



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 22, 2024 – 05:07 PM EDT

PDB ID : 4V6C
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 : 3.19 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<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	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

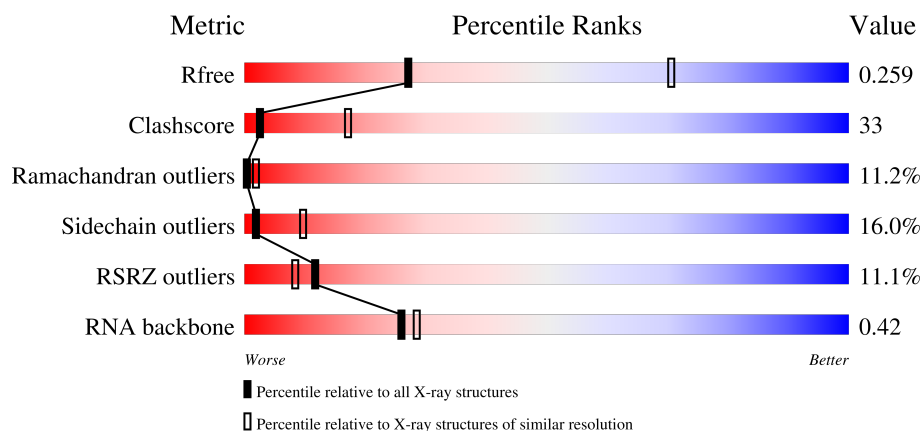
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 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}	164625	1370 (3.20-3.20)
Clashscore	180529	1497 (3.20-3.20)
Ramachandran outliers	177936	1479 (3.20-3.20)
Sidechain outliers	177891	1478 (3.20-3.20)
RSRZ outliers	164620	1371 (3.20-3.20)
RNA backbone	3690	1111 (3.50-2.90)

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	<div> <div>5%</div> <div>18% 49% 21% 10%</div> </div>
1	CB	241	<div> <div>8%</div> <div>23% 53% 14% 10%</div> </div>
2	AC	233	<div> <div>2%</div> <div>33% 43% 10% 12%</div> </div>
2	CC	233	<div> <div>6%</div> <div>34% 41% 12% 12%</div> </div>

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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	BA	2903	
22	DA	2903	
23	BB	118	
24	BC	273	
24	DC	273	
25	BD	209	
25	DD	209	
26	BE	201	
26	DE	201	
27	BF	179	
27	DF	179	
28	BG	177	
28	DG	177	

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Mol	Chain	Length	Quality of chain
29	BH	149	
29	DH	149	
30	BI	142	
30	DI	142	
31	BJ	142	
31	DJ	142	
32	BK	123	
32	DK	123	
33	BL	144	
33	DL	144	
34	BM	136	
34	DM	136	
35	BN	127	
35	DN	127	
36	BO	117	
36	DO	117	
37	BP	115	
37	DP	115	
38	BQ	118	
38	DQ	118	
39	BR	103	
39	DR	103	
40	BS	110	
40	DS	110	
41	BT	100	

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Mol	Chain	Length	Quality of chain
41	DT	100	
42	BU	104	
42	DU	104	
43	BV	94	
43	DV	94	
44	BW	85	
44	DW	85	
45	BX	78	
45	DX	78	
46	BY	63	
46	DY	63	
47	BZ	59	
47	DZ	59	
48	B0	57	
48	D0	57	
49	B1	55	
49	D1	55	
50	B2	46	
50	D2	46	
51	B3	65	
51	D3	65	
52	B4	38	
52	D4	38	
53	CA	1530	
54	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
55	MG	BA	3132	-	-	-	X
55	MG	DA	3013	-	-	-	X
55	MG	DA	3058	-	-	-	X
55	MG	DA	3063	-	-	-	X
55	MG	DA	3064	-	-	-	X
55	MG	DA	3075	-	-	-	X
55	MG	DA	3129	-	-	-	X

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 284450 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 23S rRNA.

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

- Molecule 23 is a RNA chain called 5S rRNA.

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

- Molecule 24 is a protein called 50S ribosomal protein L2.

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

- Molecule 25 is a protein called 50S ribosomal protein L3.

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

- Molecule 26 is a protein called 50S ribosomal protein L4.

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

- Molecule 27 is a protein called 50S ribosomal protein L5.

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

- Molecule 28 is a protein called 50S ribosomal protein L6.

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

- Molecule 29 is a protein called 50S ribosomal protein L9.

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

- Molecule 30 is a protein called 50S ribosomal protein L11.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 43 is a protein called 50S ribosomal protein L25.

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

- Molecule 44 is a protein called 50S ribosomal protein L27.

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

- Molecule 45 is a protein called 50S ribosomal protein L28.

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

- Molecule 46 is a protein called 50S ribosomal protein L29.

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

- Molecule 47 is a protein called 50S ribosomal protein L30.

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

- Molecule 48 is a protein called 50S ribosomal protein L32.

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

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

- Molecule 49 is a protein called 50S ribosomal protein L33.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L35.

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

- Molecule 52 is a protein called 50S ribosomal protein L36.

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

- Molecule 53 is a RNA chain called 16S rRNA.

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

- Molecule 54 is a RNA chain called 5S rRNA.

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

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	AA	43	Total	Mg	0	0
			43	43		
55	BA	137	Total	Mg	0	0
			137	137		
55	BB	4	Total	Mg	0	0
			4	4		
55	CA	42	Total	Mg	0	0
			42	42		
55	DA	135	Total	Mg	0	0
			135	135		
55	DB	1	Total	Mg	0	0
			1	1		
55	DJ	1	Total	Mg	0	0
			1	1		

- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 57 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	AE	1	Total	O	0	0
			1	1		
57	AL	3	Total	O	0	0
			3	3		
57	AN	6	Total	O	0	0
			6	6		
57	AT	2	Total	O	0	0
			2	2		
57	AU	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	AA	195	Total 195	O 195	0	0
57	BA	610	Total 610	O 610	0	0
57	BB	20	Total 20	O 20	0	0
57	BC	10	Total 10	O 10	0	0
57	BD	2	Total 2	O 2	0	0
57	BL	4	Total 4	O 4	0	0
57	BN	3	Total 3	O 3	0	0
57	BQ	1	Total 1	O 1	0	0
57	BT	2	Total 2	O 2	0	0
57	B0	1	Total 1	O 1	0	0
57	B2	1	Total 1	O 1	0	0
57	B3	3	Total 3	O 3	0	0
57	B4	3	Total 3	O 3	0	0
57	CE	5	Total 5	O 5	0	0
57	CI	1	Total 1	O 1	0	0
57	CL	1	Total 1	O 1	0	0
57	CN	3	Total 3	O 3	0	0
57	CT	3	Total 3	O 3	0	0
57	CU	2	Total 2	O 2	0	0
57	CA	192	Total 192	O 192	0	0
57	DA	599	Total 599	O 599	0	0

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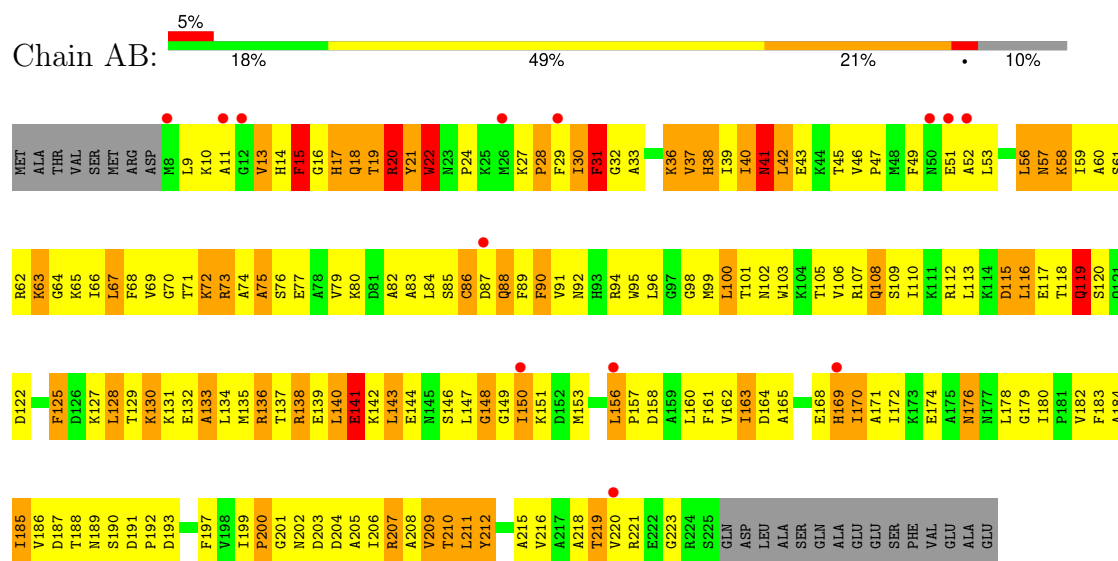
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	DB	4	Total 4	O 4	0	0
57	DC	13	Total 13	O 13	0	0
57	DD	4	Total 4	O 4	0	0
57	DE	3	Total 3	O 3	0	0
57	DJ	3	Total 3	O 3	0	0
57	DL	5	Total 5	O 5	0	0
57	DN	2	Total 2	O 2	0	0
57	DT	2	Total 2	O 2	0	0
57	DU	1	Total 1	O 1	0	0
57	DV	1	Total 1	O 1	0	0
57	D2	1	Total 1	O 1	0	0
57	D3	1	Total 1	O 1	0	0
57	D4	4	Total 4	O 4	0	0

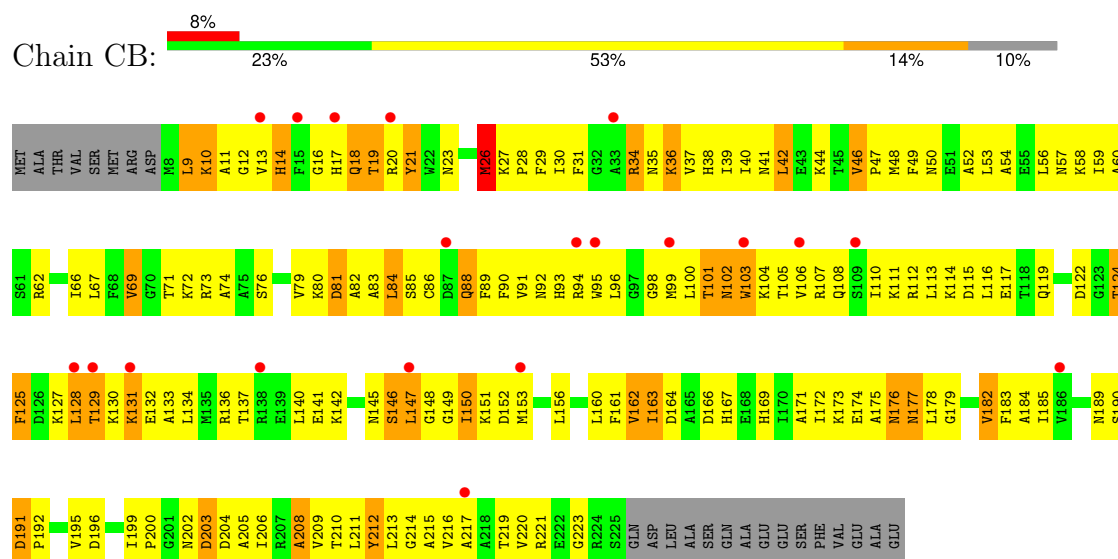
3 Residue-property plots

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.

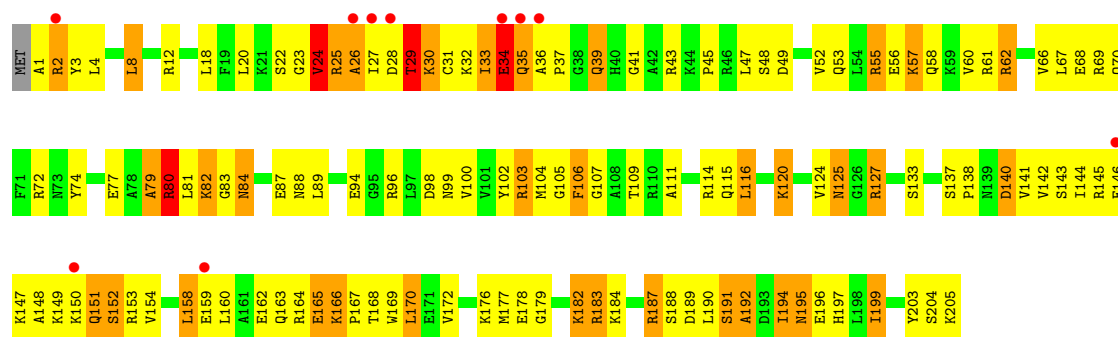
• Molecule 1: 30S ribosomal protein S2



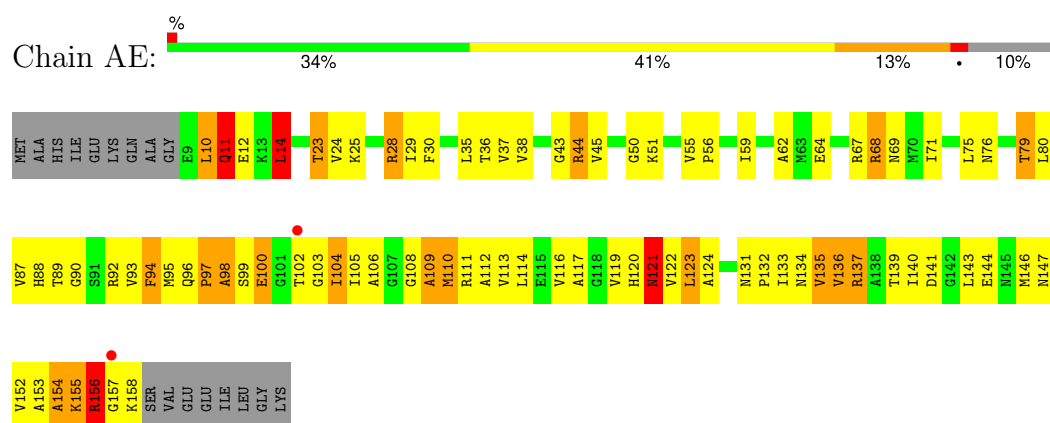
• Molecule 1: 30S ribosomal protein S2



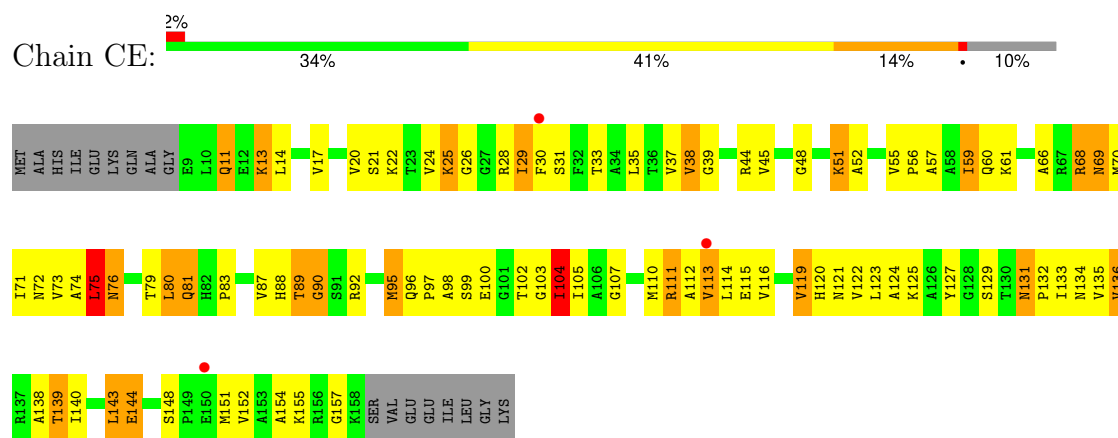
• Molecule 2: 30S ribosomal protein S3



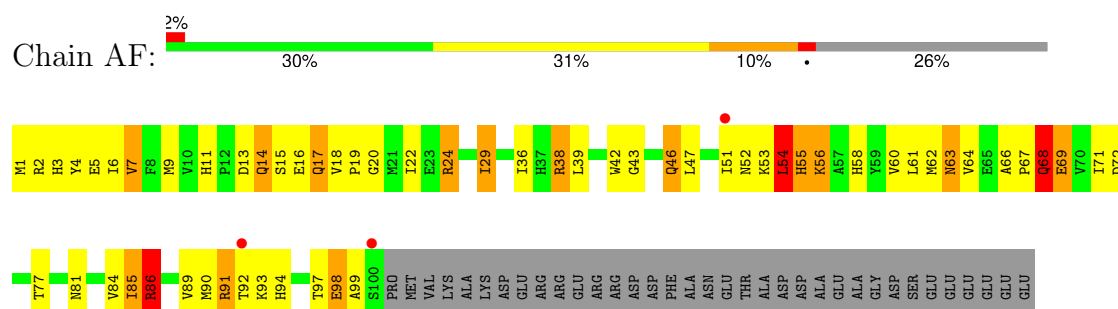
• Molecule 4: 30S ribosomal protein S5



• Molecule 4: 30S ribosomal protein S5



• Molecule 5: 30S ribosomal protein S6



Chain CF:

4% 25% 34% 14% 26%

Chain AG:

4% 32% 44% 8% 16%

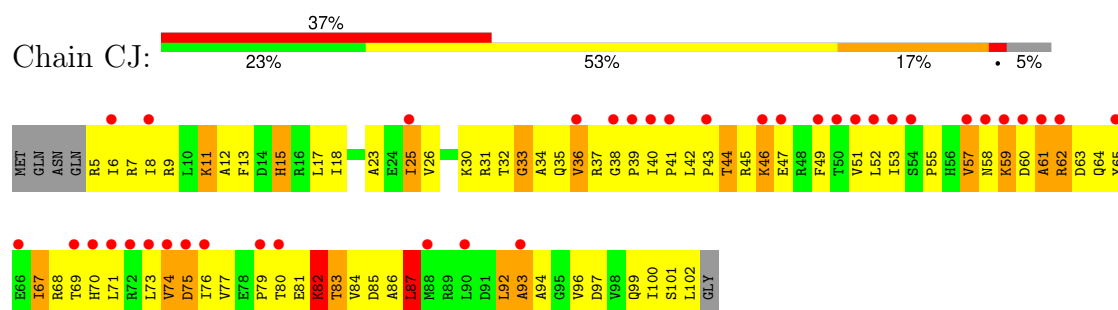
MET P R R3 R4 V G G7 Q8 L12 F13 D14 P15 K16 F17 G18 S19 E20 L21 L22 A23 K24 F25 N27 I28 L29 M30 V31 D32 G33 K34 K35 S36 T37 A38 E39 S40 I41 V42 Y43 L46 E47 T48 L49 R52 S53 G54 K55 A60 F61 E62 V63 A64 L65

V68 R69 P70 T71 S76 T83 Q84 R85 V86 F87 V88 E89 Y90 R91 F92 R93 R94 R95 R96 A99 M100 R101 M102 I103 V104 A105 A106 A107 R108 K109 R110 G111 D112 K113 S114 M115 A116 L117 R118 L119 A120 M121 E122 L123 S124 D125 E128 N129 K130 G131 T132 A133 V134 K135 K136

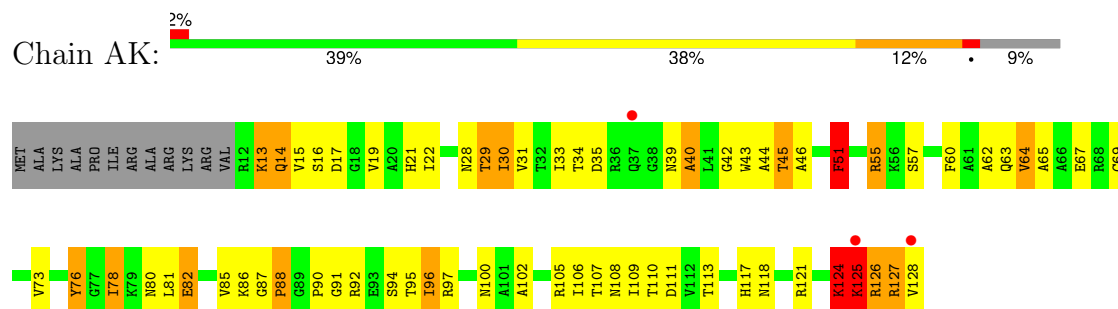
Chain CG:

Chain AH:

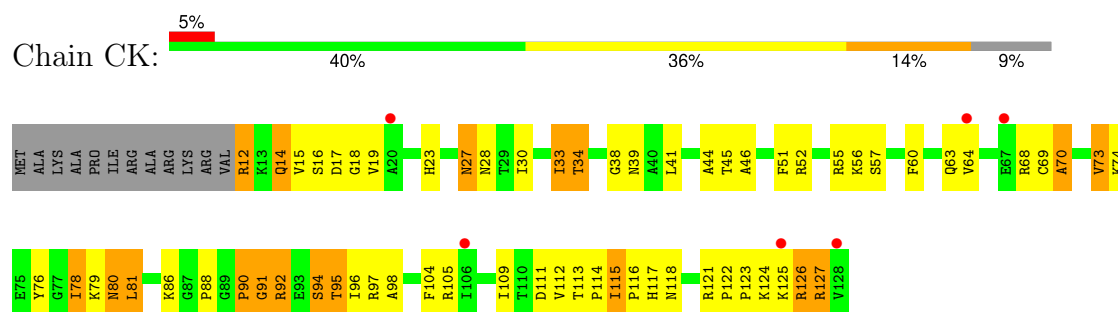
2% 44% 44% 12%



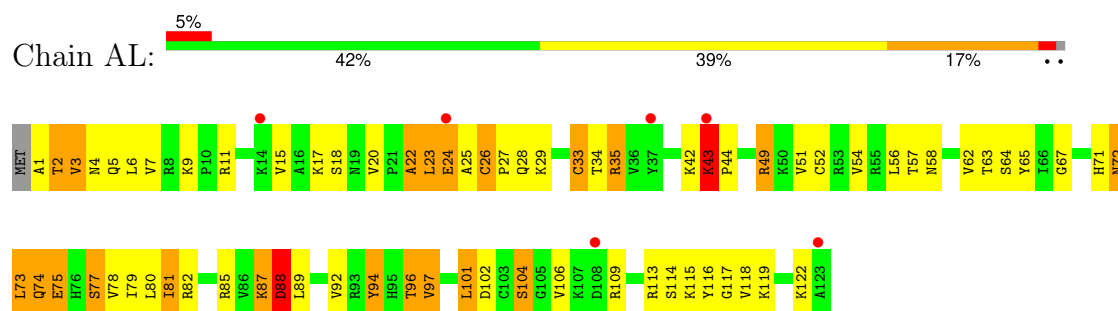
- Molecule 10: 30S ribosomal protein S11



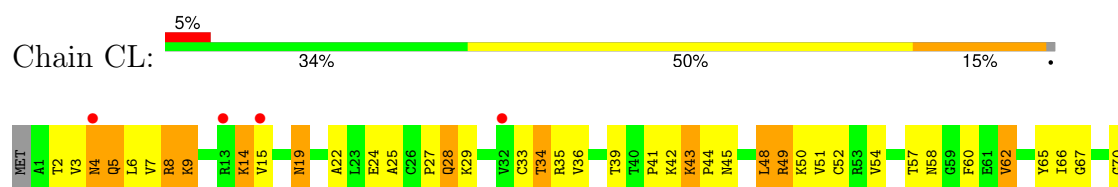
- Molecule 10: 30S ribosomal protein S11

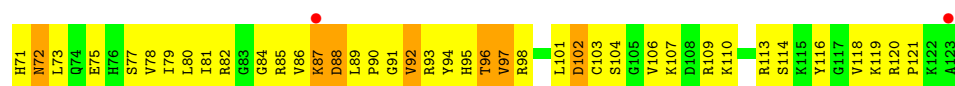


- Molecule 11: 30S ribosomal protein S12



- Molecule 11: 30S ribosomal protein S12

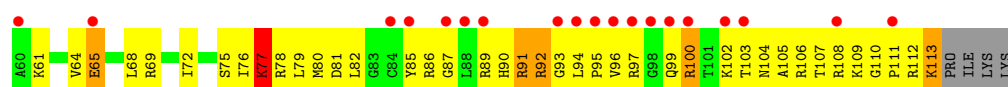
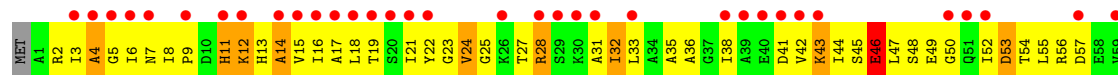




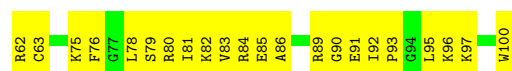
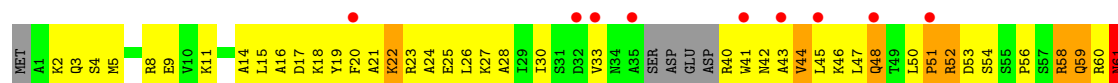
• Molecule 12: 30S ribosomal protein S13



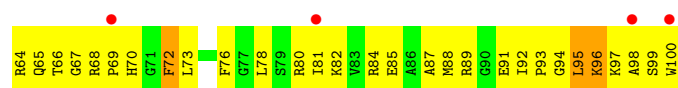
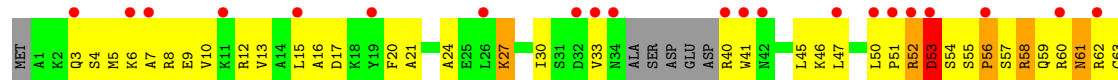
• Molecule 12: 30S ribosomal protein S13



• Molecule 13: 30S ribosomal protein S14

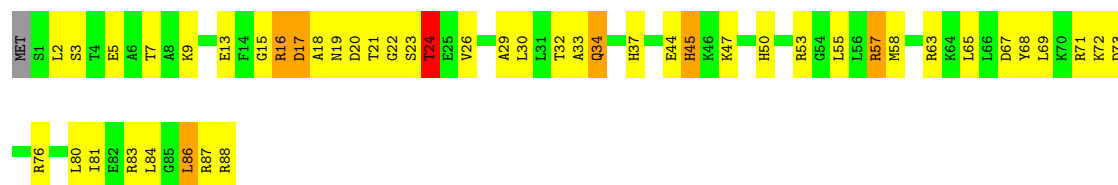


• Molecule 13: 30S ribosomal protein S14



• Molecule 14: 30S ribosomal protein S15





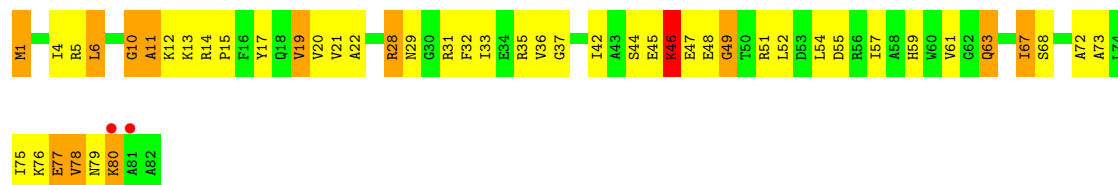
• Molecule 14: 30S ribosomal protein S15

Chain CO: 10% 52% 40% 7%



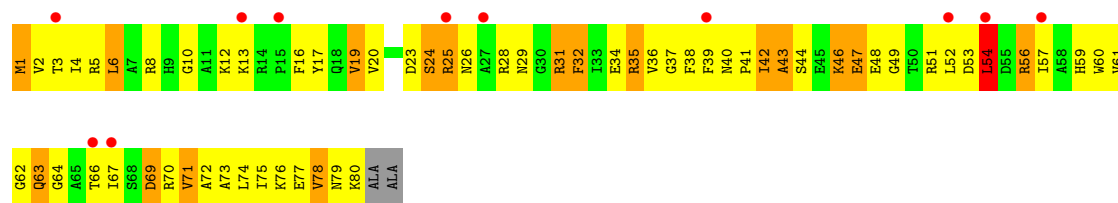
• Molecule 15: 30S ribosomal protein S16

Chain AP: 2% 41% 43% 15%



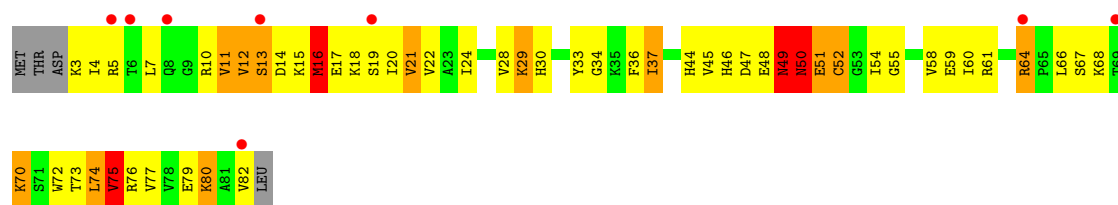
• Molecule 15: 30S ribosomal protein S16

Chain CP: 13% 21% 55% 21%

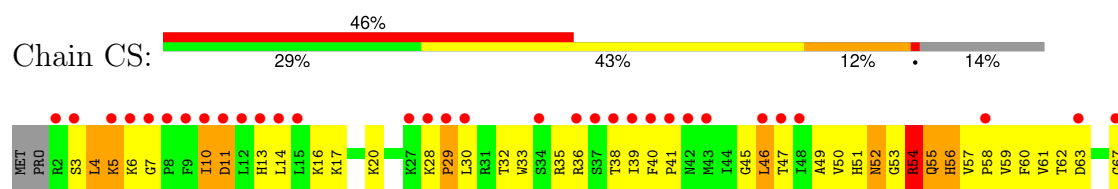


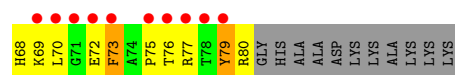
• Molecule 16: 30S ribosomal protein S17

Chain AQ: 10% 31% 45% 14% 5% 5%

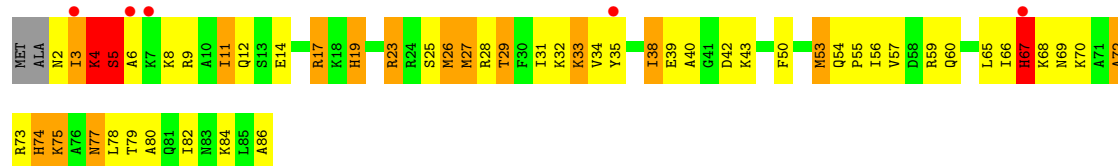


• Molecule 16: 30S ribosomal protein S17

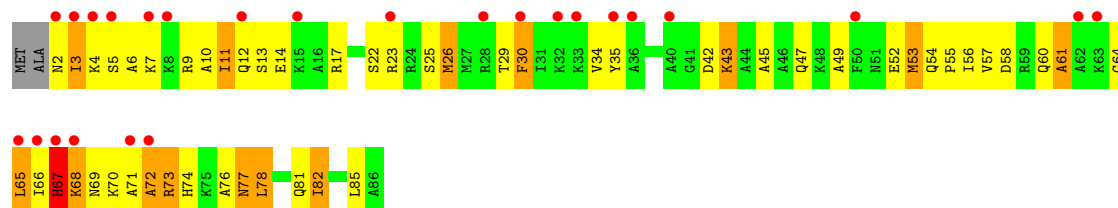




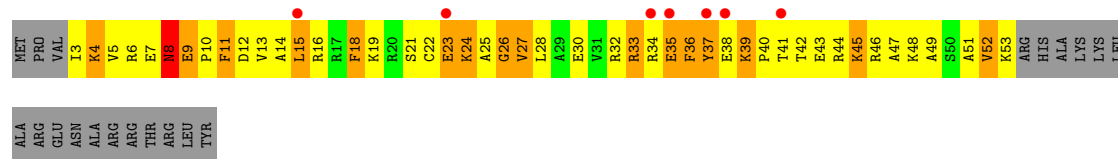
• Molecule 19: 30S ribosomal protein S20



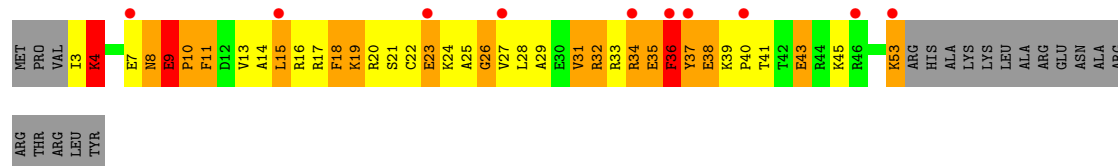
• Molecule 19: 30S ribosomal protein S20



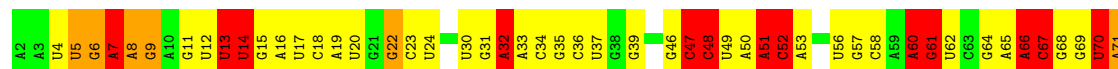
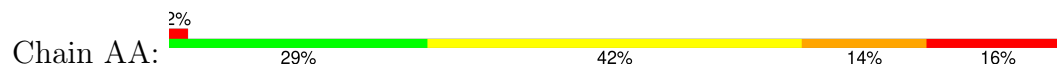
• Molecule 20: 30S ribosomal protein S21



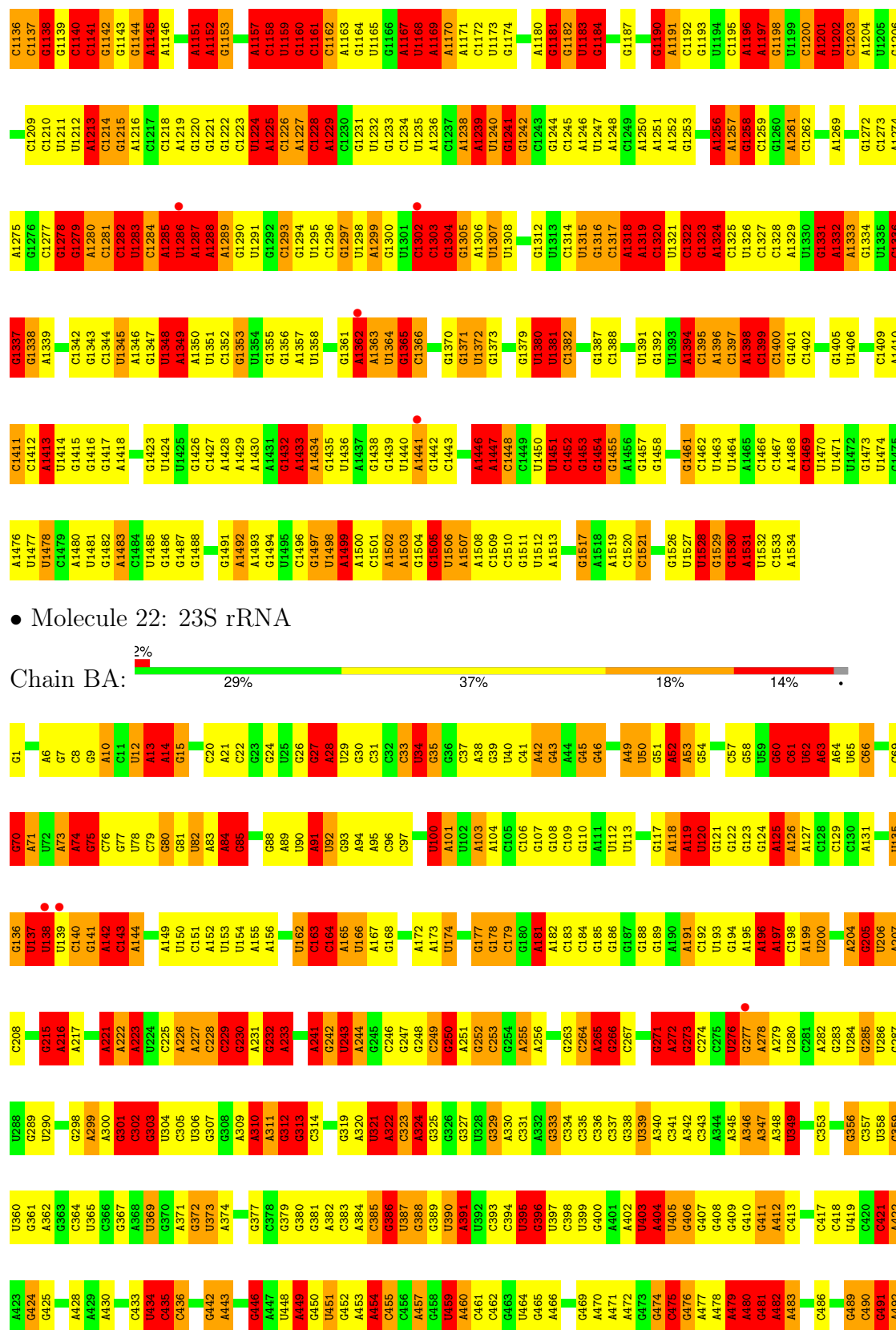
• Molecule 20: 30S ribosomal protein S21



• Molecule 21: 16S rRNA

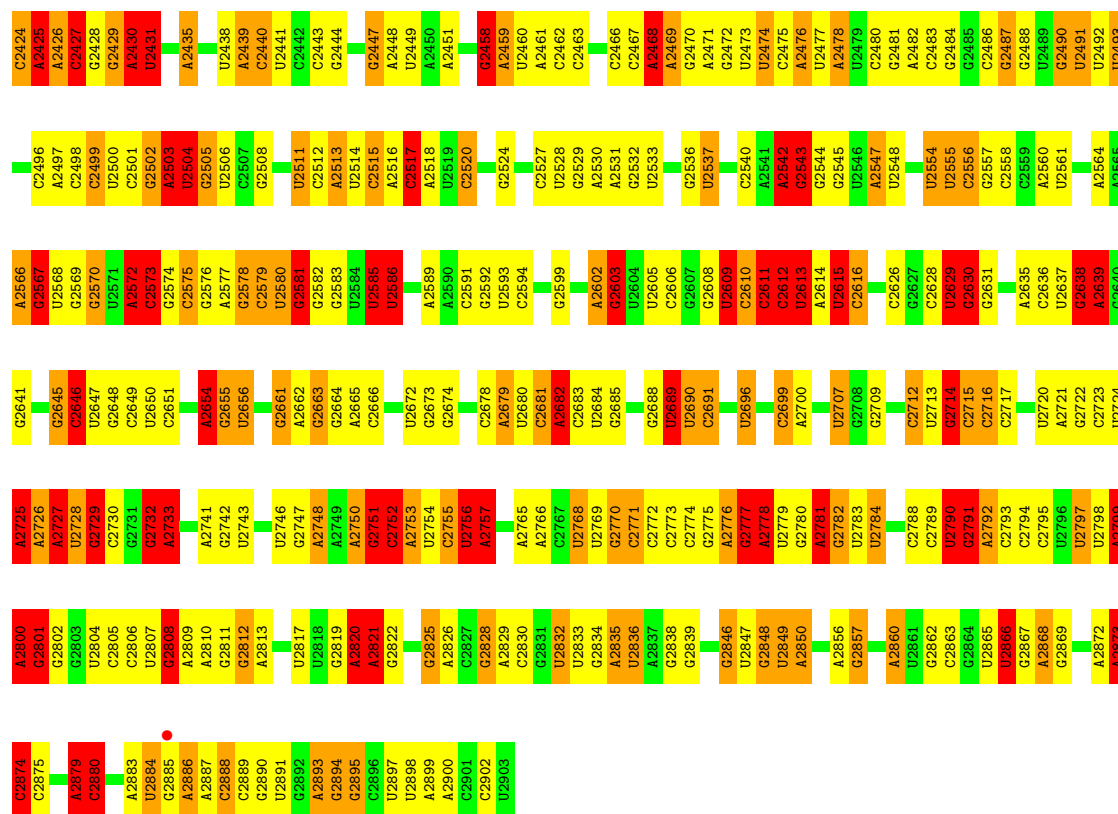




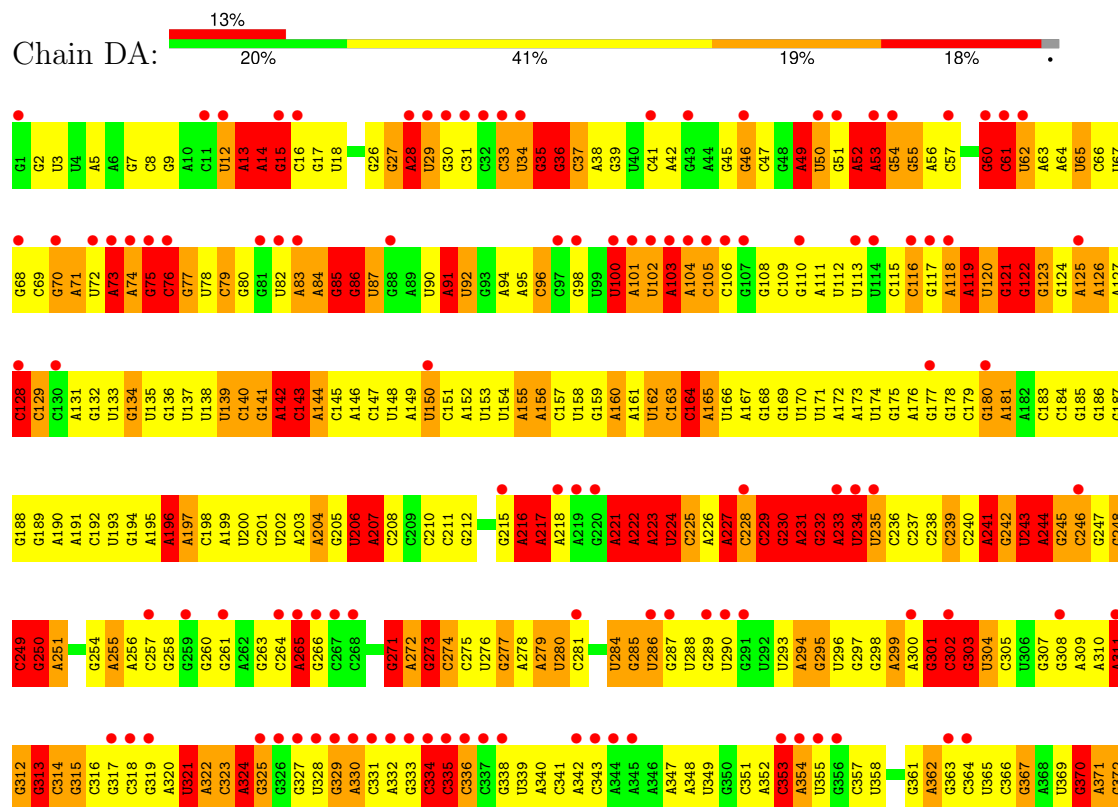






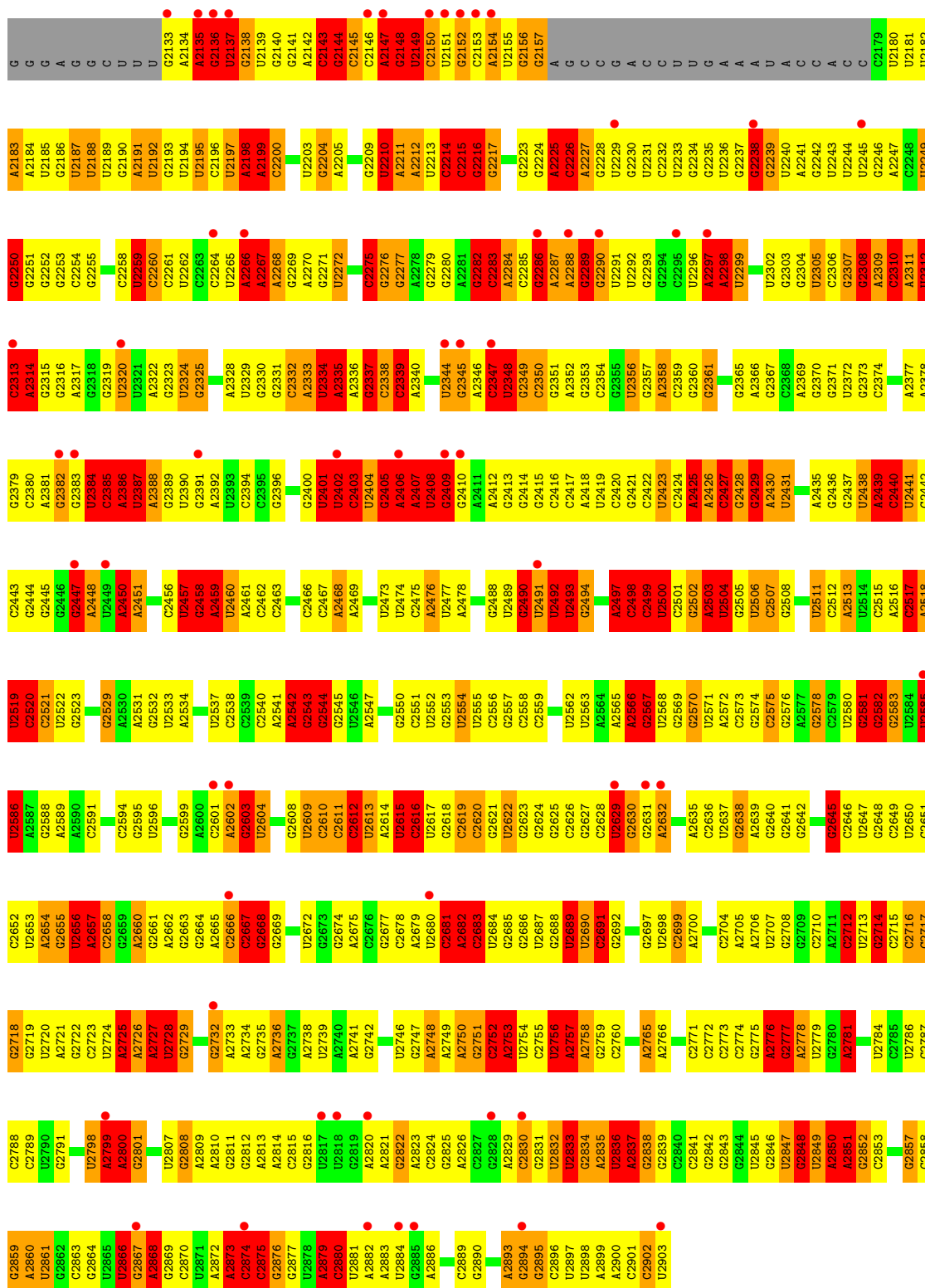


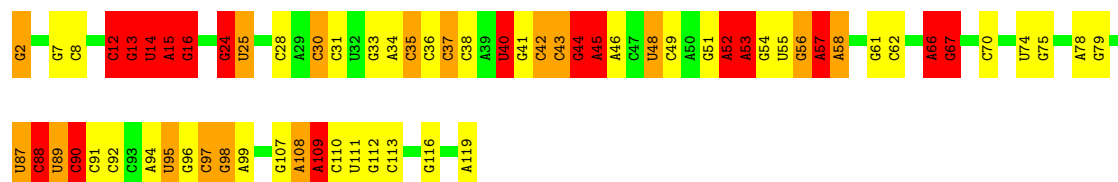
- Molecule 22: 23S rRNA



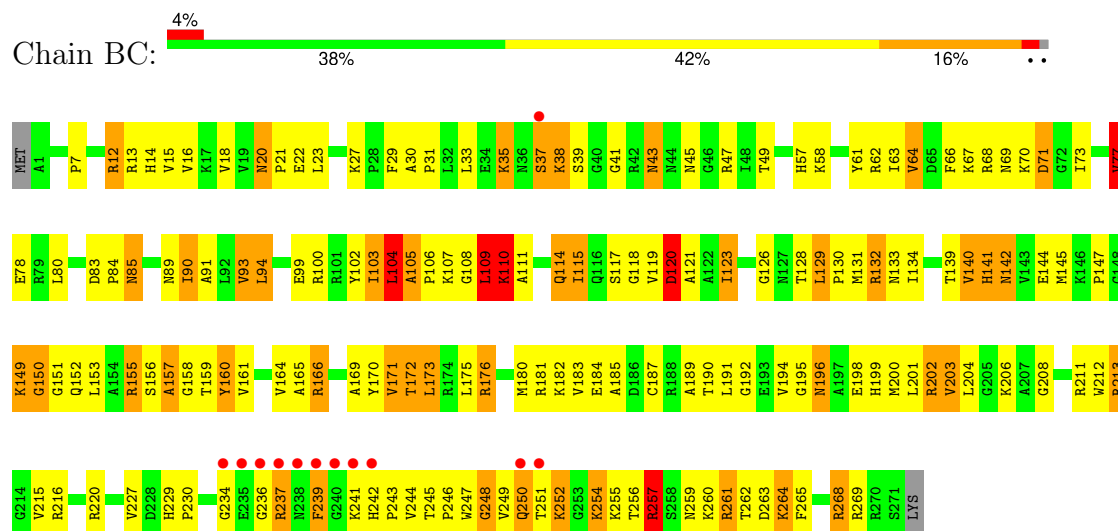


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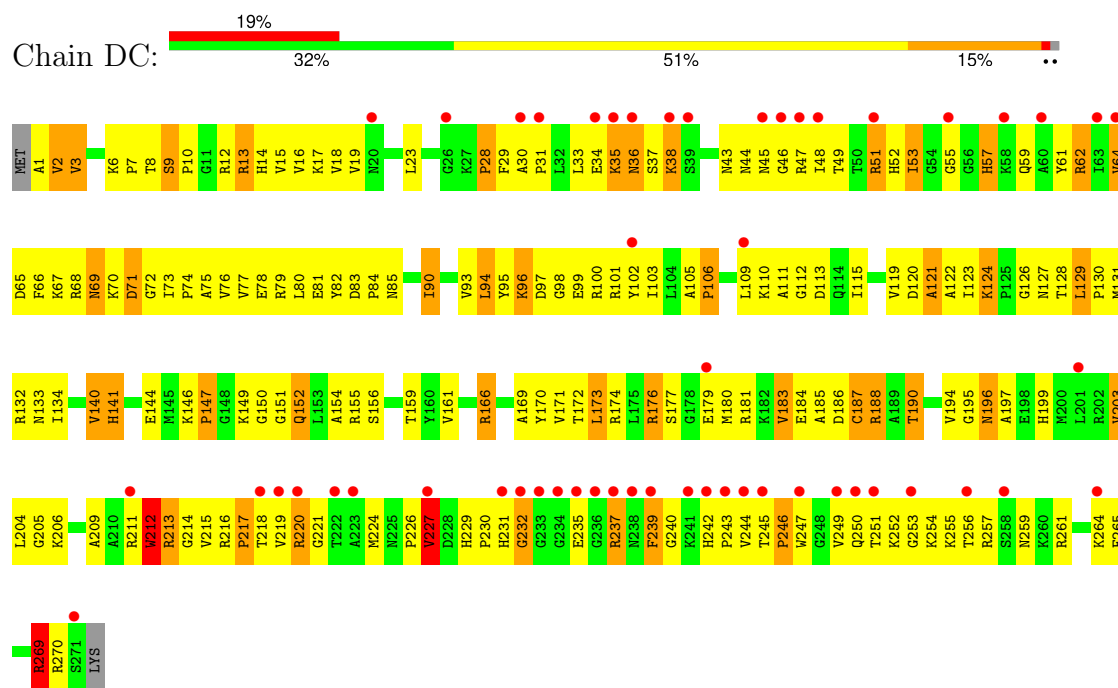




• Molecule 24: 50S ribosomal protein L2

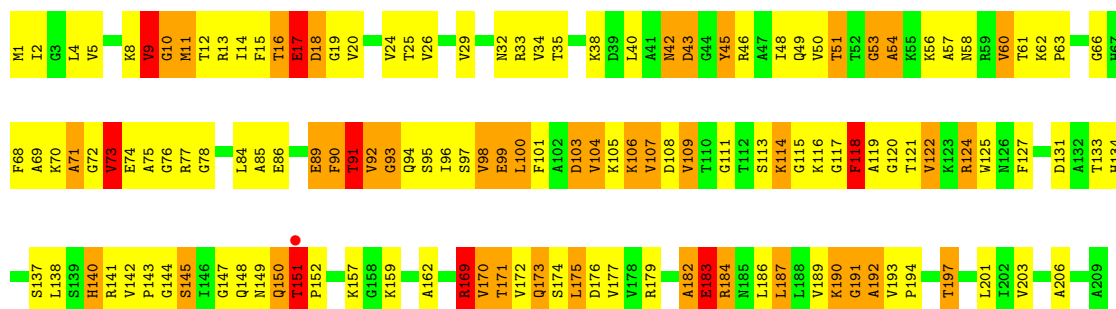


• Molecule 24: 50S ribosomal protein L2

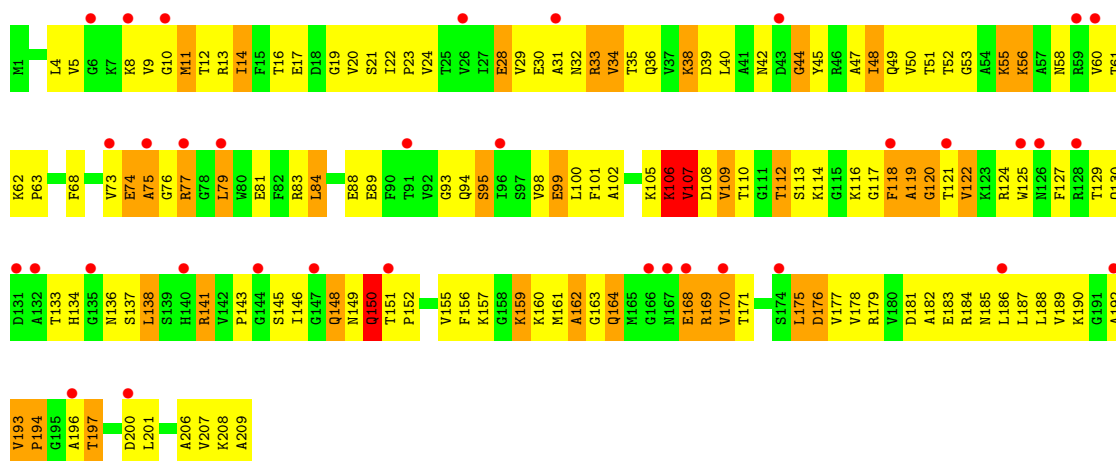


• Molecule 25: 50S ribosomal protein L3

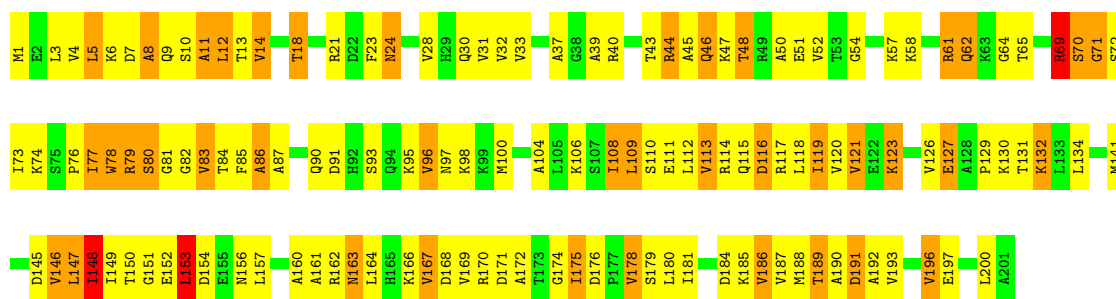




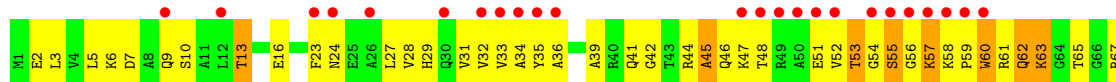
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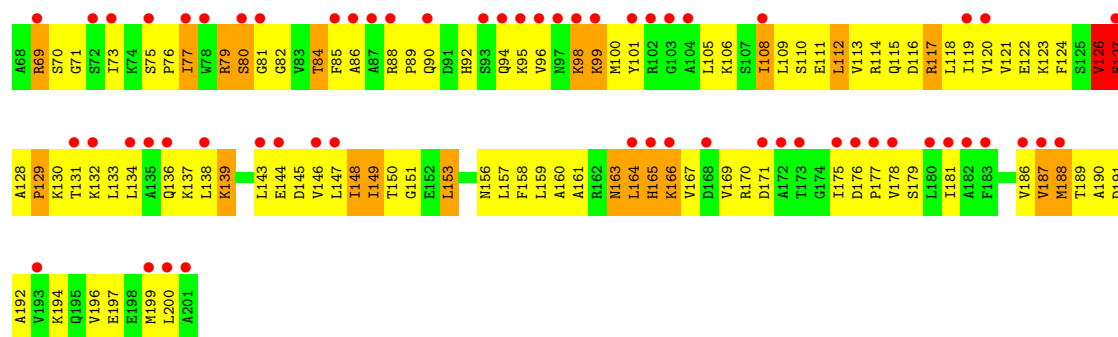


• Molecule 26: 50S ribosomal protein L4

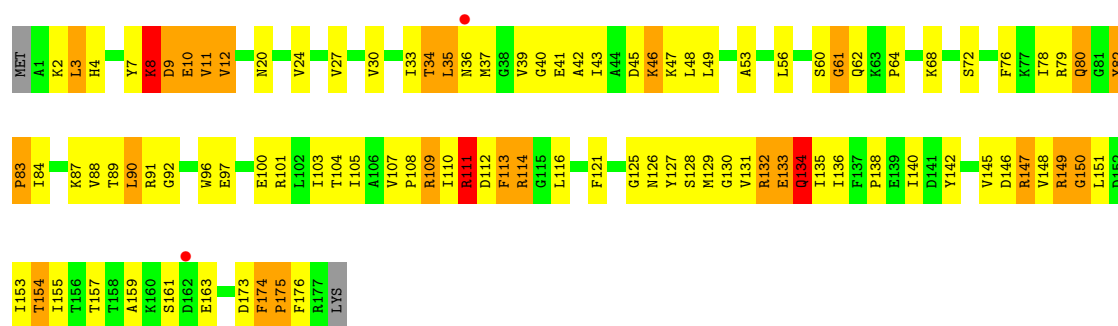
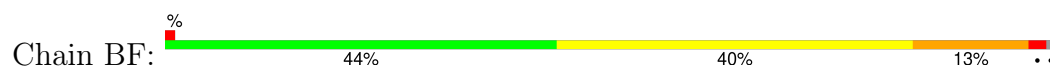


• Molecule 26: 50S ribosomal protein L4

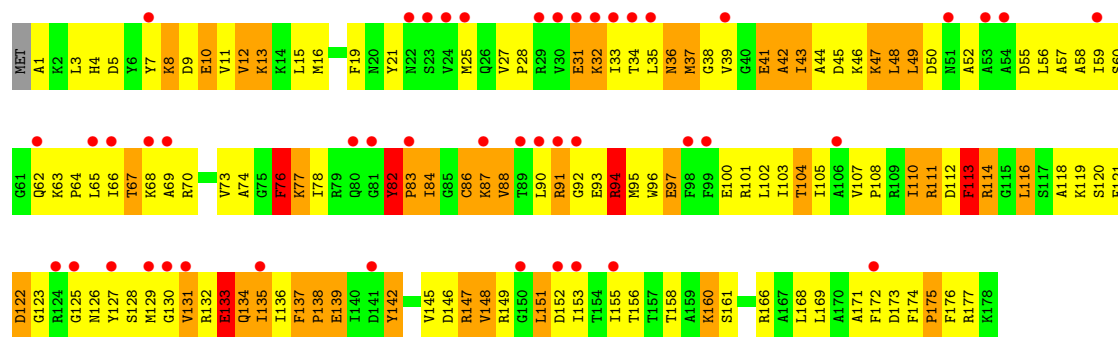




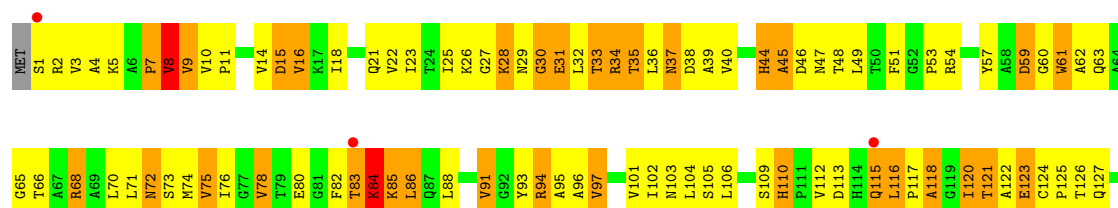
• Molecule 27: 50S ribosomal protein L5



• Molecule 27: 50S ribosomal protein L5

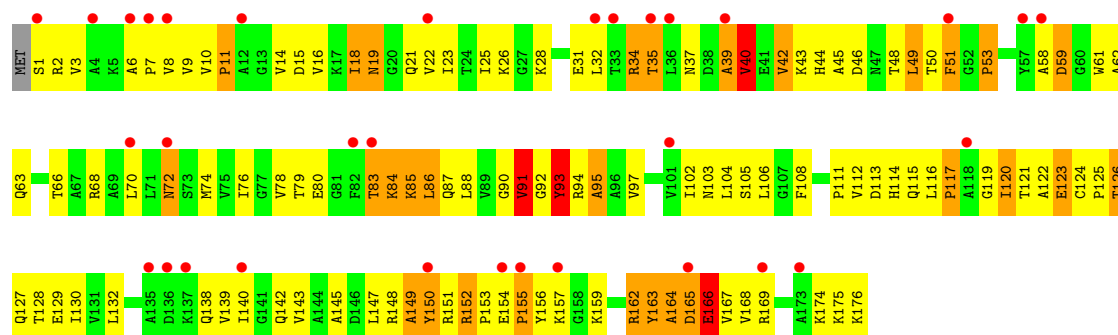


• Molecule 28: 50S ribosomal protein L6

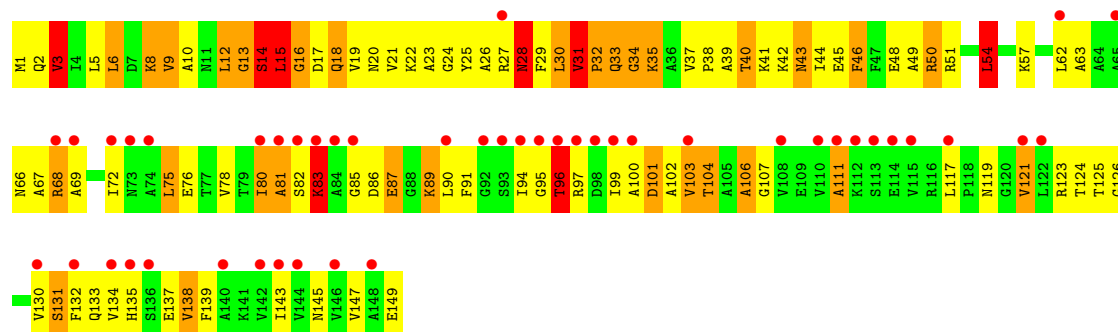




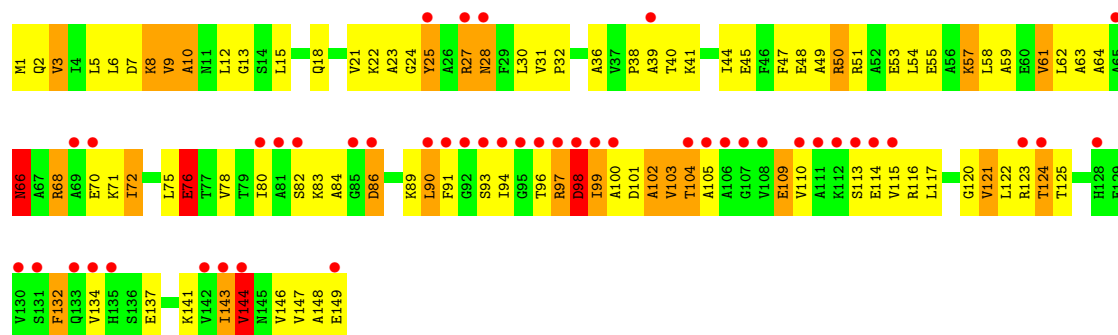
• Molecule 28: 50S ribosomal protein L6



• Molecule 29: 50S ribosomal protein L9

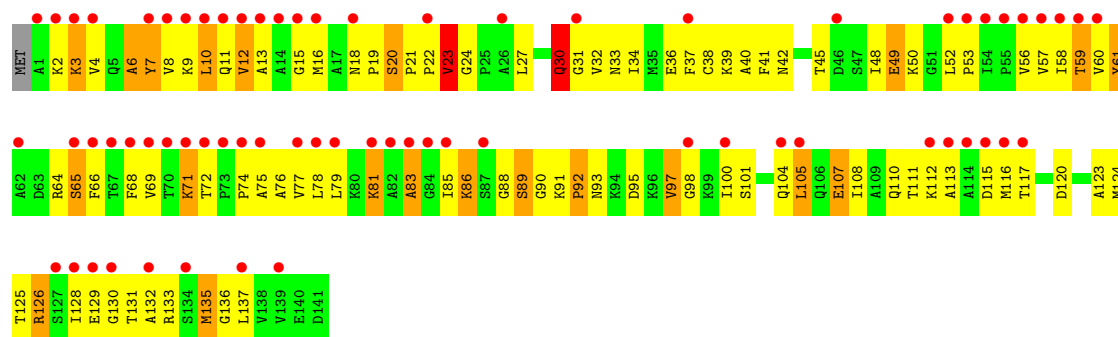


• Molecule 29: 50S ribosomal protein L9

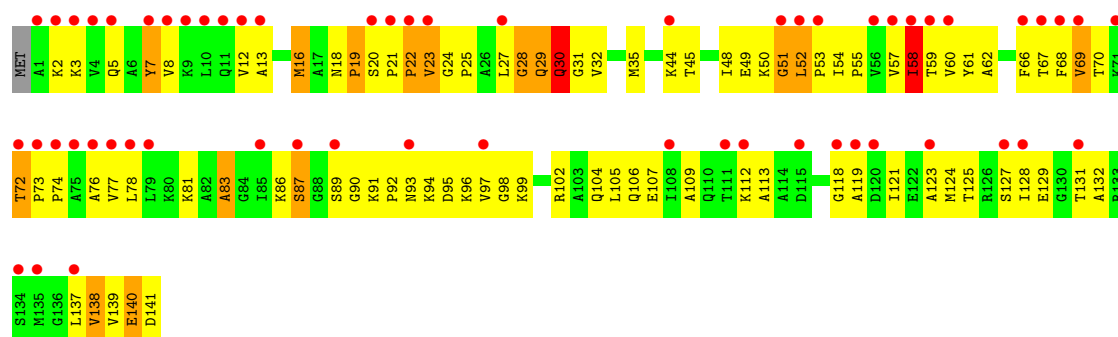


• Molecule 30: 50S ribosomal protein L11

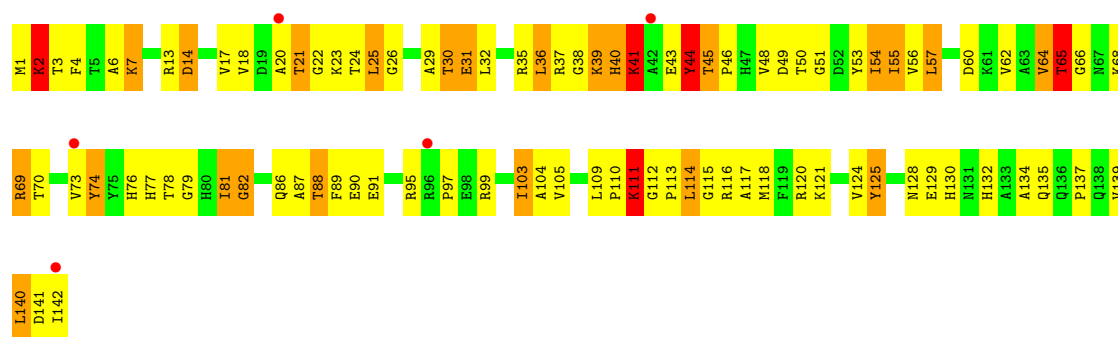




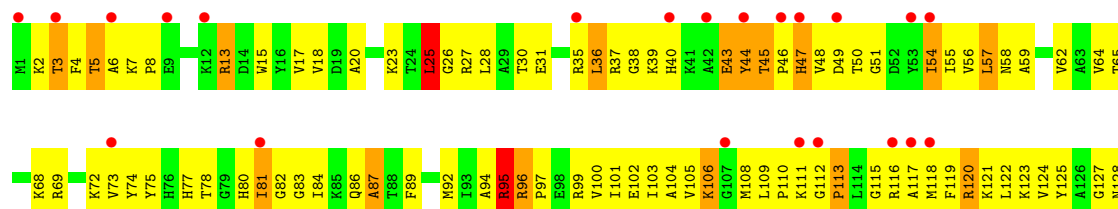
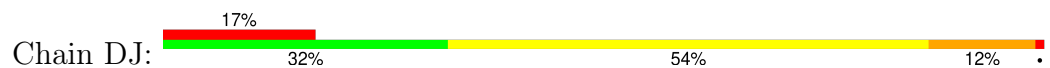
• Molecule 30: 50S ribosomal protein L11



• Molecule 31: 50S ribosomal protein L13

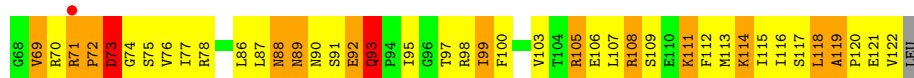
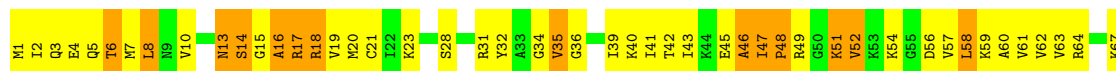


• Molecule 31: 50S ribosomal protein L13

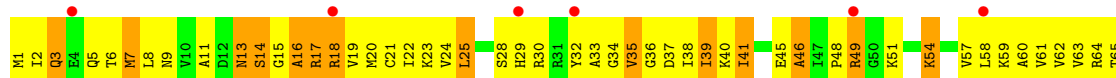




- Molecule 32: 50S ribosomal protein L14



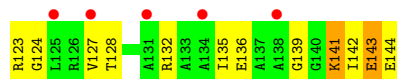
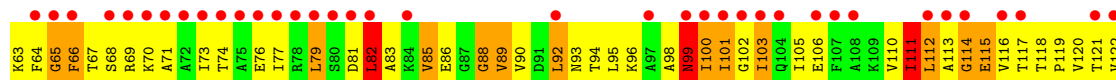
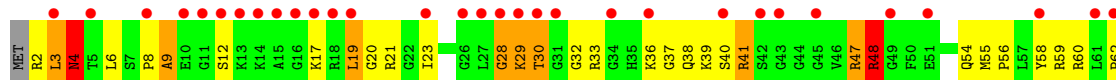
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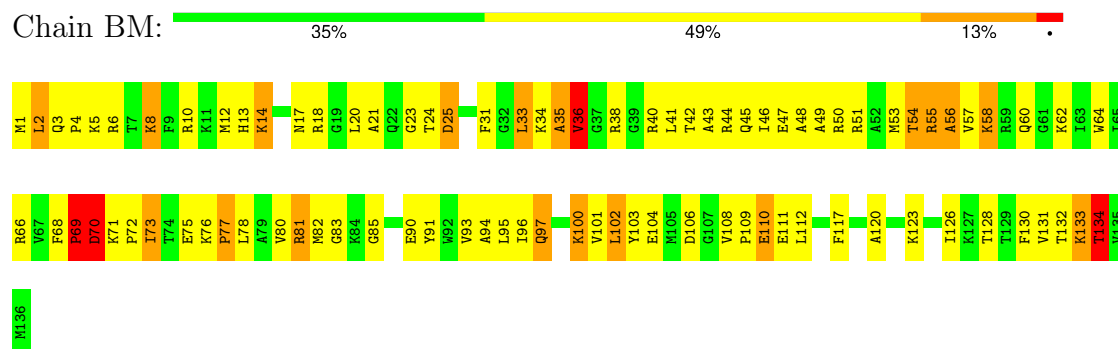
- Molecule 33: 50S ribosomal protein L15



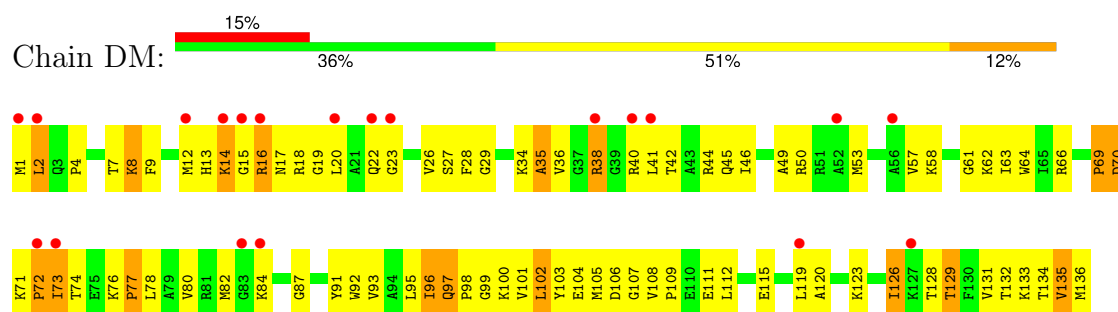
- Molecule 33: 50S ribosomal protein L15



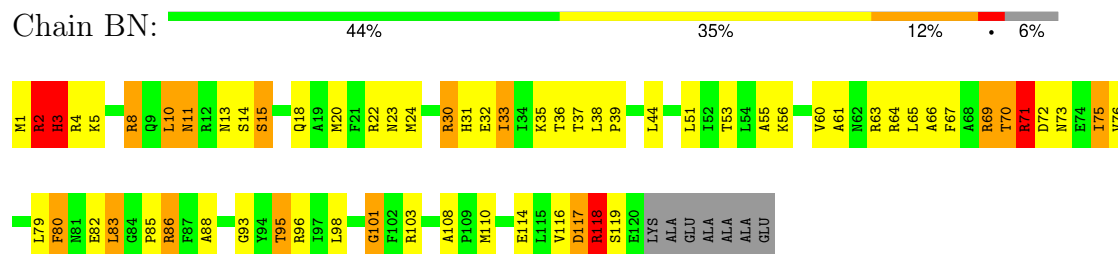
- Molecule 34: 50S ribosomal protein L16



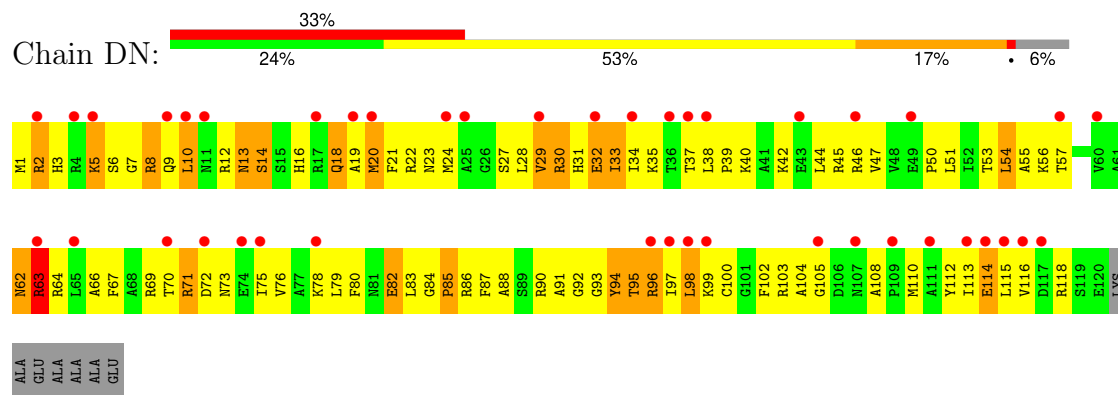
- Molecule 34: 50S ribosomal protein L16



- Molecule 35: 50S ribosomal protein L17

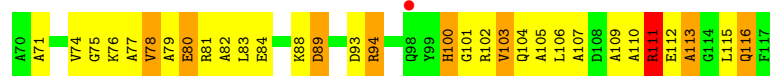


- Molecule 35: 50S ribosomal protein L17

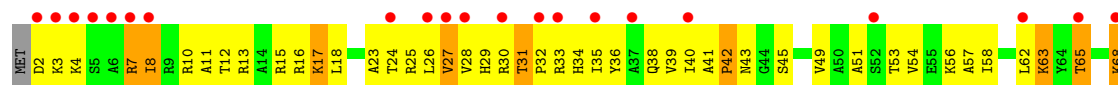


- Molecule 36: 50S ribosomal protein L18

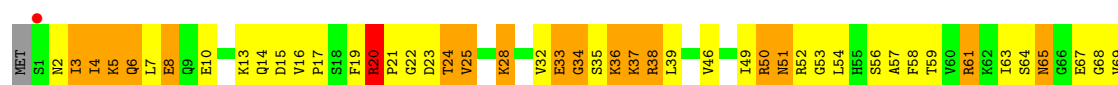




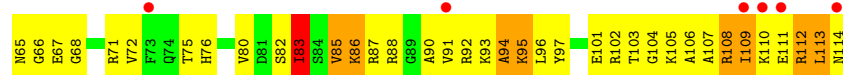
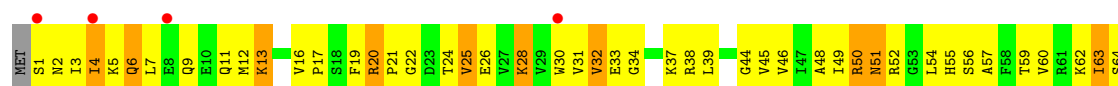
• Molecule 36: 50S ribosomal protein L18



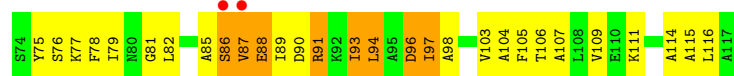
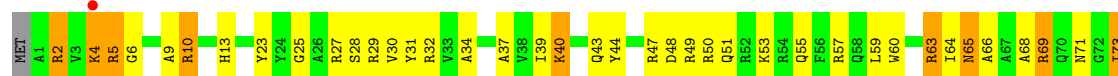
• Molecule 37: 50S ribosomal protein L19



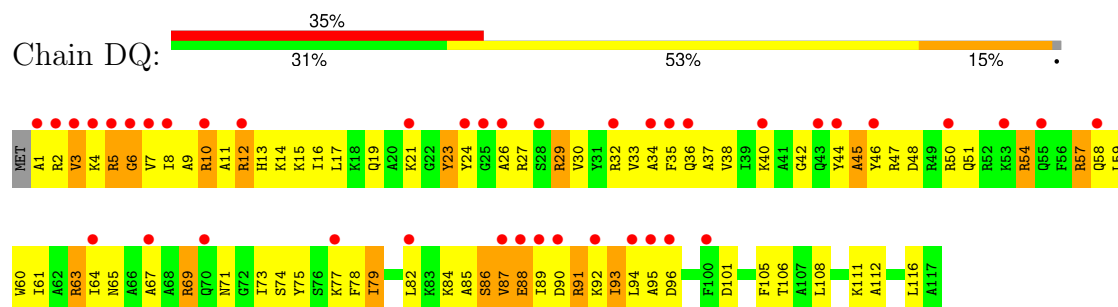
• Molecule 37: 50S ribosomal protein L19



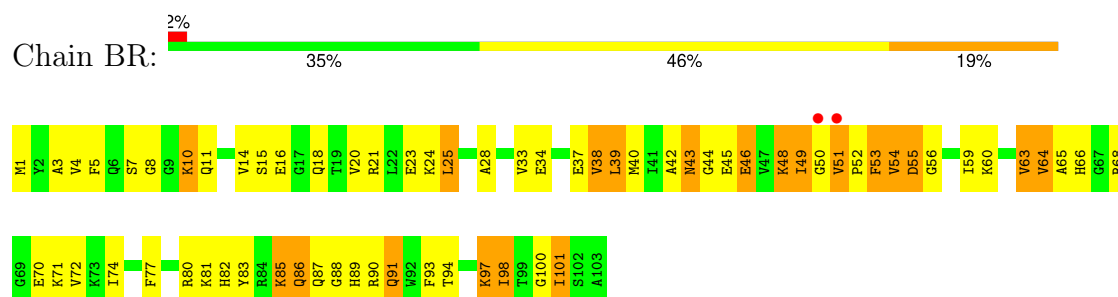
• Molecule 38: 50S ribosomal protein L20



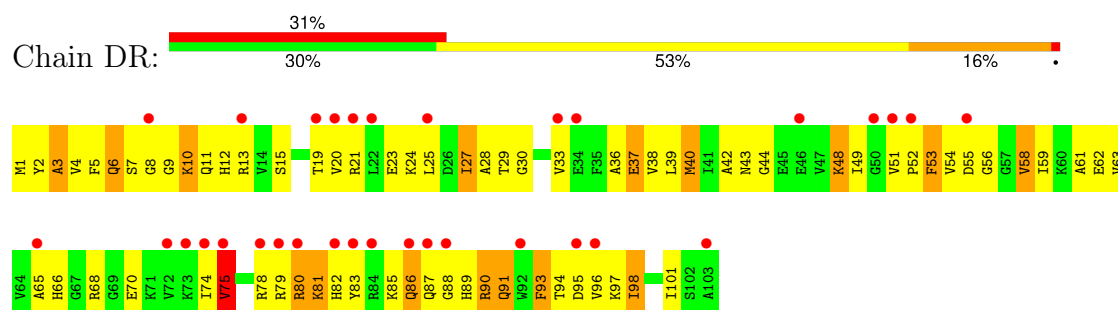
- Molecule 38: 50S ribosomal protein L20



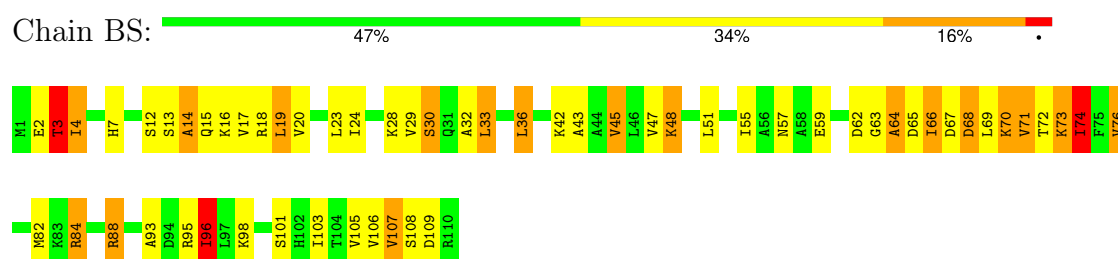
- Molecule 39: 50S ribosomal protein L21



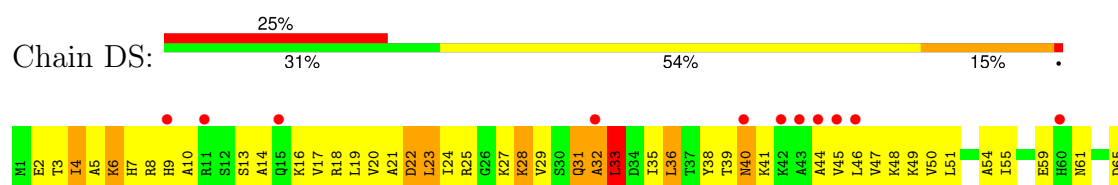
- Molecule 39: 50S ribosomal protein L21

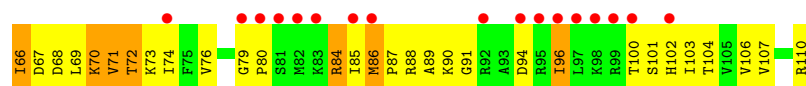


- Molecule 40: 50S ribosomal protein L22

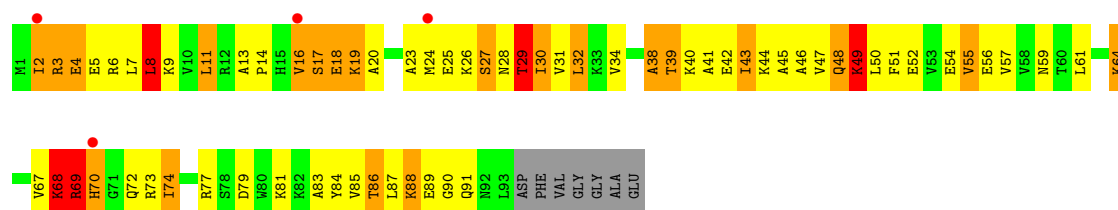


- Molecule 40: 50S ribosomal protein L22

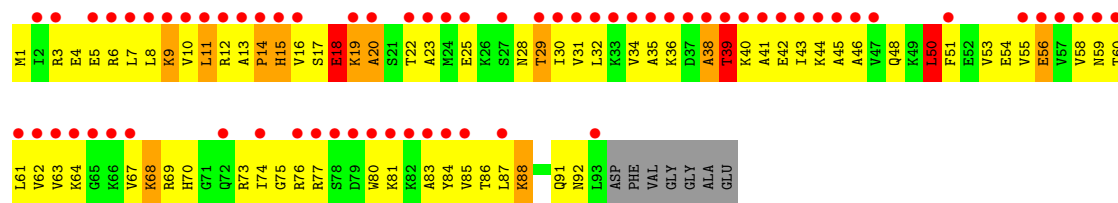




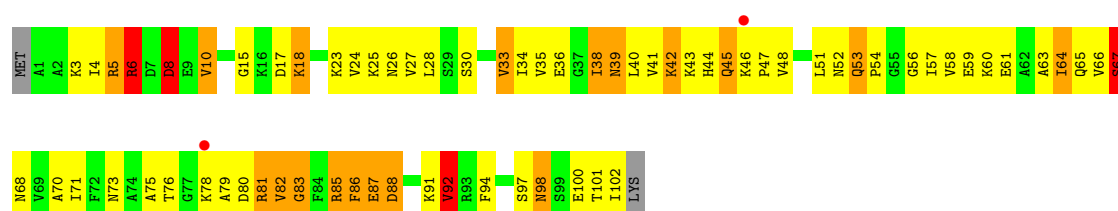
• Molecule 41: 50S ribosomal protein L23



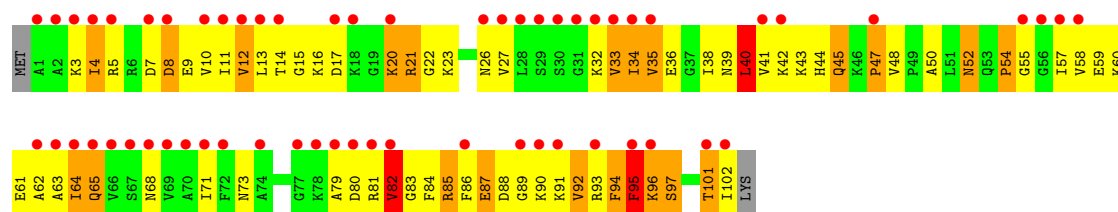
• Molecule 41: 50S ribosomal protein L23



• Molecule 42: 50S ribosomal protein L24

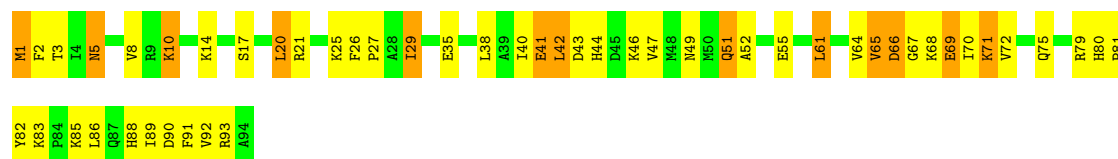


• Molecule 42: 50S ribosomal protein L24

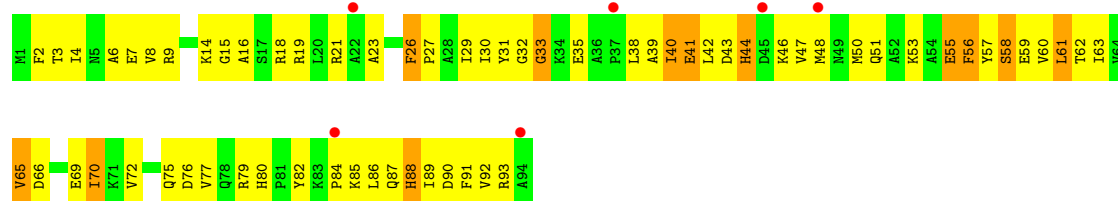
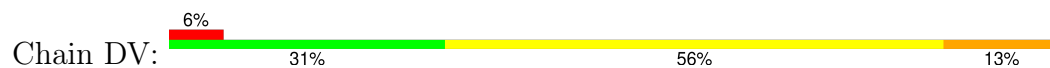


• Molecule 43: 50S ribosomal protein L25

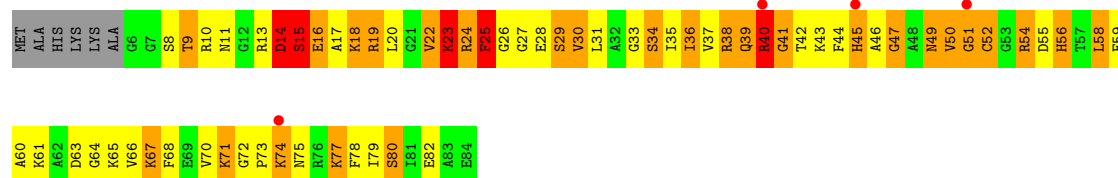
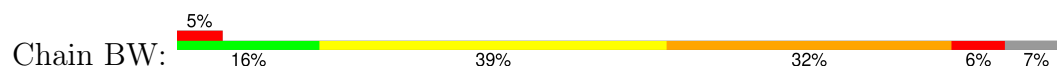




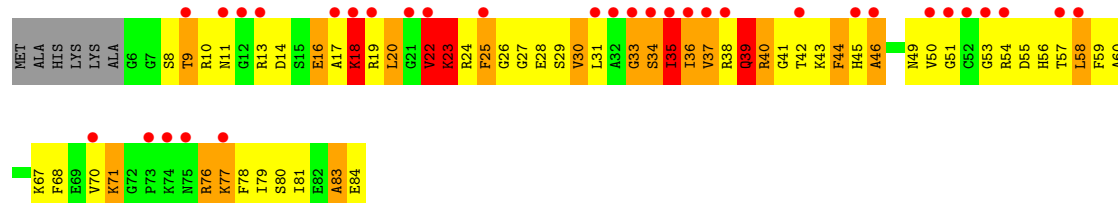
• Molecule 43: 50S ribosomal protein L25



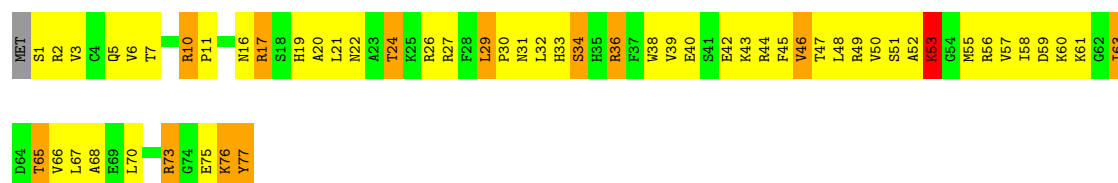
• Molecule 44: 50S ribosomal protein L27



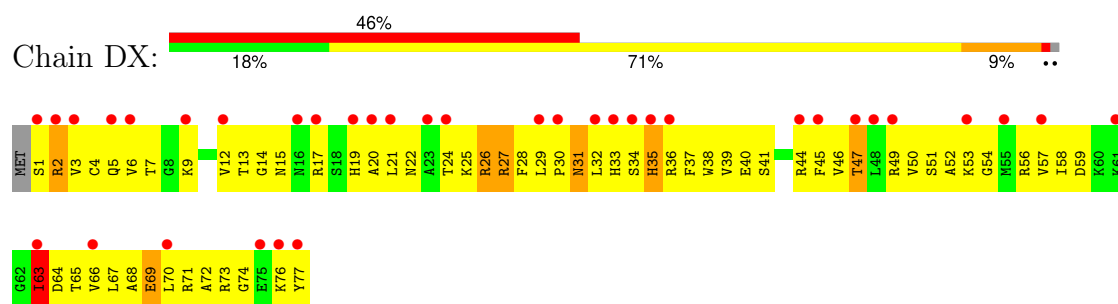
• Molecule 44: 50S ribosomal protein L27



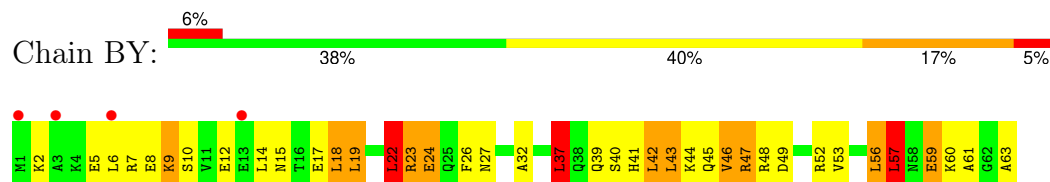
• Molecule 45: 50S ribosomal protein L28



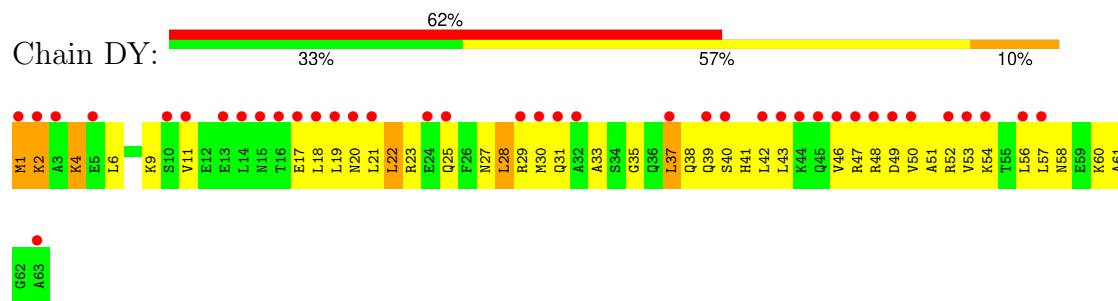
• Molecule 45: 50S ribosomal protein L28



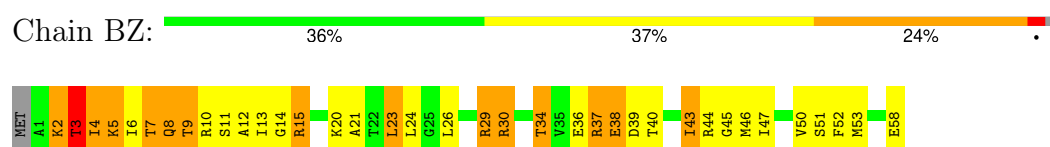
- Molecule 46: 50S ribosomal protein L29



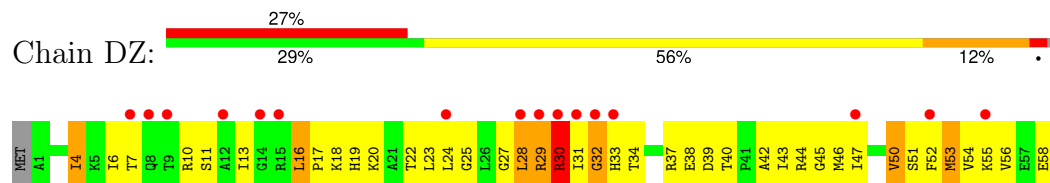
- Molecule 46: 50S ribosomal protein L29



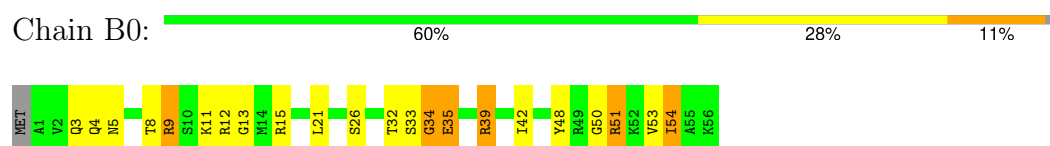
- Molecule 47: 50S ribosomal protein L30



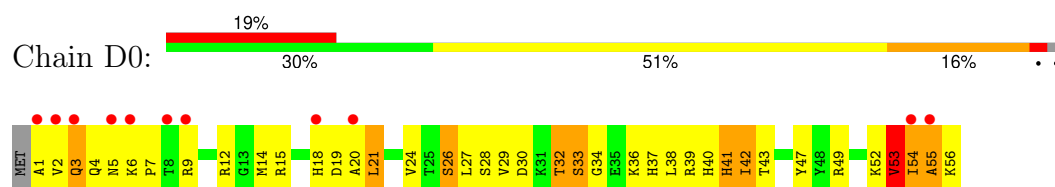
- Molecule 47: 50S ribosomal protein L30



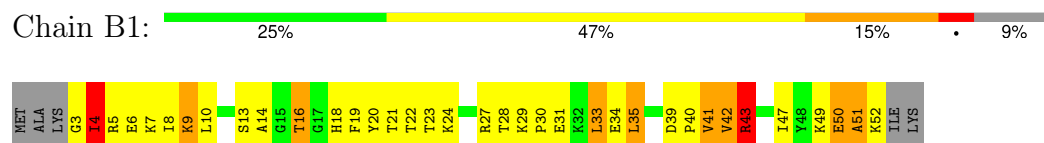
- Molecule 48: 50S ribosomal protein L32



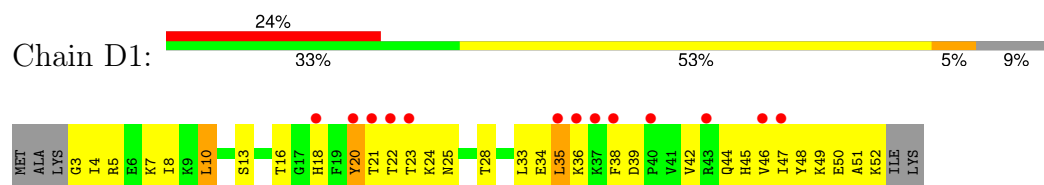
- Molecule 48: 50S ribosomal protein L32



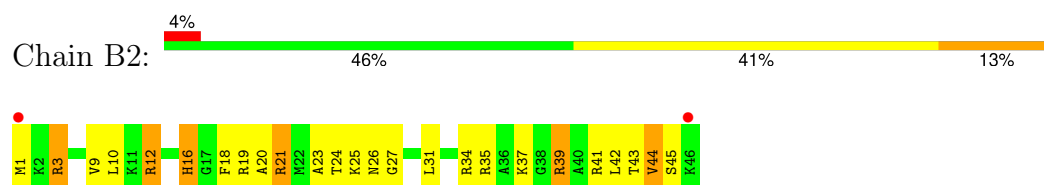
- Molecule 49: 50S ribosomal protein L33



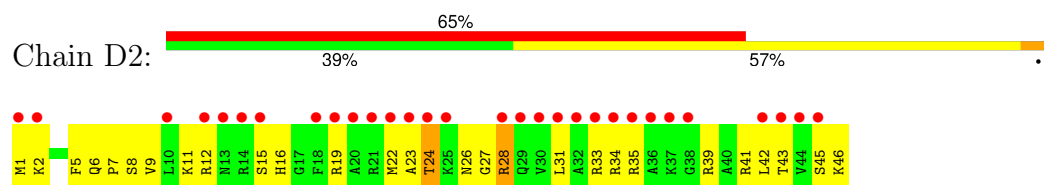
- Molecule 49: 50S ribosomal protein L33



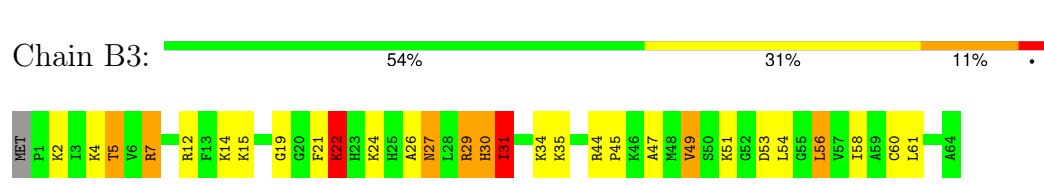
- Molecule 50: 50S ribosomal protein L34



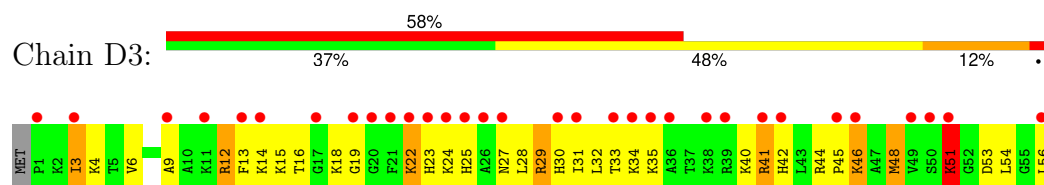
- Molecule 50: 50S ribosomal protein L34



- Molecule 51: 50S ribosomal protein L35

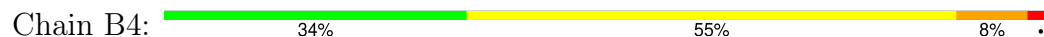


- Molecule 51: 50S ribosomal protein L35

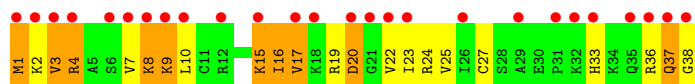
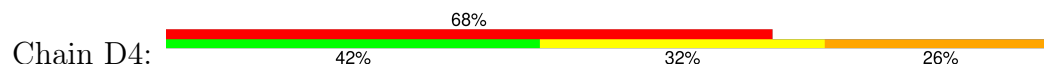




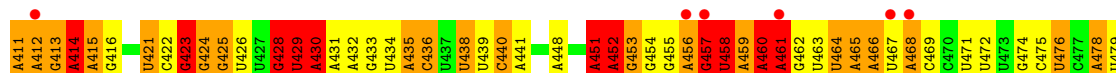
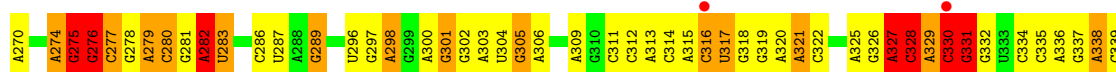
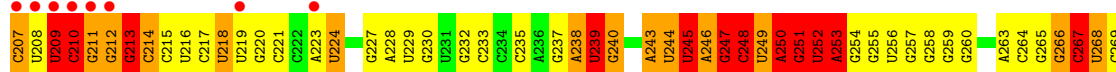
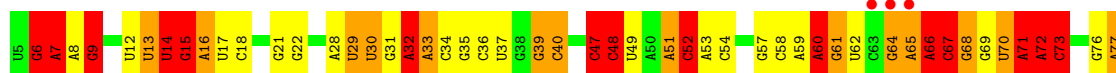
- Molecule 52: 50S ribosomal protein L36

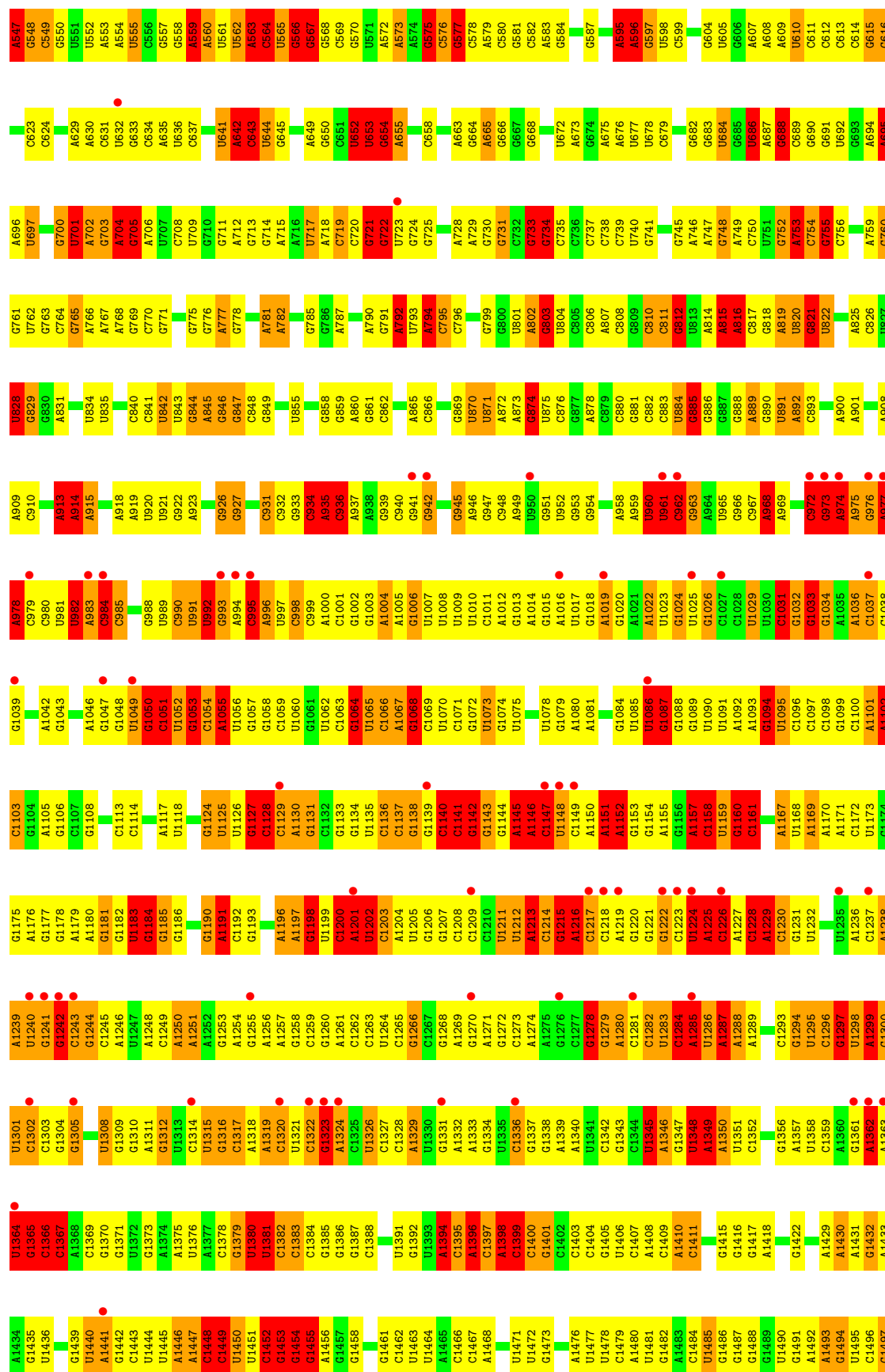


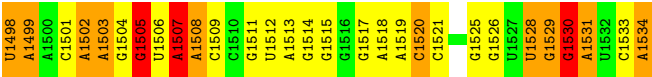
- Molecule 52: 50S ribosomal protein L36



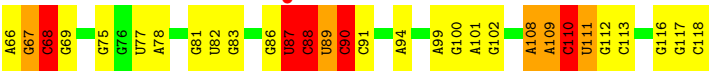
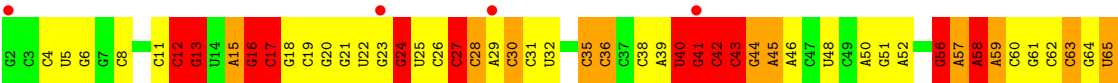
- Molecule 53: 16S rRNA







● Molecule 54: 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	211.89Å 434.93Å 622.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.88 – 3.19 39.88 – 3.19	Depositor EDS
% Data completeness (in resolution range)	95.8 (39.88-3.19) 95.8 (39.88-3.19)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 3.18Å)	Xtriage
Refinement program	PHENIX, PHENIX (phenix.refine)	Depositor
R, R_{free}	0.195 , 0.252 0.207 , 0.259	Depositor DCC
R_{free} test set	18197 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å ²)	63.6	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 76.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	284450	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.53% 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	0.30	0/1735	0.52	0/2338
1	CB	0.27	0/1735	0.49	0/2338
2	AC	0.30	0/1651	0.53	1/2225 (0.0%)
2	CC	0.25	0/1651	0.45	0/2225
3	AD	0.31	0/1665	0.52	0/2227
3	CD	0.39	0/1665	0.60	0/2227
4	AE	0.36	0/1118	0.63	1/1504 (0.1%)
4	CE	0.34	0/1118	0.54	0/1504
5	AF	0.32	0/835	0.49	0/1128
5	CF	0.28	0/835	0.50	0/1128
6	AG	0.27	0/1195	0.48	0/1602
6	CG	0.25	0/1187	0.46	0/1591
7	AH	0.33	0/989	0.55	0/1326
7	CH	0.28	0/989	0.50	0/1326
8	AI	0.27	0/1034	0.49	0/1375
8	CI	0.24	0/1034	0.43	0/1375
9	AJ	0.29	0/796	0.53	0/1077
9	CJ	0.24	0/796	0.48	0/1077
10	AK	0.31	0/893	0.56	0/1205
10	CK	0.29	0/893	0.50	0/1205
11	AL	0.39	0/969	0.69	0/1300
11	CL	0.32	0/969	0.57	0/1300
12	AM	0.26	0/892	0.49	0/1193
12	CM	0.20	0/884	0.41	0/1181
13	AN	0.30	0/785	0.54	0/1043
13	CN	0.22	0/780	0.39	0/1036
14	AO	0.30	0/722	0.49	0/964
14	CO	0.26	0/722	0.45	0/964
15	AP	0.30	0/659	0.50	0/884
15	CP	0.30	0/648	0.51	0/870
16	AQ	0.39	0/657	0.59	0/881
16	CQ	0.31	0/657	0.51	0/881

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AR	0.30	0/462	0.50	0/621
17	CR	0.30	0/462	0.47	0/621
18	AS	0.28	0/652	0.49	0/877
18	CS	0.21	0/652	0.43	0/877
19	AT	0.35	0/671	0.56	0/888
19	CT	0.27	0/671	0.50	0/888
20	AU	0.39	0/430	0.54	0/570
20	CU	0.39	0/430	0.63	0/570
21	AA	0.55	1/36834 (0.0%)	1.38	581/57462 (1.0%)
22	BA	0.78	12/68626 (0.0%)	1.59	1420/107056 (1.3%)
22	DA	0.50	0/68314	1.35	1136/106569 (1.1%)
23	BB	0.71	0/2828	1.50	45/4410 (1.0%)
24	BC	0.44	0/2121	0.70	1/2852 (0.0%)
24	DC	0.31	0/2121	0.53	0/2852
25	BD	0.53	0/1586	0.76	1/2134 (0.0%)
25	DD	0.30	0/1586	0.56	0/2134
26	BE	0.43	0/1571	0.64	0/2113
26	DE	0.26	0/1571	0.47	0/2113
27	BF	0.33	0/1434	0.54	0/1926
27	DF	0.23	0/1444	0.47	0/1937
28	BG	0.40	0/1343	0.64	0/1816
28	DG	0.24	0/1343	0.48	0/1816
29	BH	0.31	0/1122	0.50	0/1515
29	DH	0.28	0/1122	0.50	0/1515
30	BI	0.23	0/1046	0.47	0/1410
30	DI	0.21	0/1046	0.43	0/1410
31	BJ	0.57	0/1152	0.80	1/1551 (0.1%)
31	DJ	0.28	0/1152	0.55	1/1551 (0.1%)
32	BK	0.51	0/947	0.77	0/1268
32	DK	0.33	0/947	0.56	0/1268
33	BL	0.43	0/1054	0.75	0/1403
33	DL	0.27	0/1054	0.52	0/1403
34	BM	0.50	0/1093	0.70	0/1460
34	DM	0.27	0/1093	0.46	0/1460
35	BN	0.47	0/973	0.70	0/1301
35	DN	0.28	0/973	0.50	0/1301
36	BO	0.42	0/902	0.63	0/1209
36	DO	0.22	0/902	0.42	0/1209
37	BP	0.50	0/929	0.73	0/1242
37	DP	0.30	0/929	0.50	0/1242
38	BQ	0.57	0/960	0.73	0/1278
38	DQ	0.29	0/960	0.46	0/1278
39	BR	0.60	1/829 (0.1%)	0.75	0/1107

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	DR	0.28	0/829	0.49	0/1107
40	BS	0.53	0/864	0.72	0/1156
40	DS	0.29	0/864	0.52	0/1156
41	BT	0.46	0/744	0.74	0/994
41	DT	0.24	0/744	0.48	0/994
42	BU	0.44	0/787	0.70	0/1051
42	DU	0.25	0/787	0.47	0/1051
43	BV	0.42	0/766	0.58	0/1025
43	DV	0.25	0/766	0.43	0/1025
44	BW	0.56	0/603	0.87	0/797
44	DW	0.26	0/603	0.48	0/797
45	BX	0.42	0/635	0.70	1/848 (0.1%)
45	DX	0.27	0/635	0.55	0/848
46	BY	0.35	0/510	0.65	0/677
46	DY	0.22	0/510	0.45	0/677
47	BZ	0.51	0/453	0.77	0/605
47	DZ	0.26	0/453	0.49	0/605
48	B0	0.45	0/450	0.71	0/599
48	D0	0.28	0/450	0.51	0/599
49	B1	0.40	0/416	0.63	0/554
49	D1	0.27	0/416	0.46	0/554
50	B2	0.46	0/380	0.73	0/498
50	D2	0.28	0/380	0.50	0/498
51	B3	0.45	0/513	0.69	0/676
51	D3	0.27	0/513	0.51	0/676
52	B4	0.55	0/303	0.78	0/397
52	D4	0.27	0/303	0.49	0/397
53	CA	0.50	0/36762	1.32	542/57350 (0.9%)
54	DB	0.44	0/2803	1.26	34/4371 (0.8%)
All	All	0.55	14/306737 (0.0%)	1.26	3765/458565 (0.8%)

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
25	BD	0	1
32	BK	0	1
35	BN	0	1
51	B3	0	1
All	All	0	4

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1142	A	N9-C4	-10.15	1.31	1.37
22	BA	2451	A	C8-N7	8.00	1.37	1.31
22	BA	2447	G	N9-C4	7.71	1.44	1.38
22	BA	984	A	N9-C4	-6.87	1.33	1.37
22	BA	1142	A	C8-N7	6.70	1.36	1.31

The worst 5 of 3765 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2447	G	C6-N1-C2	-18.49	114.00	125.10
22	BA	919	U	N1-C2-O2	18.00	135.40	122.80
22	BA	919	U	C2-N1-C1'	16.54	137.55	117.70
22	BA	302	C	N1-C1'-C2'	-16.46	92.60	114.00
22	BA	805	G	P-O3'-C3'	15.12	137.85	119.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
51	B3	29	ARG	Peptide
25	BD	9	VAL	Peptide
32	BK	15	GLY	Peptide
35	BN	101	GLY	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	221	0
1	CB	1704	0	1732	174	0
2	AC	1624	0	1699	112	0
2	CC	1624	0	1699	143	0
3	AD	1643	0	1710	151	0
3	CD	1643	0	1710	152	0
4	AE	1105	0	1148	132	0
4	CE	1105	0	1148	99	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	AF	817	0	808	73	0
5	CF	817	0	808	66	0
6	AG	1181	0	1240	87	0
6	CG	1174	0	1230	136	0
7	AH	979	0	1034	74	0
7	CH	979	0	1034	88	0
8	AI	1022	0	1070	83	0
8	CI	1022	0	1070	98	0
9	AJ	786	0	828	74	0
9	CJ	786	0	828	97	0
10	AK	877	0	887	89	0
10	CK	877	0	887	78	0
11	AL	955	0	1019	89	0
11	CL	955	0	1019	89	0
12	AM	883	0	944	74	0
12	CM	876	0	937	107	0
13	AN	774	0	827	76	0
13	CN	769	0	822	82	0
14	AO	714	0	737	54	0
14	CO	714	0	737	36	0
15	AP	649	0	666	52	0
15	CP	638	0	656	67	0
16	AQ	648	0	691	75	0
16	CQ	648	0	691	61	0
17	AR	455	0	478	25	0
17	CR	455	0	478	35	0
18	AS	637	0	665	52	0
18	CS	637	0	665	75	0
19	AT	665	0	714	72	0
19	CT	665	0	714	52	0
20	AU	425	0	449	88	0
20	CU	425	0	449	80	0
21	AA	32895	0	16553	1203	0
22	BA	61274	0	30819	1932	0
22	DA	60995	0	30679	3174	0
23	BB	2529	0	1281	63	0
24	BC	2082	0	2157	213	0
24	DC	2082	0	2157	210	0
25	BD	1565	0	1616	186	0
25	DD	1565	0	1616	179	0
26	BE	1552	0	1619	127	0
26	DE	1552	0	1619	172	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	BF	1410	0	1447	124	0
27	DF	1420	0	1460	170	0
28	BG	1323	0	1374	169	0
28	DG	1323	0	1374	137	0
29	BH	1111	0	1148	107	0
29	DH	1111	0	1148	102	0
30	BI	1032	0	1088	108	0
30	DI	1032	0	1088	77	0
31	BJ	1129	0	1162	154	0
31	DJ	1129	0	1162	141	0
32	BK	938	0	1012	99	0
32	DK	938	0	1012	111	0
33	BL	1045	0	1117	117	0
33	DL	1045	0	1117	115	0
34	BM	1074	0	1157	102	0
34	DM	1074	0	1157	96	0
35	BN	960	0	1000	82	0
35	DN	960	0	1000	122	0
36	BO	892	0	923	74	0
36	DO	892	0	923	75	0
37	BP	917	0	965	131	0
37	DP	917	0	965	112	0
38	BQ	947	0	1022	124	0
38	DQ	947	0	1022	131	0
39	BR	816	0	839	91	0
39	DR	816	0	839	91	0
40	BS	857	0	922	67	0
40	DS	857	0	922	76	0
41	BT	738	0	807	117	0
41	DT	738	0	807	98	0
42	BU	779	0	834	57	0
42	DU	779	0	834	89	0
43	BV	753	0	780	45	0
43	DV	753	0	780	64	0
44	BW	596	0	610	187	0
44	DW	596	0	610	111	0
45	BX	625	0	655	61	0
45	DX	625	0	655	63	0
46	BY	509	0	543	55	0
46	DY	509	0	543	58	0
47	BZ	449	0	491	39	0
47	DZ	449	0	491	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	B0	444	0	461	22	0
48	D0	444	0	461	53	0
49	B1	409	0	440	44	0
49	D1	409	0	440	31	0
50	B2	377	0	418	29	0
50	D2	377	0	418	41	0
51	B3	504	0	574	41	0
51	D3	504	0	574	58	0
52	B4	302	0	340	32	0
52	D4	302	0	340	29	0
53	CA	32831	0	16521	1452	0
54	DB	2507	0	1270	121	0
55	AA	43	0	0	0	0
55	BA	137	0	0	0	0
55	BB	4	0	0	0	0
55	CA	42	0	0	0	0
55	DA	135	0	0	0	0
55	DB	1	0	0	0	0
55	DJ	1	0	0	0	0
56	B4	1	0	0	0	0
56	D4	1	0	0	0	0
57	AA	195	0	0	2	0
57	AE	1	0	0	0	0
57	AL	3	0	0	0	0
57	AN	6	0	0	0	0
57	AT	2	0	0	0	0
57	AU	1	0	0	0	0
57	B0	1	0	0	0	0
57	B2	1	0	0	0	0
57	B3	3	0	0	0	0
57	B4	3	0	0	0	0
57	BA	610	0	0	24	0
57	BB	20	0	0	1	0
57	BC	10	0	0	0	0
57	BD	2	0	0	1	0
57	BL	4	0	0	1	0
57	BN	3	0	0	0	0
57	BQ	1	0	0	0	0
57	BT	2	0	0	1	0
57	CA	192	0	0	8	0
57	CE	5	0	0	0	0
57	CI	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	CL	1	0	0	0	0
57	CN	3	0	0	0	0
57	CT	3	0	0	0	0
57	CU	2	0	0	0	0
57	D2	1	0	0	1	0
57	D3	1	0	0	0	0
57	D4	4	0	0	0	0
57	DA	599	0	0	9	0
57	DB	4	0	0	0	0
57	DC	13	0	0	1	0
57	DD	4	0	0	0	0
57	DE	3	0	0	0	0
57	DJ	3	0	0	0	0
57	DL	5	0	0	0	0
57	DN	2	0	0	2	0
57	DT	2	0	0	1	0
57	DU	1	0	0	0	0
57	DV	1	0	0	0	0
All	All	284450	0	190838	15808	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 33.

The worst 5 of 15808 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)
38:BQ:63:ARG:NH1	38:BQ:96:ASP:HA	1.49	1.26
22:DA:1439:A:C2	22:DA:1552:A:C6	2.32	1.17
22:DA:1439:A:N1	22:DA:1552:A:C5	2.12	1.17
27:BF:35:LEU:HB3	27:BF:153:ILE:HG22	1.19	1.16
33:BL:93:ASN:HD22	33:BL:94:THR:N	1.44	1.16

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%)	131 (61%)	49 (23%)	36 (17%)	0	0
1	CB	216/241 (90%)	149 (69%)	47 (22%)	20 (9%)	0	3
2	AC	204/233 (88%)	151 (74%)	35 (17%)	18 (9%)	0	3
2	CC	204/233 (88%)	144 (71%)	41 (20%)	19 (9%)	0	3
3	AD	203/206 (98%)	140 (69%)	36 (18%)	27 (13%)	0	1
3	CD	203/206 (98%)	142 (70%)	39 (19%)	22 (11%)	0	2
4	AE	148/167 (89%)	107 (72%)	25 (17%)	16 (11%)	0	2
4	CE	148/167 (89%)	111 (75%)	21 (14%)	16 (11%)	0	2
5	AF	98/135 (73%)	74 (76%)	15 (15%)	9 (9%)	0	3
5	CF	98/135 (73%)	68 (69%)	18 (18%)	12 (12%)	0	1
6	AG	149/179 (83%)	108 (72%)	34 (23%)	7 (5%)	2	14
6	CG	148/179 (83%)	99 (67%)	35 (24%)	14 (10%)	0	3
7	AH	127/130 (98%)	93 (73%)	30 (24%)	4 (3%)	3	22
7	CH	127/130 (98%)	96 (76%)	20 (16%)	11 (9%)	0	3
8	AI	125/130 (96%)	84 (67%)	31 (25%)	10 (8%)	1	5
8	CI	125/130 (96%)	90 (72%)	21 (17%)	14 (11%)	0	2
9	AJ	96/103 (93%)	67 (70%)	18 (19%)	11 (12%)	0	2
9	CJ	96/103 (93%)	55 (57%)	24 (25%)	17 (18%)	0	0
10	AK	115/129 (89%)	85 (74%)	21 (18%)	9 (8%)	1	5
10	CK	115/129 (89%)	85 (74%)	22 (19%)	8 (7%)	1	6
11	AL	121/124 (98%)	87 (72%)	20 (16%)	14 (12%)	0	1
11	CL	121/124 (98%)	85 (70%)	29 (24%)	7 (6%)	1	10
12	AM	112/118 (95%)	89 (80%)	16 (14%)	7 (6%)	1	8
12	CM	111/118 (94%)	60 (54%)	38 (34%)	13 (12%)	0	1
13	AN	92/101 (91%)	56 (61%)	24 (26%)	12 (13%)	0	1
13	CN	91/101 (90%)	60 (66%)	26 (29%)	5 (6%)	1	11
14	AO	86/89 (97%)	63 (73%)	20 (23%)	3 (4%)	3	20
14	CO	86/89 (97%)	62 (72%)	20 (23%)	4 (5%)	2	14
15	AP	80/82 (98%)	58 (72%)	14 (18%)	8 (10%)	0	2
15	CP	78/82 (95%)	50 (64%)	17 (22%)	11 (14%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	AQ	78/84 (93%)	51 (65%)	15 (19%)	12 (15%)	0	0
16	CQ	78/84 (93%)	59 (76%)	10 (13%)	9 (12%)	0	2
17	AR	53/75 (71%)	40 (76%)	11 (21%)	2 (4%)	2	18
17	CR	53/75 (71%)	39 (74%)	12 (23%)	2 (4%)	2	18
18	AS	77/92 (84%)	59 (77%)	9 (12%)	9 (12%)	0	1
18	CS	77/92 (84%)	46 (60%)	24 (31%)	7 (9%)	0	3
19	AT	83/87 (95%)	56 (68%)	20 (24%)	7 (8%)	0	4
19	CT	83/87 (95%)	59 (71%)	16 (19%)	8 (10%)	0	3
20	AU	49/71 (69%)	25 (51%)	13 (26%)	11 (22%)	0	0
20	CU	49/71 (69%)	21 (43%)	11 (22%)	17 (35%)	0	0
24	BC	269/273 (98%)	194 (72%)	50 (19%)	25 (9%)	0	3
24	DC	269/273 (98%)	174 (65%)	63 (23%)	32 (12%)	0	1
25	BD	207/209 (99%)	146 (70%)	27 (13%)	34 (16%)	0	0
25	DD	207/209 (99%)	132 (64%)	43 (21%)	32 (16%)	0	0
26	BE	199/201 (99%)	155 (78%)	24 (12%)	20 (10%)	0	2
26	DE	199/201 (99%)	130 (65%)	46 (23%)	23 (12%)	0	1
27	BF	175/179 (98%)	134 (77%)	25 (14%)	16 (9%)	0	3
27	DF	176/179 (98%)	98 (56%)	43 (24%)	35 (20%)	0	0
28	BG	174/177 (98%)	111 (64%)	38 (22%)	25 (14%)	0	1
28	DG	174/177 (98%)	106 (61%)	38 (22%)	30 (17%)	0	0
29	BH	147/149 (99%)	68 (46%)	47 (32%)	32 (22%)	0	0
29	DH	147/149 (99%)	75 (51%)	54 (37%)	18 (12%)	0	1
30	BI	139/142 (98%)	84 (60%)	41 (30%)	14 (10%)	0	2
30	DI	139/142 (98%)	81 (58%)	39 (28%)	19 (14%)	0	1
31	BJ	140/142 (99%)	107 (76%)	21 (15%)	12 (9%)	0	3
31	DJ	140/142 (99%)	91 (65%)	38 (27%)	11 (8%)	1	5
32	BK	120/123 (98%)	86 (72%)	15 (12%)	19 (16%)	0	0
32	DK	120/123 (98%)	80 (67%)	20 (17%)	20 (17%)	0	0
33	BL	141/144 (98%)	101 (72%)	32 (23%)	8 (6%)	1	11
33	DL	141/144 (98%)	81 (57%)	40 (28%)	20 (14%)	0	1
34	BM	134/136 (98%)	97 (72%)	22 (16%)	15 (11%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	DM	134/136 (98%)	92 (69%)	29 (22%)	13 (10%)	0	3
35	BN	118/127 (93%)	92 (78%)	17 (14%)	9 (8%)	1	5
35	DN	118/127 (93%)	72 (61%)	30 (25%)	16 (14%)	0	1
36	BO	114/117 (97%)	91 (80%)	12 (10%)	11 (10%)	0	3
36	DO	114/117 (97%)	77 (68%)	30 (26%)	7 (6%)	1	9
37	BP	112/115 (97%)	77 (69%)	18 (16%)	17 (15%)	0	0
37	DP	112/115 (97%)	68 (61%)	27 (24%)	17 (15%)	0	0
38	BQ	115/118 (98%)	100 (87%)	9 (8%)	6 (5%)	1	12
38	DQ	115/118 (98%)	80 (70%)	25 (22%)	10 (9%)	0	3
39	BR	101/103 (98%)	80 (79%)	13 (13%)	8 (8%)	1	5
39	DR	101/103 (98%)	70 (69%)	21 (21%)	10 (10%)	0	2
40	BS	108/110 (98%)	86 (80%)	16 (15%)	6 (6%)	1	11
40	DS	108/110 (98%)	76 (70%)	23 (21%)	9 (8%)	0	4
41	BT	91/100 (91%)	52 (57%)	24 (26%)	15 (16%)	0	0
41	DT	91/100 (91%)	46 (50%)	31 (34%)	14 (15%)	0	0
42	BU	100/104 (96%)	69 (69%)	15 (15%)	16 (16%)	0	0
42	DU	100/104 (96%)	51 (51%)	26 (26%)	23 (23%)	0	0
43	BV	92/94 (98%)	77 (84%)	13 (14%)	2 (2%)	5	30
43	DV	92/94 (98%)	61 (66%)	23 (25%)	8 (9%)	0	3
44	BW	77/85 (91%)	30 (39%)	24 (31%)	23 (30%)	0	0
44	DW	77/85 (91%)	33 (43%)	27 (35%)	17 (22%)	0	0
45	BX	75/78 (96%)	56 (75%)	14 (19%)	5 (7%)	1	7
45	DX	75/78 (96%)	47 (63%)	20 (27%)	8 (11%)	0	2
46	BY	61/63 (97%)	38 (62%)	16 (26%)	7 (12%)	0	2
46	DY	61/63 (97%)	42 (69%)	14 (23%)	5 (8%)	1	4
47	BZ	56/59 (95%)	45 (80%)	9 (16%)	2 (4%)	3	20
47	DZ	56/59 (95%)	34 (61%)	16 (29%)	6 (11%)	0	2
48	B0	54/57 (95%)	41 (76%)	9 (17%)	4 (7%)	1	6
48	D0	54/57 (95%)	39 (72%)	8 (15%)	7 (13%)	0	1
49	B1	48/55 (87%)	36 (75%)	7 (15%)	5 (10%)	0	2
49	D1	48/55 (87%)	37 (77%)	7 (15%)	4 (8%)	0	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	B2	44/46 (96%)	39 (89%)	4 (9%)	1 (2%)	5	29
50	D2	44/46 (96%)	31 (70%)	10 (23%)	3 (7%)	1	7
51	B3	62/65 (95%)	53 (86%)	5 (8%)	4 (6%)	1	8
51	D3	62/65 (95%)	39 (63%)	18 (29%)	5 (8%)	1	4
52	B4	36/38 (95%)	31 (86%)	2 (6%)	3 (8%)	0	4
52	D4	36/38 (95%)	23 (64%)	7 (19%)	6 (17%)	0	0
All	All	11238/11970 (94%)	7646 (68%)	2332 (21%)	1260 (11%)	0	2

5 of 1260 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AB	18	GLN
1	AB	20	ARG
1	AB	40	ILE
1	AB	75	ALA
1	AB	119	GLN

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%)	138 (77%)	42 (23%)	0	3
1	CB	180/199 (90%)	155 (86%)	25 (14%)	3	14
2	AC	170/190 (90%)	139 (82%)	31 (18%)	1	7
2	CC	170/190 (90%)	152 (89%)	18 (11%)	5	24
3	AD	172/173 (99%)	144 (84%)	28 (16%)	2	9
3	CD	172/173 (99%)	138 (80%)	34 (20%)	1	6
4	AE	113/126 (90%)	94 (83%)	19 (17%)	1	8
4	CE	113/126 (90%)	93 (82%)	20 (18%)	1	8
5	AF	87/116 (75%)	74 (85%)	13 (15%)	2	12
5	CF	87/116 (75%)	74 (85%)	13 (15%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	AG	124/147 (84%)	109 (88%)	15 (12%)	4	19
6	CG	123/147 (84%)	99 (80%)	24 (20%)	1	6
7	AH	104/105 (99%)	88 (85%)	16 (15%)	2	11
7	CH	104/105 (99%)	90 (86%)	14 (14%)	3	15
8	AI	105/107 (98%)	88 (84%)	17 (16%)	2	9
8	CI	105/107 (98%)	91 (87%)	14 (13%)	3	15
9	AJ	86/90 (96%)	72 (84%)	14 (16%)	2	9
9	CJ	86/90 (96%)	77 (90%)	9 (10%)	5	24
10	AK	90/99 (91%)	71 (79%)	19 (21%)	1	5
10	CK	90/99 (91%)	78 (87%)	12 (13%)	3	15
11	AL	103/104 (99%)	81 (79%)	22 (21%)	1	5
11	CL	103/104 (99%)	84 (82%)	19 (18%)	1	7
12	AM	92/96 (96%)	88 (96%)	4 (4%)	25	57
12	CM	91/96 (95%)	80 (88%)	11 (12%)	4	19
13	AN	79/84 (94%)	73 (92%)	6 (8%)	11	39
13	CN	79/84 (94%)	67 (85%)	12 (15%)	2	12
14	AO	76/77 (99%)	69 (91%)	7 (9%)	7	29
14	CO	76/77 (99%)	70 (92%)	6 (8%)	10	38
15	AP	65/65 (100%)	54 (83%)	11 (17%)	1	8
15	CP	65/65 (100%)	53 (82%)	12 (18%)	1	7
16	AQ	74/78 (95%)	61 (82%)	13 (18%)	1	8
16	CQ	74/78 (95%)	63 (85%)	11 (15%)	2	12
17	AR	48/65 (74%)	45 (94%)	3 (6%)	15	46
17	CR	48/65 (74%)	46 (96%)	2 (4%)	25	58
18	AS	70/79 (89%)	62 (89%)	8 (11%)	4	21
18	CS	70/79 (89%)	62 (89%)	8 (11%)	4	21
19	AT	65/66 (98%)	48 (74%)	17 (26%)	0	1
19	CT	65/66 (98%)	54 (83%)	11 (17%)	1	8
20	AU	44/61 (72%)	32 (73%)	12 (27%)	0	1
20	CU	44/61 (72%)	34 (77%)	10 (23%)	0	3
24	BC	216/218 (99%)	173 (80%)	43 (20%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	DC	216/218 (99%)	188 (87%)	28 (13%)	3	16
25	BD	164/164 (100%)	136 (83%)	28 (17%)	1	8
25	DD	164/164 (100%)	140 (85%)	24 (15%)	2	13
26	BE	165/165 (100%)	125 (76%)	40 (24%)	0	2
26	DE	165/165 (100%)	150 (91%)	15 (9%)	7	29
27	BF	148/150 (99%)	128 (86%)	20 (14%)	3	15
27	DF	149/150 (99%)	122 (82%)	27 (18%)	1	7
28	BG	137/138 (99%)	107 (78%)	30 (22%)	1	4
28	DG	137/138 (99%)	119 (87%)	18 (13%)	3	16
29	BH	114/114 (100%)	96 (84%)	18 (16%)	2	10
29	DH	114/114 (100%)	96 (84%)	18 (16%)	2	10
30	BI	109/110 (99%)	91 (84%)	18 (16%)	2	9
30	DI	109/110 (99%)	102 (94%)	7 (6%)	14	46
31	BJ	116/116 (100%)	89 (77%)	27 (23%)	0	3
31	DJ	116/116 (100%)	104 (90%)	12 (10%)	6	25
32	BK	103/104 (99%)	84 (82%)	19 (18%)	1	7
32	DK	103/104 (99%)	87 (84%)	16 (16%)	2	10
33	BL	102/103 (99%)	79 (78%)	23 (22%)	1	4
33	DL	102/103 (99%)	88 (86%)	14 (14%)	3	14
34	BM	109/109 (100%)	87 (80%)	22 (20%)	1	5
34	DM	109/109 (100%)	99 (91%)	10 (9%)	7	29
35	BN	100/103 (97%)	83 (83%)	17 (17%)	1	8
35	DN	100/103 (97%)	85 (85%)	15 (15%)	2	12
36	BO	86/87 (99%)	69 (80%)	17 (20%)	1	6
36	DO	86/87 (99%)	78 (91%)	8 (9%)	7	29
37	BP	99/100 (99%)	78 (79%)	21 (21%)	1	5
37	DP	99/100 (99%)	90 (91%)	9 (9%)	7	29
38	BQ	89/90 (99%)	74 (83%)	15 (17%)	1	8
38	DQ	89/90 (99%)	78 (88%)	11 (12%)	4	18
39	BR	84/84 (100%)	65 (77%)	19 (23%)	1	4
39	DR	84/84 (100%)	71 (84%)	13 (16%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	BS	93/93 (100%)	73 (78%)	20 (22%)	1	4
40	DS	93/93 (100%)	76 (82%)	17 (18%)	1	7
41	BT	80/84 (95%)	61 (76%)	19 (24%)	0	3
41	DT	80/84 (95%)	74 (92%)	6 (8%)	11	40
42	BU	83/85 (98%)	66 (80%)	17 (20%)	1	5
42	DU	83/85 (98%)	74 (89%)	9 (11%)	5	23
43	BV	78/78 (100%)	61 (78%)	17 (22%)	1	4
43	DV	78/78 (100%)	66 (85%)	12 (15%)	2	11
44	BW	59/63 (94%)	42 (71%)	17 (29%)	0	1
44	DW	59/63 (94%)	44 (75%)	15 (25%)	0	2
45	BX	67/68 (98%)	53 (79%)	14 (21%)	1	5
45	DX	67/68 (98%)	58 (87%)	9 (13%)	3	15
46	BY	55/55 (100%)	43 (78%)	12 (22%)	1	4
46	DY	55/55 (100%)	52 (94%)	3 (6%)	18	51
47	BZ	48/49 (98%)	32 (67%)	16 (33%)	0	0
47	DZ	48/49 (98%)	41 (85%)	7 (15%)	2	13
48	B0	47/48 (98%)	43 (92%)	4 (8%)	8	34
48	D0	47/48 (98%)	40 (85%)	7 (15%)	2	12
49	B1	45/49 (92%)	36 (80%)	9 (20%)	1	5
49	D1	45/49 (92%)	41 (91%)	4 (9%)	8	31
50	B2	38/38 (100%)	31 (82%)	7 (18%)	1	7
50	D2	38/38 (100%)	34 (90%)	4 (10%)	5	24
51	B3	51/52 (98%)	44 (86%)	7 (14%)	3	14
51	D3	51/52 (98%)	42 (82%)	9 (18%)	1	8
52	B4	34/34 (100%)	30 (88%)	4 (12%)	4	20
52	D4	34/34 (100%)	29 (85%)	5 (15%)	2	12
All	All	9331/9756 (96%)	7837 (84%)	1494 (16%)	2	10

5 of 1494 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	CD	170	LEU
24	DC	57	HIS

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Mol	Chain	Res	Type
4	CE	144	GLU
3	CD	168	THR
11	CL	4	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 333 such sidechains are listed below:

Mol	Chain	Res	Type
18	CS	51	HIS
36	DO	38	GLN
24	DC	43	ASN
28	DG	103	ASN
40	DS	31	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1532/1533 (99%)	471 (30%)	241 (15%)
22	BA	2850/2903 (98%)	800 (28%)	404 (14%)
22	DA	2838/2903 (97%)	1022 (36%)	515 (18%)
23	BB	117/118 (99%)	29 (24%)	19 (16%)
53	CA	1529/1530 (99%)	512 (33%)	238 (15%)
54	DB	116/117 (99%)	36 (31%)	19 (16%)
All	All	8982/9104 (98%)	2870 (31%)	1436 (15%)

5 of 2870 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	5	U
21	AA	6	G
21	AA	7	A
21	AA	8	A
21	AA	9	G

5 of 1436 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	DA	128	C
22	DA	1312	U
22	DA	271	G
22	DA	125	A

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Mol	Chain	Res	Type
22	DA	740	C

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	AB	218/241 (90%)	0.49	13 (5%) 29 19	85, 115, 146, 164	0
1	CB	218/241 (90%)	0.69	20 (9%) 16 11	90, 125, 152, 170	0
2	AC	206/233 (88%)	-0.19	4 (1%) 66 50	57, 83, 116, 147	0
2	CC	206/233 (88%)	0.56	13 (6%) 27 18	83, 129, 170, 188	0
3	AD	205/206 (99%)	0.17	10 (4%) 36 25	50, 87, 137, 176	0
3	CD	205/206 (99%)	0.21	10 (4%) 36 25	41, 63, 102, 148	0
4	AE	150/167 (89%)	-0.01	2 (1%) 74 60	51, 70, 116, 147	0
4	CE	150/167 (89%)	0.66	3 (2%) 64 49	65, 87, 122, 144	0
5	AF	100/135 (74%)	0.09	3 (3%) 52 37	60, 90, 125, 142	0
5	CF	100/135 (74%)	0.57	6 (6%) 29 19	65, 113, 147, 158	0
6	AG	151/179 (84%)	0.22	7 (4%) 38 26	69, 108, 139, 157	0
6	CG	150/179 (83%)	1.50	45 (30%) 1 1	98, 173, 223, 233	0
7	AH	129/130 (99%)	-0.11	2 (1%) 70 55	49, 71, 106, 133	0
7	CH	129/130 (99%)	0.32	4 (3%) 51 36	63, 100, 133, 159	0
8	AI	127/130 (97%)	0.55	12 (9%) 15 11	56, 115, 166, 189	0
8	CI	127/130 (97%)	1.72	41 (32%) 1 1	127, 174, 225, 239	0
9	AJ	98/103 (95%)	0.37	4 (4%) 42 28	59, 97, 152, 160	0
9	CJ	98/103 (95%)	1.82	38 (38%) 1 1	122, 160, 189, 201	0
10	AK	117/129 (90%)	0.18	3 (2%) 57 41	43, 88, 124, 137	0
10	CK	117/129 (90%)	0.60	6 (5%) 34 23	57, 99, 130, 151	0
11	AL	123/124 (99%)	-0.03	6 (4%) 36 25	33, 54, 96, 135	0
11	CL	123/124 (99%)	0.50	6 (4%) 36 25	47, 74, 110, 135	0
12	AM	114/118 (96%)	0.45	5 (4%) 39 27	70, 117, 155, 177	0
12	CM	113/118 (95%)	2.31	53 (46%) 0 1	220, 351, 413, 434	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AN	96/101 (95%)	0.45	9 (9%) 15 11	59, 86, 136, 158	0
13	CN	95/101 (94%)	1.49	25 (26%) 2 2	102, 191, 256, 269	0
14	AO	88/89 (98%)	-0.07	0 100 100	48, 75, 106, 128	0
14	CO	88/89 (98%)	0.73	9 (10%) 13 9	72, 109, 141, 167	0
15	AP	82/82 (100%)	0.02	2 (2%) 59 44	55, 79, 129, 174	0
15	CP	80/82 (97%)	0.86	11 (13%) 8 5	64, 96, 133, 152	0
16	AQ	80/84 (95%)	0.49	8 (10%) 14 10	38, 73, 112, 144	0
16	CQ	80/84 (95%)	0.48	4 (5%) 35 24	54, 96, 117, 131	0
17	AR	55/75 (73%)	0.24	4 (7%) 22 16	56, 80, 129, 146	0
17	CR	55/75 (73%)	0.68	6 (10%) 12 9	57, 89, 131, 170	0
18	AS	79/92 (85%)	0.49	9 (11%) 11 8	79, 110, 152, 161	0
18	CS	79/92 (85%)	2.42	42 (53%) 0 1	250, 307, 359, 371	0
19	AT	85/87 (97%)	0.26	5 (5%) 29 19	51, 81, 114, 133	0
19	CT	85/87 (97%)	1.64	25 (29%) 1 1	79, 125, 161, 177	0
20	AU	51/71 (71%)	0.83	7 (13%) 8 5	60, 104, 138, 148	0
20	CU	51/71 (71%)	1.04	10 (19%) 4 3	63, 97, 143, 153	0
21	AA	1533/1533 (100%)	-0.44	25 (1%) 70 55	34, 72, 169, 235	0
22	BA	2854/2903 (98%)	-0.72	67 (2%) 61 44	13, 33, 142, 320	0
22	DA	2841/2903 (97%)	1.04	382 (13%) 8 6	59, 119, 216, 320	0
23	BB	118/118 (100%)	-0.73	0 100 100	18, 47, 75, 99	0
24	BC	271/273 (99%)	-0.15	12 (4%) 39 27	20, 43, 83, 142	0
24	DC	271/273 (99%)	1.14	53 (19%) 4 3	63, 94, 128, 153	0
25	BD	209/209 (100%)	-0.53	1 (0%) 87 78	13, 29, 72, 96	0
25	DD	209/209 (100%)	1.21	35 (16%) 5 4	68, 108, 141, 168	0
26	BE	201/201 (100%)	-0.43	0 100 100	15, 42, 87, 124	0
26	DE	201/201 (100%)	2.01	84 (41%) 1 1	89, 191, 252, 282	0
27	BF	177/179 (98%)	0.06	2 (1%) 77 63	32, 67, 116, 132	0
27	DF	178/179 (99%)	1.43	46 (25%) 2 2	125, 209, 220, 232	0
28	BG	176/177 (99%)	-0.16	5 (2%) 55 39	27, 57, 103, 128	0
28	DG	176/177 (99%)	1.19	32 (18%) 4 3	120, 165, 207, 220	0
29	BH	149/149 (100%)	1.42	46 (30%) 1 1	42, 178, 213, 217	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
29	DH	149/149 (100%)	1.68	46 (30%) 1 1	104, 173, 208, 219	0
30	BI	141/142 (99%)	2.25	68 (48%) 0 1	199, 245, 286, 294	0
30	DI	141/142 (99%)	1.98	58 (41%) 1 1	264, 305, 323, 331	0
31	BJ	142/142 (100%)	-0.52	5 (3%) 47 33	12, 25, 57, 111	0
31	DJ	142/142 (100%)	1.13	24 (16%) 5 4	76, 110, 134, 153	0
32	BK	122/123 (99%)	-0.52	1 (0%) 82 70	20, 32, 76, 121	0
32	DK	122/123 (99%)	0.63	9 (7%) 22 16	71, 93, 127, 142	0
33	BL	143/144 (99%)	-0.40	2 (1%) 73 58	13, 38, 74, 100	0
33	DL	143/144 (99%)	2.15	73 (51%) 0 1	80, 150, 189, 202	0
34	BM	136/136 (100%)	-0.61	0 100 100	14, 30, 61, 99	0
34	DM	136/136 (100%)	0.88	20 (14%) 7 5	73, 117, 143, 161	0
35	BN	120/127 (94%)	-0.58	0 100 100	14, 28, 44, 97	0
35	DN	120/127 (94%)	1.75	42 (35%) 1 1	89, 121, 152, 171	0
36	BO	116/117 (99%)	-0.19	3 (2%) 57 41	30, 46, 73, 101	0
36	DO	116/117 (99%)	1.46	28 (24%) 2 2	146, 178, 207, 216	0
37	BP	114/115 (99%)	-0.50	2 (1%) 67 52	22, 39, 90, 131	0
37	DP	114/115 (99%)	0.90	10 (8%) 17 12	80, 108, 135, 143	0
38	BQ	117/118 (99%)	-0.53	3 (2%) 57 41	9, 22, 46, 96	0
38	DQ	117/118 (99%)	1.81	41 (35%) 1 1	87, 112, 154, 191	0
39	BR	103/103 (100%)	-0.45	2 (1%) 66 50	11, 33, 75, 91	0
39	DR	103/103 (100%)	1.79	32 (31%) 1 1	85, 135, 170, 190	0
40	BS	110/110 (100%)	-0.76	0 100 100	14, 23, 57, 118	0
40	DS	110/110 (100%)	1.45	28 (25%) 2 2	76, 120, 154, 170	0
41	BT	93/100 (93%)	0.19	4 (4%) 40 27	28, 51, 112, 140	0
41	DT	93/100 (93%)	2.81	68 (73%) 0 0	132, 189, 223, 233	0
42	BU	102/104 (98%)	-0.11	2 (1%) 64 49	29, 54, 100, 155	0
42	DU	102/104 (98%)	2.64	59 (57%) 0 1	153, 202, 250, 283	0
43	BV	94/94 (100%)	-0.67	0 100 100	17, 39, 79, 105	0
43	DV	94/94 (100%)	0.83	6 (6%) 27 18	113, 143, 165, 179	0
44	BW	79/85 (92%)	0.15	4 (5%) 34 23	18, 39, 94, 127	0
44	DW	79/85 (92%)	2.03	33 (41%) 1 1	99, 157, 191, 201	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
45	BX	77/78 (98%)	-0.31	0 100 100	23, 43, 80, 104	0
45	DX	77/78 (98%)	1.96	36 (46%) 0 1	84, 124, 170, 177	0
46	BY	63/63 (100%)	0.23	4 (6%) 27 18	41, 68, 113, 128	0
46	DY	63/63 (100%)	2.96	39 (61%) 0 1	180, 226, 268, 278	0
47	BZ	58/59 (98%)	-0.61	0 100 100	13, 27, 56, 97	0
47	DZ	58/59 (98%)	1.55	16 (27%) 2 1	97, 143, 180, 187	0
48	B0	56/57 (98%)	-0.69	0 100 100	12, 29, 61, 113	0
48	D0	56/57 (98%)	1.51	11 (19%) 4 3	84, 128, 163, 172	0
49	B1	50/55 (90%)	-0.35	0 100 100	29, 50, 91, 116	0
49	D1	50/55 (90%)	1.50	13 (26%) 2 2	110, 143, 159, 168	0
50	B2	46/46 (100%)	-0.24	2 (4%) 40 27	20, 30, 49, 131	0
50	D2	46/46 (100%)	2.84	30 (65%) 0 1	87, 115, 137, 147	0
51	B3	64/65 (98%)	-0.51	0 100 100	15, 30, 43, 62	0
51	D3	64/65 (98%)	2.37	38 (59%) 0 1	93, 126, 150, 169	0
52	B4	38/38 (100%)	-0.30	0 100 100	19, 33, 62, 87	0
52	D4	38/38 (100%)	2.31	26 (68%) 0 0	84, 127, 158, 161	0
53	CA	1530/1530 (100%)	0.59	102 (6%) 25 17	44, 100, 246, 325	0
54	DB	117/117 (100%)	0.75	5 (4%) 40 27	108, 175, 209, 221	0
All	All	20431/21074 (96%)	0.43	2277 (11%) 12 8	9, 93, 219, 434	0

The worst 5 of 2277 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	BA	2154	A	10.9
53	CA	1224	U	10.8
27	DF	129	MET	9.6
3	CD	27	ILE	9.4
42	DU	30	SER	9.3

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(Å ²)	Q<0.9
55	MG	DA	3063	1/1	0.23	0.46	191,191,191,191	0
55	MG	DJ	201	1/1	0.31	0.34	242,242,242,242	0
55	MG	DA	3003	1/1	0.32	0.28	210,210,210,210	0
55	MG	DA	3064	1/1	0.44	0.76	204,204,204,204	0
55	MG	DA	3075	1/1	0.52	0.68	207,207,207,207	0
55	MG	DA	3065	1/1	0.53	0.39	221,221,221,221	0
55	MG	DA	3042	1/1	0.55	0.15	139,139,139,139	0
55	MG	DA	3134	1/1	0.59	0.13	198,198,198,198	0
55	MG	DA	3006	1/1	0.61	0.16	200,200,200,200	0
55	MG	DA	3010	1/1	0.61	0.31	200,200,200,200	0
55	MG	DA	3002	1/1	0.61	0.39	179,179,179,179	0
55	MG	DA	3013	1/1	0.62	0.41	211,211,211,211	0
55	MG	CA	1617	1/1	0.62	0.15	220,220,220,220	0
55	MG	CA	1624	1/1	0.64	0.32	120,120,120,120	0
55	MG	DA	3005	1/1	0.64	0.38	208,208,208,208	0
55	MG	DA	3132	1/1	0.65	0.20	216,216,216,216	0
55	MG	DA	3129	1/1	0.67	0.42	194,194,194,194	0
55	MG	DA	3110	1/1	0.67	0.29	181,181,181,181	0
55	MG	DA	3007	1/1	0.68	0.12	198,198,198,198	0
55	MG	DA	3074	1/1	0.68	0.09	194,194,194,194	0
55	MG	DA	3015	1/1	0.68	0.34	183,183,183,183	0
55	MG	DA	3026	1/1	0.68	0.25	145,145,145,145	0
55	MG	DA	3109	1/1	0.69	0.13	165,165,165,165	0
55	MG	CA	1636	1/1	0.69	0.18	171,171,171,171	0
55	MG	DA	3020	1/1	0.70	0.21	207,207,207,207	0
55	MG	DA	3027	1/1	0.71	0.36	195,195,195,195	0
55	MG	DA	3079	1/1	0.71	0.24	184,184,184,184	0
55	MG	DA	3050	1/1	0.73	0.09	209,209,209,209	0
55	MG	DA	3124	1/1	0.73	0.28	165,165,165,165	0
55	MG	DA	3018	1/1	0.73	0.16	194,194,194,194	0
55	MG	DA	3070	1/1	0.74	0.28	209,209,209,209	0
55	MG	BA	3048	1/1	0.76	0.14	144,144,144,144	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3059	1/1	0.76	0.23	188,188,188,188	0
55	MG	DA	3126	1/1	0.77	0.17	164,164,164,164	0
55	MG	CA	1619	1/1	0.77	0.16	180,180,180,180	0
55	MG	DA	3060	1/1	0.77	0.19	198,198,198,198	0
55	MG	BA	3132	1/1	0.77	0.53	202,202,202,202	0
55	MG	CA	1629	1/1	0.77	0.09	174,174,174,174	0
55	MG	DA	3037	1/1	0.78	0.15	176,176,176,176	0
55	MG	CA	1616	1/1	0.78	0.12	192,192,192,192	0
55	MG	AA	1619	1/1	0.78	0.25	165,165,165,165	0
55	MG	CA	1615	1/1	0.78	0.13	136,136,136,136	0
55	MG	BA	3026	1/1	0.79	0.26	152,152,152,152	0
55	MG	CA	1620	1/1	0.80	0.16	172,172,172,172	0
55	MG	DA	3084	1/1	0.80	0.13	178,178,178,178	0
55	MG	CA	1628	1/1	0.80	0.20	204,204,204,204	0
55	MG	DA	3029	1/1	0.80	0.22	205,205,205,205	0
55	MG	DA	3058	1/1	0.80	0.45	171,171,171,171	0
55	MG	DA	3089	1/1	0.81	0.15	169,169,169,169	0
55	MG	AA	1611	1/1	0.82	0.25	176,176,176,176	0
55	MG	DA	3131	1/1	0.82	0.37	204,204,204,204	0
55	MG	DA	3083	1/1	0.82	0.14	144,144,144,144	0
55	MG	DA	3046	1/1	0.82	0.15	173,173,173,173	0
55	MG	DA	3016	1/1	0.82	0.13	169,169,169,169	0
55	MG	CA	1603	1/1	0.83	0.12	169,169,169,169	0
55	MG	DA	3092	1/1	0.83	0.13	157,157,157,157	0
55	MG	DA	3100	1/1	0.83	0.12	171,171,171,171	0
55	MG	CA	1612	1/1	0.84	0.21	117,117,117,117	0
55	MG	BA	3004	1/1	0.84	0.19	155,155,155,155	0
55	MG	DA	3019	1/1	0.84	0.16	161,161,161,161	0
55	MG	DA	3028	1/1	0.84	0.12	162,162,162,162	0
55	MG	DA	3115	1/1	0.84	0.17	151,151,151,151	0
55	MG	DA	3061	1/1	0.84	0.34	160,160,160,160	0
55	MG	DA	3107	1/1	0.85	0.23	169,169,169,169	0
55	MG	BA	3015	1/1	0.85	0.17	221,221,221,221	0
55	MG	DA	3039	1/1	0.85	0.12	220,220,220,220	0
55	MG	DA	3098	1/1	0.85	0.21	158,158,158,158	0
55	MG	DA	3116	1/1	0.85	0.20	154,154,154,154	0
55	MG	CA	1610	1/1	0.85	0.12	145,145,145,145	0
55	MG	AA	1636	1/1	0.86	0.19	164,164,164,164	0
55	MG	BB	201	1/1	0.86	0.17	187,187,187,187	0
55	MG	CA	1602	1/1	0.86	0.10	120,120,120,120	0
55	MG	DA	3111	1/1	0.86	0.10	166,166,166,166	0
55	MG	DA	3025	1/1	0.86	0.15	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	3049	1/1	0.86	0.12	104,104,104,104	0
55	MG	DA	3121	1/1	0.86	0.14	97,97,97,97	0
55	MG	DA	3009	1/1	0.87	0.17	107,107,107,107	0
55	MG	DA	3034	1/1	0.87	0.13	105,105,105,105	0
55	MG	DA	3099	1/1	0.87	0.15	142,142,142,142	0
55	MG	CA	1614	1/1	0.87	0.25	178,178,178,178	0
55	MG	DA	3073	1/1	0.87	0.12	141,141,141,141	0
55	MG	DA	3135	1/1	0.87	0.17	162,162,162,162	0
55	MG	CA	1632	1/1	0.87	0.13	160,160,160,160	0
55	MG	CA	1639	1/1	0.88	0.12	149,149,149,149	0
55	MG	CA	1634	1/1	0.88	0.10	112,112,112,112	0
55	MG	DA	3044	1/1	0.88	0.10	138,138,138,138	0
55	MG	CA	1607	1/1	0.88	0.10	154,154,154,154	0
55	MG	DA	3048	1/1	0.88	0.15	128,128,128,128	0
55	MG	BA	3112	1/1	0.89	0.12	121,121,121,121	0
55	MG	AA	1630	1/1	0.89	0.09	163,163,163,163	0
55	MG	DA	3087	1/1	0.89	0.12	87,87,87,87	0
55	MG	DA	3108	1/1	0.89	0.09	103,103,103,103	0
55	MG	DA	3088	1/1	0.89	0.10	160,160,160,160	0
55	MG	CA	1622	1/1	0.89	0.10	169,169,169,169	0
55	MG	DA	3076	1/1	0.89	0.26	167,167,167,167	0
55	MG	DA	3096	1/1	0.89	0.14	107,107,107,107	0
55	MG	BA	3089	1/1	0.89	0.12	134,134,134,134	0
55	MG	DA	3094	1/1	0.90	0.15	172,172,172,172	0
55	MG	DA	3072	1/1	0.90	0.14	80,80,80,80	0
55	MG	DA	3119	1/1	0.90	0.08	86,86,86,86	0
55	MG	BA	3091	1/1	0.90	0.07	47,47,47,47	0
55	MG	AA	1618	1/1	0.90	0.08	68,68,68,68	0
55	MG	DA	3011	1/1	0.90	0.16	126,126,126,126	0
55	MG	DA	3035	1/1	0.91	0.12	87,87,87,87	0
55	MG	BA	3070	1/1	0.91	0.13	164,164,164,164	0
55	MG	DA	3101	1/1	0.91	0.18	127,127,127,127	0
55	MG	CA	1625	1/1	0.91	0.17	118,118,118,118	0
55	MG	AA	1628	1/1	0.91	0.15	96,96,96,96	0
55	MG	CA	1638	1/1	0.91	0.14	155,155,155,155	0
55	MG	DA	3062	1/1	0.91	0.10	113,113,113,113	0
55	MG	DA	3033	1/1	0.91	0.11	113,113,113,113	0
55	MG	DA	3077	1/1	0.91	0.17	159,159,159,159	0
55	MG	BA	3011	1/1	0.91	0.13	120,120,120,120	0
55	MG	BA	3113	1/1	0.92	0.10	60,60,60,60	0
55	MG	DA	3123	1/1	0.92	0.09	99,99,99,99	0
55	MG	DA	3081	1/1	0.92	0.13	141,141,141,141	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3125	1/1	0.92	0.11	77,77,77,77	0
55	MG	DA	3030	1/1	0.92	0.17	144,144,144,144	0
55	MG	DA	3127	1/1	0.92	0.14	97,97,97,97	0
55	MG	DA	3051	1/1	0.92	0.07	140,140,140,140	0
55	MG	DA	3130	1/1	0.92	0.28	102,102,102,102	0
55	MG	BA	3056	1/1	0.92	0.16	187,187,187,187	0
55	MG	DA	3112	1/1	0.92	0.08	148,148,148,148	0
55	MG	CA	1627	1/1	0.92	0.16	166,166,166,166	0
55	MG	BA	3060	1/1	0.92	0.19	129,129,129,129	0
55	MG	DA	3102	1/1	0.92	0.10	83,83,83,83	0
55	MG	BA	3077	1/1	0.93	0.13	90,90,90,90	0
55	MG	AA	1620	1/1	0.93	0.07	107,107,107,107	0
55	MG	DA	3031	1/1	0.93	0.10	113,113,113,113	0
55	MG	BA	3134	1/1	0.93	0.23	137,137,137,137	0
55	MG	DA	3128	1/1	0.93	0.15	153,153,153,153	0
55	MG	DA	3004	1/1	0.93	0.16	118,118,118,118	0
55	MG	DA	3085	1/1	0.93	0.22	169,169,169,169	0
55	MG	DA	3047	1/1	0.93	0.08	82,82,82,82	0
55	MG	CA	1631	1/1	0.93	0.13	92,92,92,92	0
55	MG	DA	3120	1/1	0.93	0.09	84,84,84,84	0
55	MG	DA	3106	1/1	0.93	0.14	69,69,69,69	0
55	MG	DA	3049	1/1	0.93	0.10	99,99,99,99	0
55	MG	BA	3092	1/1	0.94	0.10	75,75,75,75	0
55	MG	CA	1637	1/1	0.94	0.11	100,100,100,100	0
55	MG	CA	1611	1/1	0.94	0.10	108,108,108,108	0
55	MG	BA	3100	1/1	0.94	0.07	47,47,47,47	0
55	MG	CA	1640	1/1	0.94	0.18	161,161,161,161	0
55	MG	DA	3066	1/1	0.94	0.07	94,94,94,94	0
55	MG	AA	1616	1/1	0.94	0.08	126,126,126,126	0
55	MG	AA	1640	1/1	0.94	0.07	109,109,109,109	0
55	MG	BA	3117	1/1	0.94	0.09	23,23,23,23	0
55	MG	BA	3120	1/1	0.94	0.18	156,156,156,156	0
55	MG	BA	3062	1/1	0.94	0.34	193,193,193,193	0
55	MG	BA	3035	1/1	0.94	0.19	168,168,168,168	0
55	MG	DA	3040	1/1	0.94	0.07	117,117,117,117	0
55	MG	DA	3008	1/1	0.94	0.10	100,100,100,100	0
55	MG	DA	3043	1/1	0.94	0.08	104,104,104,104	0
55	MG	BA	3136	1/1	0.94	0.22	150,150,150,150	0
55	MG	BA	3137	1/1	0.94	0.30	188,188,188,188	0
55	MG	BA	3072	1/1	0.94	0.23	94,94,94,94	0
55	MG	DA	3086	1/1	0.94	0.12	122,122,122,122	0
55	MG	CA	1601	1/1	0.94	0.09	124,124,124,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	3037	1/1	0.94	0.25	171,171,171,171	0
55	MG	AA	1615	1/1	0.94	0.13	164,164,164,164	0
55	MG	DA	3091	1/1	0.94	0.06	95,95,95,95	0
55	MG	CA	1630	1/1	0.94	0.07	121,121,121,121	0
55	MG	DA	3057	1/1	0.94	0.09	104,104,104,104	0
55	MG	CA	1606	1/1	0.94	0.08	64,64,64,64	0
55	MG	AA	1631	1/1	0.94	0.08	165,165,165,165	0
55	MG	CA	1608	1/1	0.94	0.13	60,60,60,60	0
56	ZN	D4	101	1/1	0.94	0.06	156,156,156,156	0
55	MG	BA	3058	1/1	0.95	0.20	164,164,164,164	0
55	MG	AA	1641	1/1	0.95	0.17	131,131,131,131	0
55	MG	DA	3114	1/1	0.95	0.06	95,95,95,95	0
55	MG	DA	3041	1/1	0.95	0.09	77,77,77,77	0
55	MG	DA	3022	1/1	0.95	0.09	155,155,155,155	0
55	MG	DA	3117	1/1	0.95	0.12	67,67,67,67	0
55	MG	BA	3003	1/1	0.95	0.07	63,63,63,63	0
55	MG	BA	3105	1/1	0.95	0.14	16,16,16,16	0
55	MG	DA	3093	1/1	0.95	0.13	121,121,121,121	0
55	MG	AA	1609	1/1	0.95	0.16	71,71,71,71	0
55	MG	BA	3071	1/1	0.95	0.15	132,132,132,132	0
55	MG	DA	3097	1/1	0.95	0.09	110,110,110,110	0
55	MG	AA	1639	1/1	0.95	0.07	96,96,96,96	0
55	MG	BA	3014	1/1	0.95	0.12	64,64,64,64	0
55	MG	CA	1623	1/1	0.95	0.10	96,96,96,96	0
55	MG	BA	3125	1/1	0.95	0.37	162,162,162,162	0
55	MG	DA	3052	1/1	0.95	0.08	110,110,110,110	0
55	MG	DA	3105	1/1	0.95	0.13	62,62,62,62	0
55	MG	DA	3054	1/1	0.95	0.14	75,75,75,75	0
55	MG	BA	3088	1/1	0.95	0.11	81,81,81,81	0
55	MG	DA	3001	1/1	0.95	0.06	109,109,109,109	0
55	MG	DB	201	1/1	0.95	0.08	117,117,117,117	0
55	MG	AA	1613	1/1	0.95	0.08	102,102,102,102	0
55	MG	DA	3038	1/1	0.95	0.10	97,97,97,97	0
55	MG	BA	3093	1/1	0.96	0.11	110,110,110,110	0
55	MG	BA	3007	1/1	0.96	0.06	67,67,67,67	0
55	MG	DA	3045	1/1	0.96	0.15	102,102,102,102	0
55	MG	AA	1627	1/1	0.96	0.12	86,86,86,86	0
55	MG	BA	3106	1/1	0.96	0.09	37,37,37,37	0
55	MG	DA	3095	1/1	0.96	0.07	114,114,114,114	0
55	MG	AA	1603	1/1	0.96	0.08	124,124,124,124	0
55	MG	CA	1618	1/1	0.96	0.07	90,90,90,90	0
55	MG	AA	1608	1/1	0.96	0.07	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3032	1/1	0.96	0.07	71,71,71,71	0
55	MG	BA	3057	1/1	0.96	0.23	219,219,219,219	0
55	MG	CA	1605	1/1	0.96	0.10	48,48,48,48	0
55	MG	DA	3080	1/1	0.96	0.08	74,74,74,74	0
55	MG	DA	3104	1/1	0.96	0.13	109,109,109,109	0
55	MG	BA	3119	1/1	0.96	0.10	88,88,88,88	0
55	MG	DA	3082	1/1	0.96	0.09	83,83,83,83	0
55	MG	DA	3017	1/1	0.96	0.08	86,86,86,86	0
55	MG	AA	1623	1/1	0.96	0.11	70,70,70,70	0
55	MG	BA	3032	1/1	0.96	0.05	31,31,31,31	0
55	MG	BA	3127	1/1	0.96	0.13	43,43,43,43	0
55	MG	AA	1624	1/1	0.96	0.07	101,101,101,101	0
55	MG	DA	3023	1/1	0.96	0.06	71,71,71,71	0
55	MG	BA	3002	1/1	0.97	0.12	81,81,81,81	0
55	MG	BA	3116	1/1	0.97	0.09	133,133,133,133	0
55	MG	DA	3067	1/1	0.97	0.05	70,70,70,70	0
55	MG	CA	1613	1/1	0.97	0.05	96,96,96,96	0
55	MG	AA	1621	1/1	0.97	0.06	139,139,139,139	0
55	MG	DA	3036	1/1	0.97	0.10	97,97,97,97	0
55	MG	AA	1605	1/1	0.97	0.07	123,123,123,123	0
55	MG	BA	3075	1/1	0.97	0.19	119,119,119,119	0
55	MG	BA	3124	1/1	0.97	0.06	39,39,39,39	0
55	MG	BA	3047	1/1	0.97	0.10	20,20,20,20	0
55	MG	BA	3084	1/1	0.97	0.08	58,58,58,58	0
55	MG	BA	3085	1/1	0.97	0.08	116,116,116,116	0
55	MG	CA	1621	1/1	0.97	0.11	40,40,40,40	0
55	MG	AA	1635	1/1	0.97	0.06	64,64,64,64	0
55	MG	AA	1606	1/1	0.97	0.09	38,38,38,38	0
55	MG	DA	3014	1/1	0.97	0.15	151,151,151,151	0
55	MG	AA	1607	1/1	0.97	0.07	62,62,62,62	0
55	MG	DA	3122	1/1	0.97	0.15	113,113,113,113	0
55	MG	AA	1602	1/1	0.97	0.07	121,121,121,121	0
55	MG	BB	202	1/1	0.97	0.06	67,67,67,67	0
55	MG	BB	203	1/1	0.97	0.06	37,37,37,37	0
55	MG	BA	3019	1/1	0.97	0.05	39,39,39,39	0
55	MG	BA	3094	1/1	0.97	0.06	37,37,37,37	0
55	MG	BA	3098	1/1	0.97	0.08	60,60,60,60	0
55	MG	DA	3056	1/1	0.97	0.08	103,103,103,103	0
55	MG	CA	1604	1/1	0.97	0.05	71,71,71,71	0
55	MG	CA	1633	1/1	0.97	0.06	61,61,61,61	0
55	MG	AA	1629	1/1	0.97	0.05	58,58,58,58	0
55	MG	DA	3133	1/1	0.97	0.06	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	1635	1/1	0.97	0.06	76,76,76,76	0
55	MG	BA	3061	1/1	0.97	0.16	171,171,171,171	0
55	MG	BA	3029	1/1	0.97	0.05	43,43,43,43	0
55	MG	BA	3110	1/1	0.97	0.12	11,11,11,11	0
55	MG	BA	3063	1/1	0.97	0.05	42,42,42,42	0
55	MG	BA	3108	1/1	0.98	0.09	30,30,30,30	0
55	MG	AA	1632	1/1	0.98	0.05	81,81,81,81	0
55	MG	CA	1609	1/1	0.98	0.07	83,83,83,83	0
55	MG	DA	3103	1/1	0.98	0.10	62,62,62,62	0
55	MG	BA	3111	1/1	0.98	0.05	47,47,47,47	0
55	MG	BA	3074	1/1	0.98	0.05	59,59,59,59	0
55	MG	CA	1641	1/1	0.98	0.06	68,68,68,68	0
55	MG	DA	3068	1/1	0.98	0.06	65,65,65,65	0
55	MG	DA	3069	1/1	0.98	0.06	79,79,79,79	0
55	MG	AA	1633	1/1	0.98	0.09	78,78,78,78	0
55	MG	AA	1601	1/1	0.98	0.06	82,82,82,82	0
55	MG	BA	3078	1/1	0.98	0.06	26,26,26,26	0
55	MG	BA	3079	1/1	0.98	0.06	99,99,99,99	0
55	MG	DA	3113	1/1	0.98	0.04	59,59,59,59	0
55	MG	BA	3080	1/1	0.98	0.04	31,31,31,31	0
55	MG	BA	3121	1/1	0.98	0.04	12,12,12,12	0
55	MG	BA	3081	1/1	0.98	0.04	32,32,32,32	0
55	MG	BA	3083	1/1	0.98	0.07	42,42,42,42	0
55	MG	DA	3118	1/1	0.98	0.09	77,77,77,77	0
55	MG	BA	3005	1/1	0.98	0.05	86,86,86,86	0
55	MG	AA	1617	1/1	0.98	0.04	83,83,83,83	0
55	MG	BA	3133	1/1	0.98	0.13	103,103,103,103	0
55	MG	BA	3086	1/1	0.98	0.06	45,45,45,45	0
55	MG	AA	1638	1/1	0.98	0.05	29,29,29,29	0
55	MG	AA	1614	1/1	0.98	0.05	55,55,55,55	0
55	MG	CA	1626	1/1	0.98	0.13	40,40,40,40	0
55	MG	AA	1604	1/1	0.98	0.06	98,98,98,98	0
55	MG	AA	1625	1/1	0.98	0.06	67,67,67,67	0
55	MG	BA	3024	1/1	0.98	0.04	16,16,16,16	0
55	MG	DA	3090	1/1	0.98	0.09	90,90,90,90	0
55	MG	AA	1642	1/1	0.98	0.12	40,40,40,40	0
55	MG	DA	3021	1/1	0.98	0.15	66,66,66,66	0
55	MG	DA	3055	1/1	0.98	0.04	75,75,75,75	0
55	MG	BA	3095	1/1	0.98	0.05	38,38,38,38	0
55	MG	BA	3028	1/1	0.98	0.09	100,100,100,100	0
55	MG	DA	3024	1/1	0.98	0.04	85,85,85,85	0
55	MG	BA	3001	1/1	0.98	0.07	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	3030	1/1	0.98	0.08	57,57,57,57	0
56	ZN	B4	101	1/1	0.98	0.04	51,51,51,51	0
55	MG	BA	3031	1/1	0.98	0.06	11,11,11,11	0
55	MG	BA	3018	1/1	0.99	0.03	35,35,35,35	0
55	MG	BA	3090	1/1	0.99	0.04	28,28,28,28	0
55	MG	AA	1626	1/1	0.99	0.17	39,39,39,39	0
55	MG	BA	3022	1/1	0.99	0.03	37,37,37,37	0
55	MG	BA	3064	1/1	0.99	0.04	38,38,38,38	0
55	MG	BA	3065	1/1	0.99	0.02	26,26,26,26	0
55	MG	BA	3067	1/1	0.99	0.04	21,21,21,21	0
55	MG	BA	3039	1/1	0.99	0.04	9,9,9,9	0
55	MG	BB	204	1/1	0.99	0.04	40,40,40,40	0
55	MG	BA	3099	1/1	0.99	0.07	82,82,82,82	0
55	MG	BA	3040	1/1	0.99	0.04	27,27,27,27	0
55	MG	DA	3071	1/1	0.99	0.06	64,64,64,64	0
55	MG	BA	3102	1/1	0.99	0.03	36,36,36,36	0
55	MG	BA	3103	1/1	0.99	0.08	60,60,60,60	0
55	MG	BA	3041	1/1	0.99	0.10	19,19,19,19	0
55	MG	BA	3044	1/1	0.99	0.04	34,34,34,34	0
55	MG	CA	1642	1/1	0.99	0.06	78,78,78,78	0
55	MG	BA	3107	1/1	0.99	0.06	11,11,11,11	0
55	MG	DA	3078	1/1	0.99	0.10	68,68,68,68	0
55	MG	BA	3046	1/1	0.99	0.06	23,23,23,23	0
55	MG	BA	3076	1/1	0.99	0.05	16,16,16,16	0
55	MG	BA	3010	1/1	0.99	0.04	29,29,29,29	0
55	MG	BA	3025	1/1	0.99	0.05	21,21,21,21	0
55	MG	AA	1610	1/1	0.99	0.04	33,33,33,33	0
55	MG	BA	3114	1/1	0.99	0.08	86,86,86,86	0
55	MG	BA	3115	1/1	0.99	0.05	49,49,49,49	0
55	MG	BA	3051	1/1	0.99	0.04	71,71,71,71	0
55	MG	BA	3053	1/1	0.99	0.05	30,30,30,30	0
55	MG	BA	3082	1/1	0.99	0.04	30,30,30,30	0
55	MG	DA	3012	1/1	0.99	0.07	75,75,75,75	0
55	MG	BA	3012	1/1	0.99	0.04	8,8,8,8	0
55	MG	AA	1643	1/1	0.99	0.03	35,35,35,35	0
55	MG	AA	1637	1/1	0.99	0.05	85,85,85,85	0
55	MG	DA	3053	1/1	0.99	0.04	59,59,59,59	0
55	MG	BA	3059	1/1	0.99	0.03	36,36,36,36	0
55	MG	BA	3126	1/1	0.99	0.05	21,21,21,21	0
55	MG	BA	3016	1/1	0.99	0.07	64,64,64,64	0
55	MG	BA	3129	1/1	0.99	0.04	31,31,31,31	0
55	MG	BA	3130	1/1	0.99	0.04	8,8,8,8	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	3131	1/1	0.99	0.05	17,17,17,17	0
55	MG	BA	3096	1/1	1.00	0.04	40,40,40,40	0
55	MG	BA	3097	1/1	1.00	0.02	18,18,18,18	0
55	MG	BA	3135	1/1	1.00	0.03	12,12,12,12	0
55	MG	BA	3068	1/1	1.00	0.04	11,11,11,11	0
55	MG	BA	3069	1/1	1.00	0.03	14,14,14,14	0
55	MG	BA	3008	1/1	1.00	0.06	17,17,17,17	0
55	MG	BA	3101	1/1	1.00	0.03	27,27,27,27	0
55	MG	BA	3045	1/1	1.00	0.11	21,21,21,21	0
55	MG	BA	3027	1/1	1.00	0.08	31,31,31,31	0
55	MG	BA	3104	1/1	1.00	0.04	22,22,22,22	0
55	MG	BA	3073	1/1	1.00	0.04	12,12,12,12	0
55	MG	BA	3009	1/1	1.00	0.04	13,13,13,13	0
55	MG	BA	3017	1/1	1.00	0.02	9,9,9,9	0
55	MG	AA	1622	1/1	1.00	0.07	30,30,30,30	0
55	MG	BA	3109	1/1	1.00	0.07	13,13,13,13	0
55	MG	BA	3050	1/1	1.00	0.02	16,16,16,16	0
55	MG	AA	1612	1/1	1.00	0.04	60,60,60,60	0
55	MG	BA	3052	1/1	1.00	0.02	25,25,25,25	0
55	MG	BA	3020	1/1	1.00	0.19	16,16,16,16	0
55	MG	BA	3054	1/1	1.00	0.02	14,14,14,14	0
55	MG	BA	3055	1/1	1.00	0.02	25,25,25,25	0
55	MG	BA	3033	1/1	1.00	0.03	9,9,9,9	0
55	MG	BA	3034	1/1	1.00	0.07	8,8,8,8	0
55	MG	BA	3118	1/1	1.00	0.05	13,13,13,13	0
55	MG	BA	3021	1/1	1.00	0.06	17,17,17,17	0
55	MG	BA	3036	1/1	1.00	0.06	11,11,11,11	0
55	MG	BA	3087	1/1	1.00	0.04	13,13,13,13	0
55	MG	BA	3122	1/1	1.00	0.04	64,64,64,64	0
55	MG	BA	3123	1/1	1.00	0.04	10,10,10,10	0
55	MG	BA	3006	1/1	1.00	0.01	32,32,32,32	0
55	MG	BA	3038	1/1	1.00	0.06	30,30,30,30	0
55	MG	BA	3023	1/1	1.00	0.03	11,11,11,11	0
55	MG	BA	3013	1/1	1.00	0.04	8,8,8,8	0
55	MG	BA	3128	1/1	1.00	0.04	18,18,18,18	0
55	MG	AA	1634	1/1	1.00	0.05	59,59,59,59	0
55	MG	BA	3042	1/1	1.00	0.08	18,18,18,18	0
55	MG	BA	3066	1/1	1.00	0.03	18,18,18,18	0
55	MG	BA	3043	1/1	1.00	0.03	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.