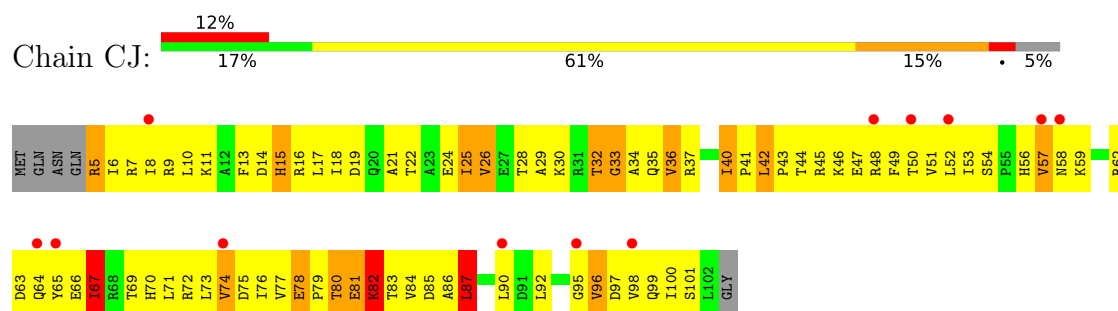
• Molecule 8: 30S ribosomal protein S9



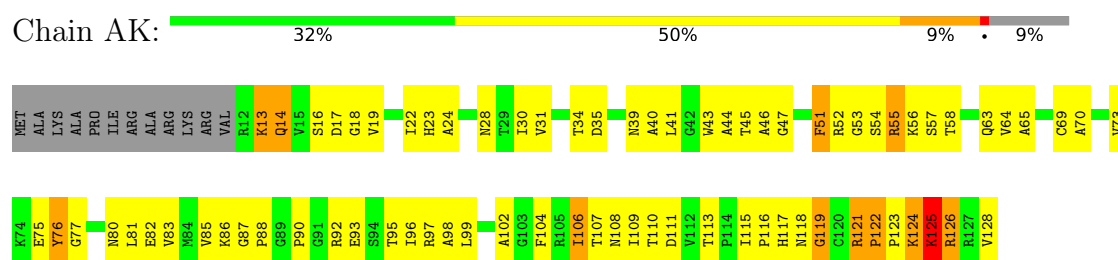
- Molecule 9: 30S ribosomal protein S10



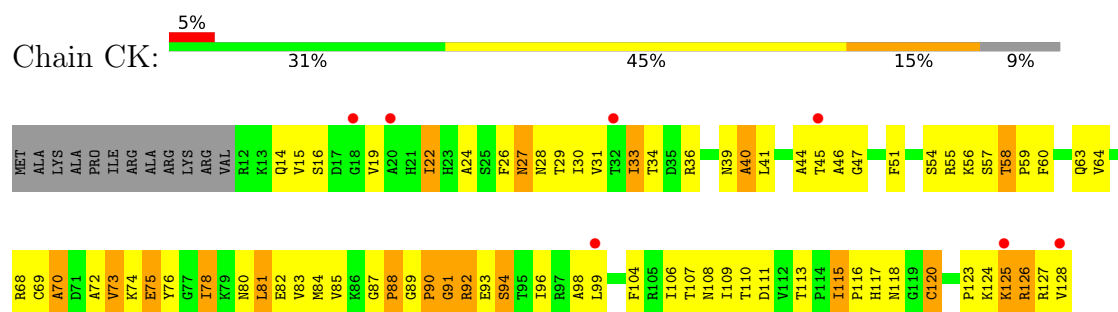
- Molecule 9: 30S ribosomal protein S10



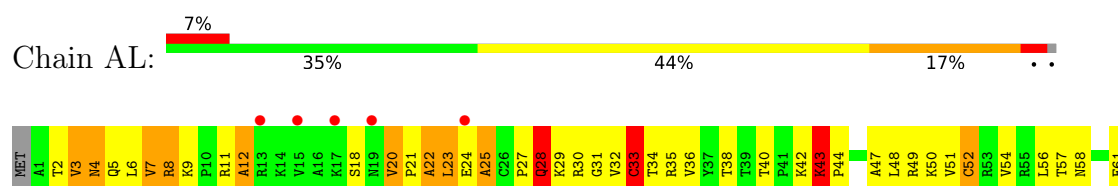
- Molecule 10: 30S ribosomal protein S11

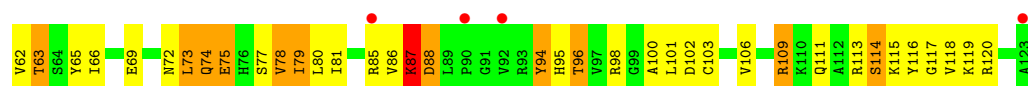


- Molecule 10: 30S ribosomal protein S11

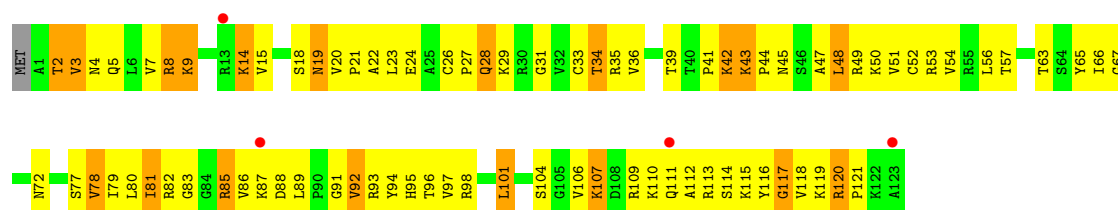


- Molecule 11: 30S ribosomal protein S12

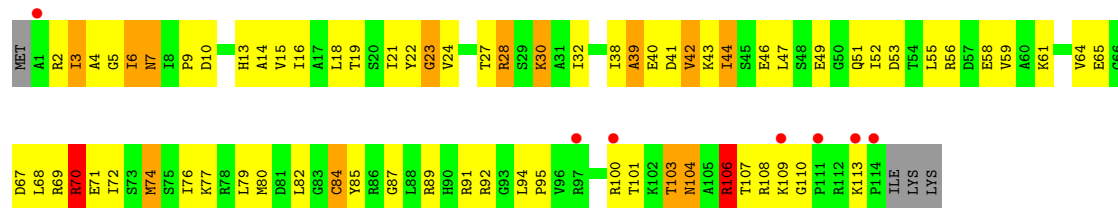




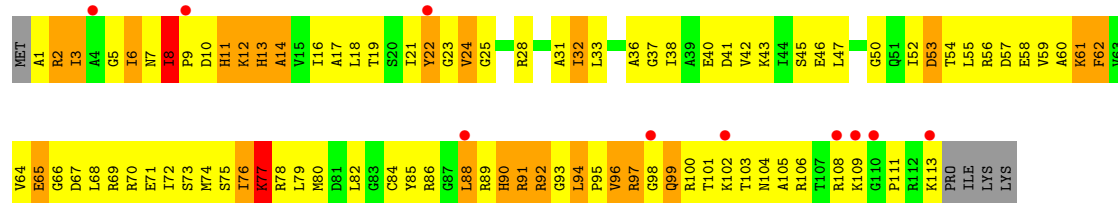
• Molecule 11: 30S ribosomal protein S12



• Molecule 12: 30S ribosomal protein S13



• Molecule 12: 30S ribosomal protein S13

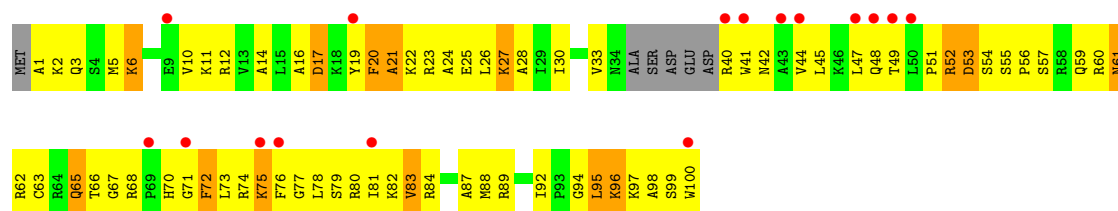


• Molecule 13: 30S ribosomal protein S14



• Molecule 13: 30S ribosomal protein S14





• Molecule 14: 30S ribosomal protein S15



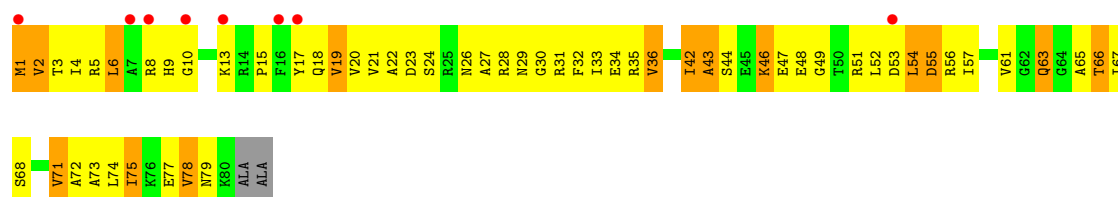
• Molecule 14: 30S ribosomal protein S15



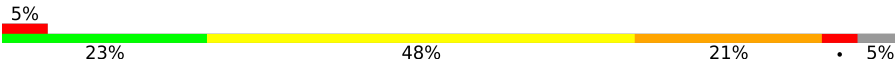
• Molecule 15: 30S ribosomal protein S16



• Molecule 15: 30S ribosomal protein S16



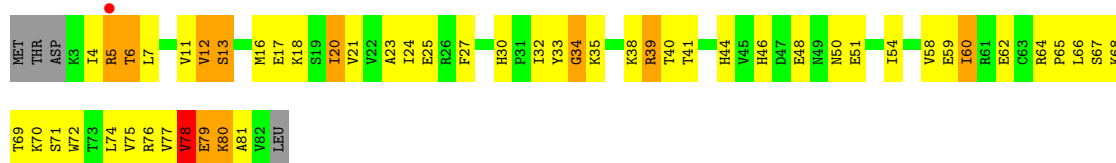
- Molecule 16: 30S ribosomal protein S17

Chain AQ: 

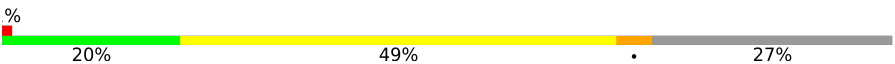


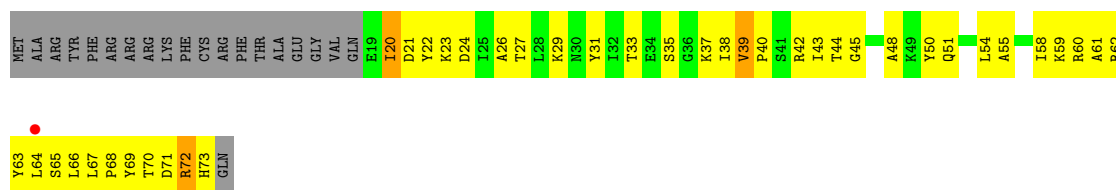
- Molecule 16: 30S ribosomal protein S17

Chain CQ: 



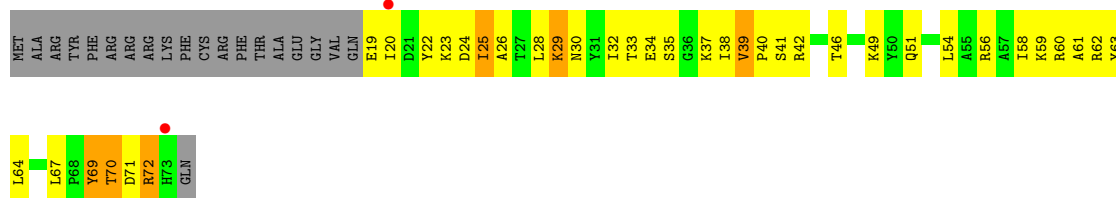
- Molecule 17: 30S ribosomal protein S18

Chain AR: 

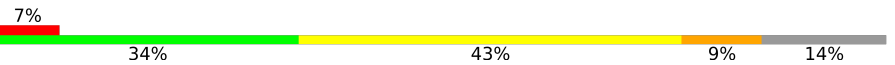


- Molecule 17: 30S ribosomal protein S18

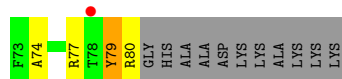
Chain CR: 



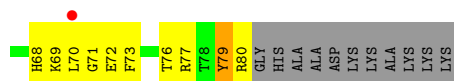
- Molecule 18: 30S ribosomal protein S19

Chain AS: 

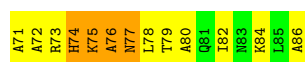




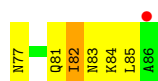
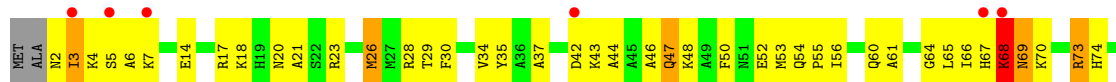
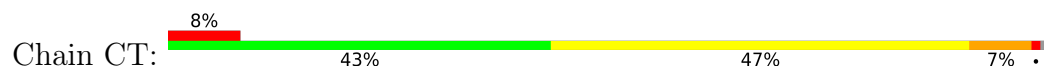
- Molecule 18: 30S ribosomal protein S19



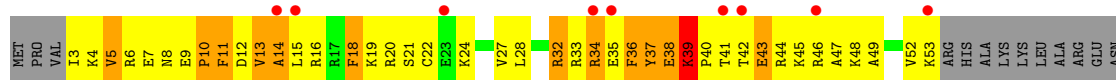
- Molecule 19: 30S ribosomal protein S20



- Molecule 19: 30S ribosomal protein S20

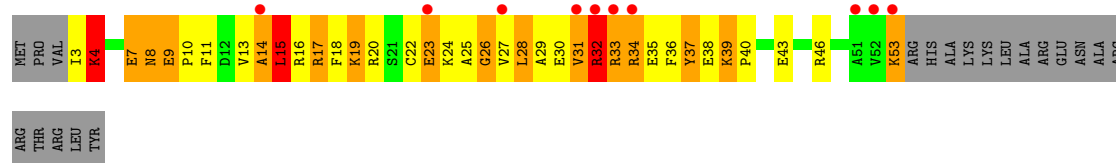


- Molecule 20: 30S ribosomal protein S21

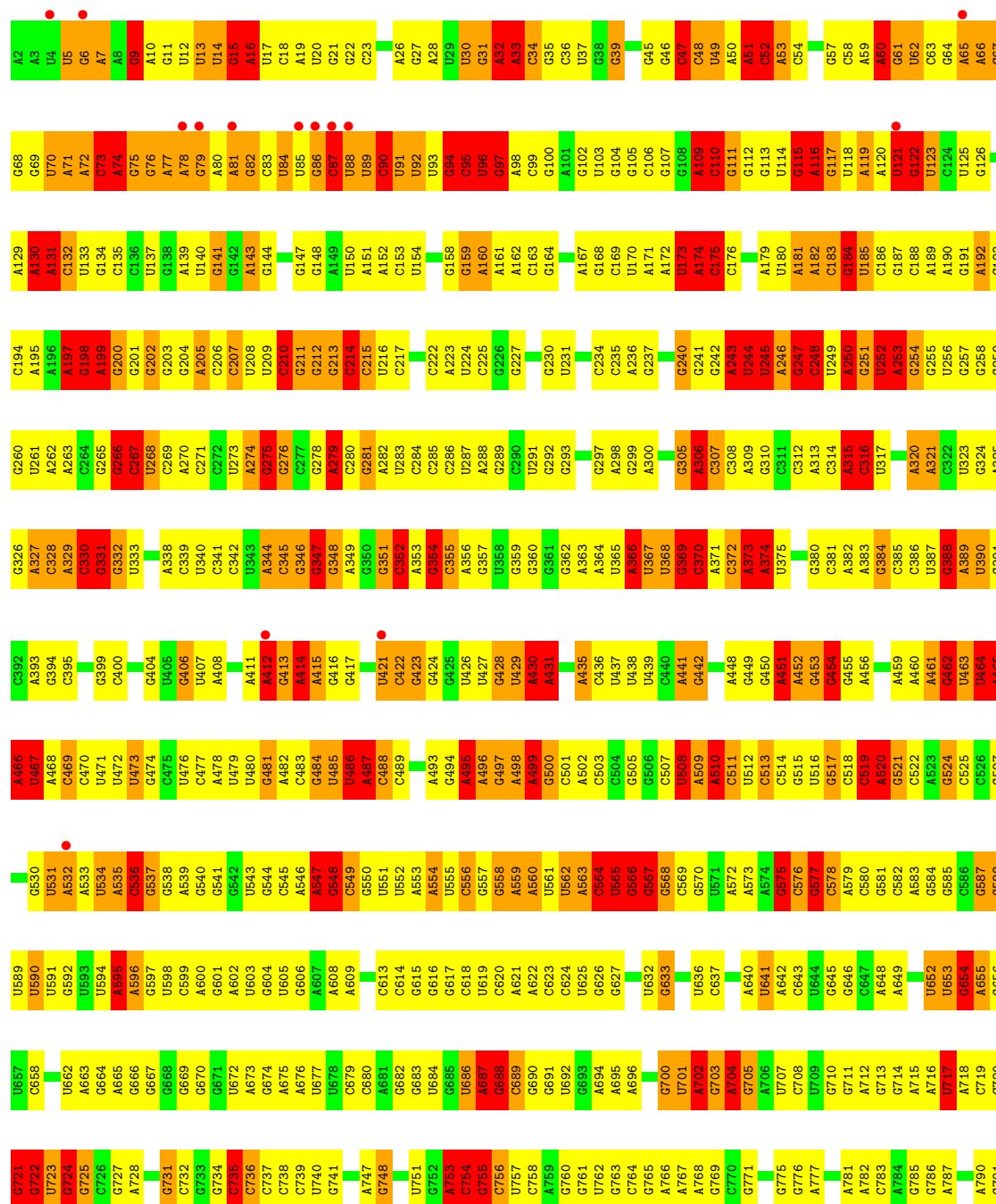
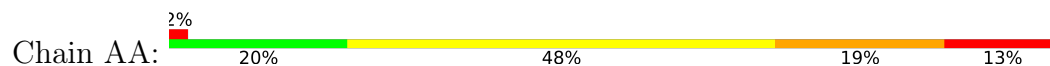


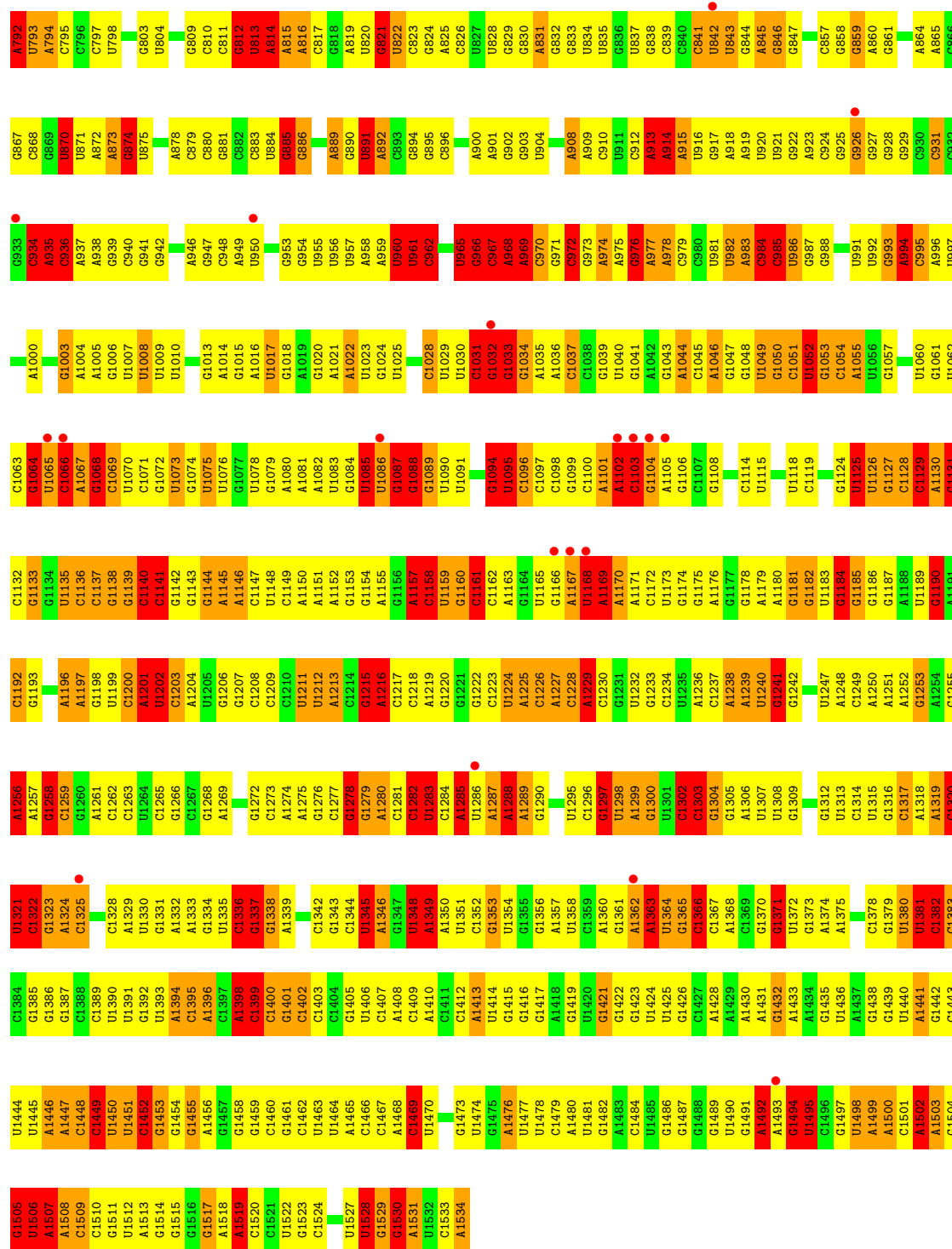
- Molecule 20: 30S ribosomal protein S21



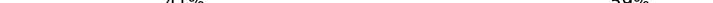


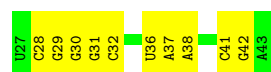
• Molecule 21: 16S rRNA



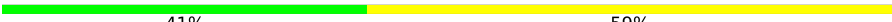


- Molecule 22: P-site tRNA ASL fragment

Chain AV:  41% 59%



- Molecule 22: P-site tRNA ASL fragment

Chain CV:  41% 59%



- Molecule 23: messenger RNA

Chain AW:  67% 33%



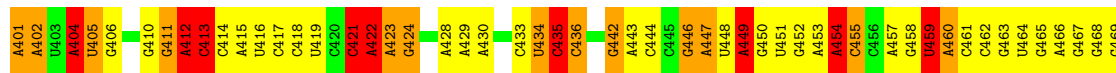
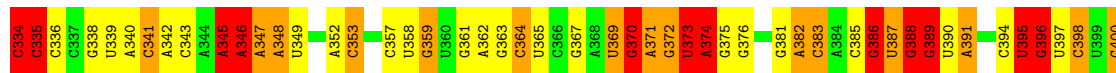
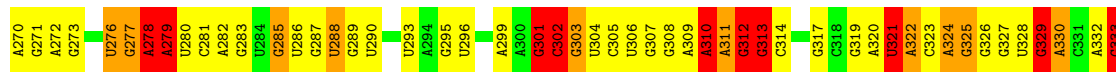
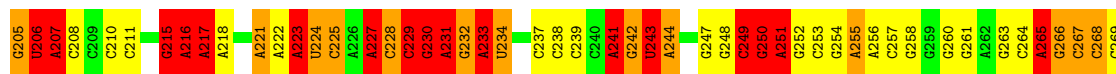
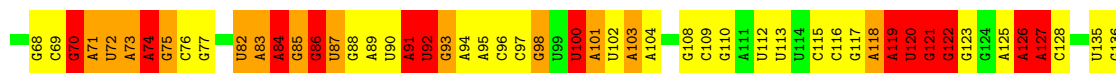
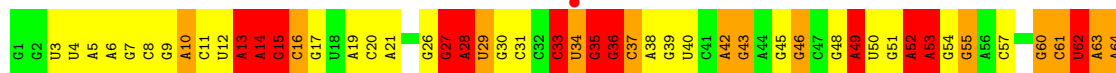
- Molecule 23: messenger RNA

Chain CW:  67% 33%



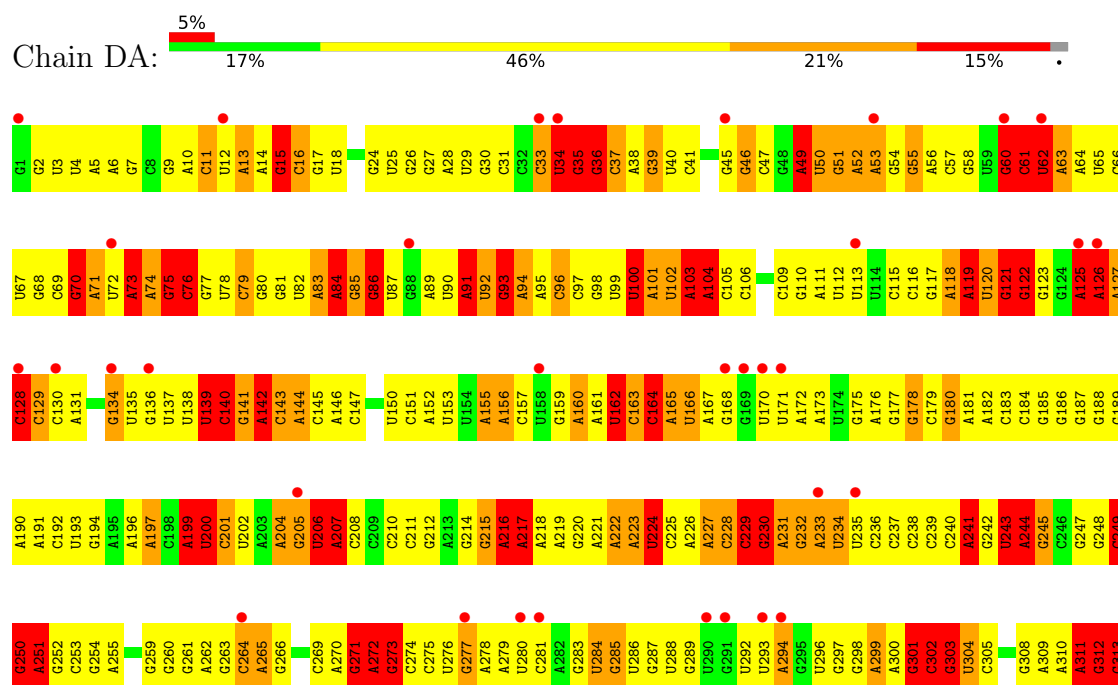
- Molecule 24: 23S rRNA

Chain BA:  2% 19% 44% 20% 15%



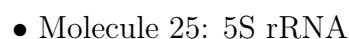
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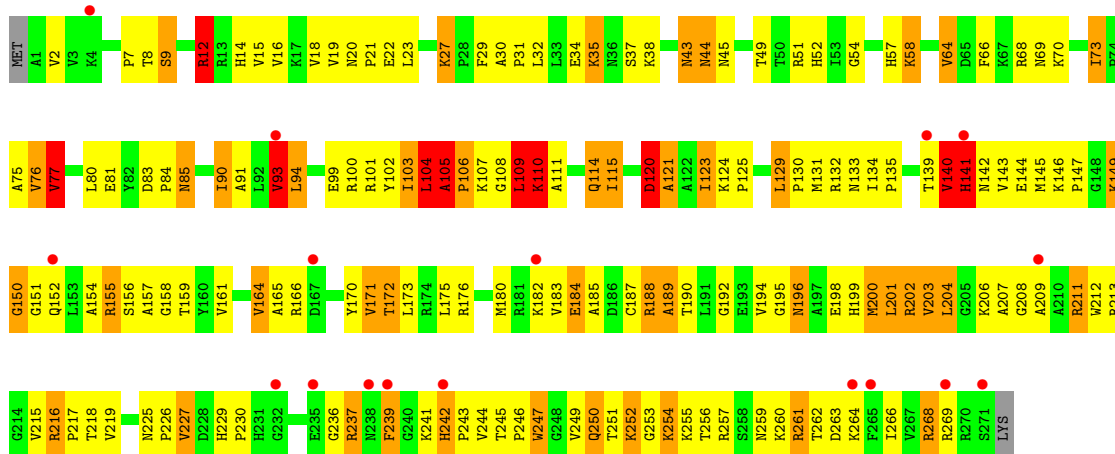
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G2035	C1967	G1904	G1775	U1776	G1708	G1643	A1579	C1518	G1456	A1393	G1332	C1270	A1205
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G2046	A1978	U1917	G1849	A1786	G1654	A1590	A1590	G1529	U1467	C1404	A1343	G1281	U1219
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G2049	A1981	C1920	A1854	A1789	U1657	U1657	U1657	A1532	A1470	G1407	G1346	A1284	C1221
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G2061	G1936	G1937	G1867	A1802	U1735	U1671	C1607	A1544	G1483	G1422	G1358	C1298	G1236
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U2075	G1848	G1817	U1751	C1696	C1696	C1697	C1697	G1560	C1498	G1437	U1375	C1314	G1253
G2076	U1885	A1818	G1752	U1687	C1625	A1626	U1562	U1438	C1499	U1438	C1376	C1315	A1254
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G2083	U1825	G1818	G1761	G1696	A1633	G1633	A1508	G1445	A1384	C1323	C1323	A1264	A1265
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G2086	G1828	A1817	G1763	A1698	A1635	A1635	A1572	G1448	C1388	U1326	A1388	A1268	G1267
A2087	A1829	A1818	C1764	G1699	U1636	A1637	A1573	C1451	G1389	A1328	A1328	A1269	G1268
U2088	G1830	A1819	U1770	A1700	A1637	A1637	C1574	G1452	G1389	A1328	A1328	A1270	G1269
G2089	G1831	A1820	G1770	A1701	A1638	A1638	C1575	C1575	G1390	A1329	A1329	A1271	G1269
C2090	A1832	A1821	C1771	G1702	C1639	C1639	C1576	C1576	G1391	A1330	A1330	A1272	G1270
U2091	G1833	A1822	U1772	A1703	C1640	C1640	C1577	C1577	G1392	A1331	A1331	A1273	G1271
G2092	A1834	G1823	A1773	C1641	C1641	C1641	C1578	C1578	G1393	A1332	A1332	A1274	G1272
C2093	G1835	A1824	U1774	C1642	C1642	C1642	C1579	C1579	G1394	A1333	A1333	A1275	G1273
U2094	U1836	A1825	U1775	G1643	G1643	G1643	C1580	C1580	G1395	A1334	A1334	A1276	G1274
G2095	G1837	G1826	U1776	G1644	G1644	G1644	A1581	U1521	U1458	A1395	G1335	A1277	G1275
U2096	C1838	A1815	U1777	G1645	G1645	G1645	C1582	G1522	G1459	U1396	C1336	A1278	G1276
A2097	A1839	A1816	U1778	C1646	C1646	C1646	A1583	A1523	U1460	U1397	A1337	A1279	G1277
G2098	G1840	G1817	U1779	U1647	U1647	U1647	U1584	U1522	A1461	U1398	G1338	A1280	G1278
U2099	U1841	A1818	U1780	U1648	U1648	U1648	A1585	G1524	C1462	C1399	G1339	A1281	G1279
A2100	C1843	U1781	U1781	G1649	G1649	G1649	A1586	A1525	C1463	U1400	U1340	A1282	G1280
G2101	G1844	A1782	U1782	A1650	A1586	A1586	G1587	G1526	G1464	U1401	U1341	A1283	G1281
U2102	A1845	A1783	A1783	G1651	G1587	G1587	G1588	G1527	G1465	U1402	U1342	A1284	G1282
G2103	A1846	A1784	G1718	G1652	G1588	G1588	U1589	A1528	U1466	A1403	A1342	A1285	G1283
U2104	G1719	G1719	G1719	G1653	U1589	U1589	A1590	G1529	U1467	U1404	A1343	A1286	G1284
A2105	U1720	U1720	U1720	A1654	A1591	A1591	A1591	G1530	U1468	U1405	U1344	A1287	G1285
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U2110	U1725	U1725	U1725	U1660	A1597	A1597	A1597	A1535	U1475	A1413	C1350	C1292	G1290
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G2112	C1727	C1727	C1727	U1662	U1599	U1599	U1599	G1537	U1477	U1415	C1352	C1294	G1292
U2113	G1728	G1728	G1728	A1663	G1600	G1600	G1600	U1538	A1478	G1416	A1353	C1295	G1293
A2114	U1729	U1729	U1729	G1664	G1601	G1601	U1602	G1415	U1479	C1417	A1354	C1296	G1294
G2115	G1730	G1730	G1730	G1665	U1602	U1602	A1603	U1539	G1478	G1418	G1355	C1297	G1295
U2116	C1731	C1731	C1731	G1666	A1603	A1603	A1603	G1540	U1479	G1419	G1356	C1298	G1296
A2117	G1732	G1732	G1732	U1667	C1604	C1604	C1604	C1541	C1480	A1419	C1357	C1299	A1237
G2118	U1733	U1733	U1733	A1668	C1605	C1605	C1605	U1542	U1481	G1420	G1358	G1300	G1238
U2119	G1734	G1734	G1734	A1669	G1606	G1606	G1606	G1543	G1482	G1421	A1359	G1299	G1239
A2120	A1800	A1800	A1800	C1670	C1607	C1607	C1607	A1544	G1483	G1422	G1360	A1301	U1240
G2121	G1801	G1801	G1801	U1671	U1671	U1671	U1671	U1545	U1484	G1423	G1361	A1302	U1241
U2122	A1802	A1802	A1802	A1672	A1608	A1608	A1608	U1552	U1485	G1424	G1362	G1303	U1242
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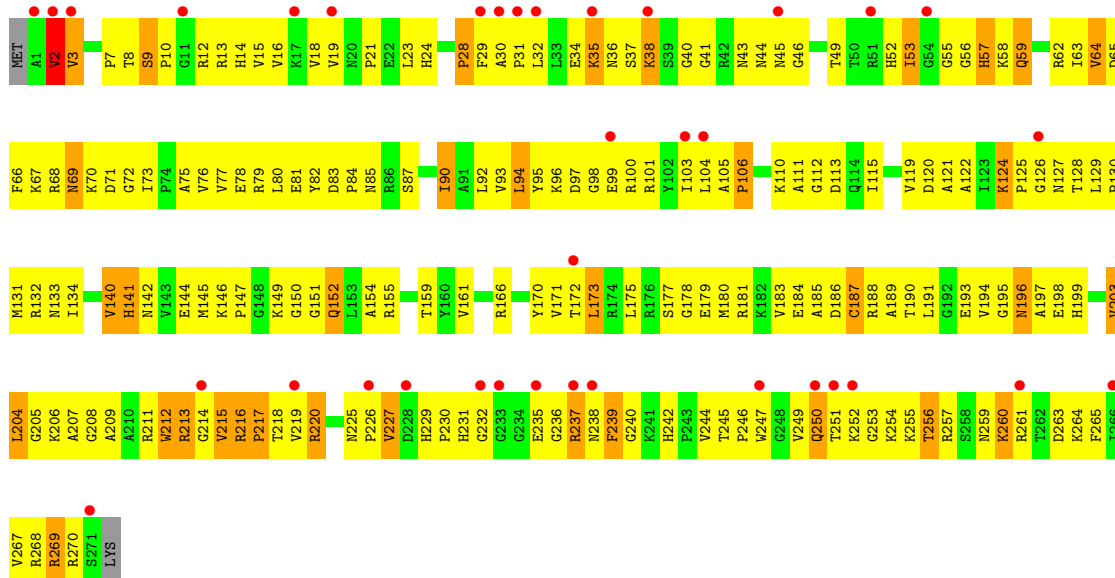




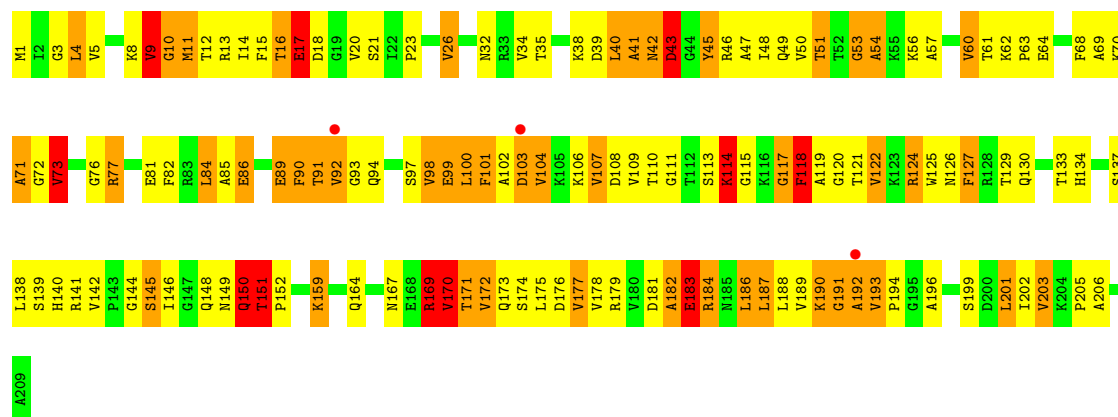
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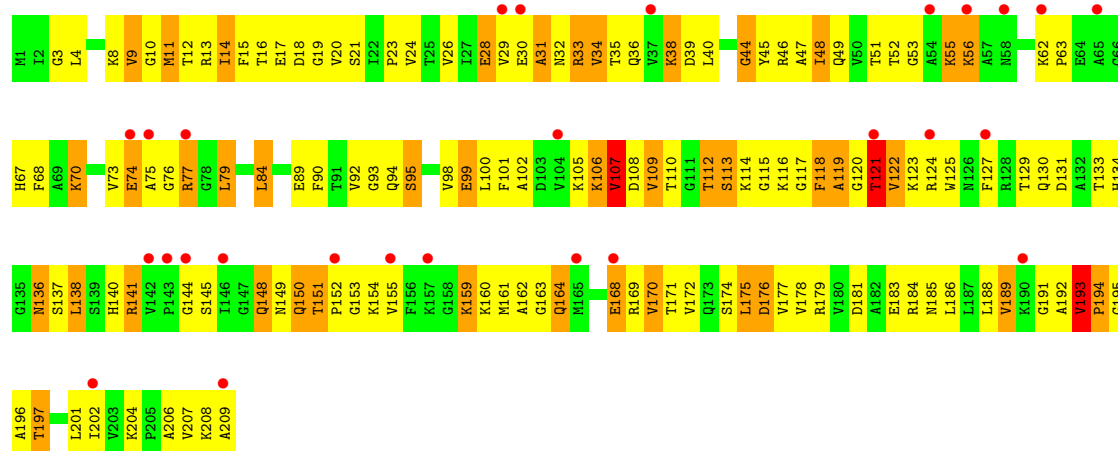
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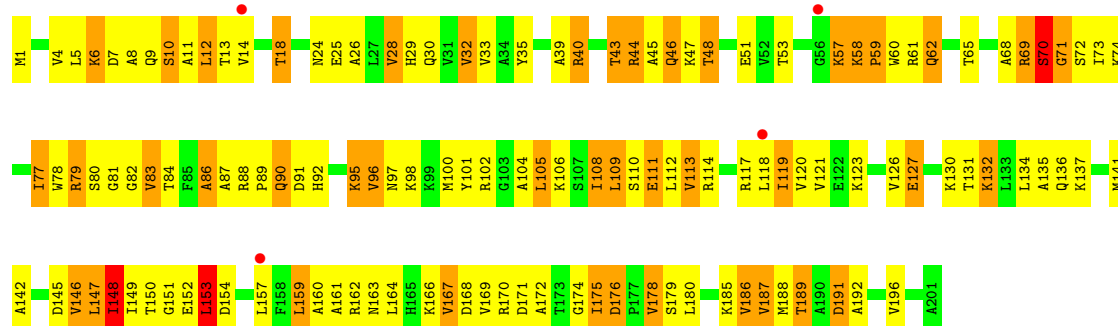
Chain BD: %



• Molecule 27: 50S ribosomal protein L3

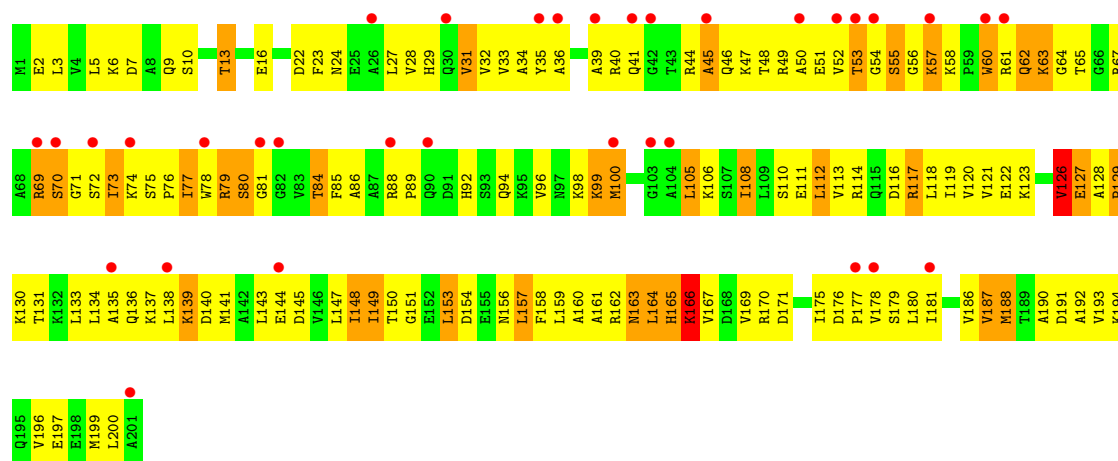


• Molecule 28: 50S ribosomal protein L4

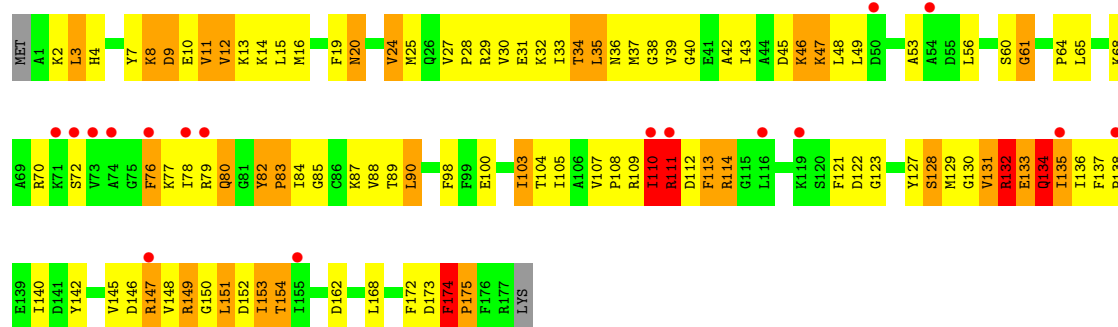


• Molecule 28: 50S ribosomal protein L4

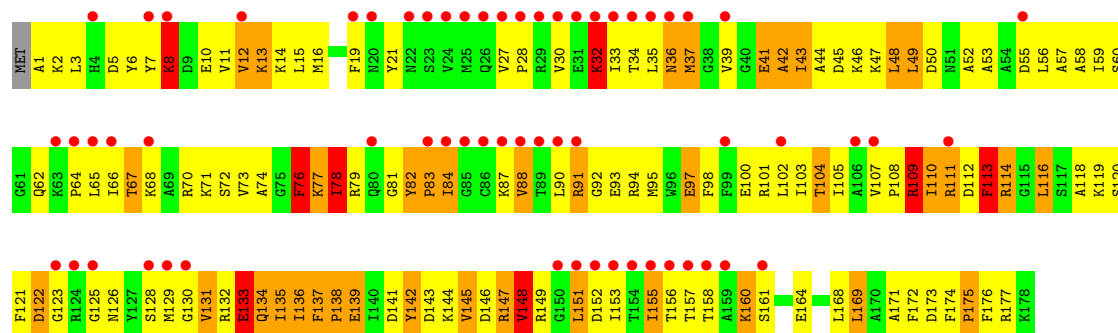




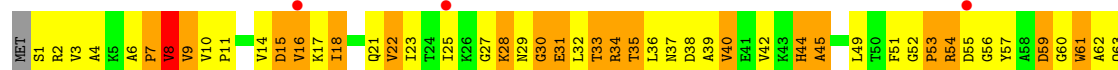
• Molecule 29: 50S ribosomal protein L5

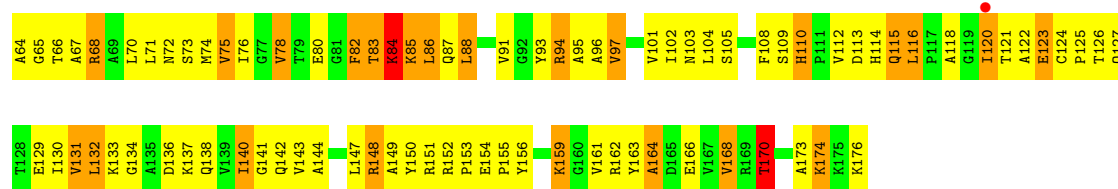


• Molecule 29: 50S ribosomal protein L5

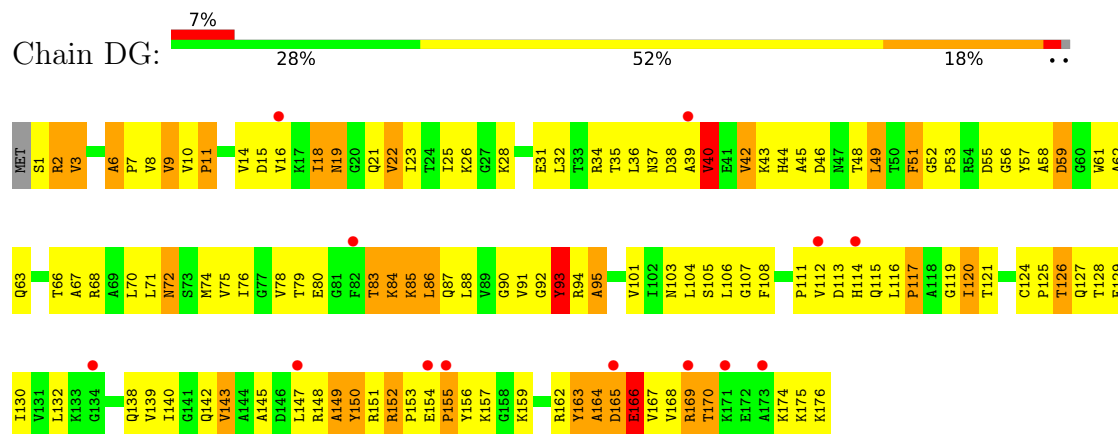


• Molecule 30: 50S ribosomal protein L6

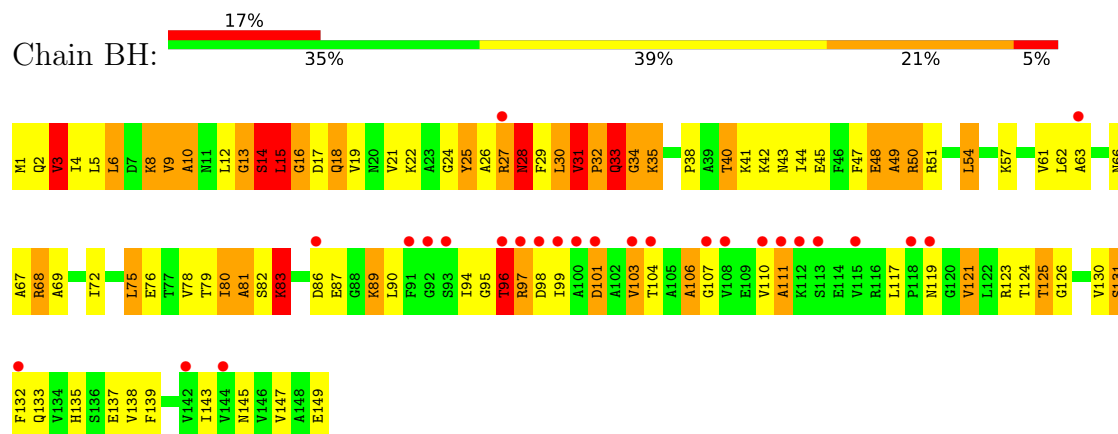




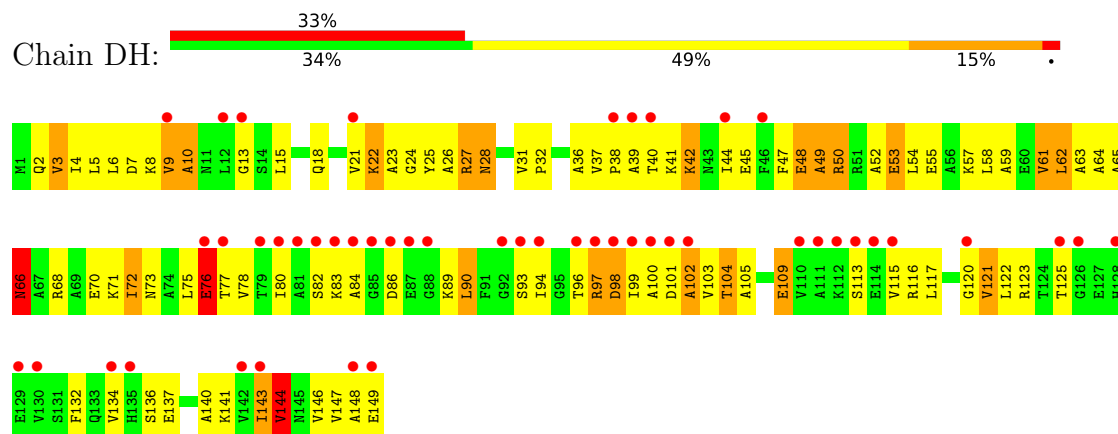
• Molecule 30: 50S ribosomal protein L6



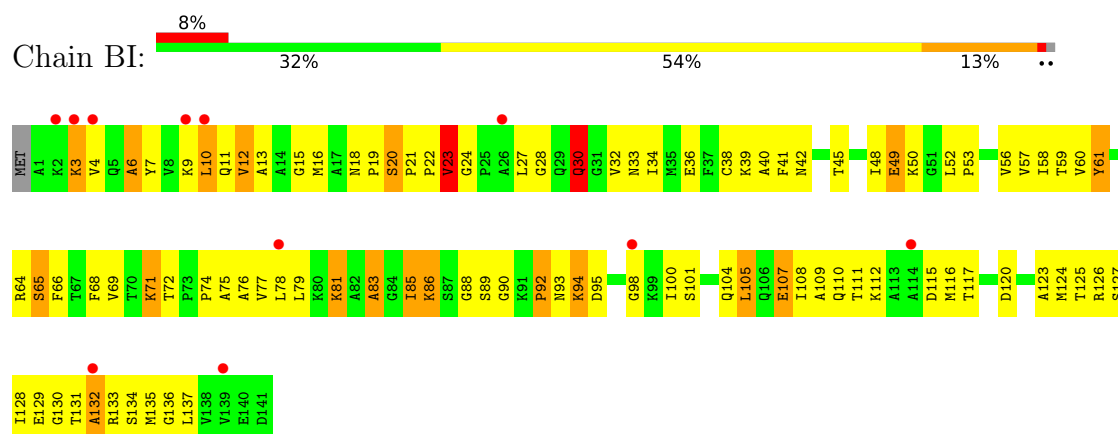
• Molecule 31: 50S ribosomal protein L9



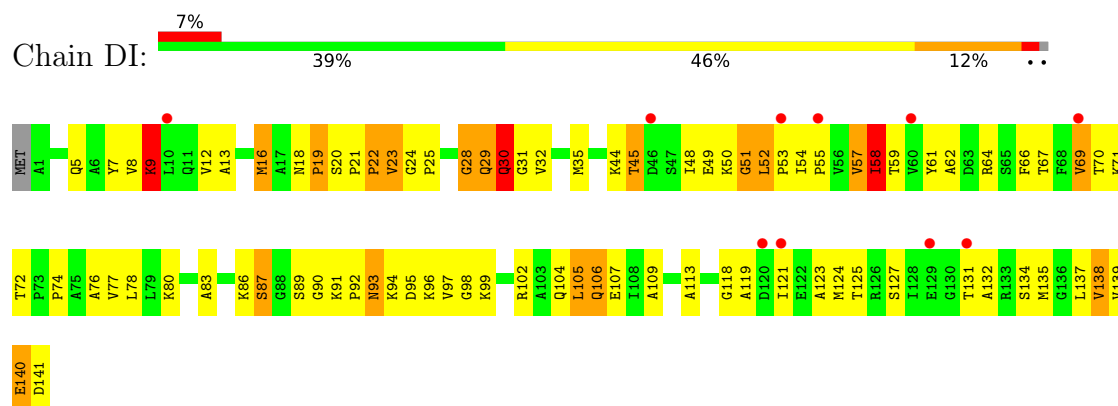
• Molecule 31: 50S ribosomal protein L9



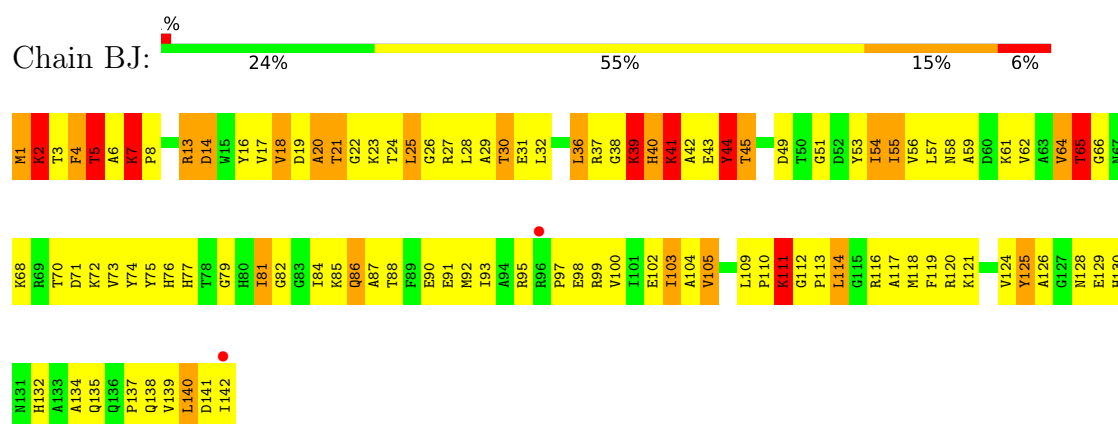
• Molecule 32: 50S ribosomal protein L11



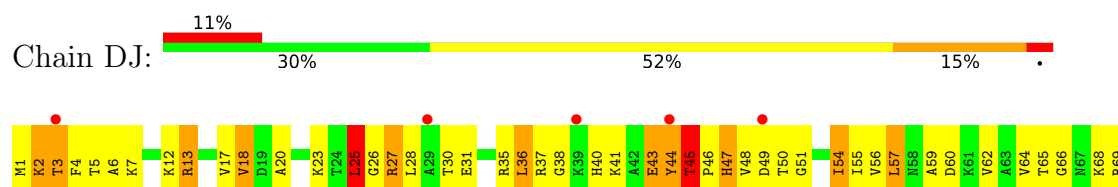
• Molecule 32: 50S ribosomal protein L11

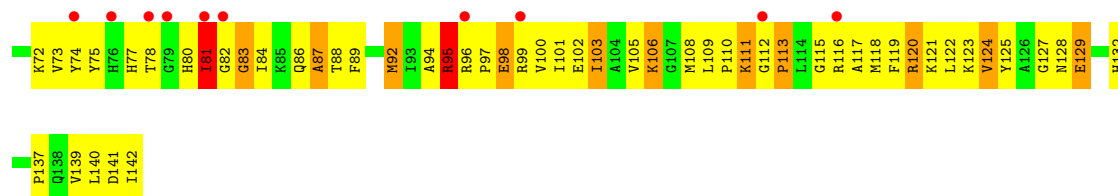


• Molecule 33: 50S ribosomal protein L13

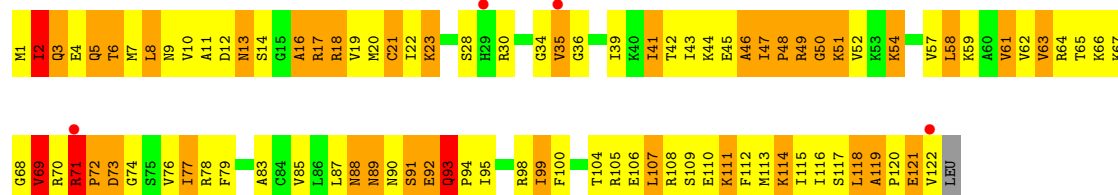
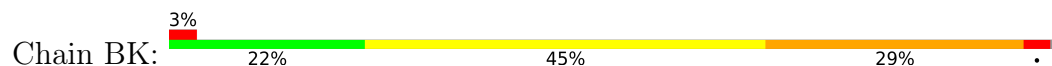


• Molecule 33: 50S ribosomal protein L13

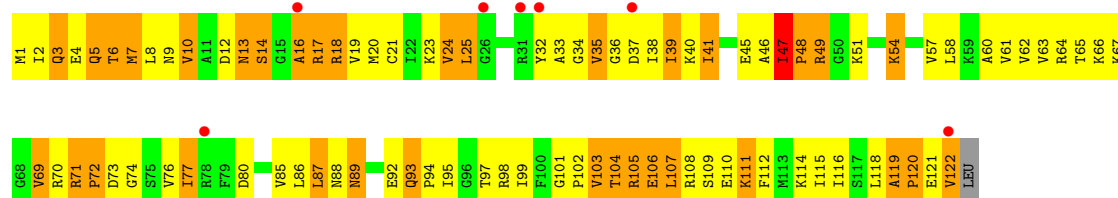




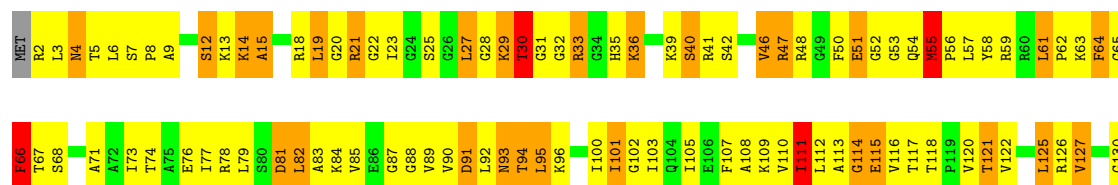
• Molecule 34: 50S ribosomal protein L14



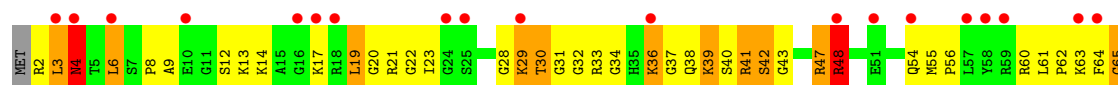
• Molecule 34: 50S ribosomal protein L14

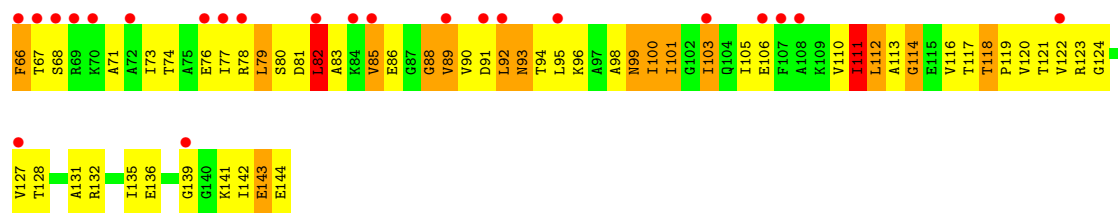


• Molecule 35: 50S ribosomal protein L15

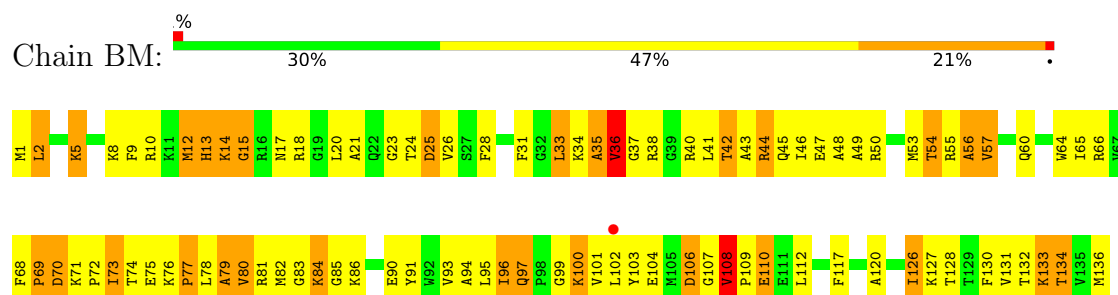


• Molecule 35: 50S ribosomal protein L15

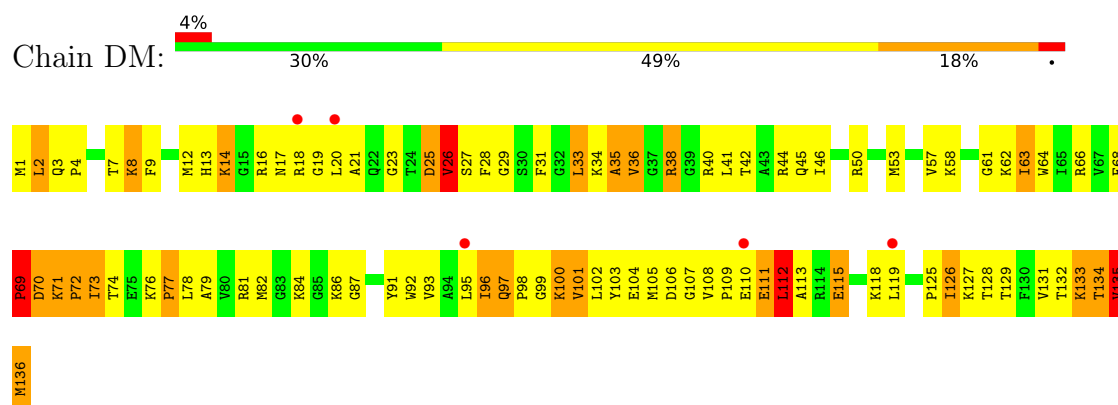




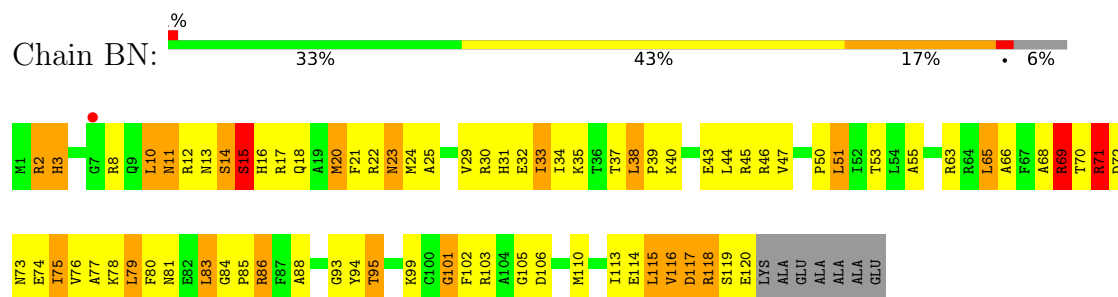
• Molecule 36: 50S ribosomal protein L16



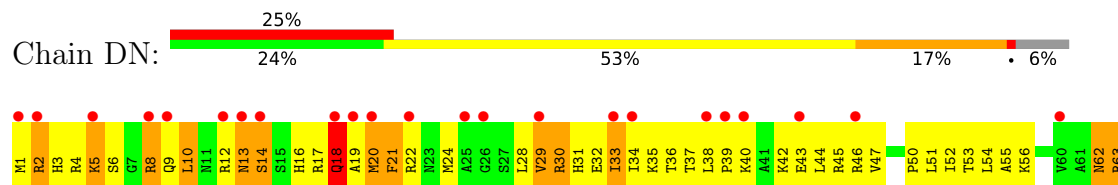
• Molecule 36: 50S ribosomal protein L16

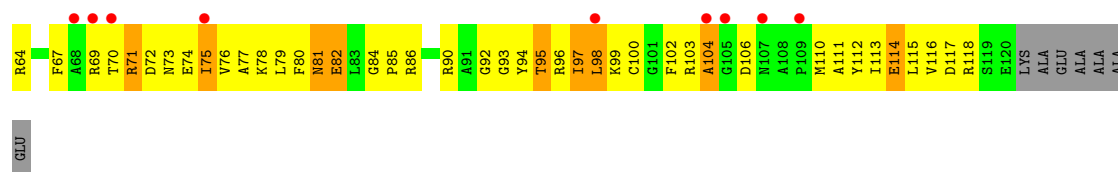


• Molecule 37: 50S ribosomal protein L17

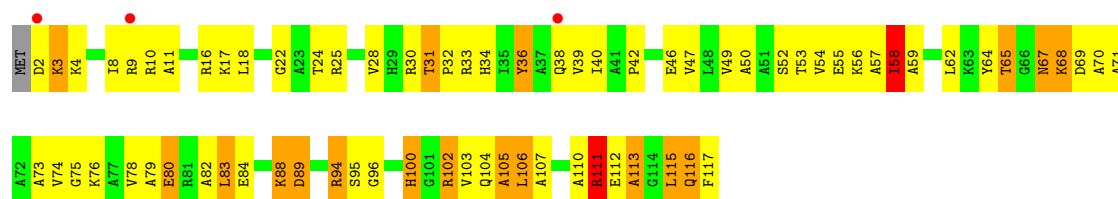


• Molecule 37: 50S ribosomal protein L17

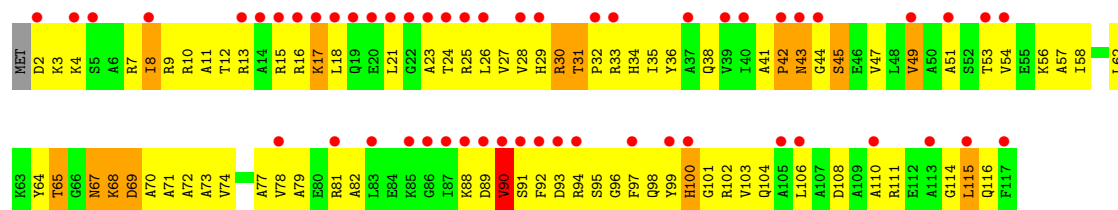




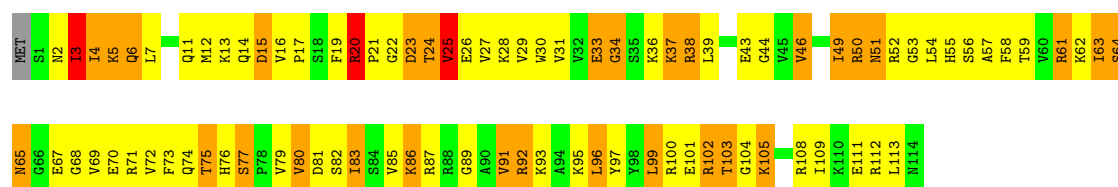
- Molecule 38: 50S ribosomal protein L18



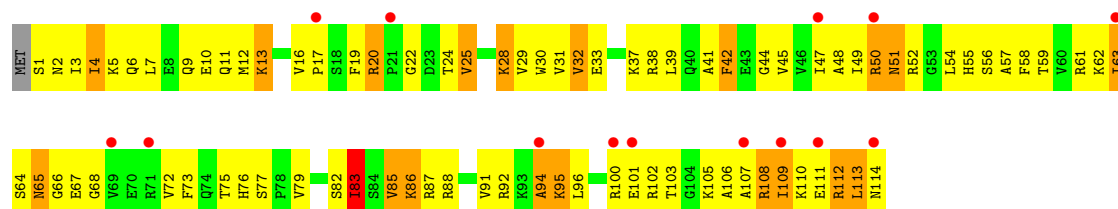
- Molecule 38: 50S ribosomal protein L18



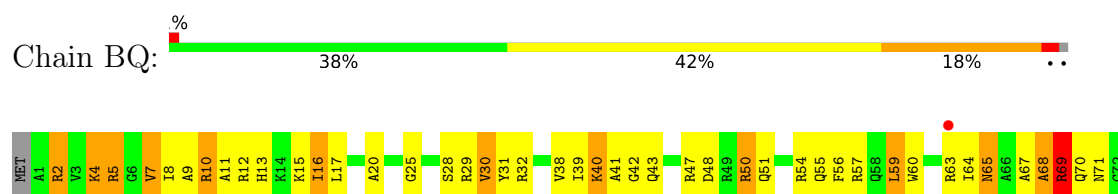
- Molecule 39: 50S ribosomal protein L19



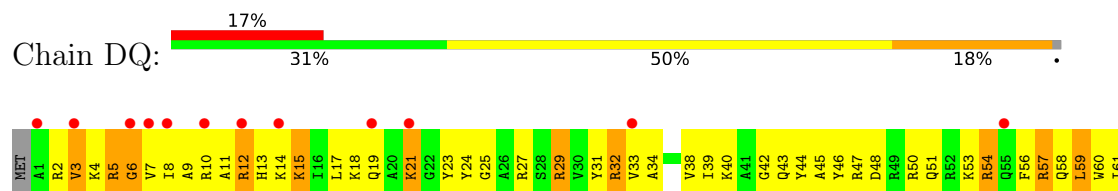
- Molecule 39: 50S ribosomal protein L19



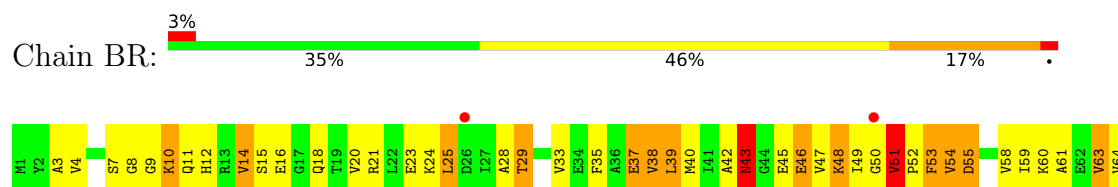
- Molecule 40: 50S ribosomal protein L20



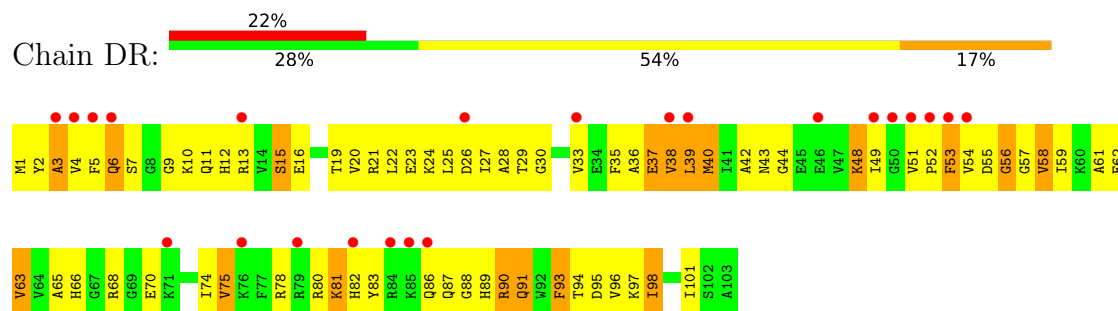
• Molecule 40: 50S ribosomal protein L20



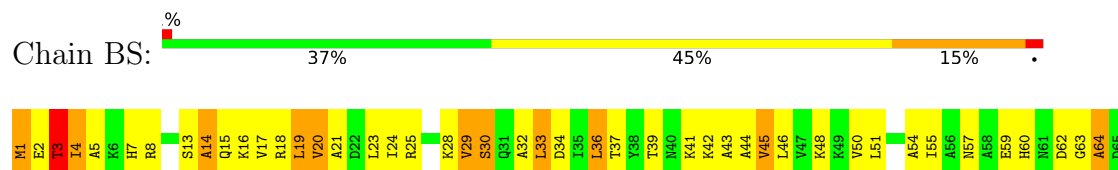
• Molecule 41: 50S ribosomal protein L21

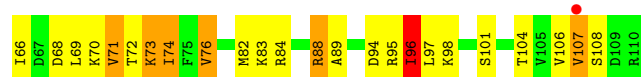


• Molecule 41: 50S ribosomal protein L21

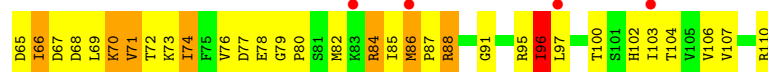


• Molecule 42: 50S ribosomal protein L22

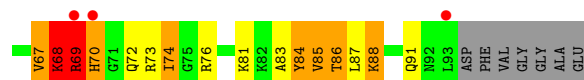
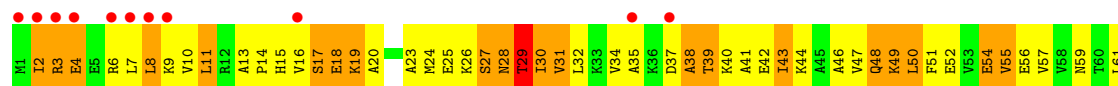
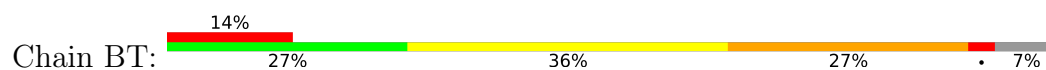




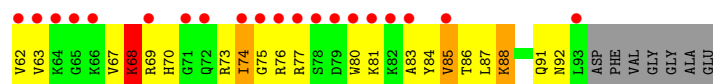
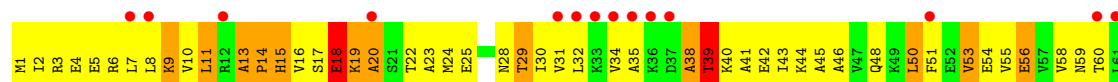
• Molecule 42: 50S ribosomal protein L22



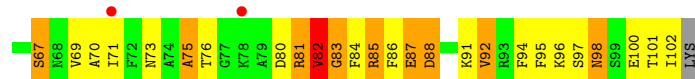
• Molecule 43: 50S ribosomal protein L23



• Molecule 43: 50S ribosomal protein L23

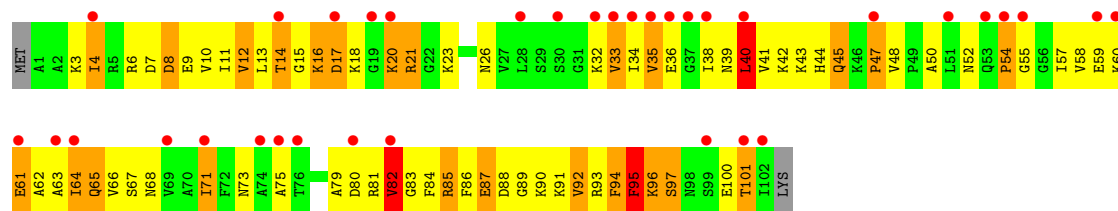


• Molecule 44: 50S ribosomal protein L24

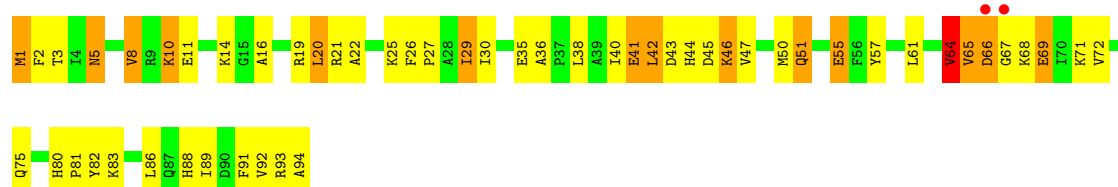
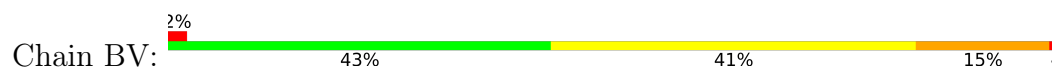


• Molecule 44: 50S ribosomal protein L24

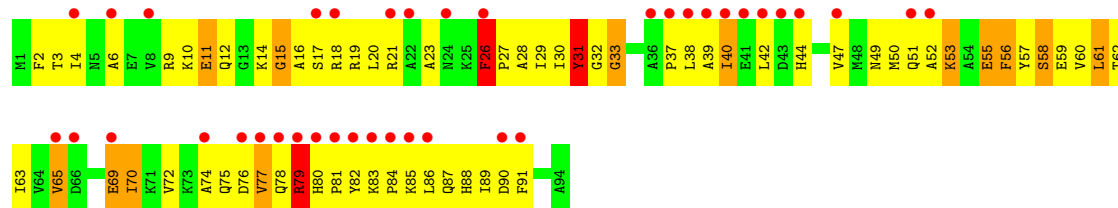




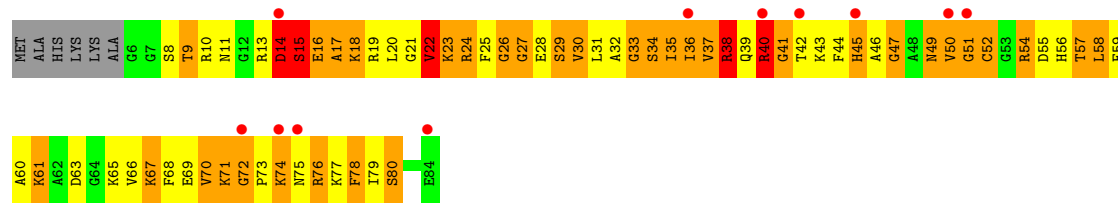
• Molecule 45: 50S ribosomal protein L25



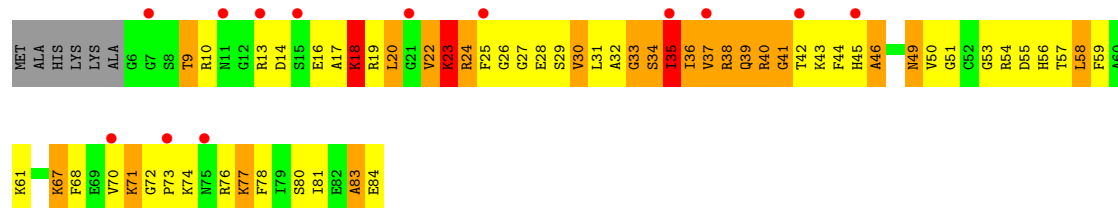
• Molecule 45: 50S ribosomal protein L25



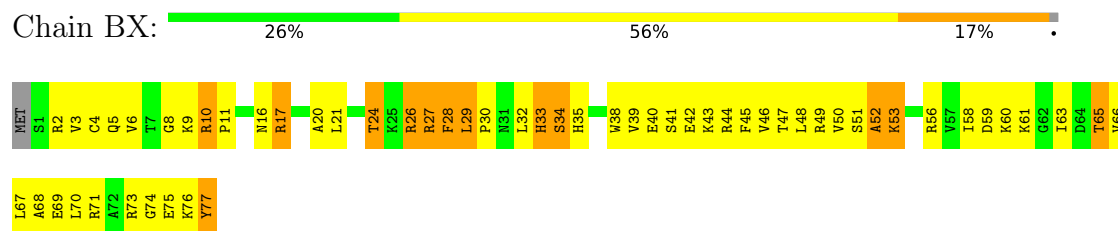
• Molecule 46: 50S ribosomal protein L27



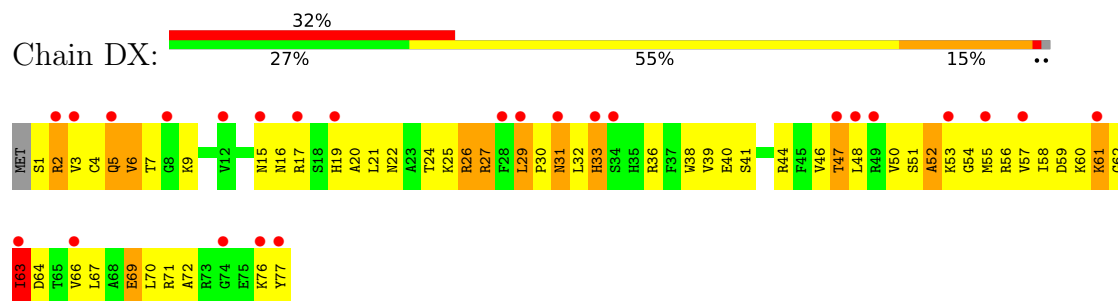
• Molecule 46: 50S ribosomal protein L27



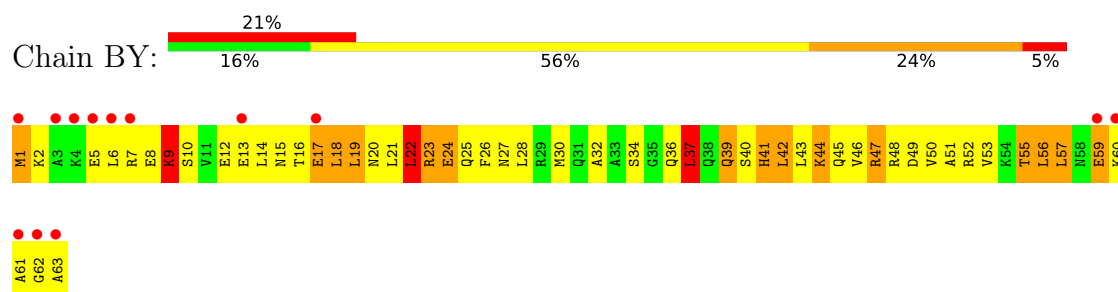
- Molecule 47: 50S ribosomal protein L28



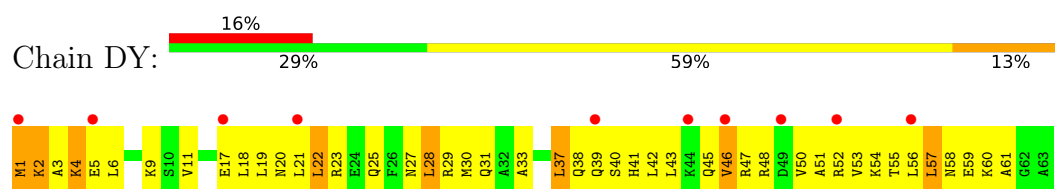
- Molecule 47: 50S ribosomal protein L28



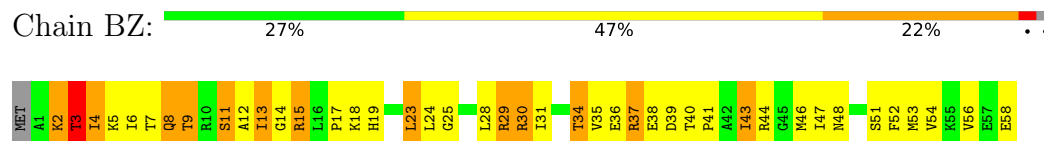
- Molecule 48: 50S ribosomal protein L29



- Molecule 48: 50S ribosomal protein L29

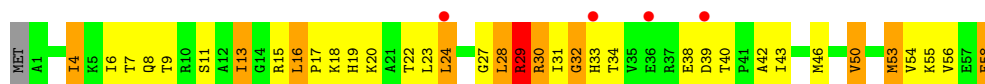


- Molecule 49: 50S ribosomal protein L30



- Molecule 49: 50S ribosomal protein L30

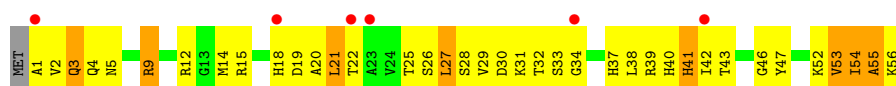




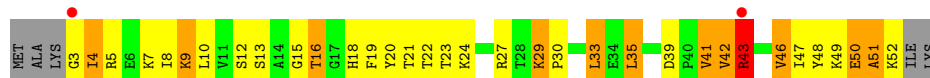
- Molecule 50: 50S ribosomal protein L32



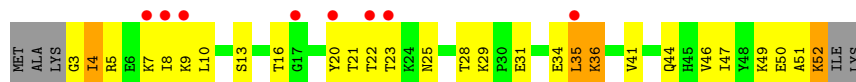
- Molecule 50: 50S ribosomal protein L32



- Molecule 51: 50S ribosomal protein L33



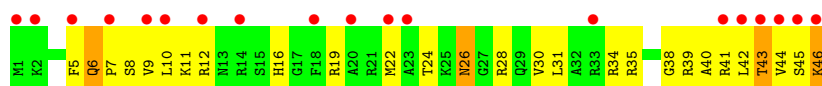
- Molecule 51: 50S ribosomal protein L33



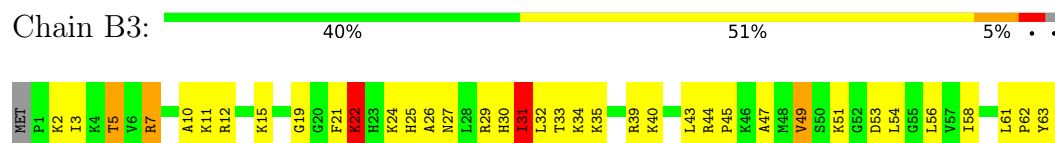
- Molecule 52: 50S ribosomal protein L34



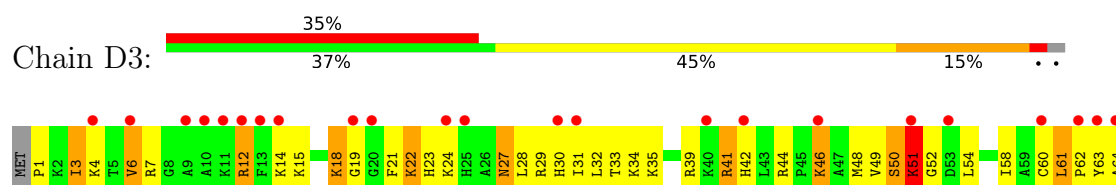
- Molecule 52: 50S ribosomal protein L34



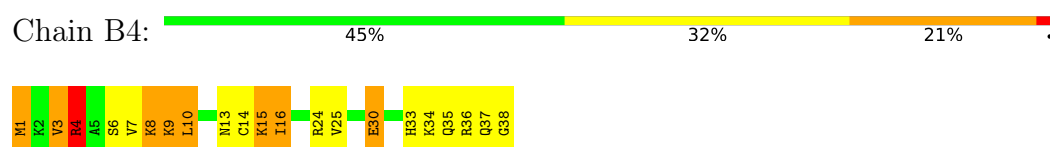
- Molecule 53: 50S ribosomal protein L35



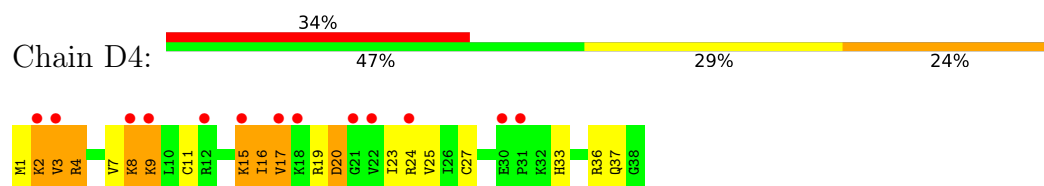
- Molecule 53: 50S ribosomal protein L35



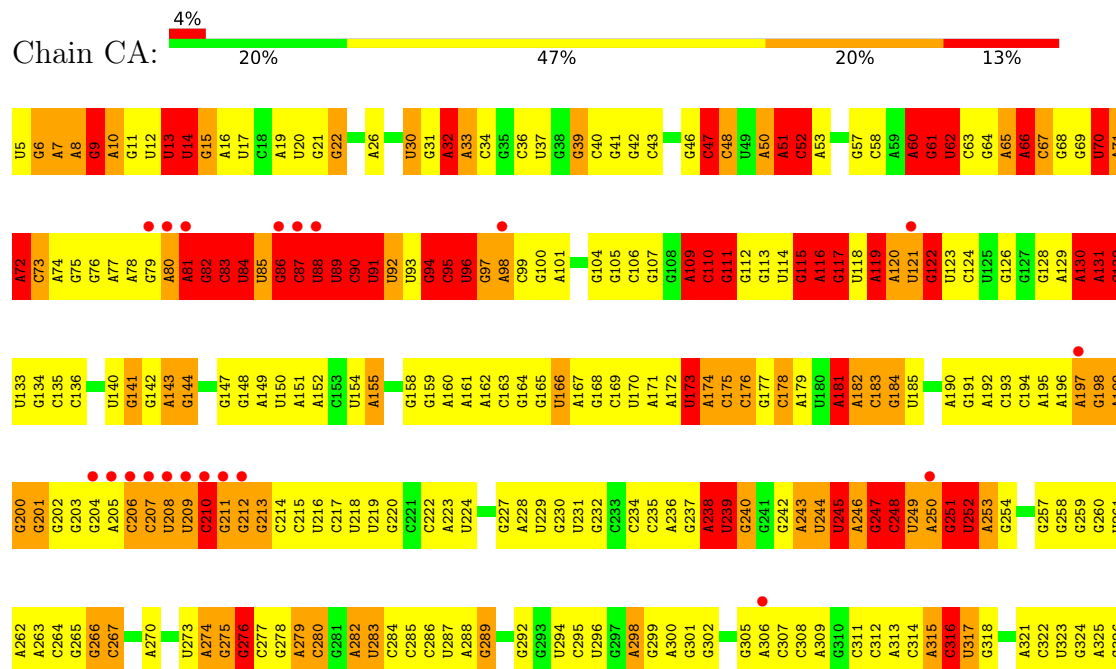
- Molecule 54: 50S ribosomal protein L36

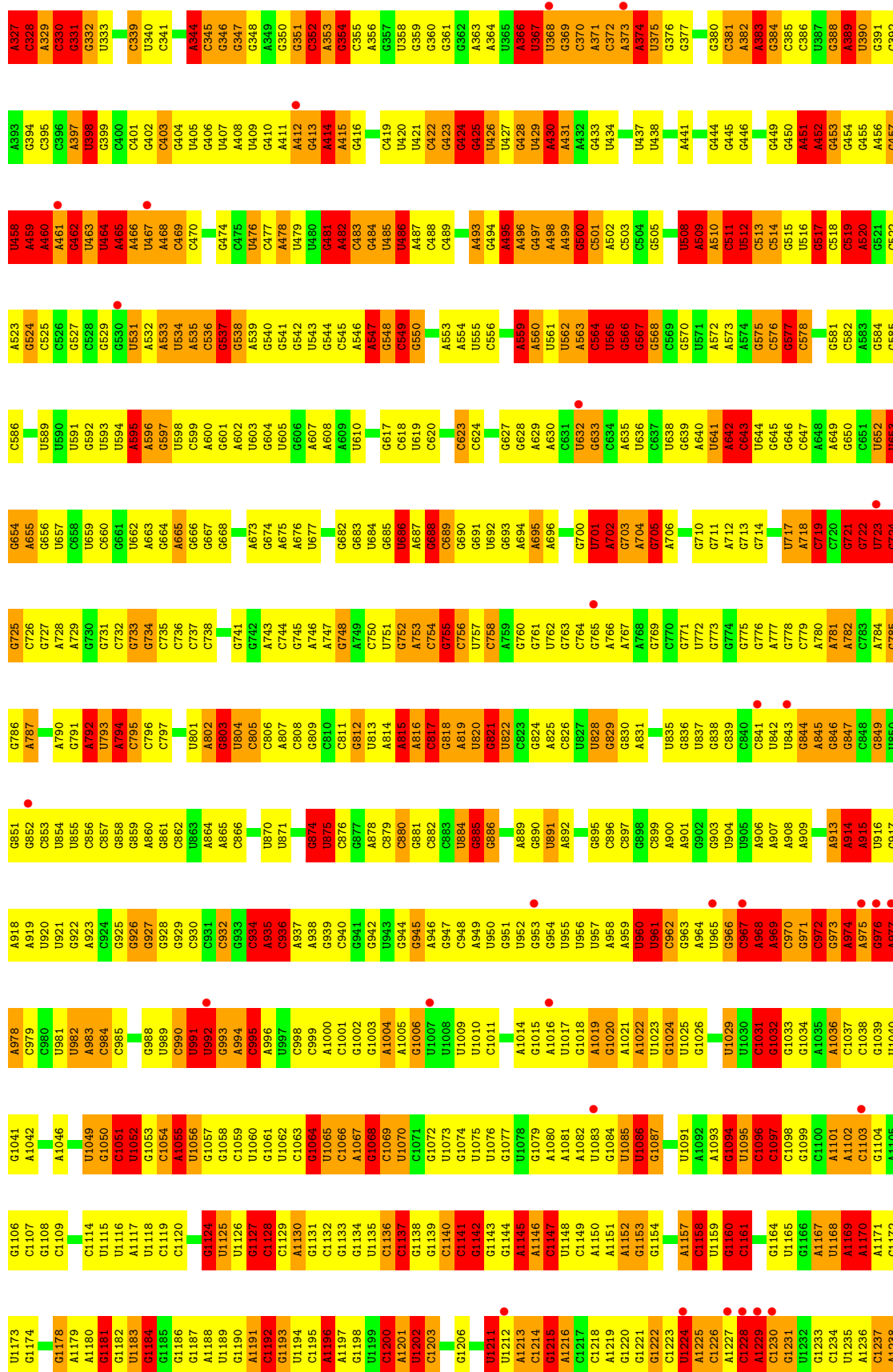


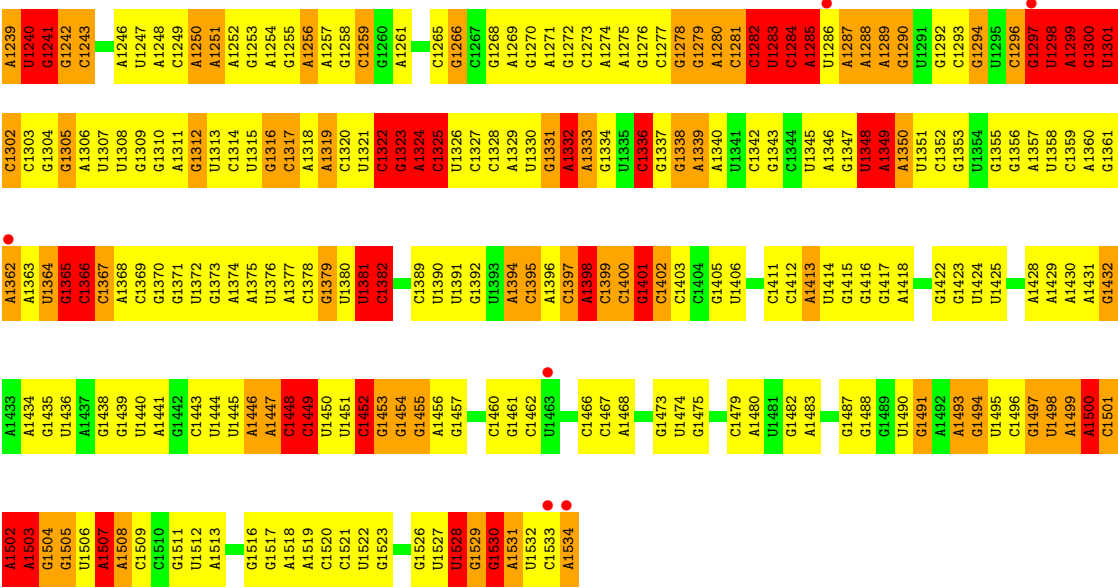
- Molecule 54: 50S ribosomal protein L36



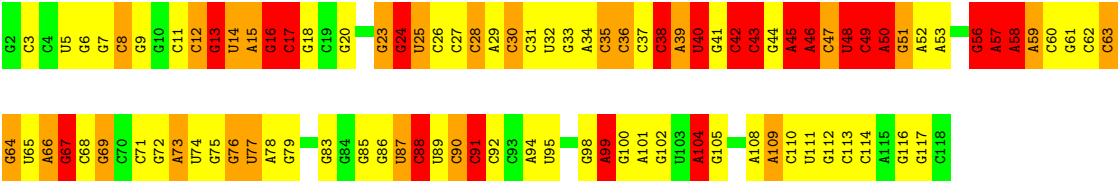
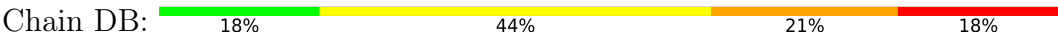
- Molecule 55: 16S rRNA







● Molecule 56: 5S rRNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.72Å 435.07Å 628.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	75.71 – 3.81 75.71 – 3.81	Depositor EDS
% Data completeness (in resolution range)	78.6 (75.71-3.81) 78.6 (75.71-3.81)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 3.77Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.207 , 0.253 0.226 , 0.269	Depositor DCC
R_{free} test set	8842 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å ²)	99.2	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 67.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	285420	wwPDB-VP
Average B, all atoms (Å ²)	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	AB	0.38	0/1735	0.86	5/2338 (0.2%)
1	CB	0.38	0/1735	0.89	4/2338 (0.2%)
2	AC	0.39	0/1651	0.84	2/2225 (0.1%)
2	CC	0.39	0/1651	0.81	2/2225 (0.1%)
3	AD	0.38	0/1665	0.77	1/2227 (0.0%)
3	CD	0.45	0/1665	0.85	2/2227 (0.1%)
4	AE	0.53	0/1118	1.02	6/1504 (0.4%)
4	CE	0.47	0/1118	0.87	2/1504 (0.1%)
5	AF	0.37	0/835	0.80	2/1128 (0.2%)
5	CF	0.35	0/835	0.83	3/1128 (0.3%)
6	AG	0.35	0/1195	0.77	0/1602
6	CG	0.38	0/1187	0.80	2/1591 (0.1%)
7	AH	0.38	0/989	0.80	1/1326 (0.1%)
7	CH	0.40	0/989	0.87	1/1326 (0.1%)
8	AI	0.34	0/1034	0.78	1/1375 (0.1%)
8	CI	0.33	0/1034	0.77	0/1375
9	AJ	0.35	0/796	0.84	2/1077 (0.2%)
9	CJ	0.35	0/796	0.84	2/1077 (0.2%)
10	AK	0.36	0/893	0.88	4/1205 (0.3%)
10	CK	0.40	0/893	0.85	0/1205
11	AL	0.45	0/969	0.93	2/1300 (0.2%)
11	CL	0.41	0/969	0.94	2/1300 (0.2%)
12	AM	0.38	0/892	0.87	4/1193 (0.3%)
12	CM	0.45	1/884 (0.1%)	1.04	7/1181 (0.6%)
13	AN	0.35	0/785	0.84	2/1043 (0.2%)
13	CN	0.34	0/780	0.83	2/1036 (0.2%)
14	AO	0.34	0/722	0.79	2/964 (0.2%)
14	CO	0.35	0/722	0.83	2/964 (0.2%)
15	AP	0.39	0/659	0.89	5/884 (0.6%)
15	CP	0.43	0/648	0.82	0/870
16	AQ	0.40	0/657	0.88	0/881
16	CQ	0.37	0/657	0.84	2/881 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AR	0.33	0/462	0.83	2/621 (0.3%)
17	CR	0.39	0/462	0.83	0/621
18	AS	0.33	0/652	0.76	0/877
18	CS	0.31	0/652	0.84	2/877 (0.2%)
19	AT	0.40	0/671	0.89	3/888 (0.3%)
19	CT	0.35	0/671	0.81	2/888 (0.2%)
20	AU	0.35	0/430	0.86	2/570 (0.4%)
20	CU	0.39	0/430	0.89	1/570 (0.2%)
21	AA	0.38	0/36834	1.04	312/57462 (0.5%)
22	AV	0.38	0/401	0.79	0/622
22	CV	0.32	0/401	0.72	0/622
23	AW	0.56	0/138	1.24	3/212 (1.4%)
23	CW	0.60	0/138	1.50	2/212 (0.9%)
24	BA	0.46	6/68626 (0.0%)	1.18	808/107056 (0.8%)
24	DA	0.38	1/68314 (0.0%)	1.08	649/106569 (0.6%)
25	BB	0.43	0/2828	1.11	31/4410 (0.7%)
26	BC	0.63	0/2121	1.09	17/2852 (0.6%)
26	DC	0.47	0/2121	0.96	6/2852 (0.2%)
27	BD	0.69	0/1586	1.12	4/2134 (0.2%)
27	DD	0.42	0/1586	0.95	7/2134 (0.3%)
28	BE	0.58	0/1571	1.02	7/2113 (0.3%)
28	DE	0.45	0/1571	0.87	2/2113 (0.1%)
29	BF	0.53	1/1434 (0.1%)	0.93	5/1926 (0.3%)
29	DF	0.67	3/1444 (0.2%)	0.99	4/1937 (0.2%)
30	BG	0.53	0/1343	1.00	8/1816 (0.4%)
30	DG	0.38	0/1343	0.85	4/1816 (0.2%)
31	BH	0.70	3/1122 (0.3%)	0.94	2/1515 (0.1%)
31	DH	0.55	2/1122 (0.2%)	0.80	0/1515
32	BI	0.38	0/1046	0.90	2/1410 (0.1%)
32	DI	0.36	0/1046	0.80	2/1410 (0.1%)
33	BJ	0.73	0/1152	1.14	5/1551 (0.3%)
33	DJ	0.50	0/1152	0.97	5/1551 (0.3%)
34	BK	0.72	0/947	1.17	5/1268 (0.4%)
34	DK	0.44	0/947	0.96	3/1268 (0.2%)
35	BL	0.63	0/1054	1.15	5/1403 (0.4%)
35	DL	0.43	0/1054	0.83	0/1403
36	BM	0.63	0/1093	1.11	10/1460 (0.7%)
36	DM	0.56	0/1093	0.99	7/1460 (0.5%)
37	BN	0.65	0/973	1.05	8/1301 (0.6%)
37	DN	0.42	0/973	0.93	2/1301 (0.2%)
38	BO	0.56	0/902	0.92	3/1209 (0.2%)
38	DO	0.59	1/902 (0.1%)	0.95	1/1209 (0.1%)
39	BP	0.60	0/929	1.08	5/1242 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	DP	0.41	0/929	0.81	1/1242 (0.1%)
40	BQ	0.79	1/960 (0.1%)	1.05	2/1278 (0.2%)
40	DQ	0.48	0/960	0.86	1/1278 (0.1%)
41	BR	0.72	0/829	1.09	3/1107 (0.3%)
41	DR	0.45	0/829	0.86	0/1107
42	BS	0.77	0/864	1.08	1/1156 (0.1%)
42	DS	0.40	0/864	0.84	1/1156 (0.1%)
43	BT	0.57	0/744	1.02	2/994 (0.2%)
43	DT	0.36	0/744	0.84	2/994 (0.2%)
44	BU	0.56	0/787	1.13	4/1051 (0.4%)
44	DU	0.42	0/787	0.86	0/1051
45	BV	0.61	0/766	1.04	5/1025 (0.5%)
45	DV	0.65	1/766 (0.1%)	0.99	3/1025 (0.3%)
46	BW	0.67	0/603	1.20	4/797 (0.5%)
46	DW	0.44	0/603	0.83	2/797 (0.3%)
47	BX	0.57	0/635	0.98	2/848 (0.2%)
47	DX	0.43	0/635	0.92	4/848 (0.5%)
48	BY	0.58	0/510	0.96	2/677 (0.3%)
48	DY	0.38	0/510	0.81	0/677
49	BZ	0.66	0/453	1.04	1/605 (0.2%)
49	DZ	0.42	0/453	0.82	0/605
50	B0	0.54	0/450	1.00	2/599 (0.3%)
50	D0	0.38	0/450	0.87	0/599
51	B1	0.50	0/416	0.97	2/554 (0.4%)
51	D1	0.38	0/416	0.83	0/554
52	B2	0.61	0/380	1.14	3/498 (0.6%)
52	D2	0.41	0/380	0.96	2/498 (0.4%)
53	B3	0.60	0/513	0.98	0/676
53	D3	0.50	0/513	0.89	0/676
54	B4	0.76	0/303	1.29	3/397 (0.8%)
54	D4	0.57	0/303	0.84	0/397
55	CA	0.37	2/36762 (0.0%)	1.05	311/57350 (0.5%)
56	DB	0.43	1/2803 (0.0%)	1.23	45/4371 (1.0%)
All	All	0.43	23/307815 (0.0%)	1.06	2426/460233 (0.5%)

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
27	BD	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
29	DF	0	1
36	DM	0	1
All	All	0	4

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	DF	78	ILE	CA-CB	14.39	1.68	1.54
31	BH	48	GLU	C-O	-10.48	1.11	1.23
31	BH	48	GLU	CA-C	-8.49	1.42	1.52
31	DH	53	GLU	N-CA	-6.38	1.38	1.46
45	DV	31	TYR	CE1-CZ	6.07	1.52	1.38

The worst 5 of 2426 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	DF	78	ILE	CB-CA-C	-15.63	88.10	111.08
44	BU	82	VAL	N-CA-C	14.12	124.58	111.45
24	BA	1330	C	N1-C1'-C2'	-13.65	91.53	112.00
56	DB	49	C	O3'-P-O5'	12.90	123.35	104.00
12	CM	2	ARG	NE-CZ-NH1	-12.44	109.06	121.50

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	BD	10	GLY	Peptide
27	BD	9	VAL	Peptide
29	DF	78	ILE	Peptide
36	DM	135	VAL	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AB	1704	0	1732	284	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CB	1704	0	1732	222	0
2	AC	1624	0	1699	148	0
2	CC	1624	0	1699	164	0
3	AD	1643	0	1710	184	0
3	CD	1643	0	1710	157	0
4	AE	1105	0	1148	255	0
4	CE	1105	0	1148	131	0
5	AF	817	0	808	89	0
5	CF	817	0	808	84	0
6	AG	1181	0	1240	105	0
6	CG	1174	0	1230	162	0
7	AH	979	0	1034	122	0
7	CH	979	0	1034	99	0
8	AI	1022	0	1070	125	0
8	CI	1022	0	1070	149	0
9	AJ	786	0	828	79	0
9	CJ	786	0	828	124	0
10	AK	877	0	887	89	0
10	CK	877	0	887	105	0
11	AL	955	0	1019	101	0
11	CL	955	0	1019	103	0
12	AM	883	0	944	75	0
12	CM	876	0	937	144	0
13	AN	774	0	827	87	0
13	CN	769	0	822	96	0
14	AO	714	0	737	60	0
14	CO	714	0	737	41	0
15	AP	649	0	666	56	0
15	CP	638	0	656	70	0
16	AQ	648	0	691	84	0
16	CQ	648	0	691	49	0
17	AR	455	0	478	46	0
17	CR	455	0	478	45	0
18	AS	637	0	665	52	0
18	CS	637	0	665	82	0
19	AT	665	0	714	68	0
19	CT	665	0	714	53	0
20	AU	425	0	449	70	0
20	CU	425	0	449	78	0
21	AA	32895	0	16553	1702	0
22	AV	360	0	185	10	0
22	CV	360	0	185	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	AW	125	0	63	4	0
23	CW	125	0	63	6	0
24	BA	61274	0	30819	3140	0
24	DA	60995	0	30677	3532	0
25	BB	2529	0	1281	108	0
26	BC	2082	0	2157	212	0
26	DC	2082	0	2157	228	0
27	BD	1565	0	1616	204	0
27	DD	1565	0	1616	172	0
28	BE	1552	0	1619	158	0
28	DE	1552	0	1619	176	0
29	BF	1410	0	1447	130	0
29	DF	1420	0	1460	204	0
30	BG	1323	0	1374	176	0
30	DG	1323	0	1374	149	0
31	BH	1111	0	1148	123	0
31	DH	1111	0	1148	113	0
32	BI	1032	0	1088	116	0
32	DI	1032	0	1088	72	0
33	BJ	1129	0	1162	167	0
33	DJ	1129	0	1162	124	0
34	BK	938	0	1012	118	0
34	DK	938	0	1012	114	0
35	BL	1045	0	1117	134	0
35	DL	1045	0	1117	149	0
36	BM	1074	0	1157	114	0
36	DM	1074	0	1157	118	0
37	BN	960	0	1000	101	0
37	DN	960	0	1000	119	0
38	BO	892	0	923	73	0
38	DO	892	0	923	157	0
39	BP	917	0	965	143	0
39	DP	917	0	965	107	0
40	BQ	947	0	1022	129	0
40	DQ	947	0	1022	137	0
41	BR	816	0	839	93	0
41	DR	816	0	839	98	0
42	BS	857	0	922	73	0
42	DS	857	0	922	72	0
43	BT	738	0	807	112	0
43	DT	738	0	807	100	0
44	BU	779	0	834	60	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	DU	779	0	834	112	0
45	BV	753	0	780	59	0
45	DV	753	0	780	123	0
46	BW	596	0	610	186	0
46	DW	596	0	610	124	0
47	BX	625	0	655	73	0
47	DX	625	0	655	76	0
48	BY	509	0	543	72	0
48	DY	509	0	543	71	0
49	BZ	449	0	491	49	0
49	DZ	449	0	491	41	0
50	B0	444	0	461	36	0
50	D0	444	0	461	52	0
51	B1	409	0	440	40	0
51	D1	409	0	440	34	0
52	B2	377	0	418	33	0
52	D2	377	0	418	36	0
53	B3	504	0	574	51	0
53	D3	504	0	574	51	0
54	B4	302	0	340	33	0
54	D4	302	0	340	26	0
55	CA	32831	0	16521	1803	0
56	DB	2507	0	1270	203	0
57	AA	43	0	0	0	0
57	BA	136	0	0	0	0
57	BB	4	0	0	0	0
57	BD	1	0	0	0	0
57	CA	42	0	0	0	0
57	DA	134	0	0	0	0
57	DB	1	0	0	0	0
57	DC	1	0	0	0	0
57	DJ	1	0	0	0	0
58	B4	1	0	0	0	0
58	D4	1	0	0	0	0
59	AA	195	0	0	7	0
59	AE	1	0	0	0	0
59	AL	3	0	0	1	0
59	AN	5	0	0	0	0
59	AT	3	0	0	0	0
59	AU	1	0	0	0	0
59	B2	2	0	0	0	0
59	B3	3	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	B4	2	0	0	0	0
59	BA	615	0	0	31	0
59	BB	19	0	0	0	0
59	BC	7	0	0	1	0
59	BD	2	0	0	3	0
59	BE	1	0	0	1	0
59	BL	4	0	0	1	0
59	BN	2	0	0	0	0
59	BQ	1	0	0	0	0
59	BT	1	0	0	1	0
59	BV	1	0	0	1	0
59	CA	196	0	0	4	0
59	CE	3	0	0	1	0
59	CI	1	0	0	0	0
59	CL	1	0	0	0	0
59	CN	2	0	0	0	0
59	CT	2	0	0	0	0
59	CU	2	0	0	0	0
59	D2	1	0	0	0	0
59	D3	1	0	0	0	0
59	D4	5	0	0	0	0
59	DA	598	0	0	14	0
59	DB	4	0	0	0	0
59	DC	14	0	0	2	0
59	DD	4	0	0	1	0
59	DE	2	0	0	0	0
59	DJ	3	0	0	0	0
59	DL	5	0	0	0	0
59	DN	2	0	0	0	0
59	DT	2	0	0	0	0
59	DU	1	0	0	0	0
59	DV	1	0	0	0	0
All	All	285420	0	191332	19508	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 41.

The worst 5 of 19508 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)
24:DA:1439:A:C2	24:DA:1552:A:C6	2.21	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:DA:1439:A:N1	24:DA:1552:A:C5	2.03	1.26
24:DA:1439:A:C2	24:DA:1552:A:C5	2.25	1.25
38:DO:100:HIS:CE1	56:DB:48:U:O2'	1.89	1.25
38:DO:30:ARG:HB2	38:DO:30:ARG:NH1	1.53	1.21

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AB	216/241 (90%)	128 (59%)	60 (28%)	28 (13%)	0	3
1	CB	216/241 (90%)	145 (67%)	49 (23%)	22 (10%)	0	7
2	AC	204/233 (88%)	139 (68%)	51 (25%)	14 (7%)	1	13
2	CC	204/233 (88%)	146 (72%)	41 (20%)	17 (8%)	0	10
3	AD	203/206 (98%)	126 (62%)	52 (26%)	25 (12%)	0	4
3	CD	203/206 (98%)	141 (70%)	40 (20%)	22 (11%)	0	6
4	AE	148/167 (89%)	100 (68%)	31 (21%)	17 (12%)	0	5
4	CE	148/167 (89%)	98 (66%)	37 (25%)	13 (9%)	0	9
5	AF	98/135 (73%)	62 (63%)	25 (26%)	11 (11%)	0	5
5	CF	98/135 (73%)	65 (66%)	21 (21%)	12 (12%)	0	4
6	AG	149/179 (83%)	109 (73%)	29 (20%)	11 (7%)	1	12
6	CG	148/179 (83%)	80 (54%)	44 (30%)	24 (16%)	0	2
7	AH	127/130 (98%)	97 (76%)	22 (17%)	8 (6%)	1	14
7	CH	127/130 (98%)	96 (76%)	24 (19%)	7 (6%)	1	16
8	AI	125/130 (96%)	80 (64%)	34 (27%)	11 (9%)	0	9
8	CI	125/130 (96%)	86 (69%)	33 (26%)	6 (5%)	2	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	AJ	96/103 (93%)	69 (72%)	12 (12%)	15 (16%)	0	2
9	CJ	96/103 (93%)	61 (64%)	20 (21%)	15 (16%)	0	2
10	AK	115/129 (89%)	86 (75%)	22 (19%)	7 (6%)	1	15
10	CK	115/129 (89%)	74 (64%)	31 (27%)	10 (9%)	0	9
11	AL	121/124 (98%)	80 (66%)	24 (20%)	17 (14%)	0	3
11	CL	121/124 (98%)	86 (71%)	25 (21%)	10 (8%)	0	10
12	AM	112/118 (95%)	87 (78%)	16 (14%)	9 (8%)	1	11
12	CM	111/118 (94%)	65 (59%)	30 (27%)	16 (14%)	0	3
13	AN	92/101 (91%)	58 (63%)	25 (27%)	9 (10%)	0	7
13	CN	91/101 (90%)	59 (65%)	24 (26%)	8 (9%)	0	9
14	AO	86/89 (97%)	64 (74%)	17 (20%)	5 (6%)	1	15
14	CO	86/89 (97%)	72 (84%)	13 (15%)	1 (1%)	10	40
15	AP	80/82 (98%)	54 (68%)	15 (19%)	11 (14%)	0	3
15	CP	78/82 (95%)	56 (72%)	14 (18%)	8 (10%)	0	7
16	AQ	78/84 (93%)	48 (62%)	21 (27%)	9 (12%)	0	5
16	CQ	78/84 (93%)	59 (76%)	13 (17%)	6 (8%)	1	11
17	AR	53/75 (71%)	40 (76%)	11 (21%)	2 (4%)	2	21
17	CR	53/75 (71%)	44 (83%)	6 (11%)	3 (6%)	1	16
18	AS	77/92 (84%)	67 (87%)	6 (8%)	4 (5%)	1	17
18	CS	77/92 (84%)	54 (70%)	19 (25%)	4 (5%)	1	17
19	AT	83/87 (95%)	55 (66%)	21 (25%)	7 (8%)	0	9
19	CT	83/87 (95%)	59 (71%)	21 (25%)	3 (4%)	2	22
20	AU	49/71 (69%)	22 (45%)	18 (37%)	9 (18%)	0	1
20	CU	49/71 (69%)	20 (41%)	17 (35%)	12 (24%)	0	0
26	BC	269/273 (98%)	184 (68%)	59 (22%)	26 (10%)	0	8
26	DC	269/273 (98%)	181 (67%)	60 (22%)	28 (10%)	0	6
27	BD	207/209 (99%)	141 (68%)	32 (16%)	34 (16%)	0	2
27	DD	207/209 (99%)	132 (64%)	45 (22%)	30 (14%)	0	3
28	BE	199/201 (99%)	151 (76%)	24 (12%)	24 (12%)	0	4
28	DE	199/201 (99%)	130 (65%)	43 (22%)	26 (13%)	0	3
29	BF	175/179 (98%)	133 (76%)	25 (14%)	17 (10%)	0	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	DF	176/179 (98%)	97 (55%)	45 (26%)	34 (19%)	0	1
30	BG	174/177 (98%)	112 (64%)	35 (20%)	27 (16%)	0	2
30	DG	174/177 (98%)	105 (60%)	41 (24%)	28 (16%)	0	2
31	BH	147/149 (99%)	62 (42%)	54 (37%)	31 (21%)	0	1
31	DH	147/149 (99%)	76 (52%)	50 (34%)	21 (14%)	0	3
32	BI	139/142 (98%)	84 (60%)	44 (32%)	11 (8%)	1	11
32	DI	139/142 (98%)	81 (58%)	39 (28%)	19 (14%)	0	3
33	BJ	140/142 (99%)	106 (76%)	20 (14%)	14 (10%)	0	7
33	DJ	140/142 (99%)	95 (68%)	33 (24%)	12 (9%)	0	9
34	BK	120/123 (98%)	84 (70%)	18 (15%)	18 (15%)	0	2
34	DK	120/123 (98%)	80 (67%)	21 (18%)	19 (16%)	0	2
35	BL	141/144 (98%)	101 (72%)	28 (20%)	12 (8%)	0	9
35	DL	141/144 (98%)	83 (59%)	37 (26%)	21 (15%)	0	3
36	BM	134/136 (98%)	94 (70%)	25 (19%)	15 (11%)	0	5
36	DM	134/136 (98%)	92 (69%)	25 (19%)	17 (13%)	0	4
37	BN	118/127 (93%)	87 (74%)	21 (18%)	10 (8%)	0	9
37	DN	118/127 (93%)	71 (60%)	35 (30%)	12 (10%)	0	7
38	BO	114/117 (97%)	79 (69%)	26 (23%)	9 (8%)	1	11
38	DO	114/117 (97%)	76 (67%)	29 (25%)	9 (8%)	1	11
39	BP	112/115 (97%)	71 (63%)	22 (20%)	19 (17%)	0	2
39	DP	112/115 (97%)	67 (60%)	28 (25%)	17 (15%)	0	2
40	BQ	115/118 (98%)	88 (76%)	18 (16%)	9 (8%)	1	11
40	DQ	115/118 (98%)	79 (69%)	26 (23%)	10 (9%)	0	9
41	BR	101/103 (98%)	79 (78%)	14 (14%)	8 (8%)	1	11
41	DR	101/103 (98%)	72 (71%)	19 (19%)	10 (10%)	0	7
42	BS	108/110 (98%)	76 (70%)	27 (25%)	5 (5%)	2	19
42	DS	108/110 (98%)	81 (75%)	18 (17%)	9 (8%)	0	10
43	BT	91/100 (91%)	53 (58%)	23 (25%)	15 (16%)	0	2
43	DT	91/100 (91%)	48 (53%)	28 (31%)	15 (16%)	0	2
44	BU	100/104 (96%)	71 (71%)	13 (13%)	16 (16%)	0	2
44	DU	100/104 (96%)	51 (51%)	28 (28%)	21 (21%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	BV	92/94 (98%)	75 (82%)	15 (16%)	2 (2%)	5	30
45	DV	92/94 (98%)	59 (64%)	26 (28%)	7 (8%)	1	11
46	BW	77/85 (91%)	29 (38%)	22 (29%)	26 (34%)	0	0
46	DW	77/85 (91%)	32 (42%)	27 (35%)	18 (23%)	0	0
47	BX	75/78 (96%)	59 (79%)	13 (17%)	3 (4%)	2	21
47	DX	75/78 (96%)	48 (64%)	21 (28%)	6 (8%)	1	11
48	BY	61/63 (97%)	36 (59%)	17 (28%)	8 (13%)	0	3
48	DY	61/63 (97%)	44 (72%)	12 (20%)	5 (8%)	0	10
49	BZ	56/59 (95%)	39 (70%)	13 (23%)	4 (7%)	1	12
49	DZ	56/59 (95%)	31 (55%)	18 (32%)	7 (12%)	0	4
50	B0	54/57 (95%)	39 (72%)	9 (17%)	6 (11%)	0	5
50	D0	54/57 (95%)	40 (74%)	8 (15%)	6 (11%)	0	5
51	B1	48/55 (87%)	37 (77%)	7 (15%)	4 (8%)	0	10
51	D1	48/55 (87%)	35 (73%)	9 (19%)	4 (8%)	0	10
52	B2	44/46 (96%)	35 (80%)	8 (18%)	1 (2%)	5	30
52	D2	44/46 (96%)	32 (73%)	7 (16%)	5 (11%)	0	5
53	B3	62/65 (95%)	49 (79%)	11 (18%)	2 (3%)	3	25
53	D3	62/65 (95%)	39 (63%)	17 (27%)	6 (10%)	0	8
54	B4	36/38 (95%)	29 (81%)	4 (11%)	3 (8%)	0	10
54	D4	36/38 (95%)	22 (61%)	9 (25%)	5 (14%)	0	3
All	All	11238/11970 (94%)	7499 (67%)	2485 (22%)	1254 (11%)	0	5

5 of 1254 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AB	20	ARG
1	AB	22	TRP
1	AB	40	ILE
1	AB	71	THR
1	AB	72	LYS

5.3.2 Protein sidechains ⓘ

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AB	180/199 (90%)	150 (83%)	30 (17%)	2	13
1	CB	180/199 (90%)	158 (88%)	22 (12%)	5	21
2	AC	170/190 (90%)	143 (84%)	27 (16%)	2	15
2	CC	170/190 (90%)	154 (91%)	16 (9%)	8	30
3	AD	172/173 (99%)	145 (84%)	27 (16%)	2	15
3	CD	172/173 (99%)	146 (85%)	26 (15%)	3	16
4	AE	113/126 (90%)	86 (76%)	27 (24%)	1	5
4	CE	113/126 (90%)	93 (82%)	20 (18%)	2	12
5	AF	87/116 (75%)	78 (90%)	9 (10%)	7	27
5	CF	87/116 (75%)	79 (91%)	8 (9%)	8	31
6	AG	124/147 (84%)	115 (93%)	9 (7%)	13	38
6	CG	123/147 (84%)	94 (76%)	29 (24%)	1	5
7	AH	104/105 (99%)	91 (88%)	13 (12%)	4	21
7	CH	104/105 (99%)	86 (83%)	18 (17%)	2	12
8	AI	105/107 (98%)	88 (84%)	17 (16%)	2	14
8	CI	105/107 (98%)	90 (86%)	15 (14%)	3	18
9	AJ	86/90 (96%)	73 (85%)	13 (15%)	3	16
9	CJ	86/90 (96%)	75 (87%)	11 (13%)	4	21
10	AK	90/99 (91%)	81 (90%)	9 (10%)	7	28
10	CK	90/99 (91%)	77 (86%)	13 (14%)	3	17
11	AL	103/104 (99%)	85 (82%)	18 (18%)	2	12
11	CL	103/104 (99%)	88 (85%)	15 (15%)	3	17
12	AM	92/96 (96%)	83 (90%)	9 (10%)	7	29
12	CM	91/96 (95%)	74 (81%)	17 (19%)	1	10
13	AN	79/84 (94%)	73 (92%)	6 (8%)	12	37
13	CN	79/84 (94%)	68 (86%)	11 (14%)	3	18
14	AO	76/77 (99%)	73 (96%)	3 (4%)	28	52
14	CO	76/77 (99%)	73 (96%)	3 (4%)	28	52
15	AP	65/65 (100%)	56 (86%)	9 (14%)	3	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	CP	65/65 (100%)	57 (88%)	8 (12%)	4	21
16	AQ	74/78 (95%)	56 (76%)	18 (24%)	1	4
16	CQ	74/78 (95%)	62 (84%)	12 (16%)	2	14
17	AR	48/65 (74%)	47 (98%)	1 (2%)	47	64
17	CR	48/65 (74%)	44 (92%)	4 (8%)	10	34
18	AS	70/79 (89%)	61 (87%)	9 (13%)	4	20
18	CS	70/79 (89%)	60 (86%)	10 (14%)	3	18
19	AT	65/66 (98%)	57 (88%)	8 (12%)	4	21
19	CT	65/66 (98%)	58 (89%)	7 (11%)	6	25
20	AU	44/61 (72%)	37 (84%)	7 (16%)	2	15
20	CU	44/61 (72%)	33 (75%)	11 (25%)	0	4
26	BC	216/218 (99%)	176 (82%)	40 (18%)	1	11
26	DC	216/218 (99%)	191 (88%)	25 (12%)	5	22
27	BD	164/164 (100%)	127 (77%)	37 (23%)	1	5
27	DD	164/164 (100%)	141 (86%)	23 (14%)	3	18
28	BE	165/165 (100%)	124 (75%)	41 (25%)	1	4
28	DE	165/165 (100%)	148 (90%)	17 (10%)	7	27
29	BF	148/150 (99%)	123 (83%)	25 (17%)	2	13
29	DF	149/150 (99%)	118 (79%)	31 (21%)	1	7
30	BG	137/138 (99%)	110 (80%)	27 (20%)	1	8
30	DG	137/138 (99%)	118 (86%)	19 (14%)	3	18
31	BH	114/114 (100%)	97 (85%)	17 (15%)	3	16
31	DH	114/114 (100%)	100 (88%)	14 (12%)	4	21
32	BI	109/110 (99%)	95 (87%)	14 (13%)	4	21
32	DI	109/110 (99%)	102 (94%)	7 (6%)	16	42
33	BJ	116/116 (100%)	90 (78%)	26 (22%)	1	5
33	DJ	116/116 (100%)	94 (81%)	22 (19%)	1	10
34	BK	103/104 (99%)	75 (73%)	28 (27%)	0	3
34	DK	103/104 (99%)	81 (79%)	22 (21%)	1	6
35	BL	102/103 (99%)	72 (71%)	30 (29%)	0	2
35	DL	102/103 (99%)	87 (85%)	15 (15%)	3	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	BM	109/109 (100%)	89 (82%)	20 (18%)	2	11
36	DM	109/109 (100%)	90 (83%)	19 (17%)	2	12
37	BN	100/103 (97%)	80 (80%)	20 (20%)	1	8
37	DN	100/103 (97%)	85 (85%)	15 (15%)	3	16
38	BO	86/87 (99%)	65 (76%)	21 (24%)	1	4
38	DO	86/87 (99%)	75 (87%)	11 (13%)	4	21
39	BP	99/100 (99%)	80 (81%)	19 (19%)	1	9
39	DP	99/100 (99%)	92 (93%)	7 (7%)	13	39
40	BQ	89/90 (99%)	72 (81%)	17 (19%)	1	10
40	DQ	89/90 (99%)	77 (86%)	12 (14%)	4	19
41	BR	84/84 (100%)	65 (77%)	19 (23%)	1	5
41	DR	84/84 (100%)	70 (83%)	14 (17%)	2	13
42	BS	93/93 (100%)	71 (76%)	22 (24%)	1	5
42	DS	93/93 (100%)	73 (78%)	20 (22%)	1	6
43	BT	80/84 (95%)	62 (78%)	18 (22%)	1	5
43	DT	80/84 (95%)	74 (92%)	6 (8%)	12	38
44	BU	83/85 (98%)	65 (78%)	18 (22%)	1	6
44	DU	83/85 (98%)	69 (83%)	14 (17%)	2	13
45	BV	78/78 (100%)	61 (78%)	17 (22%)	1	6
45	DV	78/78 (100%)	65 (83%)	13 (17%)	2	13
46	BW	59/63 (94%)	43 (73%)	16 (27%)	0	3
46	DW	59/63 (94%)	46 (78%)	13 (22%)	1	6
47	BX	67/68 (98%)	56 (84%)	11 (16%)	2	14
47	DX	67/68 (98%)	59 (88%)	8 (12%)	5	22
48	BY	55/55 (100%)	39 (71%)	16 (29%)	0	2
48	DY	55/55 (100%)	51 (93%)	4 (7%)	13	38
49	BZ	48/49 (98%)	35 (73%)	13 (27%)	0	3
49	DZ	48/49 (98%)	40 (83%)	8 (17%)	2	13
50	B0	47/48 (98%)	42 (89%)	5 (11%)	6	26
50	D0	47/48 (98%)	40 (85%)	7 (15%)	3	16
51	B1	45/49 (92%)	34 (76%)	11 (24%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
51	D1	45/49 (92%)	41 (91%)	4 (9%)	9 32
52	B2	38/38 (100%)	31 (82%)	7 (18%)	1 11
52	D2	38/38 (100%)	35 (92%)	3 (8%)	11 36
53	B3	51/52 (98%)	45 (88%)	6 (12%)	5 22
53	D3	51/52 (98%)	42 (82%)	9 (18%)	2 12
54	B4	34/34 (100%)	28 (82%)	6 (18%)	2 12
54	D4	34/34 (100%)	30 (88%)	4 (12%)	5 22
All	All	9331/9756 (96%)	7833 (84%)	1498 (16%)	2 14

5 of 1498 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	CF	86	ARG
27	DD	62	LYS
6	CG	105	GLU
5	CF	85	ILE
12	CM	90	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 349 such sidechains are listed below:

Mol	Chain	Res	Type
14	CO	37	HIS
34	DK	89	ASN
18	CS	68	HIS
28	DE	41	GLN
39	DP	2	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1532/1533 (99%)	497 (32%)	255 (16%)
22	AV	16/17 (94%)	0	0
22	CV	16/17 (94%)	1 (6%)	0
23	AW	5/6 (83%)	3 (60%)	1 (20%)
23	CW	5/6 (83%)	3 (60%)	1 (20%)
24	BA	2850/2903 (98%)	1011 (35%)	492 (17%)
24	DA	2838/2903 (97%)	1038 (36%)	519 (18%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
25	BB	117/118 (99%)	36 (30%)	19 (16%)
55	CA	1530/1530 (100%)	533 (34%)	252 (16%)
56	DB	116/117 (99%)	43 (37%)	18 (15%)
All	All	9025/9150 (98%)	3165 (35%)	1557 (17%)

5 of 3165 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	5	U
21	AA	6	G
21	AA	7	A
21	AA	9	G
21	AA	13	U

5 of 1557 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
55	CA	913	A
24	DA	655	A
55	CA	1085	U
55	CA	889	A
24	DA	103	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 365 ligands modelled in this entry, 365 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AB	218/241 (90%)	1.62	63 (28%) 1 2	206, 268, 283, 298	0
1	CB	218/241 (90%)	0.93	21 (9%) 13 16	146, 174, 199, 216	0
2	AC	206/233 (88%)	0.07	1 (0%) 87 71	106, 135, 169, 198	0
2	CC	206/233 (88%)	0.17	3 (1%) 72 50	111, 140, 177, 195	0
3	AD	205/206 (99%)	0.46	13 (6%) 26 22	102, 139, 185, 204	0
3	CD	205/206 (99%)	0.37	8 (3%) 43 31	86, 109, 140, 157	0
4	AE	150/167 (89%)	2.78	86 (57%) 0 0	102, 214, 237, 255	0
4	CE	150/167 (89%)	1.20	30 (20%) 3 5	86, 134, 166, 209	0
5	AF	100/135 (74%)	0.50	8 (8%) 18 18	140, 166, 186, 192	0
5	CF	100/135 (74%)	0.55	4 (4%) 42 30	140, 170, 200, 208	0
6	AG	151/179 (84%)	0.34	5 (3%) 49 34	128, 157, 186, 202	0
6	CG	150/179 (83%)	1.17	32 (21%) 2 4	115, 165, 204, 219	0
7	AH	129/130 (99%)	0.16	4 (3%) 51 35	102, 134, 158, 182	0
7	CH	129/130 (99%)	0.56	7 (5%) 31 24	106, 135, 159, 174	0
8	AI	127/130 (97%)	0.65	8 (6%) 26 22	108, 158, 190, 210	0
8	CI	127/130 (97%)	0.89	16 (12%) 8 12	114, 174, 206, 221	0
9	AJ	98/103 (95%)	0.48	6 (6%) 27 22	105, 150, 194, 211	0
9	CJ	98/103 (95%)	0.77	12 (12%) 8 12	113, 165, 210, 220	0
10	AK	117/129 (90%)	0.07	0 100 100	100, 149, 183, 200	0
10	CK	117/129 (90%)	0.58	7 (5%) 27 22	89, 133, 167, 192	0
11	AL	123/124 (99%)	0.34	9 (7%) 21 19	75, 95, 132, 157	0
11	CL	123/124 (99%)	0.28	4 (3%) 49 34	83, 101, 132, 151	0
12	AM	114/118 (96%)	0.41	7 (6%) 27 22	122, 182, 213, 232	0
12	CM	113/118 (95%)	0.83	10 (8%) 15 17	133, 193, 225, 235	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AN	96/101 (95%)	0.46	2 (2%) 63 44	111, 142, 184, 210	0
13	CN	95/101 (94%)	1.13	16 (16%) 4 7	117, 149, 199, 207	0
14	AO	88/89 (98%)	0.03	1 (1%) 78 57	105, 133, 163, 199	0
14	CO	88/89 (98%)	0.32	2 (2%) 61 43	113, 141, 174, 197	0
15	AP	82/82 (100%)	0.67	9 (10%) 10 14	95, 127, 165, 208	0
15	CP	80/82 (97%)	0.72	8 (10%) 12 15	98, 122, 156, 189	0
16	AQ	80/84 (95%)	0.28	4 (5%) 34 26	69, 100, 142, 159	0
16	CQ	80/84 (95%)	0.15	1 (1%) 75 53	72, 111, 142, 159	0
17	AR	55/75 (73%)	0.20	1 (1%) 67 47	129, 148, 180, 190	0
17	CR	55/75 (73%)	0.31	2 (3%) 46 32	131, 150, 170, 182	0
18	AS	79/92 (85%)	0.68	6 (7%) 20 18	140, 176, 210, 235	0
18	CS	79/92 (85%)	0.61	4 (5%) 33 25	151, 182, 215, 230	0
19	AT	85/87 (97%)	0.28	3 (3%) 47 33	89, 121, 149, 180	0
19	CT	85/87 (97%)	0.57	7 (8%) 17 17	115, 153, 185, 206	0
20	AU	51/71 (71%)	1.02	9 (17%) 4 6	98, 145, 201, 208	0
20	CU	51/71 (71%)	1.14	10 (19%) 3 5	104, 139, 173, 193	0
21	AA	1533/1533 (100%)	-0.04	33 (2%) 62 44	65, 123, 208, 301	0
22	AV	17/17 (100%)	-0.44	0 100 100	102, 112, 149, 197	0
22	CV	17/17 (100%)	-0.08	0 100 100	99, 104, 145, 179	0
23	AW	6/6 (100%)	0.35	0 100 100	100, 109, 120, 155	0
23	CW	6/6 (100%)	0.43	0 100 100	98, 105, 123, 130	0
24	BA	2854/2903 (98%)	-0.16	64 (2%) 62 44	36, 66, 188, 342	0
24	DA	2841/2903 (97%)	0.60	151 (5%) 32 24	79, 132, 236, 340	0
25	BB	118/118 (100%)	-0.11	1 (0%) 82 63	52, 81, 113, 162	0
26	BC	271/273 (99%)	0.49	17 (6%) 26 22	44, 80, 122, 159	0
26	DC	271/273 (99%)	1.14	36 (13%) 7 10	89, 133, 164, 189	0
27	BD	209/209 (100%)	0.15	3 (1%) 73 52	37, 59, 105, 146	0
27	DD	209/209 (100%)	0.97	27 (12%) 7 11	83, 131, 164, 186	0
28	BE	201/201 (100%)	0.12	4 (1%) 65 45	38, 84, 131, 164	0
28	DE	201/201 (100%)	0.96	34 (16%) 4 7	95, 171, 212, 250	0
29	BF	177/179 (98%)	0.83	17 (9%) 13 16	90, 148, 201, 218	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
29	DF	178/179 (99%)	1.87	61 (34%) 1 1	250, 278, 301, 305	0
30	BG	176/177 (99%)	0.17	4 (2%) 61 43	66, 90, 135, 160	0
30	DG	176/177 (99%)	0.73	13 (7%) 20 19	120, 148, 177, 204	0
31	BH	149/149 (100%)	1.02	26 (17%) 4 6	89, 262, 290, 299	0
31	DH	149/149 (100%)	1.64	49 (32%) 1 2	156, 244, 279, 286	0
32	BI	141/142 (99%)	0.88	11 (7%) 19 18	237, 306, 364, 376	0
32	DI	141/142 (99%)	0.95	10 (7%) 22 19	277, 331, 367, 378	0
33	BJ	142/142 (100%)	0.03	2 (1%) 73 52	41, 57, 102, 157	0
33	DJ	142/142 (100%)	0.75	15 (10%) 11 14	92, 115, 142, 181	0
34	BK	122/123 (99%)	0.14	4 (3%) 49 34	41, 56, 110, 177	0
34	DK	122/123 (99%)	0.64	7 (5%) 29 23	93, 115, 144, 173	0
35	BL	143/144 (99%)	0.20	1 (0%) 84 66	38, 77, 119, 160	0
35	DL	143/144 (99%)	1.53	42 (29%) 1 2	93, 155, 197, 209	0
36	BM	136/136 (100%)	0.17	1 (0%) 84 66	41, 67, 114, 152	0
36	DM	136/136 (100%)	0.50	5 (3%) 45 32	80, 107, 142, 164	0
37	BN	120/127 (94%)	0.16	1 (0%) 82 63	46, 63, 84, 138	0
37	DN	120/127 (94%)	1.32	32 (26%) 1 3	122, 154, 180, 217	0
38	BO	116/117 (99%)	0.18	3 (2%) 57 39	73, 84, 124, 149	0
38	DO	116/117 (99%)	2.09	54 (46%) 0 1	165, 197, 217, 225	0
39	BP	114/115 (99%)	0.00	0 100 100	49, 67, 123, 152	0
39	DP	114/115 (99%)	0.98	14 (12%) 8 12	117, 137, 163, 182	0
40	BQ	117/118 (99%)	-0.06	1 (0%) 81 61	40, 58, 100, 127	0
40	DQ	117/118 (99%)	1.08	20 (17%) 4 7	97, 119, 143, 172	0
41	BR	103/103 (100%)	0.31	3 (2%) 53 37	39, 70, 116, 158	0
41	DR	103/103 (100%)	1.32	23 (22%) 2 4	96, 133, 157, 164	0
42	BS	110/110 (100%)	0.13	1 (0%) 81 61	41, 58, 95, 161	0
42	DS	110/110 (100%)	1.06	15 (13%) 7 10	98, 141, 173, 188	0
43	BT	93/100 (93%)	0.86	14 (15%) 5 8	56, 95, 135, 165	0
43	DT	93/100 (93%)	1.83	34 (36%) 1 1	144, 196, 226, 237	0
44	BU	102/104 (98%)	0.64	8 (7%) 19 18	77, 105, 139, 194	0
44	DU	102/104 (98%)	1.75	35 (34%) 1 1	174, 208, 248, 279	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
45	BV	94/94 (100%)	0.27	2 (2%) 63 44	60, 81, 115, 143	0
45	DV	94/94 (100%)	1.97	38 (40%) 0 1	125, 188, 226, 239	0
46	BW	79/85 (92%)	0.91	11 (13%) 6 10	50, 75, 131, 168	0
46	DW	79/85 (92%)	1.17	13 (16%) 4 7	88, 134, 164, 184	0
47	BX	77/78 (98%)	0.25	0 100 100	50, 84, 126, 147	0
47	DX	77/78 (98%)	1.72	25 (32%) 1 2	110, 157, 187, 203	0
48	BY	63/63 (100%)	0.96	13 (20%) 2 5	87, 109, 154, 163	0
48	DY	63/63 (100%)	1.12	10 (15%) 5 8	196, 218, 251, 257	0
49	BZ	58/59 (98%)	0.19	0 100 100	49, 63, 106, 145	0
49	DZ	58/59 (98%)	0.73	4 (6%) 23 20	97, 116, 142, 155	0
50	B0	56/57 (98%)	0.06	0 100 100	40, 63, 119, 143	0
50	D0	56/57 (98%)	0.84	6 (10%) 11 14	93, 152, 190, 202	0
51	B1	50/55 (90%)	-0.00	2 (4%) 42 30	63, 91, 117, 156	0
51	D1	50/55 (90%)	0.80	8 (16%) 5 8	113, 142, 173, 179	0
52	B2	46/46 (100%)	0.24	2 (4%) 40 29	50, 61, 80, 165	0
52	D2	46/46 (100%)	1.81	19 (41%) 0 1	118, 137, 161, 174	0
53	B3	64/65 (98%)	-0.00	0 100 100	45, 63, 98, 133	0
53	D3	64/65 (98%)	1.65	23 (35%) 1 1	105, 123, 146, 174	0
54	B4	38/38 (100%)	0.33	0 100 100	54, 68, 100, 118	0
54	D4	38/38 (100%)	1.60	13 (34%) 1 2	95, 117, 138, 142	0
55	CA	1530/1530 (100%)	0.31	55 (3%) 46 32	77, 126, 214, 305	0
56	DB	117/117 (100%)	0.23	0 100 100	87, 166, 194, 210	0
All	All	20477/21120 (96%)	0.49	1589 (7%) 19 18	36, 125, 246, 378	0

The worst 5 of 1589 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
48	BY	63	ALA	12.1
29	DF	129	MET	10.8
29	DF	153	ILE	10.8
38	DO	28	VAL	10.5
4	AE	114	LEU	9.8

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3062	1/1	-0.31	0.66	85,85,85,85	0
57	MG	AA	1619	1/1	-0.13	0.33	136,136,136,136	0
57	MG	DA	3076	1/1	-0.07	0.67	109,109,109,109	0
57	MG	CA	1624	1/1	0.08	0.49	79,79,79,79	0
57	MG	DA	3134	1/1	0.17	0.55	126,126,126,126	0
57	MG	DA	3065	1/1	0.22	0.61	84,84,84,84	0
57	MG	DA	3016	1/1	0.28	0.59	96,96,96,96	0
57	MG	BA	3015	1/1	0.30	0.53	38,38,38,38	0
57	MG	DA	3071	1/1	0.31	0.39	94,94,94,94	0
57	MG	DA	3131	1/1	0.39	0.42	103,103,103,103	0
57	MG	CA	1612	1/1	0.41	0.31	86,86,86,86	0
57	MG	BA	3058	1/1	0.42	0.37	44,44,44,44	0
57	MG	DA	3060	1/1	0.43	0.30	96,96,96,96	0
57	MG	CA	1617	1/1	0.51	0.25	130,130,130,130	0
57	MG	DA	3133	1/1	0.51	0.29	115,115,115,115	0
57	MG	DC	301	1/1	0.51	0.20	103,103,103,103	0
57	MG	DA	3004	1/1	0.53	0.42	150,150,150,150	0
57	MG	DA	3093	1/1	0.54	0.28	93,93,93,93	0
57	MG	DA	3040	1/1	0.54	0.37	102,102,102,102	0
57	MG	DA	3110	1/1	0.57	0.56	82,82,82,82	0
57	MG	BB	201	1/1	0.60	0.31	105,105,105,105	0
57	MG	DA	3084	1/1	0.61	0.15	157,157,157,157	0
57	MG	DA	3077	1/1	0.61	0.38	86,86,86,86	0
57	MG	DA	3075	1/1	0.64	0.10	255,255,255,255	0
57	MG	DA	3021	1/1	0.66	0.27	132,132,132,132	0
57	MG	BA	3075	1/1	0.68	0.38	40,40,40,40	0
57	MG	DA	3086	1/1	0.68	0.18	148,148,148,148	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3112	1/1	0.68	0.25	115,115,115,115	0
57	MG	CA	1629	1/1	0.69	0.26	111,111,111,111	0
57	MG	BA	3135	1/1	0.69	0.36	43,43,43,43	0
57	MG	CA	1625	1/1	0.69	0.21	86,86,86,86	0
57	MG	BA	3077	1/1	0.70	0.24	45,45,45,45	0
57	MG	AA	1607	1/1	0.70	0.22	88,88,88,88	0
57	MG	DA	3090	1/1	0.70	0.21	92,92,92,92	0
57	MG	DB	201	1/1	0.70	0.18	108,108,108,108	0
57	MG	DA	3047	1/1	0.71	0.15	148,148,148,148	0
57	MG	AA	1636	1/1	0.71	0.18	120,120,120,120	0
57	MG	BA	3133	1/1	0.71	0.44	53,53,53,53	0
57	MG	DA	3064	1/1	0.72	0.30	87,87,87,87	0
57	MG	DA	3100	1/1	0.72	0.21	149,149,149,149	0
57	MG	CA	1602	1/1	0.73	0.22	106,106,106,106	0
57	MG	DA	3007	1/1	0.74	0.12	192,192,192,192	0
57	MG	DA	3011	1/1	0.74	0.35	110,110,110,110	0
57	MG	DA	3051	1/1	0.74	0.10	177,177,177,177	0
57	MG	DA	3128	1/1	0.74	0.27	100,100,100,100	0
57	MG	BA	3085	1/1	0.75	0.39	42,42,42,42	0
57	MG	DA	3107	1/1	0.75	0.16	130,130,130,130	0
57	MG	DA	3066	1/1	0.75	0.21	92,92,92,92	0
57	MG	BA	3070	1/1	0.76	0.13	140,140,140,140	0
57	MG	BA	3131	1/1	0.76	0.50	48,48,48,48	0
57	MG	DA	3126	1/1	0.77	0.17	99,99,99,99	0
57	MG	BA	3132	1/1	0.77	0.42	42,42,42,42	0
57	MG	BA	3014	1/1	0.78	0.32	38,38,38,38	0
57	MG	DA	3041	1/1	0.78	0.14	113,113,113,113	0
57	MG	CA	1615	1/1	0.78	0.20	118,118,118,118	0
57	MG	DA	3006	1/1	0.79	0.11	149,149,149,149	0
57	MG	BA	3115	1/1	0.79	0.27	49,49,49,49	0
57	MG	BA	3061	1/1	0.79	0.35	39,39,39,39	0
57	MG	BA	3112	1/1	0.79	0.12	46,46,46,46	0
57	MG	DA	3054	1/1	0.80	0.27	88,88,88,88	0
57	MG	DA	3019	1/1	0.80	0.11	150,150,150,150	0
57	MG	DA	3027	1/1	0.80	0.14	87,87,87,87	0
57	MG	DA	3108	1/1	0.81	0.19	82,82,82,82	0
57	MG	DA	3109	1/1	0.81	0.12	92,92,92,92	0
57	MG	DA	3015	1/1	0.81	0.19	88,88,88,88	0
57	MG	CA	1619	1/1	0.81	0.23	119,119,119,119	0
57	MG	CA	1607	1/1	0.81	0.13	89,89,89,89	0
57	MG	DA	3020	1/1	0.81	0.17	153,153,153,153	0
57	MG	CA	1613	1/1	0.81	0.15	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3099	1/1	0.81	0.39	98,98,98,98	0
57	MG	DA	3059	1/1	0.81	0.26	88,88,88,88	0
57	MG	DA	3014	1/1	0.81	0.17	90,90,90,90	0
57	MG	CA	1634	1/1	0.82	0.15	97,97,97,97	0
57	MG	BA	3062	1/1	0.82	0.42	38,38,38,38	0
57	MG	AA	1641	1/1	0.82	0.25	89,89,89,89	0
57	MG	DA	3003	1/1	0.83	0.13	94,94,94,94	0
57	MG	BA	3060	1/1	0.83	0.29	39,39,39,39	0
57	MG	DA	3088	1/1	0.83	0.14	101,101,101,101	0
57	MG	AA	1620	1/1	0.83	0.11	144,144,144,144	0
57	MG	DA	3028	1/1	0.83	0.37	103,103,103,103	0
57	MG	DA	3032	1/1	0.83	0.19	87,87,87,87	0
57	MG	DA	3080	1/1	0.84	0.29	84,84,84,84	0
57	MG	BA	3037	1/1	0.84	0.36	42,42,42,42	0
57	MG	DA	3085	1/1	0.84	0.09	190,190,190,190	0
57	MG	CA	1614	1/1	0.84	0.12	114,114,114,114	0
57	MG	DA	3017	1/1	0.84	0.20	102,102,102,102	0
57	MG	DA	3048	1/1	0.85	0.14	131,131,131,131	0
57	MG	DA	3045	1/1	0.85	0.12	141,141,141,141	0
57	MG	BA	3124	1/1	0.85	0.40	41,41,41,41	0
57	MG	DA	3094	1/1	0.86	0.09	126,126,126,126	0
57	MG	DA	3120	1/1	0.86	0.25	96,96,96,96	0
57	MG	DA	3124	1/1	0.86	0.12	133,133,133,133	0
57	MG	AA	1626	1/1	0.86	0.12	107,107,107,107	0
57	MG	BA	3084	1/1	0.86	0.36	49,49,49,49	0
57	MG	AA	1637	1/1	0.86	0.11	87,87,87,87	0
57	MG	BA	3056	1/1	0.86	0.26	45,45,45,45	0
57	MG	DA	3029	1/1	0.86	0.12	108,108,108,108	0
57	MG	DA	3002	1/1	0.86	0.14	125,125,125,125	0
57	MG	CA	1636	1/1	0.87	0.32	88,88,88,88	0
57	MG	DA	3012	1/1	0.87	0.25	96,96,96,96	0
57	MG	CA	1606	1/1	0.87	0.09	85,85,85,85	0
57	MG	DA	3001	1/1	0.87	0.12	115,115,115,115	0
57	MG	BA	3118	1/1	0.87	0.23	42,42,42,42	0
57	MG	BA	3102	1/1	0.87	0.33	40,40,40,40	0
57	MG	BA	3026	1/1	0.87	0.31	41,41,41,41	0
57	MG	BA	3007	1/1	0.87	0.15	90,90,90,90	0
57	MG	CA	1603	1/1	0.87	0.23	92,92,92,92	0
57	MG	DA	3009	1/1	0.87	0.10	121,121,121,121	0
57	MG	DA	3058	1/1	0.87	0.11	96,96,96,96	0
57	MG	CA	1616	1/1	0.88	0.09	136,136,136,136	0
57	MG	DA	3042	1/1	0.88	0.10	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	AA	1606	1/1	0.88	0.10	96,96,96,96	0
57	MG	BA	3098	1/1	0.88	0.42	52,52,52,52	0
57	MG	CA	1622	1/1	0.88	0.08	138,138,138,138	0
57	MG	AA	1628	1/1	0.88	0.12	107,107,107,107	0
57	MG	AA	1631	1/1	0.88	0.20	98,98,98,98	0
57	MG	CA	1628	1/1	0.88	0.24	79,79,79,79	0
57	MG	DA	3101	1/1	0.88	0.14	82,82,82,82	0
57	MG	DA	3035	1/1	0.88	0.12	88,88,88,88	0
57	MG	AA	1625	1/1	0.88	0.12	90,90,90,90	0
57	MG	BB	202	1/1	0.89	0.12	114,114,114,114	0
57	MG	CA	1638	1/1	0.89	0.09	141,141,141,141	0
57	MG	DA	3010	1/1	0.89	0.11	108,108,108,108	0
57	MG	DA	3050	1/1	0.89	0.12	148,148,148,148	0
57	MG	DA	3030	1/1	0.89	0.23	101,101,101,101	0
57	MG	DA	3031	1/1	0.89	0.20	98,98,98,98	0
57	MG	DA	3081	1/1	0.89	0.08	87,87,87,87	0
57	MG	DA	3096	1/1	0.89	0.13	120,120,120,120	0
57	MG	DA	3005	1/1	0.90	0.09	157,157,157,157	0
57	MG	DA	3061	1/1	0.90	0.22	84,84,84,84	0
57	MG	BA	3095	1/1	0.90	0.15	75,75,75,75	0
57	MG	BA	3046	1/1	0.90	0.10	63,63,63,63	0
57	MG	DA	3008	1/1	0.90	0.06	177,177,177,177	0
57	MG	CA	1639	1/1	0.90	0.07	165,165,165,165	0
57	MG	BA	3123	1/1	0.90	0.11	63,63,63,63	0
57	MG	DJ	201	1/1	0.90	0.20	101,101,101,101	0
57	MG	DA	3129	1/1	0.90	0.18	83,83,83,83	0
57	MG	CA	1627	1/1	0.90	0.10	106,106,106,106	0
57	MG	BA	3071	1/1	0.90	0.29	38,38,38,38	0
57	MG	CA	1609	1/1	0.90	0.09	96,96,96,96	0
57	MG	AA	1604	1/1	0.90	0.06	126,126,126,126	0
57	MG	DA	3070	1/1	0.91	0.08	94,94,94,94	0
57	MG	DA	3122	1/1	0.91	0.09	142,142,142,142	0
57	MG	BA	3045	1/1	0.91	0.16	62,62,62,62	0
57	MG	BA	3004	1/1	0.91	0.17	69,69,69,69	0
57	MG	DA	3023	1/1	0.91	0.21	101,101,101,101	0
57	MG	DA	3089	1/1	0.91	0.09	110,110,110,110	0
57	MG	DA	3043	1/1	0.91	0.18	107,107,107,107	0
57	MG	AA	1627	1/1	0.91	0.22	109,109,109,109	0
57	MG	BA	3001	1/1	0.91	0.20	45,45,45,45	0
57	MG	DA	3095	1/1	0.91	0.12	159,159,159,159	0
57	MG	CA	1601	1/1	0.92	0.09	142,142,142,142	0
57	MG	DA	3082	1/1	0.92	0.19	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	CA	1631	1/1	0.92	0.11	91,91,91,91	0
57	MG	AA	1610	1/1	0.92	0.07	125,125,125,125	0
57	MG	BA	3099	1/1	0.92	0.13	41,41,41,41	0
57	MG	DA	3116	1/1	0.92	0.14	98,98,98,98	0
57	MG	CA	1637	1/1	0.92	0.14	83,83,83,83	0
57	MG	BA	3030	1/1	0.92	0.35	41,41,41,41	0
57	MG	AA	1632	1/1	0.92	0.10	95,95,95,95	0
57	MG	CA	1640	1/1	0.92	0.27	87,87,87,87	0
57	MG	DA	3049	1/1	0.92	0.14	150,150,150,150	0
57	MG	DA	3074	1/1	0.92	0.08	98,98,98,98	0
57	MG	DA	3130	1/1	0.92	0.37	85,85,85,85	0
57	MG	BA	3025	1/1	0.92	0.09	41,41,41,41	0
57	MG	BA	3074	1/1	0.92	0.11	38,38,38,38	0
57	MG	BA	3119	1/1	0.92	0.28	52,52,52,52	0
57	MG	BA	3121	1/1	0.92	0.12	45,45,45,45	0
57	MG	BA	3035	1/1	0.93	0.20	55,55,55,55	0
57	MG	DA	3115	1/1	0.93	0.14	84,84,84,84	0
57	MG	BA	3107	1/1	0.93	0.11	49,49,49,49	0
57	MG	DA	3034	1/1	0.93	0.13	89,89,89,89	0
57	MG	BA	3047	1/1	0.93	0.08	63,63,63,63	0
57	MG	CA	1604	1/1	0.93	0.06	106,106,106,106	0
57	MG	DA	3078	1/1	0.93	0.21	79,79,79,79	0
57	MG	BA	3113	1/1	0.93	0.15	38,38,38,38	0
57	MG	BA	3091	1/1	0.93	0.08	69,69,69,69	0
57	MG	AA	1630	1/1	0.93	0.10	79,79,79,79	0
57	MG	CA	1626	1/1	0.93	0.08	110,110,110,110	0
57	MG	BA	3136	1/1	0.93	0.31	47,47,47,47	0
57	MG	AA	1618	1/1	0.93	0.08	104,104,104,104	0
57	MG	BA	3080	1/1	0.93	0.07	74,74,74,74	0
57	MG	BA	3011	1/1	0.94	0.32	44,44,44,44	0
57	MG	AA	1614	1/1	0.94	0.07	113,113,113,113	0
57	MG	BA	3055	1/1	0.94	0.17	44,44,44,44	0
57	MG	BA	3005	1/1	0.94	0.14	73,73,73,73	0
57	MG	DA	3111	1/1	0.94	0.10	164,164,164,164	0
57	MG	BA	3109	1/1	0.94	0.11	42,42,42,42	0
57	MG	BA	3126	1/1	0.94	0.13	57,57,57,57	0
57	MG	BA	3111	1/1	0.94	0.10	38,38,38,38	0
57	MG	BA	3019	1/1	0.94	0.07	70,70,70,70	0
57	MG	DA	3121	1/1	0.94	0.13	97,97,97,97	0
57	MG	DA	3067	1/1	0.94	0.07	86,86,86,86	0
57	MG	DA	3068	1/1	0.94	0.07	86,86,86,86	0
57	MG	DA	3026	1/1	0.94	0.09	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	CA	1623	1/1	0.94	0.09	89,89,89,89	0
57	MG	DA	3072	1/1	0.94	0.07	84,84,84,84	0
57	MG	BA	3092	1/1	0.94	0.08	108,108,108,108	0
57	MG	DA	3098	1/1	0.94	0.09	87,87,87,87	0
57	MG	AA	1638	1/1	0.94	0.08	81,81,81,81	0
57	MG	CA	1610	1/1	0.94	0.06	129,129,129,129	0
57	MG	DA	3013	1/1	0.94	0.08	93,93,93,93	0
57	MG	DA	3025	1/1	0.95	0.12	105,105,105,105	0
57	MG	BA	3076	1/1	0.95	0.09	47,47,47,47	0
57	MG	BA	3059	1/1	0.95	0.14	50,50,50,50	0
57	MG	AA	1633	1/1	0.95	0.07	107,107,107,107	0
57	MG	DA	3052	1/1	0.95	0.08	118,118,118,118	0
57	MG	BA	3081	1/1	0.95	0.19	40,40,40,40	0
57	MG	CA	1642	1/1	0.95	0.07	102,102,102,102	0
57	MG	BA	3002	1/1	0.95	0.27	47,47,47,47	0
57	MG	AA	1624	1/1	0.95	0.11	94,94,94,94	0
57	MG	DA	3119	1/1	0.95	0.10	138,138,138,138	0
57	MG	AA	1608	1/1	0.95	0.11	82,82,82,82	0
57	MG	BA	3114	1/1	0.95	0.08	73,73,73,73	0
57	MG	DA	3036	1/1	0.95	0.08	84,84,84,84	0
57	MG	DA	3037	1/1	0.95	0.08	83,83,83,83	0
57	MG	DA	3038	1/1	0.95	0.15	108,108,108,108	0
57	MG	BA	3006	1/1	0.95	0.06	88,88,88,88	0
57	MG	BA	3094	1/1	0.95	0.09	75,75,75,75	0
57	MG	CA	1632	1/1	0.95	0.05	125,125,125,125	0
57	MG	DA	3097	1/1	0.95	0.10	119,119,119,119	0
57	MG	DA	3132	1/1	0.95	0.06	94,94,94,94	0
57	MG	AA	1616	1/1	0.95	0.06	126,126,126,126	0
57	MG	AA	1617	1/1	0.95	0.07	123,123,123,123	0
57	MG	DA	3024	1/1	0.95	0.09	90,90,90,90	0
57	MG	AA	1643	1/1	0.96	0.06	81,81,81,81	0
57	MG	BA	3093	1/1	0.96	0.16	84,84,84,84	0
57	MG	BA	3042	1/1	0.96	0.08	56,56,56,56	0
57	MG	BA	3065	1/1	0.96	0.12	38,38,38,38	0
57	MG	DA	3069	1/1	0.96	0.09	86,86,86,86	0
57	MG	AA	1601	1/1	0.96	0.05	111,111,111,111	0
57	MG	DA	3103	1/1	0.96	0.10	91,91,91,91	0
57	MG	DA	3104	1/1	0.96	0.10	107,107,107,107	0
57	MG	DA	3106	1/1	0.96	0.06	92,92,92,92	0
57	MG	DA	3018	1/1	0.96	0.07	106,106,106,106	0
57	MG	AA	1629	1/1	0.96	0.12	129,129,129,129	0
57	MG	DA	3073	1/1	0.96	0.18	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3044	1/1	0.96	0.05	116,116,116,116	0
57	MG	BA	3003	1/1	0.96	0.06	73,73,73,73	0
57	MG	DA	3046	1/1	0.96	0.09	142,142,142,142	0
57	MG	DA	3114	1/1	0.96	0.07	98,98,98,98	0
57	MG	CA	1618	1/1	0.96	0.09	108,108,108,108	0
57	MG	BA	3048	1/1	0.96	0.06	74,74,74,74	0
57	MG	BA	3049	1/1	0.96	0.09	45,45,45,45	0
57	MG	BA	3052	1/1	0.96	0.09	38,38,38,38	0
57	MG	BB	204	1/1	0.96	0.10	57,57,57,57	0
57	MG	BA	3024	1/1	0.96	0.08	42,42,42,42	0
57	MG	AA	1605	1/1	0.96	0.06	103,103,103,103	0
57	MG	DA	3125	1/1	0.96	0.09	90,90,90,90	0
57	MG	DA	3055	1/1	0.96	0.06	85,85,85,85	0
57	MG	DA	3127	1/1	0.96	0.14	104,104,104,104	0
57	MG	DA	3087	1/1	0.96	0.07	88,88,88,88	0
57	MG	AA	1611	1/1	0.96	0.07	91,91,91,91	0
57	MG	AA	1621	1/1	0.96	0.10	67,67,67,67	0
57	MG	BA	3089	1/1	0.96	0.14	50,50,50,50	0
57	MG	DA	3091	1/1	0.96	0.06	93,93,93,93	0
57	MG	BA	3090	1/1	0.96	0.07	47,47,47,47	0
57	MG	CA	1608	1/1	0.96	0.11	86,86,86,86	0
57	MG	AA	1642	1/1	0.96	0.07	74,74,74,74	0
57	MG	BA	3086	1/1	0.97	0.08	43,43,43,43	0
57	MG	BA	3088	1/1	0.97	0.07	58,58,58,58	0
57	MG	DA	3057	1/1	0.97	0.07	92,92,92,92	0
57	MG	AA	1635	1/1	0.97	0.05	114,114,114,114	0
57	MG	DA	3083	1/1	0.97	0.10	121,121,121,121	0
57	MG	BA	3028	1/1	0.97	0.19	39,39,39,39	0
57	MG	BA	3029	1/1	0.97	0.13	38,38,38,38	0
57	MG	DA	3113	1/1	0.97	0.09	86,86,86,86	0
57	MG	CA	1620	1/1	0.97	0.12	93,93,93,93	0
57	MG	DA	3039	1/1	0.97	0.12	104,104,104,104	0
57	MG	DA	3063	1/1	0.97	0.09	92,92,92,92	0
57	MG	DA	3117	1/1	0.97	0.09	90,90,90,90	0
57	MG	AA	1609	1/1	0.97	0.07	91,91,91,91	0
57	MG	BA	3032	1/1	0.97	0.05	40,40,40,40	0
57	MG	AA	1615	1/1	0.97	0.05	117,117,117,117	0
57	MG	DA	3092	1/1	0.97	0.09	102,102,102,102	0
57	MG	AA	1603	1/1	0.97	0.07	76,76,76,76	0
57	MG	BA	3097	1/1	0.97	0.06	49,49,49,49	0
57	MG	BA	3079	1/1	0.97	0.05	89,89,89,89	0
57	MG	AA	1640	1/1	0.97	0.06	132,132,132,132	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3044	1/1	0.97	0.07	71,71,71,71	0
57	MG	CA	1630	1/1	0.97	0.25	79,79,79,79	0
57	MG	AA	1602	1/1	0.97	0.15	79,79,79,79	0
57	MG	BA	3134	1/1	0.97	0.06	38,38,38,38	0
57	MG	AA	1623	1/1	0.97	0.08	108,108,108,108	0
57	MG	CA	1635	1/1	0.97	0.04	114,114,114,114	0
57	MG	DA	3053	1/1	0.97	0.10	101,101,101,101	0
57	MG	DA	3105	1/1	0.97	0.10	91,91,91,91	0
57	MG	BA	3101	1/1	0.98	0.05	38,38,38,38	0
57	MG	BA	3009	1/1	0.98	0.06	46,46,46,46	0
57	MG	BA	3105	1/1	0.98	0.07	38,38,38,38	0
57	MG	BA	3034	1/1	0.98	0.05	40,40,40,40	0
57	MG	BA	3063	1/1	0.98	0.10	37,37,37,37	0
57	MG	BA	3110	1/1	0.98	0.07	50,50,50,50	0
57	MG	BA	3010	1/1	0.98	0.05	46,46,46,46	0
57	MG	BA	3067	1/1	0.98	0.07	40,40,40,40	0
57	MG	DA	3118	1/1	0.98	0.15	99,99,99,99	0
57	MG	DA	3022	1/1	0.98	0.14	105,105,105,105	0
57	MG	BB	203	1/1	0.98	0.05	57,57,57,57	0
57	MG	AA	1639	1/1	0.98	0.05	119,119,119,119	0
57	MG	BD	301	1/1	0.98	0.11	39,39,39,39	0
57	MG	BA	3051	1/1	0.98	0.11	39,39,39,39	0
57	MG	BA	3039	1/1	0.98	0.06	40,40,40,40	0
57	MG	BA	3053	1/1	0.98	0.09	41,41,41,41	0
57	MG	BA	3040	1/1	0.98	0.04	41,41,41,41	0
57	MG	DA	3102	1/1	0.98	0.07	84,84,84,84	0
57	MG	AA	1612	1/1	0.98	0.05	82,82,82,82	0
57	MG	BA	3122	1/1	0.98	0.05	40,40,40,40	0
57	MG	BA	3043	1/1	0.98	0.06	56,56,56,56	0
57	MG	AA	1634	1/1	0.98	0.05	102,102,102,102	0
57	MG	AA	1613	1/1	0.98	0.04	74,74,74,74	0
57	MG	CA	1633	1/1	0.98	0.09	101,101,101,101	0
57	MG	CA	1611	1/1	0.98	0.06	93,93,93,93	0
57	MG	BA	3038	1/1	0.99	0.06	42,42,42,42	0
57	MG	DA	3056	1/1	0.99	0.08	101,101,101,101	0
57	MG	BA	3127	1/1	0.99	0.08	40,40,40,40	0
57	MG	BA	3128	1/1	0.99	0.05	52,52,52,52	0
57	MG	BA	3130	1/1	0.99	0.09	49,49,49,49	0
57	MG	BA	3027	1/1	0.99	0.06	41,41,41,41	0
57	MG	BA	3072	1/1	0.99	0.17	38,38,38,38	0
57	MG	BA	3073	1/1	0.99	0.04	43,43,43,43	0
57	MG	AA	1622	1/1	0.99	0.08	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3041	1/1	0.99	0.12	43,43,43,43	0
57	MG	BA	3100	1/1	0.99	0.03	59,59,59,59	0
57	MG	BA	3020	1/1	0.99	0.04	46,46,46,46	0
57	MG	BA	3057	1/1	0.99	0.22	42,42,42,42	0
57	MG	BA	3103	1/1	0.99	0.06	64,64,64,64	0
57	MG	BA	3104	1/1	0.99	0.09	38,38,38,38	0
57	MG	BA	3078	1/1	0.99	0.07	86,86,86,86	0
57	MG	BA	3106	1/1	0.99	0.05	40,40,40,40	0
57	MG	DA	3033	1/1	0.99	0.08	94,94,94,94	0
57	MG	BA	3021	1/1	0.99	0.07	42,42,42,42	0
57	MG	BA	3108	1/1	0.99	0.06	40,40,40,40	0
57	MG	BA	3022	1/1	0.99	0.05	38,38,38,38	0
57	MG	CA	1605	1/1	0.99	0.14	89,89,89,89	0
57	MG	BA	3033	1/1	0.99	0.05	40,40,40,40	0
57	MG	BA	3082	1/1	0.99	0.05	38,38,38,38	0
57	MG	DA	3079	1/1	0.99	0.11	90,90,90,90	0
57	MG	BA	3083	1/1	0.99	0.06	43,43,43,43	0
57	MG	BA	3013	1/1	0.99	0.05	38,38,38,38	0
57	MG	BA	3016	1/1	0.99	0.25	39,39,39,39	0
57	MG	DA	3123	1/1	0.99	0.05	93,93,93,93	0
57	MG	BA	3036	1/1	0.99	0.03	47,47,47,47	0
57	MG	BA	3116	1/1	0.99	0.07	38,38,38,38	0
57	MG	BA	3117	1/1	0.99	0.06	56,56,56,56	0
57	MG	BA	3087	1/1	0.99	0.03	45,45,45,45	0
57	MG	BA	3064	1/1	0.99	0.04	38,38,38,38	0
57	MG	BA	3120	1/1	0.99	0.04	41,41,41,41	0
57	MG	BA	3018	1/1	0.99	0.04	67,67,67,67	0
57	MG	BA	3066	1/1	0.99	0.04	43,43,43,43	0
57	MG	BA	3050	1/1	0.99	0.04	40,40,40,40	0
57	MG	BA	3069	1/1	0.99	0.04	52,52,52,52	0
57	MG	CA	1621	1/1	0.99	0.07	85,85,85,85	0
57	MG	BA	3125	1/1	0.99	0.07	40,40,40,40	0
58	ZN	B4	101	1/1	0.99	0.04	79,79,79,79	0
58	ZN	D4	101	1/1	0.99	0.09	79,79,79,79	0
57	MG	BA	3096	1/1	1.00	0.09	45,45,45,45	0
57	MG	BA	3129	1/1	1.00	0.02	39,39,39,39	0
57	MG	BA	3068	1/1	1.00	0.09	52,52,52,52	0
57	MG	BA	3012	1/1	1.00	0.06	38,38,38,38	0
57	MG	BA	3031	1/1	1.00	0.04	42,42,42,42	0
57	MG	BA	3023	1/1	1.00	0.04	41,41,41,41	0
57	MG	BA	3017	1/1	1.00	0.03	39,39,39,39	0
57	MG	BA	3054	1/1	1.00	0.06	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3008	1/1	1.00	0.05	43,43,43,43	0
57	MG	CA	1641	1/1	1.00	0.08	91,91,91,91	0

6.5 Other polymers [i](#)

There are no such residues in this entry.