



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 29, 2026 – 11:54 AM UTC

PDB ID : 4V6E / pdb_00004v6e
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 : 2009-06-28
Resolution : 3.71 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

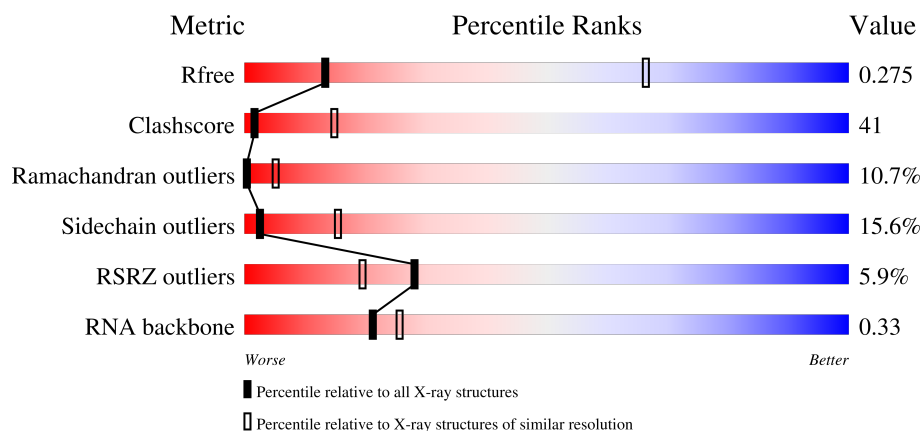
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.71 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1182 (3.84-3.60)
Clashscore	190562	1222 (3.84-3.60)
Ramachandran outliers	187476	1178 (3.84-3.60)
Sidechain outliers	187428	1174 (3.84-3.60)
RSRZ outliers	180081	1181 (3.84-3.60)
RNA backbone	3983	1007 (4.30-3.08)

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	14% 19% 52% 17% • 10%
1	CB	241	4% 21% 56% 13% • 10%
2	AC	233	29% 47% 12% • 12%
2	CC	233	29% 47% 13% 12%

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

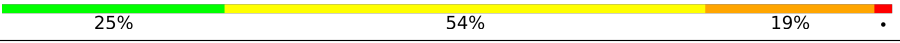
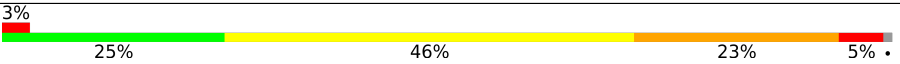
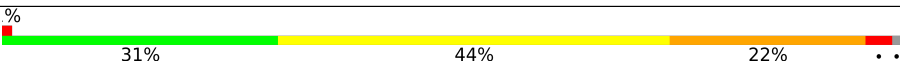
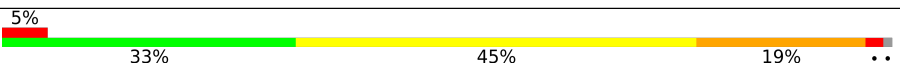
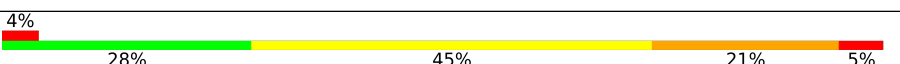
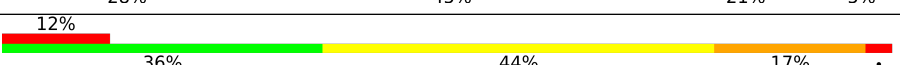
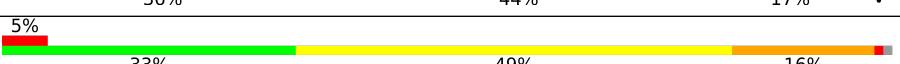
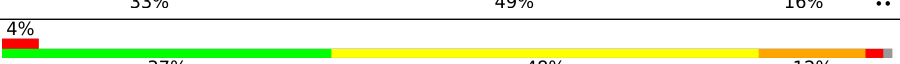
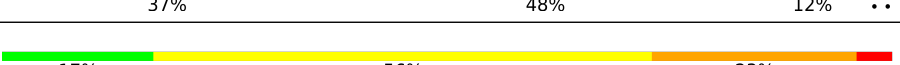
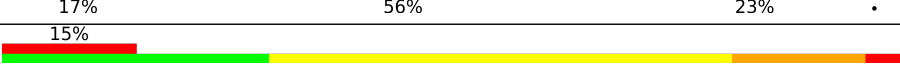
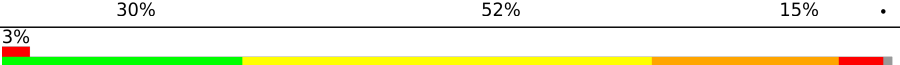
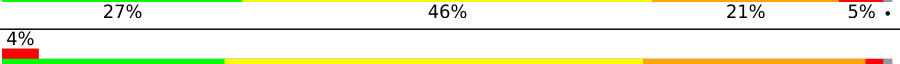
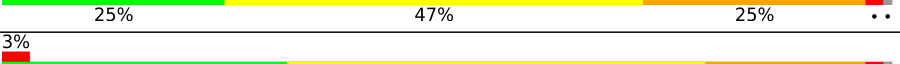
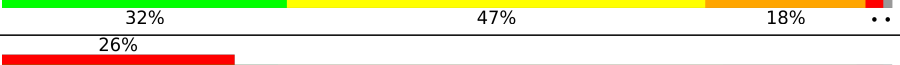
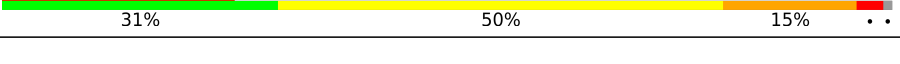
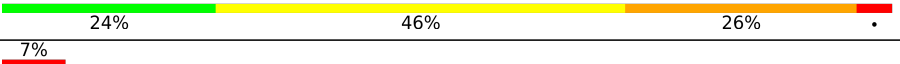
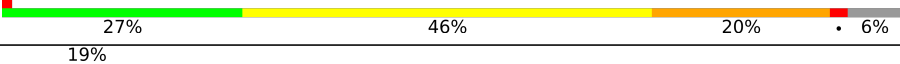
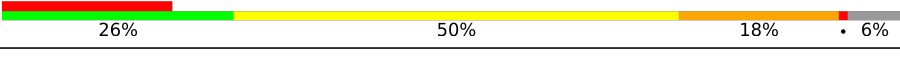
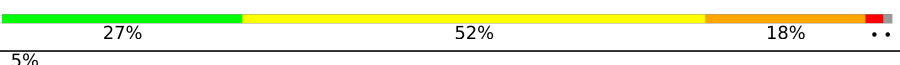
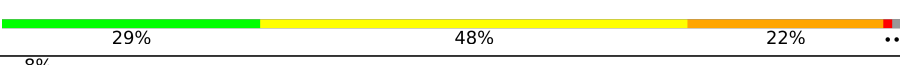
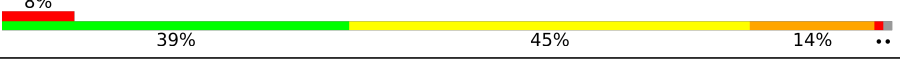
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Mol	Chain	Length	Quality of chain
15	CP	82	
16	AQ	84	
16	CQ	84	
17	AR	75	
17	CR	75	
18	AS	92	
18	CS	92	
19	AT	87	
19	CT	87	
20	AU	71	
20	CU	71	
21	AA	1533	
22	AV	17	
22	AX	17	
22	CV	17	
22	CX	17	
23	AW	6	
23	CW	6	
24	BA	2903	
24	DA	2903	
25	BB	118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

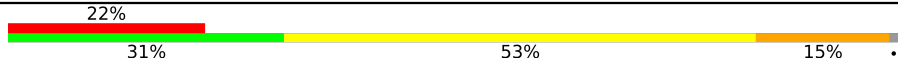
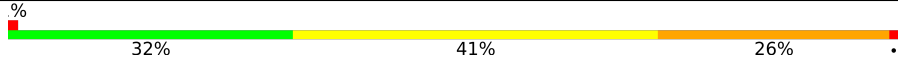
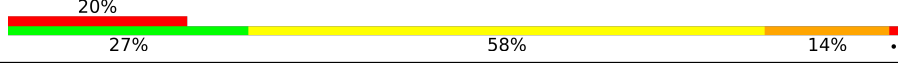
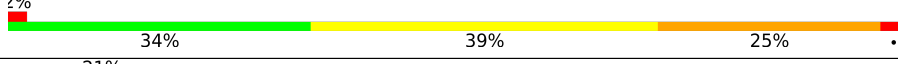
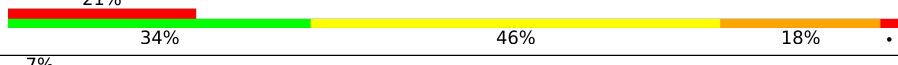
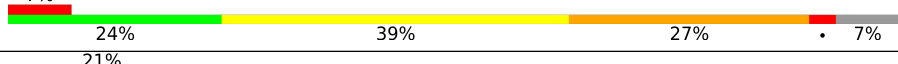
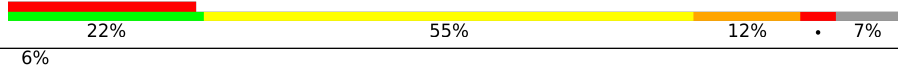
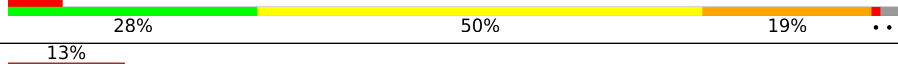
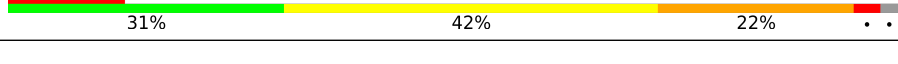
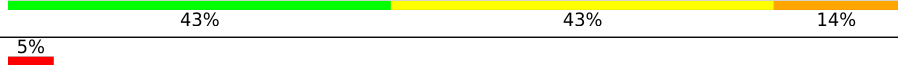
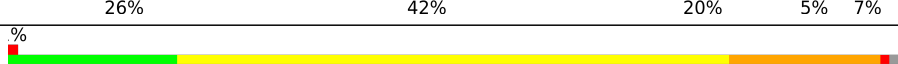
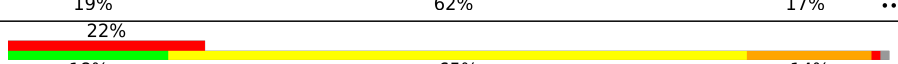
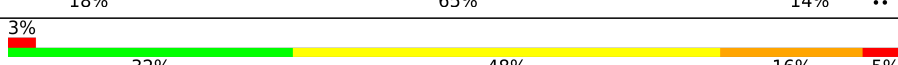
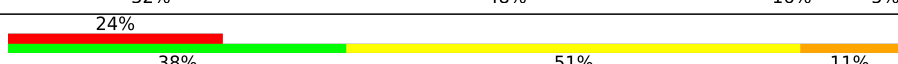
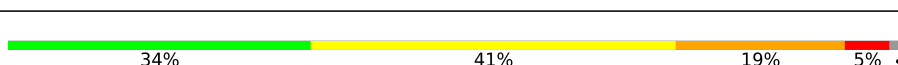
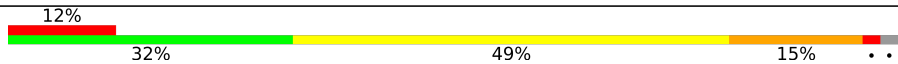
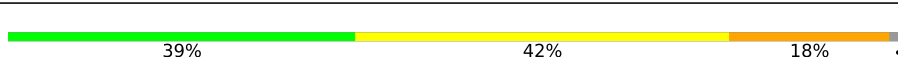
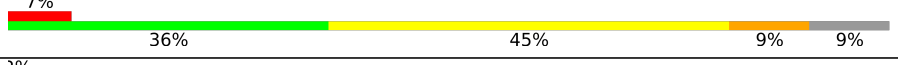
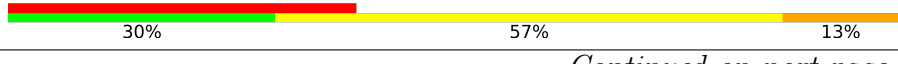
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Mol	Chain	Length	Quality of chain
28	BE	201	
28	DE	201	
29	BF	179	
29	DF	179	
30	BG	177	
30	DG	177	
31	BH	149	
31	DH	149	
32	BI	142	
32	DI	142	
33	BJ	142	
33	DJ	142	
34	BK	123	
34	DK	123	
35	BL	144	
35	DL	144	
36	BM	136	
36	DM	136	
37	BN	127	
37	DN	127	
38	BO	117	
38	DO	117	
39	BP	115	
39	DP	115	
40	BQ	118	

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Mol	Chain	Length	Quality of chain
40	DQ	118	
41	BR	103	
41	DR	103	
42	BS	110	
42	DS	110	
43	BT	100	
43	DT	100	
44	BU	104	
44	DU	104	
45	BV	94	
45	DV	94	
46	BW	85	
46	DW	85	
47	BX	78	
47	DX	78	
48	BY	63	
48	DY	63	
49	BZ	59	
49	DZ	59	
50	B0	57	
50	D0	57	
51	B1	55	
51	D1	55	
52	B2	46	
52	D2	46	

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Mol	Chain	Length	Quality of chain
53	B3	65	
53	D3	65	
54	B4	38	
54	D4	38	
55	CA	1530	
56	DB	117	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	AA	1627	-	-	-	X
57	MG	BA	3058	-	-	-	X
57	MG	BA	3062	-	-	-	X
57	MG	BA	3124	-	-	-	X
57	MG	BA	3131	-	-	-	X
57	MG	CA	1636	-	-	-	X
57	MG	DA	3058	-	-	-	X
57	MG	DA	3060	-	-	-	X
57	MG	DA	3063	-	-	-	X
57	MG	DA	3128	-	-	-	X
57	MG	DA	3129	-	-	-	X

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 286150 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AG	151	Total	C	N	O	S	0	0	0
			1181	735	227	215	4			
6	CG	150	Total	C	N	O	S	0	0	0
			1174	730	226	214	4			

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 13 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			
13	CN	95	Total	C	N	O	S	0	0	0
			769	480	159	127	3			

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 20 is a protein called 30S ribosomal protein S21.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	17	Total	C	N	O	P	0	0	0
			365	163	68	117	17			
22	AX	17	Total	C	N	O	P	0	0	0
			365	163	68	117	17			
22	CV	17	Total	C	N	O	P	0	0	0
			365	163	68	117	17			
22	CX	17	Total	C	N	O	P	0	0	0
			365	163	68	117	17			

- Molecule 23 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	6	Total	C	N	O	P	0	0	0
			120	54	12	48	6			
23	CW	6	Total	C	N	O	P	0	0	0
			120	54	12	48	6			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	AA	43	Total	Mg	0	0
			43	43		
57	BA	136	Total	Mg	0	0
			136	136		
57	BB	4	Total	Mg	0	0
			4	4		
57	BD	1	Total	Mg	0	0
			1	1		
57	CA	42	Total	Mg	0	0
			42	42		
57	DA	132	Total	Mg	0	0
			132	132		
57	DB	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	DC	2	Total	Mg	0	0
			2	2		
57	DJ	1	Total	Mg	0	0
			1	1		
57	D4	1	Total	Mg	0	0
			1	1		

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

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

- Molecule 59 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	AE	1	Total	O	0	0
			1	1		
59	AL	3	Total	O	0	0
			3	3		
59	AN	6	Total	O	0	0
			6	6		
59	AT	1	Total	O	0	0
			1	1		
59	AU	1	Total	O	0	0
			1	1		
59	AA	196	Total	O	0	0
			196	196		
59	BA	615	Total	O	0	0
			615	615		
59	BB	20	Total	O	0	0
			20	20		
59	BC	8	Total	O	0	0
			8	8		
59	BD	3	Total	O	0	0
			3	3		
59	BE	1	Total	O	0	0
			1	1		
59	BL	3	Total	O	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	BN	3	Total 3	O 3	0	0
59	BT	1	Total 1	O 1	0	0
59	B2	1	Total 1	O 1	0	0
59	B3	3	Total 3	O 3	0	0
59	B4	2	Total 2	O 2	0	0
59	CE	4	Total 4	O 4	0	0
59	CI	1	Total 1	O 1	0	0
59	CL	1	Total 1	O 1	0	0
59	CN	2	Total 2	O 2	0	0
59	CT	2	Total 2	O 2	0	0
59	CU	2	Total 2	O 2	0	0
59	CA	195	Total 195	O 195	0	0
59	DA	600	Total 600	O 600	0	0
59	DB	4	Total 4	O 4	0	0
59	DC	12	Total 12	O 12	0	0
59	DD	2	Total 2	O 2	0	0
59	DE	3	Total 3	O 3	0	0
59	DJ	3	Total 3	O 3	0	0
59	DL	6	Total 6	O 6	0	0
59	DN	2	Total 2	O 2	0	0
59	DT	2	Total 2	O 2	0	0

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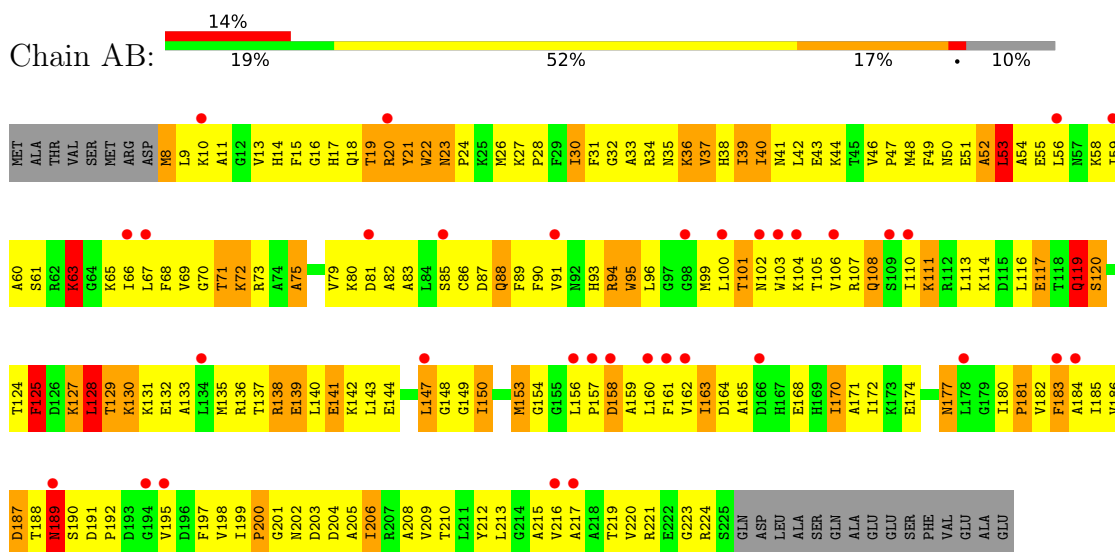
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	DU	1	Total 1	O 1	0	0
59	DV	1	Total 1	O 1	0	0
59	D2	1	Total 1	O 1	0	0
59	D3	1	Total 1	O 1	0	0
59	D4	5	Total 5	O 5	0	0

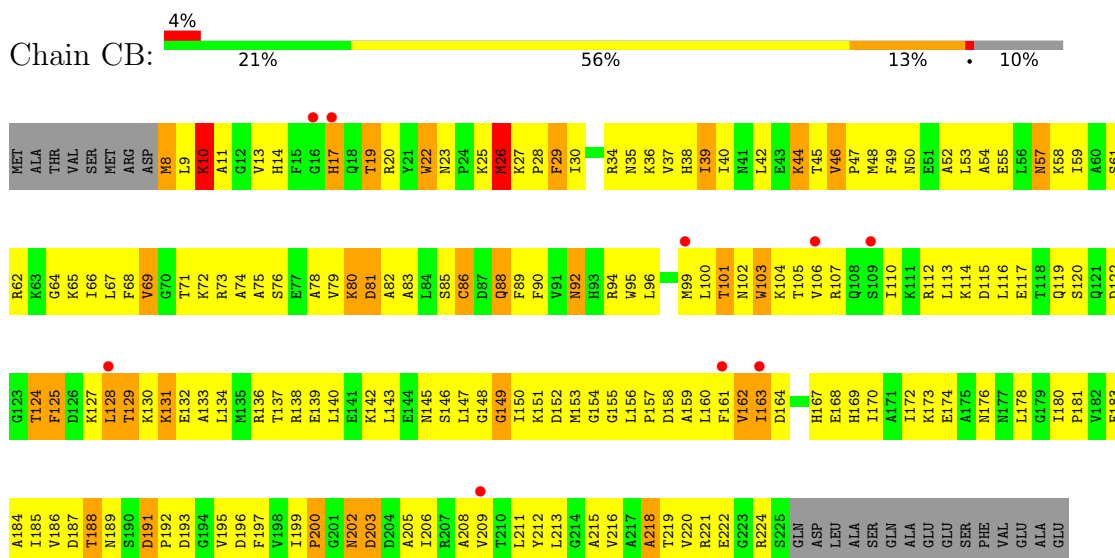
3 Residue-property plots

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

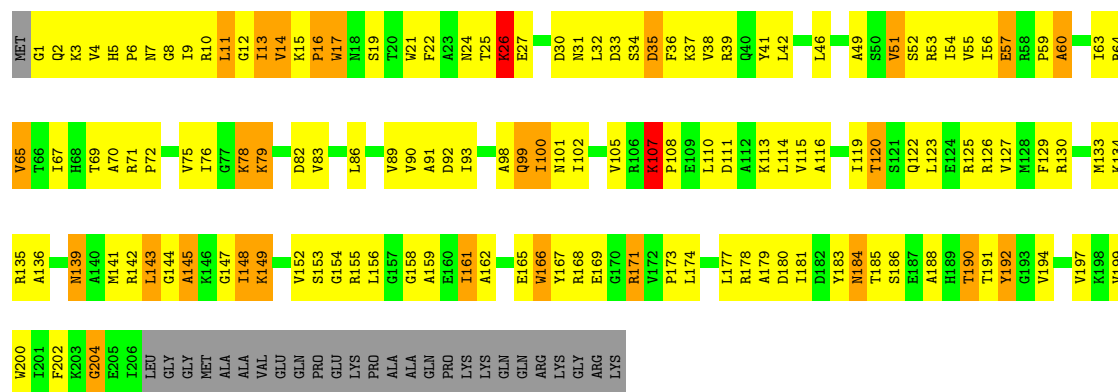


• Molecule 1: 30S ribosomal protein S2



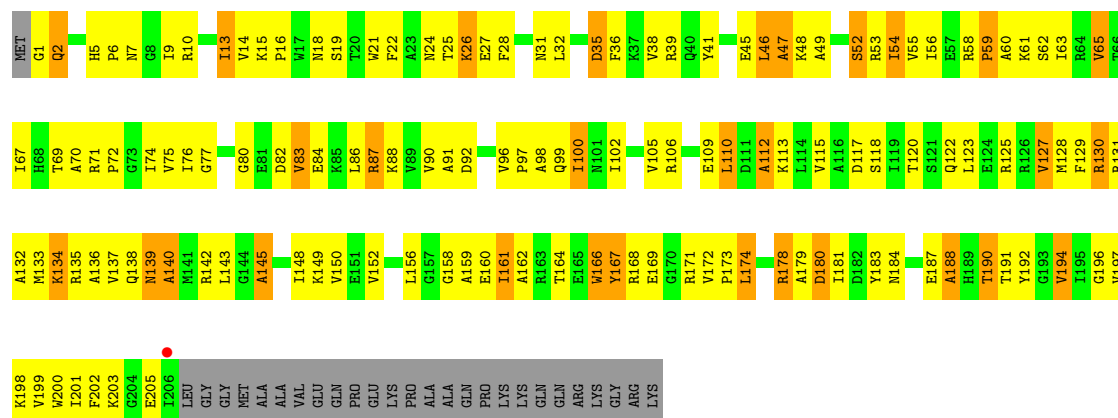
• Molecule 2: 30S ribosomal protein S3





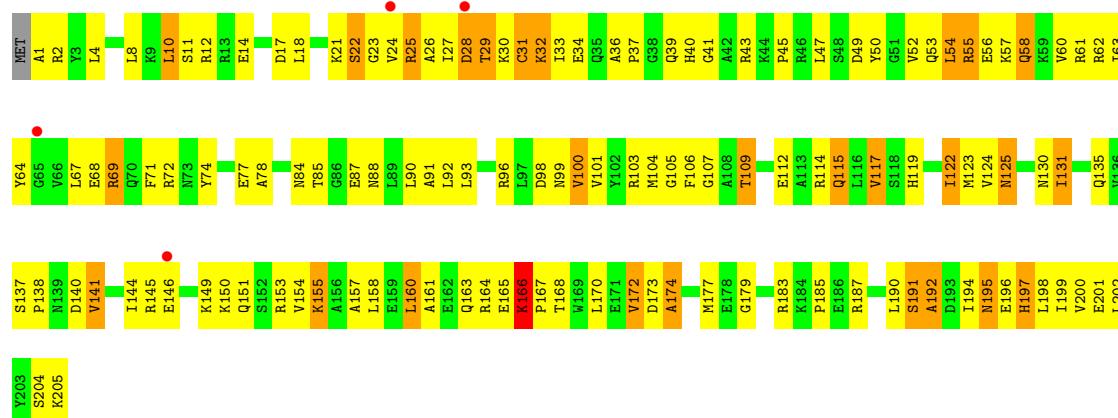
• Molecule 2: 30S ribosomal protein S3

Chain CC: 29% 47% 13% 12%



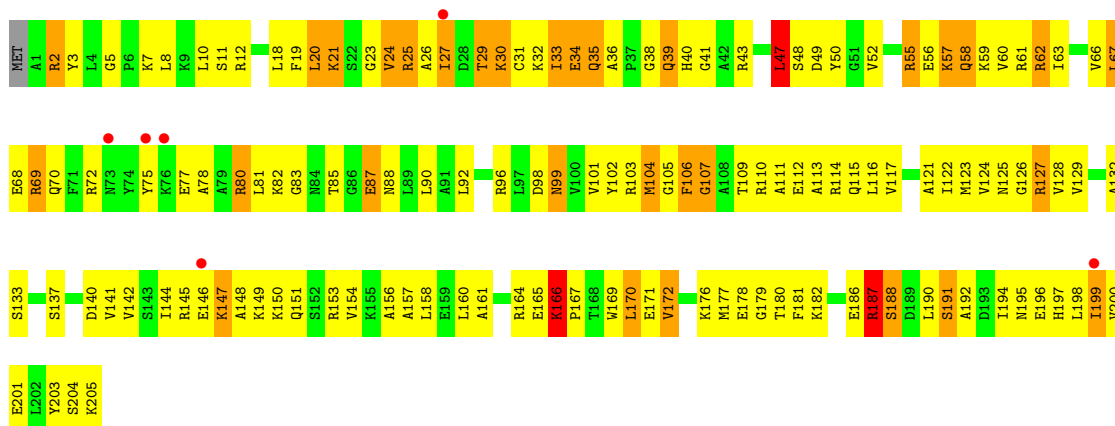
• Molecule 3: 30S ribosomal protein S4

Chain AD: 2% 36% 50% 13%

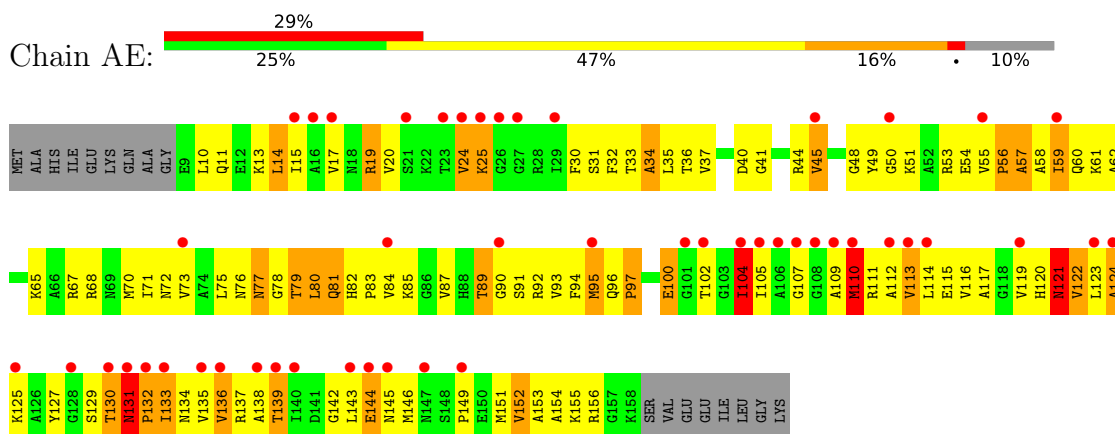


• Molecule 3: 30S ribosomal protein S4

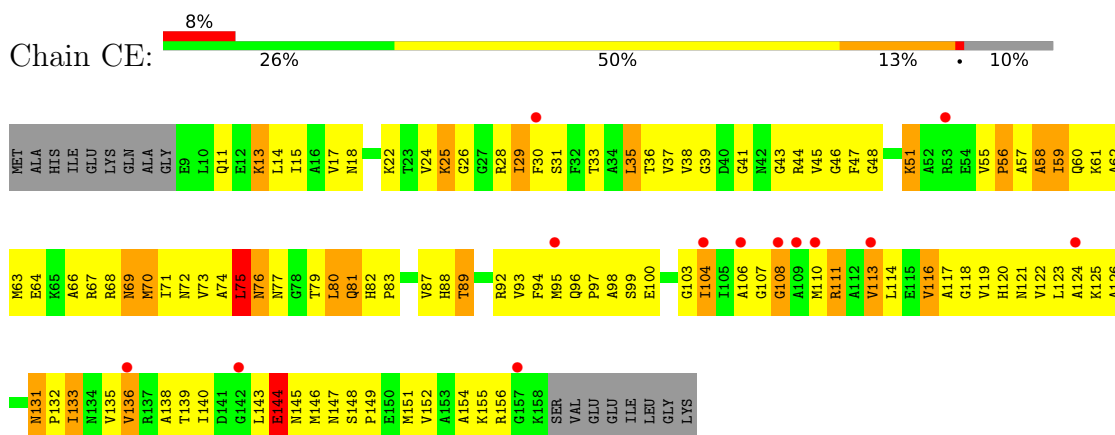
Chain CD: 3% 30% 53% 15%



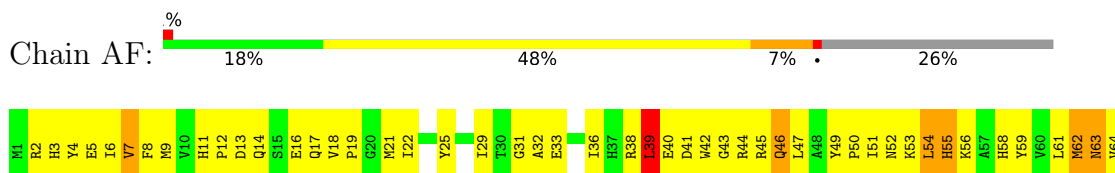
- Molecule 4: 30S ribosomal protein S5

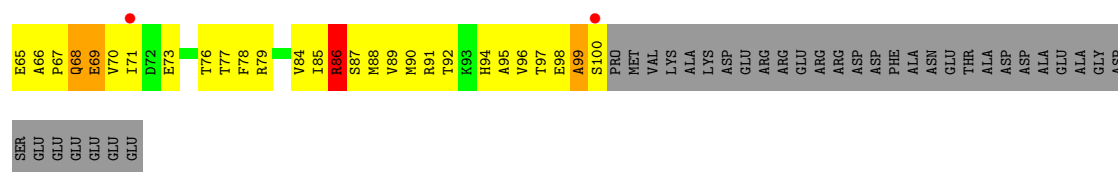


- Molecule 4: 30S ribosomal protein S5

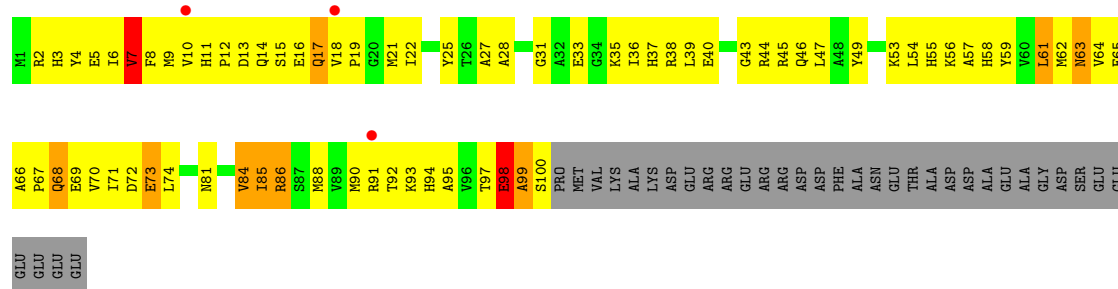
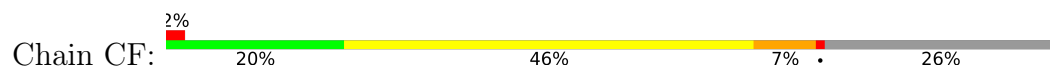


- Molecule 5: 30S ribosomal protein S6

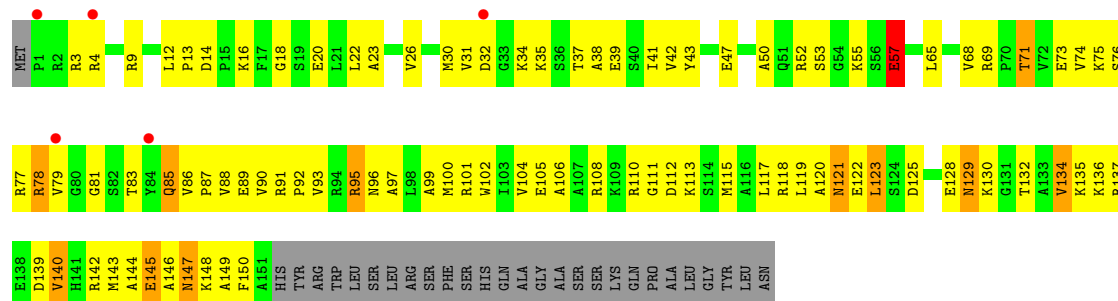




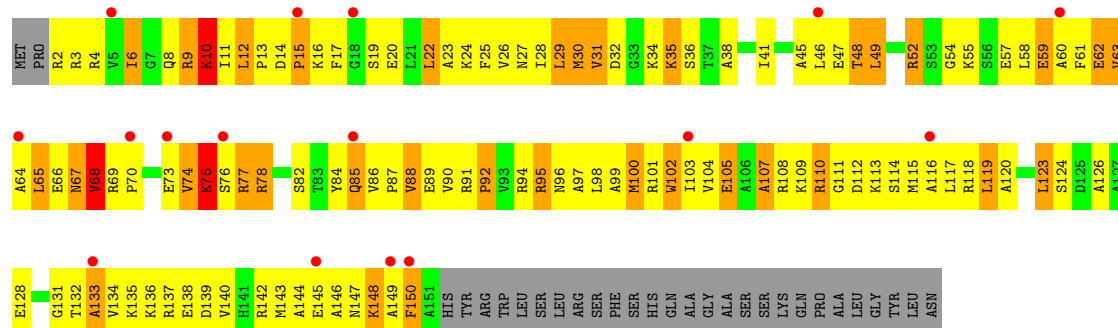
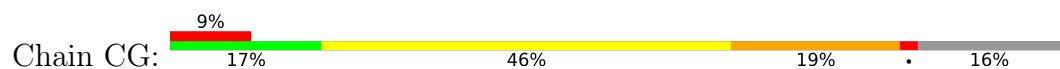
• Molecule 5: 30S ribosomal protein S6



• Molecule 6: 30S ribosomal protein S7

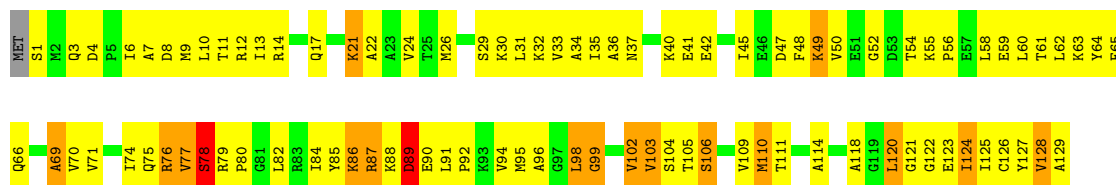


• Molecule 6: 30S ribosomal protein S7



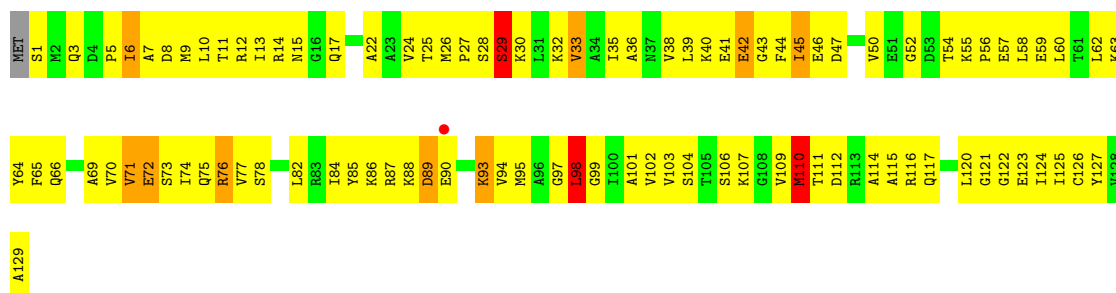
• Molecule 7: 30S ribosomal protein S8

Chain AH: 28% 57% 12% ..



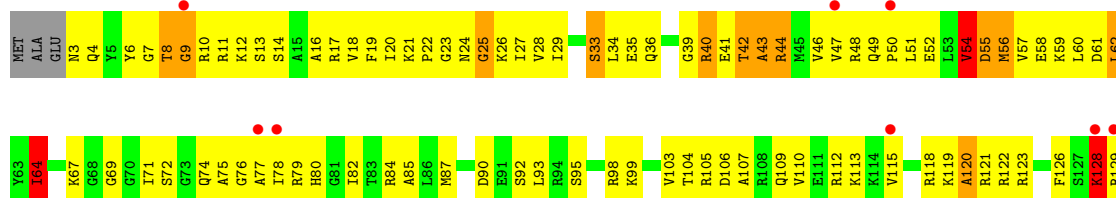
• Molecule 7: 30S ribosomal protein S8

Chain CH: 25% 65% 7% ..



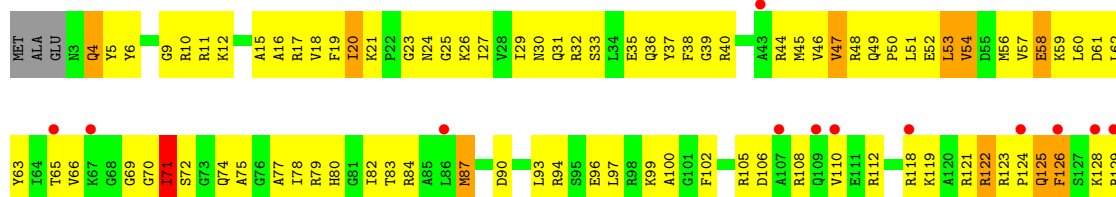
• Molecule 8: 30S ribosomal protein S9

Chain AI: 6% 27% 59% 9% ..



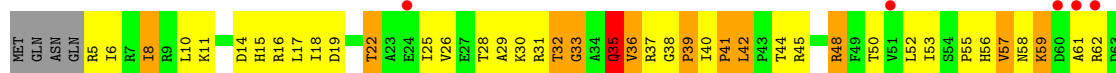
• Molecule 8: 30S ribosomal protein S9

Chain CI: 9% 30% 59% 8% ..



• Molecule 9: 30S ribosomal protein S10

Chain AJ: 6% 30% 49% 16% 5%





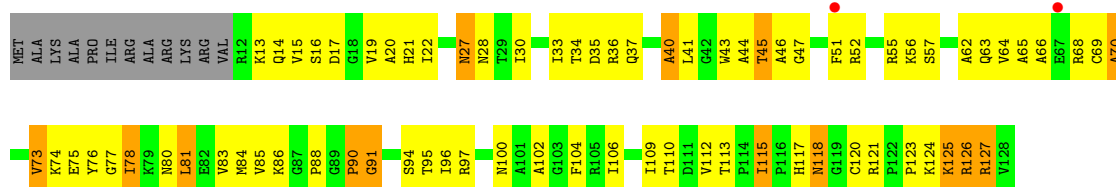
- Molecule 9: 30S ribosomal protein S10



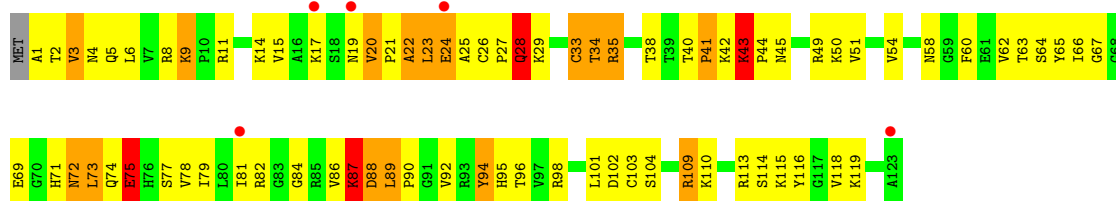
- Molecule 10: 30S ribosomal protein S11



- Molecule 10: 30S ribosomal protein S11

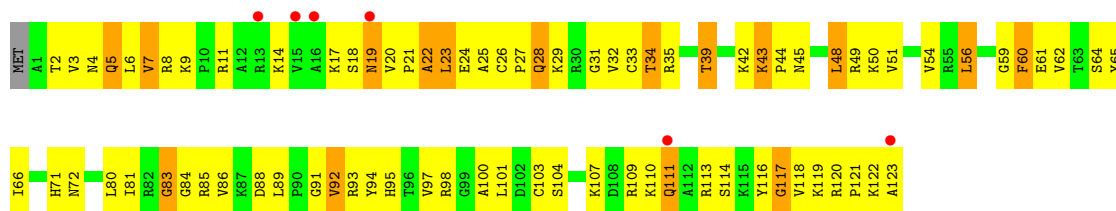


- Molecule 11: 30S ribosomal protein S12

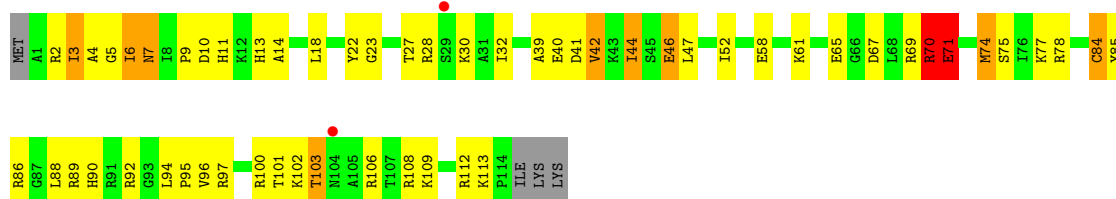


- Molecule 11: 30S ribosomal protein S12

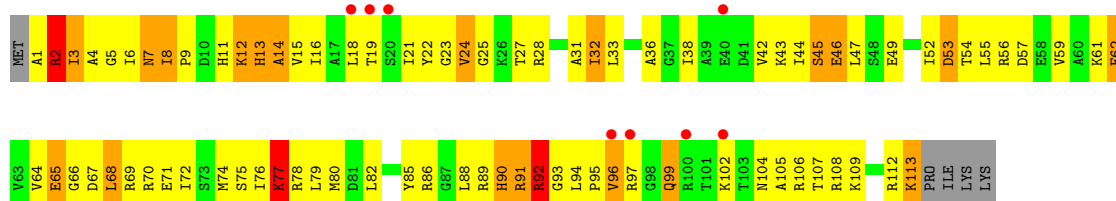




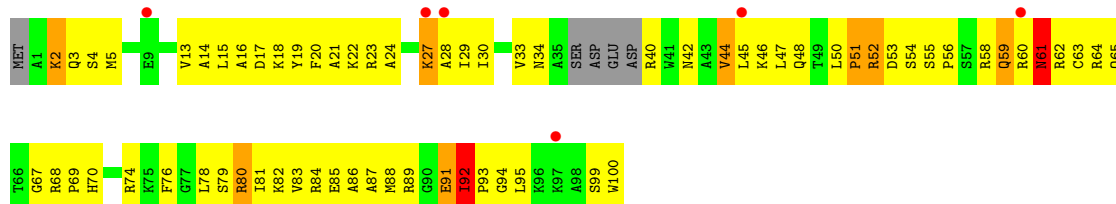
• Molecule 12: 30S ribosomal protein S13



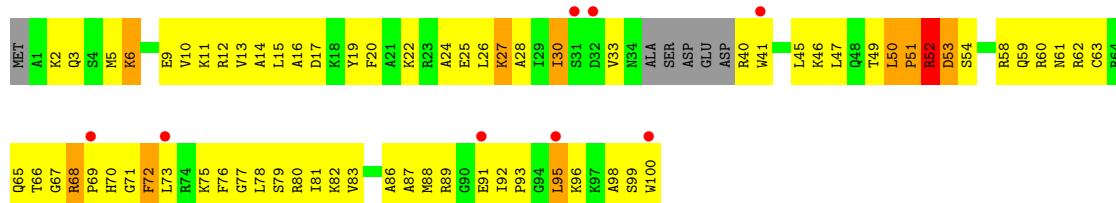
• Molecule 12: 30S ribosomal protein S13



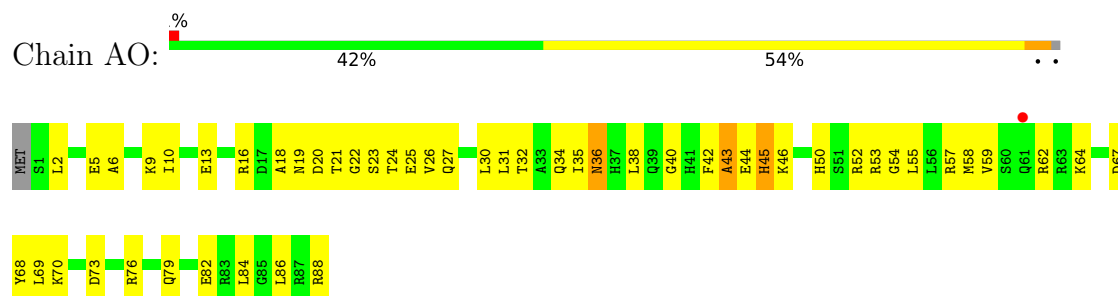
• Molecule 13: 30S ribosomal protein S14



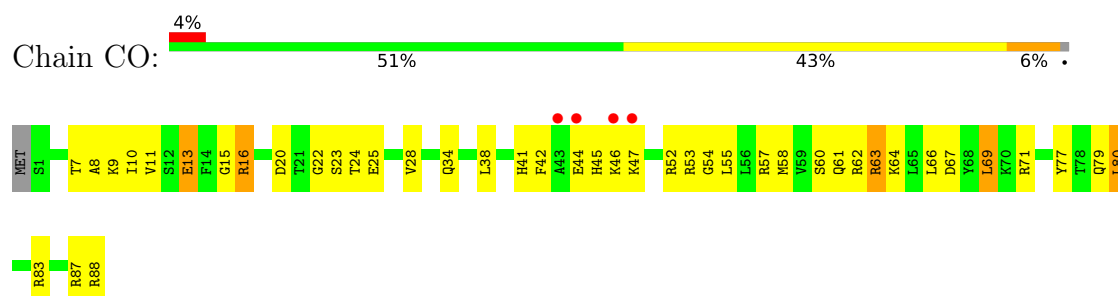
• Molecule 13: 30S ribosomal protein S14



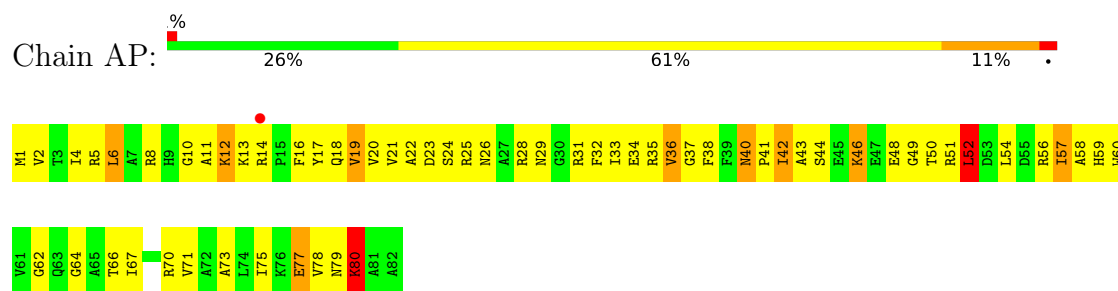
• Molecule 14: 30S ribosomal protein S15



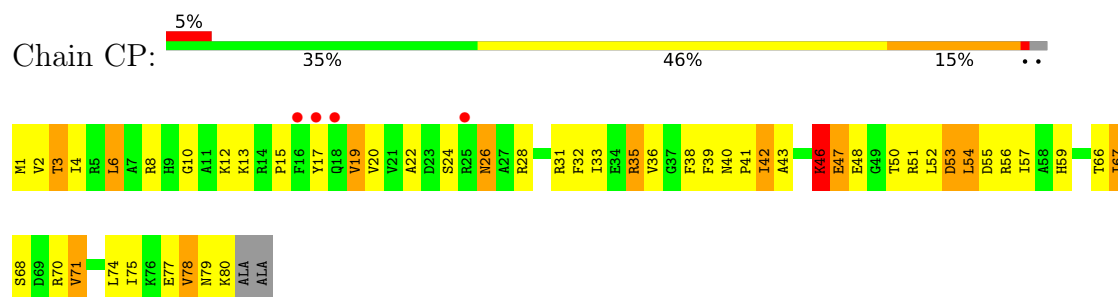
• Molecule 14: 30S ribosomal protein S15



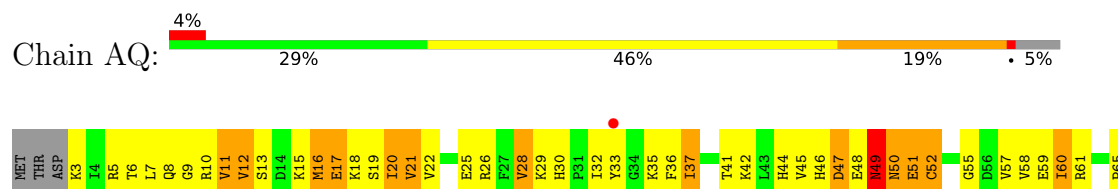
• Molecule 15: 30S ribosomal protein S16



• Molecule 15: 30S ribosomal protein S16

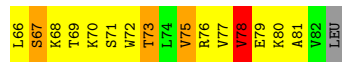
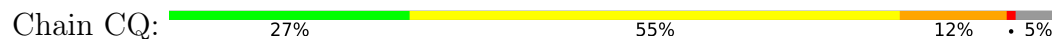


• Molecule 16: 30S ribosomal protein S17





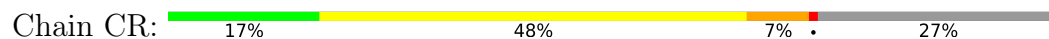
- Molecule 16: 30S ribosomal protein S17



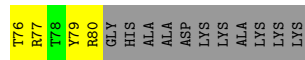
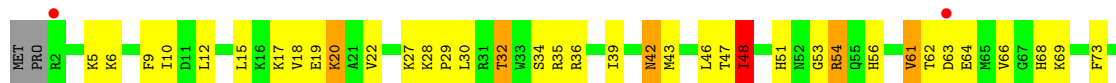
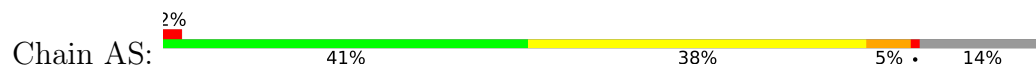
- Molecule 17: 30S ribosomal protein S18



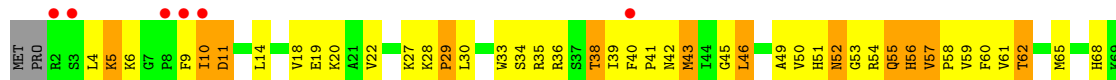
- Molecule 17: 30S ribosomal protein S18

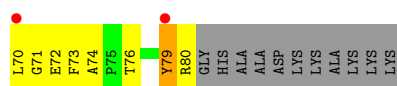


- Molecule 18: 30S ribosomal protein S19

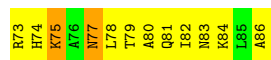


- Molecule 18: 30S ribosomal protein S19

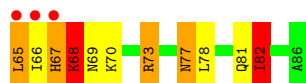
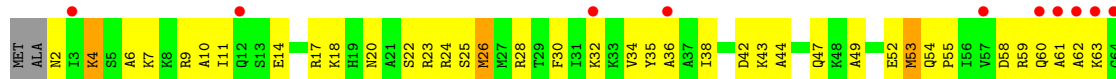




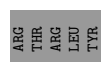
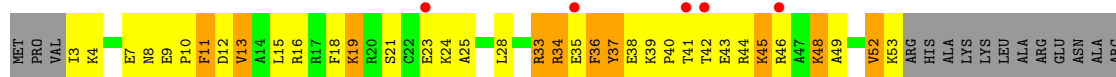
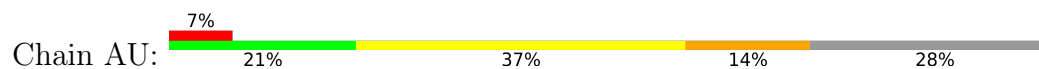
• Molecule 19: 30S ribosomal protein S20



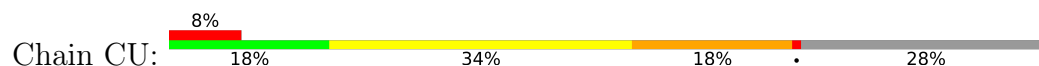
• Molecule 19: 30S ribosomal protein S20



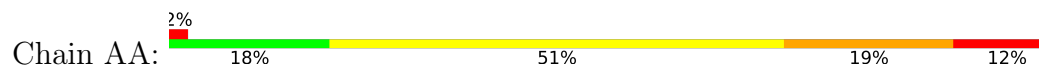
• Molecule 20: 30S ribosomal protein S21



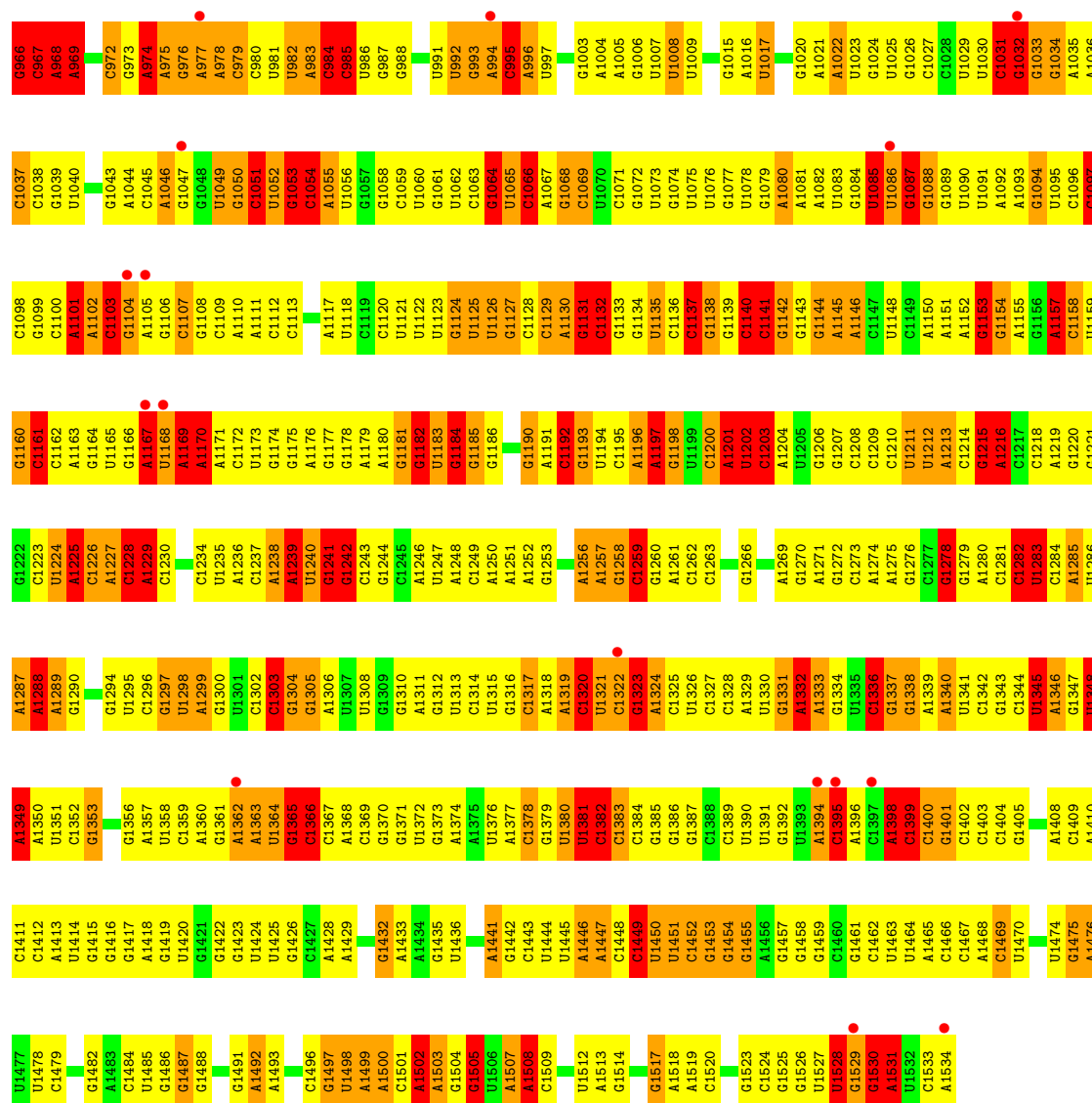
• Molecule 20: 30S ribosomal protein S21



• Molecule 21: 16S rRNA



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A2	A3	U4	U5	G6	A7	A8	G9	A10	U11	U12	U13	U14	G15	A16	U17	C18	A19	U20	G21	G22	C23	U24	C25	A26	U30	G31	A32	A33	C34	C35	C36	U37	G38	G39	C40	G41	G42	C43	A44	G45	G46	C47	C48	U49	A50	A51	G52	A53	G57	C58	A59	A60	G61	U62	C63	G64	A65																				
A66	C67	G68	G69	U70	A71	A72	G73	A74	G75	G76	U77	A78	G79	A80	A81	C82	C83	U84	U85	G86	C87	U88	U89	C90	U91	U92	U93	A94	C95	U96	C97	A98	C99	G100	G101	G102	U103	G104	C105	C106	A109	C110	G111	G112	U114	G115	A116	G117	U118	A119	A120	U121	G122	U123	U124	G125	G126																				
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C575	C576	G577	C578	A579	C580	G581	C582	A583	C586	G587	G588	U589	U590	C593	U594	A595	A596	G597	U598	C599	A600	G601	A602	U603	G604	U605	G606	A607	C608	C613	C614	G615	G616	U619	A622	C623	G624	C625	U626	G627	G628	A629	A630	C631	U632	G633	C636	U637	G638	U639	A640	U641	A642	C643																							
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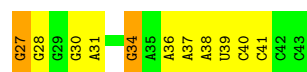
• Molecule 22: P-site tRNA ASL fragment

Chain AV: 24% 53% 24%



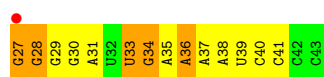
• Molecule 22: P-site tRNA ASL fragment

Chain AX: 35% 53% 12%

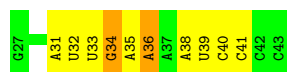


• Molecule 22: P-site tRNA ASL fragment

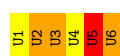
Chain CV: 6% 18% 53% 29%



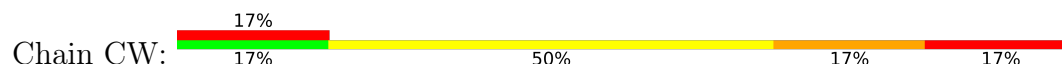
- Molecule 22: P-site tRNA ASL fragment



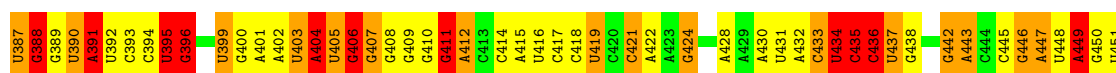
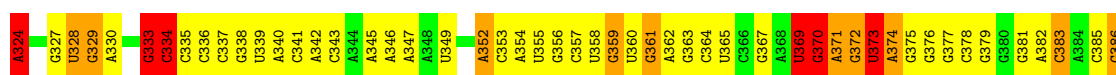
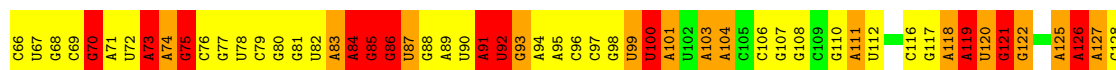
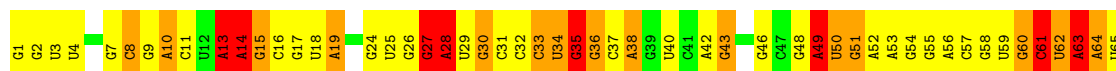
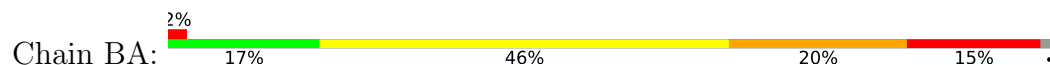
- Molecule 23: messenger RNA



- Molecule 23: messenger RNA

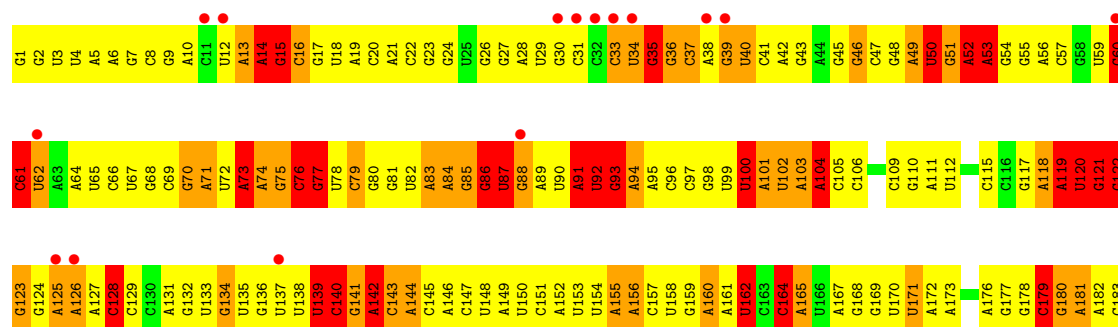
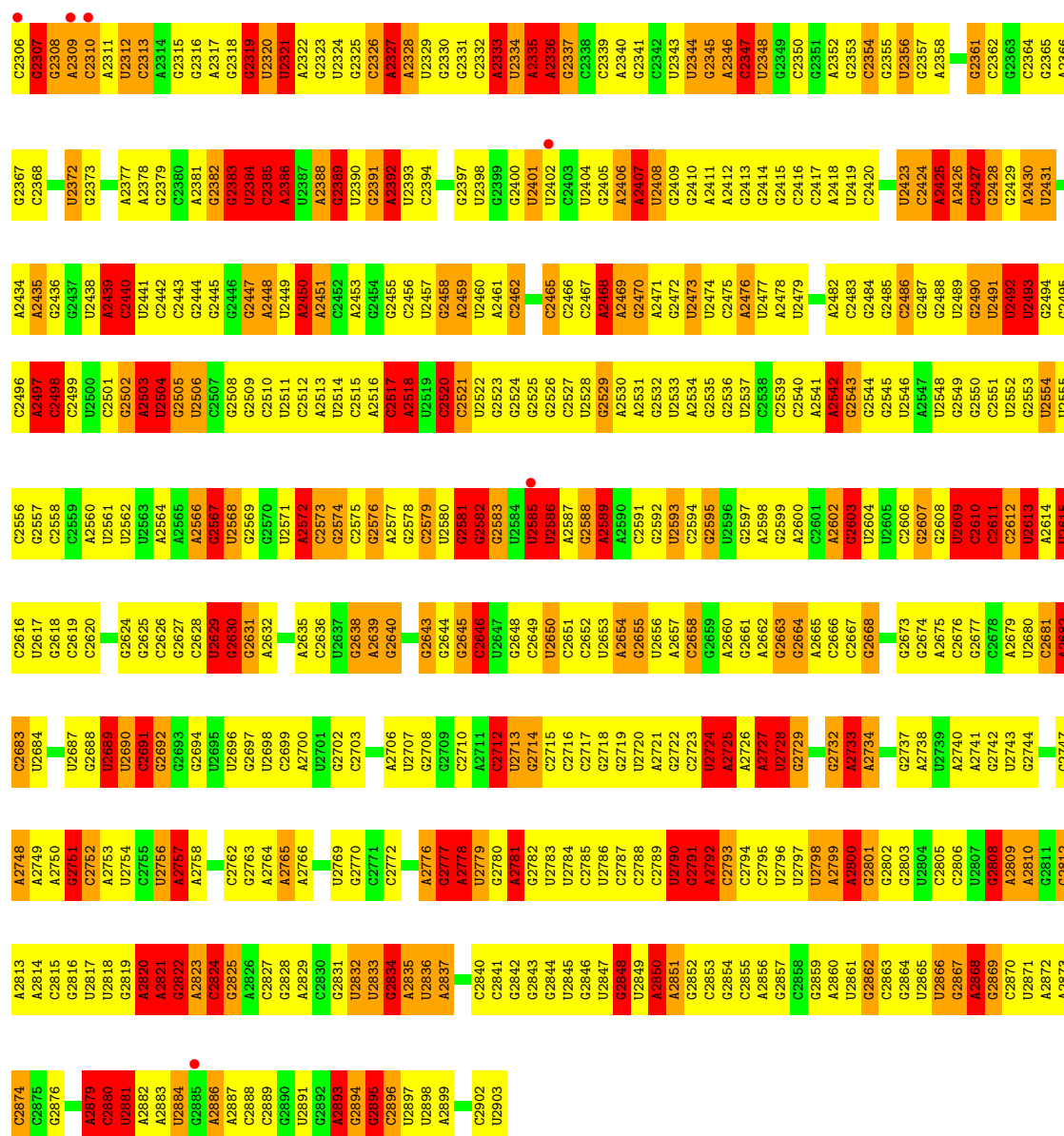


- Molecule 24: 23S rRNA



U1344	G1345	G1346	G1347	G1348	G1349	G1350	G1351	G1352	G1353	G1354	G1355	G1356	G1357	G1360	G1361	G1362	G1363	G1364	A1365	G1368	G1369	G1370	G1371	G1372	G1373	G1374	G1375	A1378	U1379	G1380	G1381	G1382	A1383	A1384	A1385	G1386	A1387	G1388	G1389	A1392	A1393	U1394	A1395	U1396	U1397	G1398	G1399	U1400	G1401	U1402	A1403	G1404	U1405	U1406	G1407								
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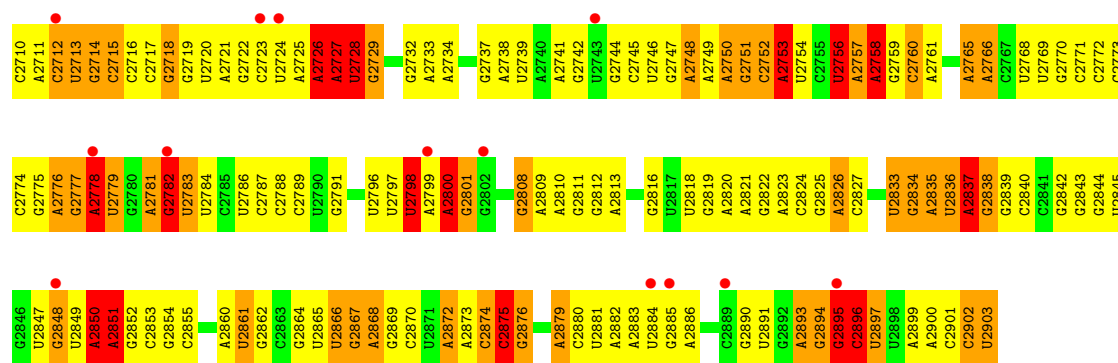






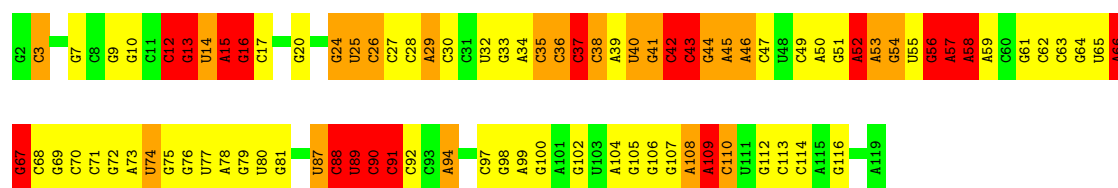


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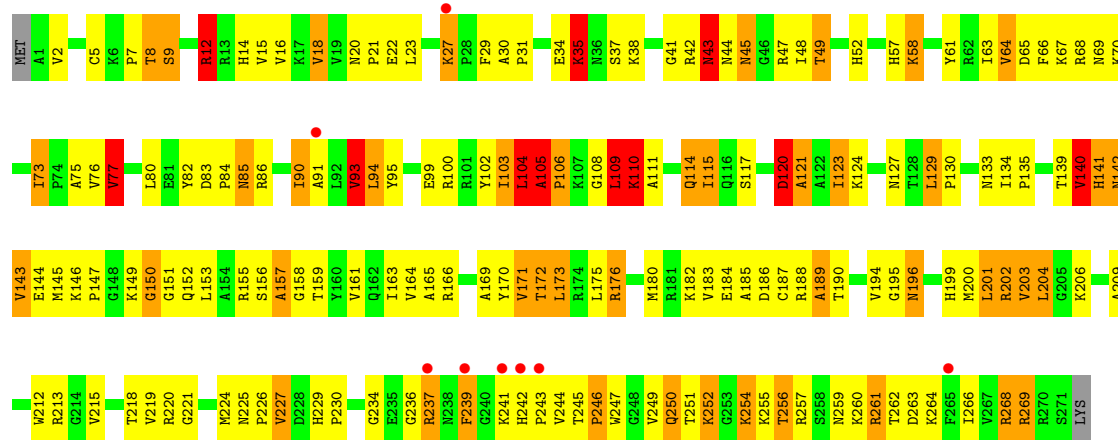
• Molecule 25: 5S rRNA

Chain BB: 25% 42% 18% 15%



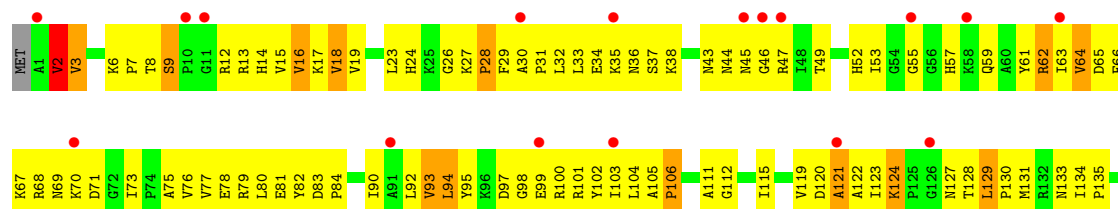
• Molecule 26: 50S ribosomal protein L2

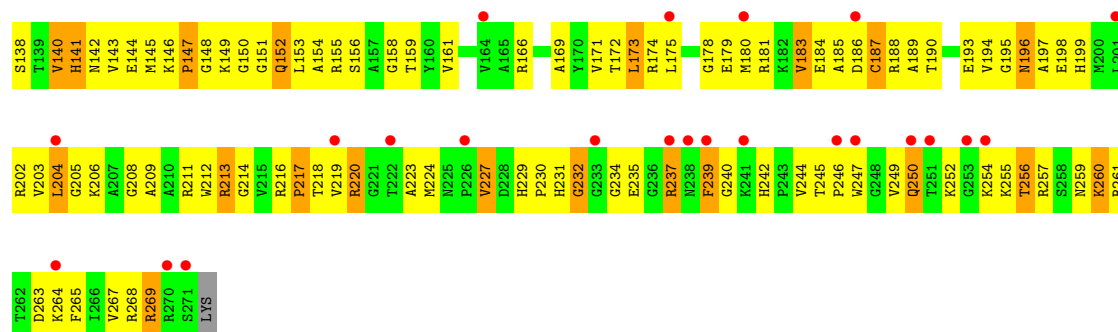
Chain BC: 3% 36% 43% 16%



• Molecule 26: 50S ribosomal protein L2

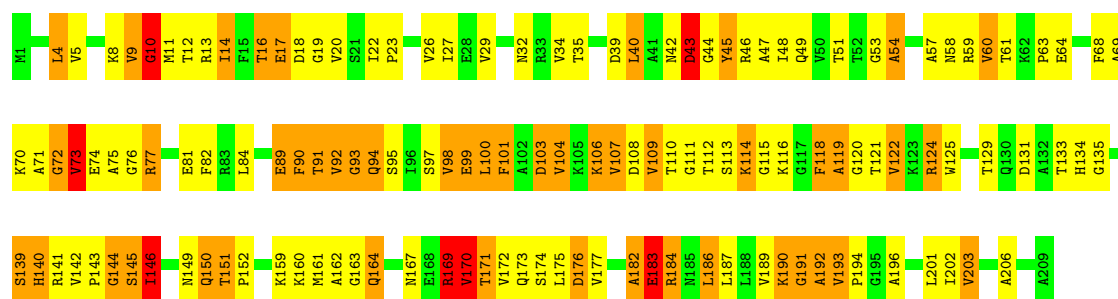
Chain DC: 15% 30% 57% 12%





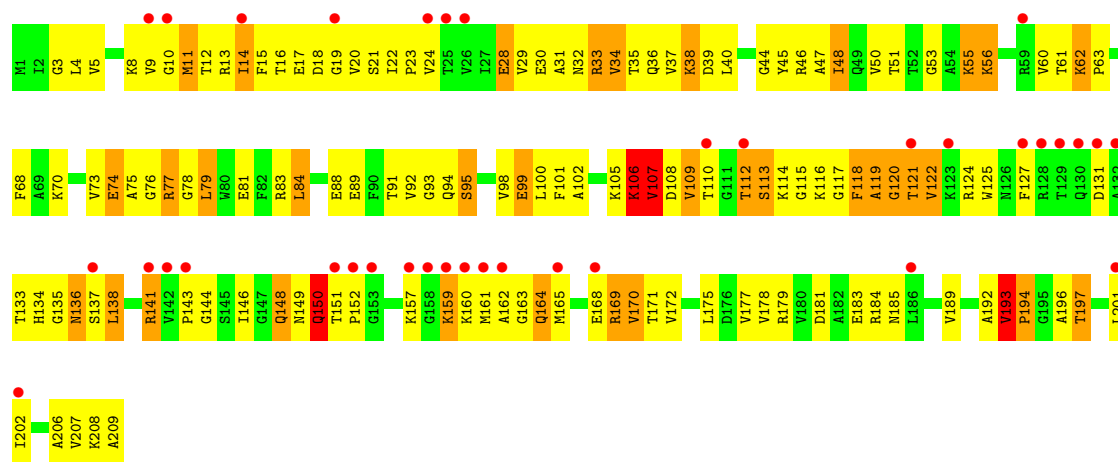
• Molecule 27: 50S ribosomal protein L3

Chain BD: 35% 39% 23% .



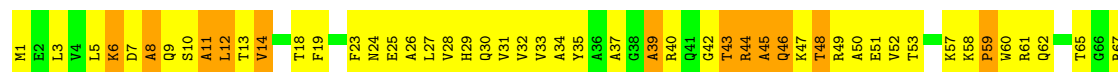
• Molecule 27: 50S ribosomal protein L3

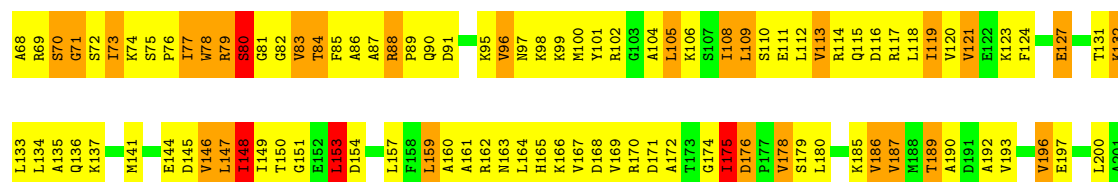
Chain DD: 17% 33% 49% 16% .



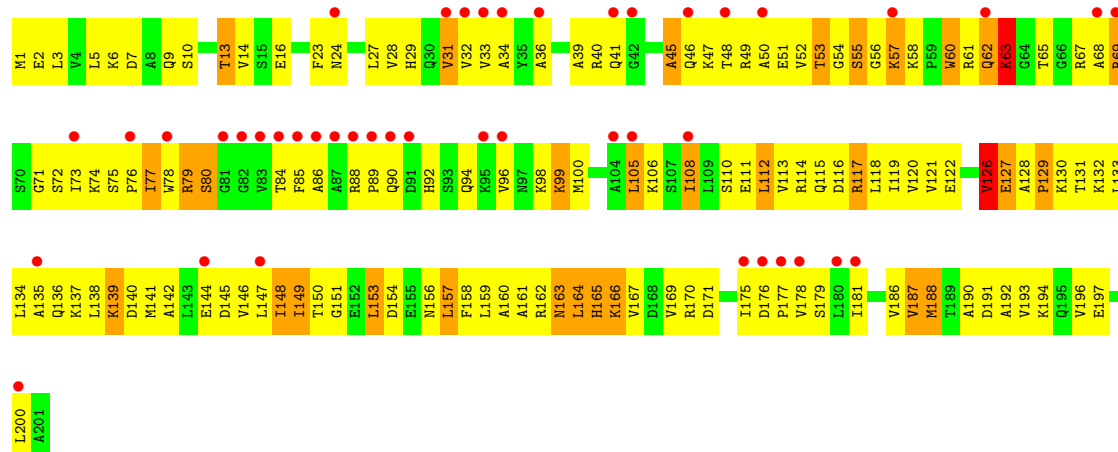
• Molecule 28: 50S ribosomal protein L4

Chain BE: 25% 54% 19% .

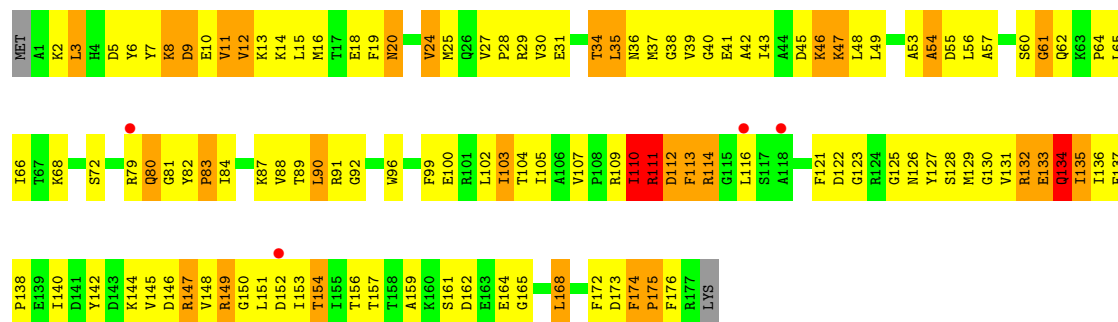




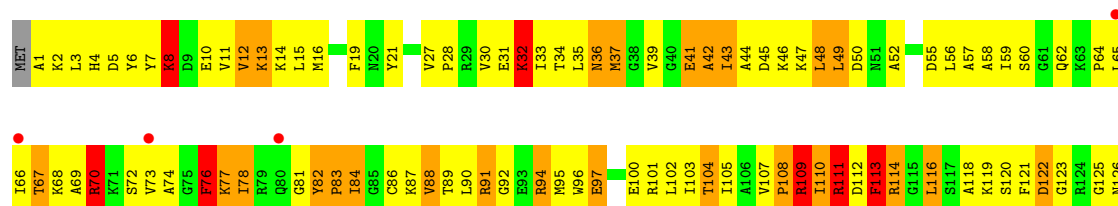
• Molecule 28: 50S ribosomal protein L4



• Molecule 29: 50S ribosomal protein L5

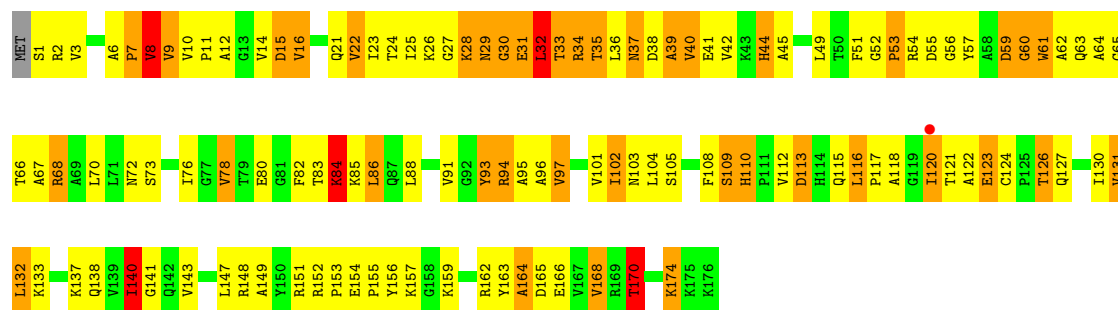


• Molecule 29: 50S ribosomal protein L5

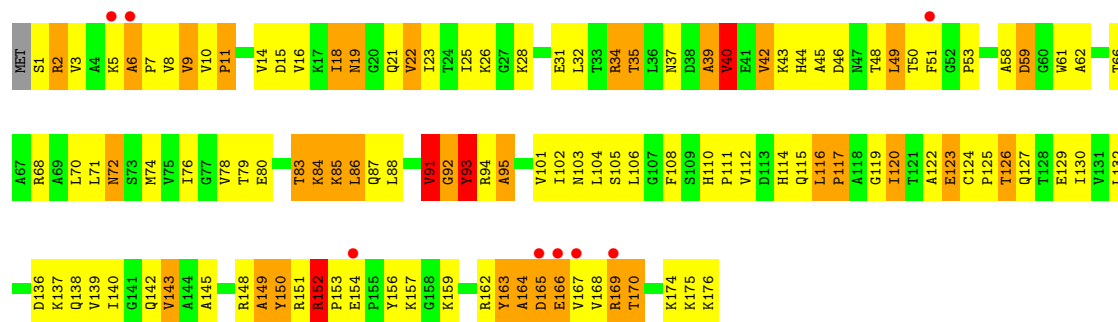




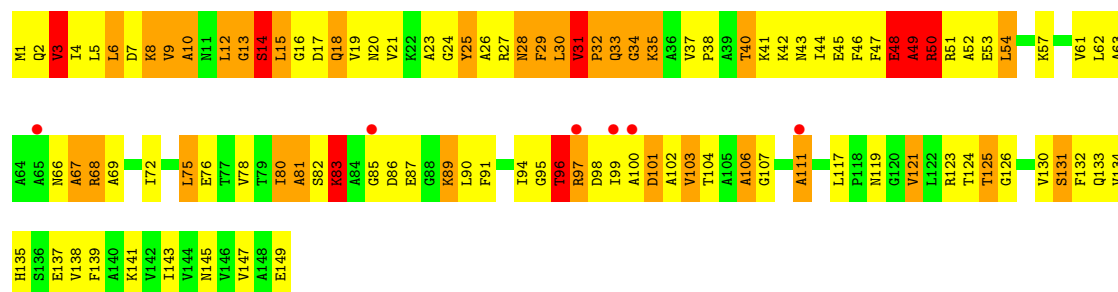
• Molecule 30: 50S ribosomal protein L6



• Molecule 30: 50S ribosomal protein L6



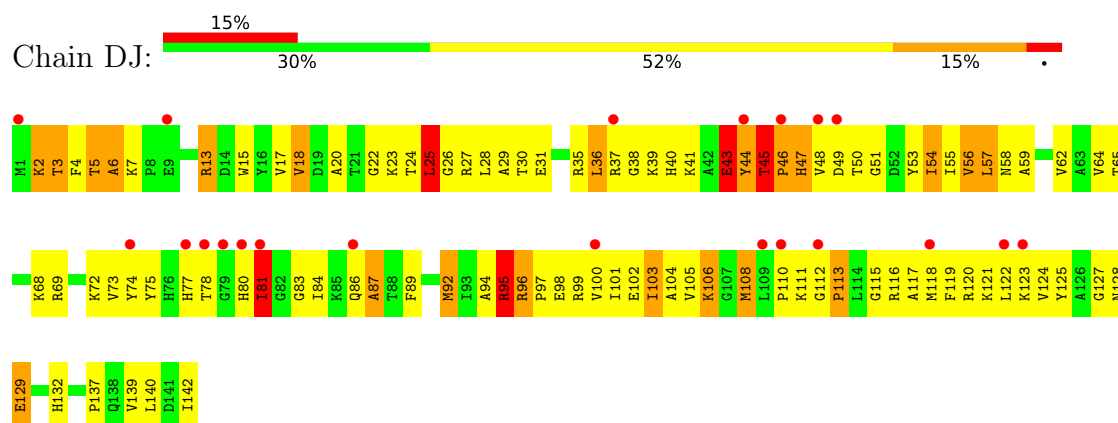
• Molecule 31: 50S ribosomal protein L9



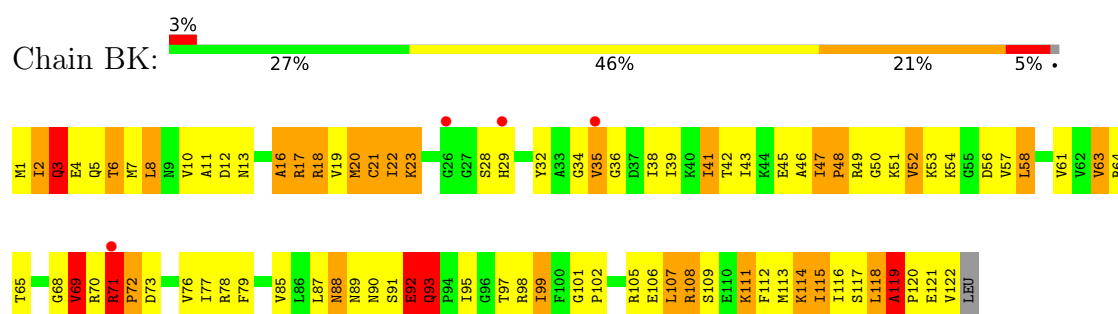
• Molecule 31: 50S ribosomal protein L9



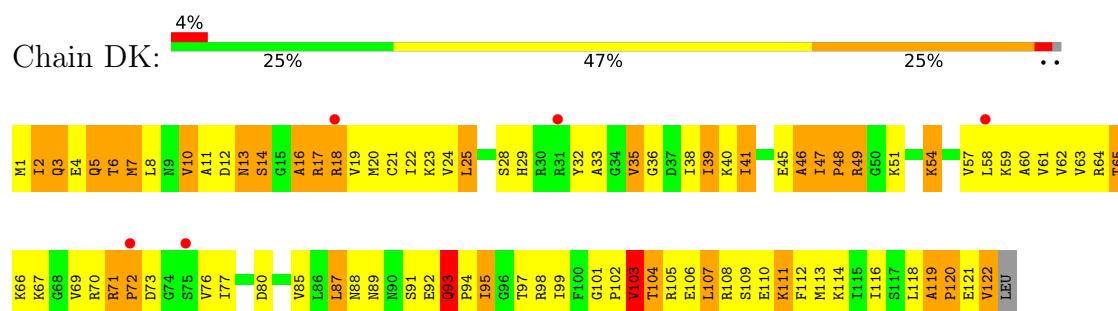
- Molecule 33: 50S ribosomal protein L13



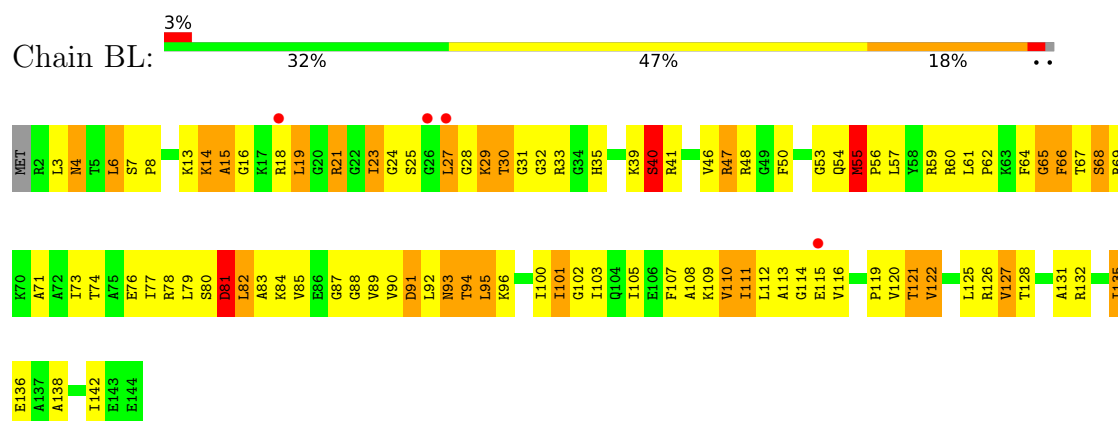
- Molecule 34: 50S ribosomal protein L14



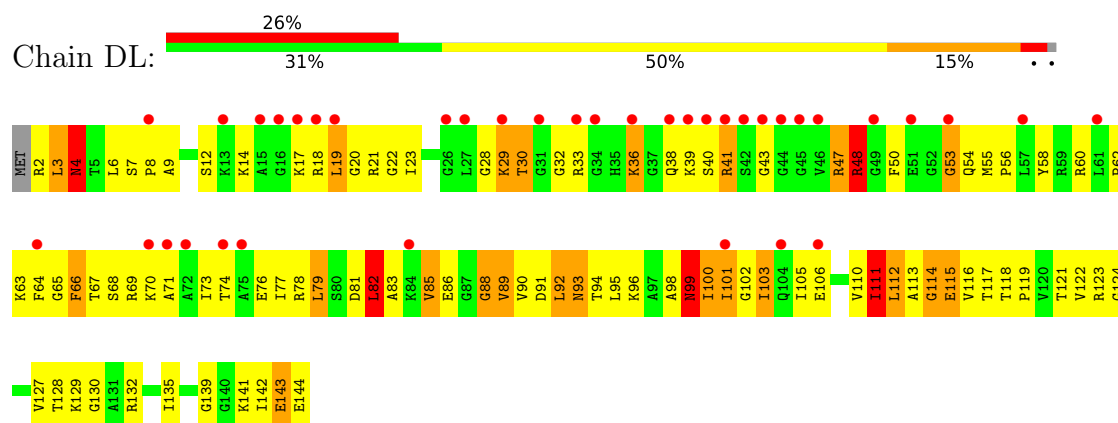
- Molecule 34: 50S ribosomal protein L14



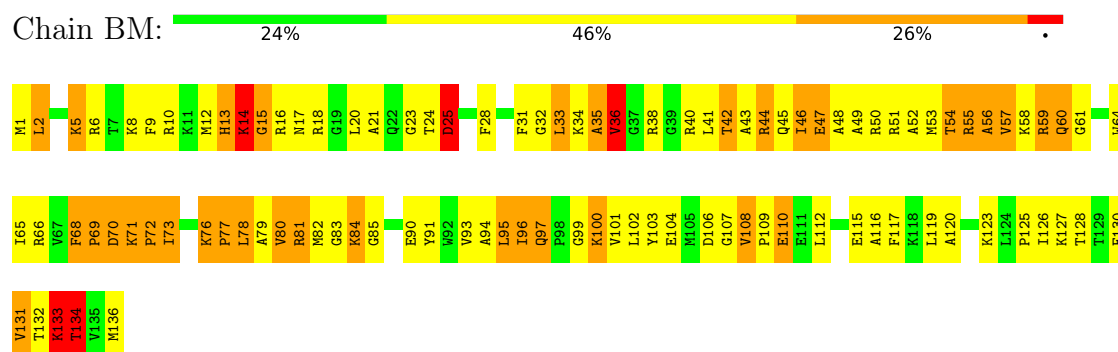
- Molecule 35: 50S ribosomal protein L15



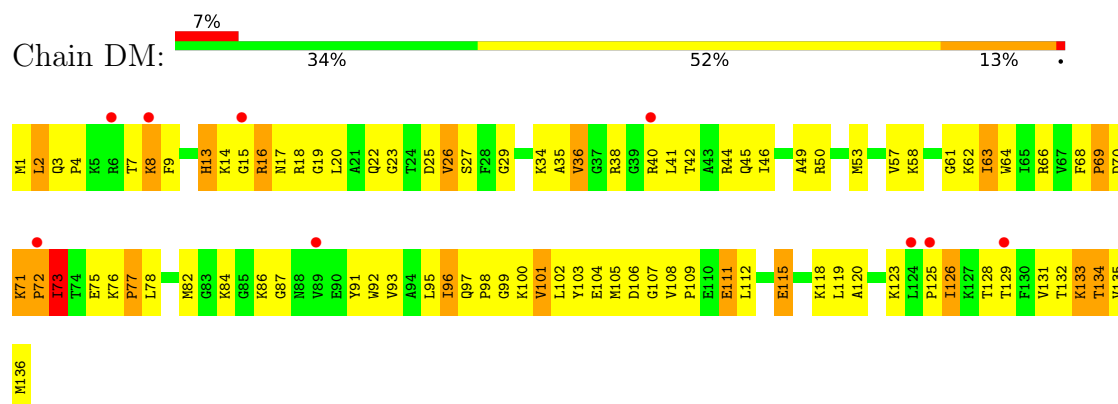
- Molecule 35: 50S ribosomal protein L15



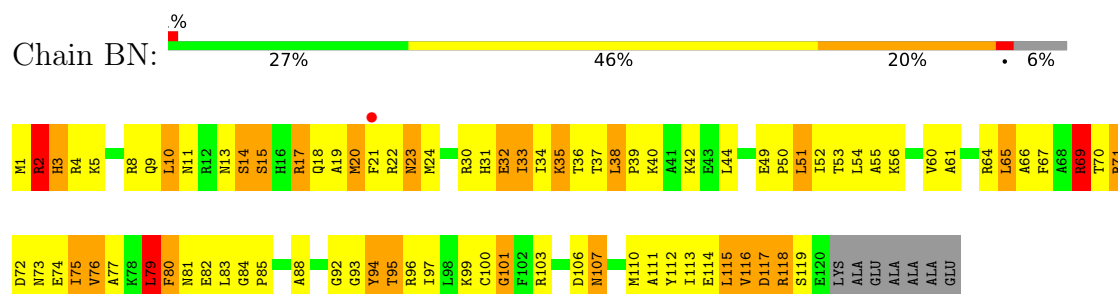
- Molecule 36: 50S ribosomal protein L16



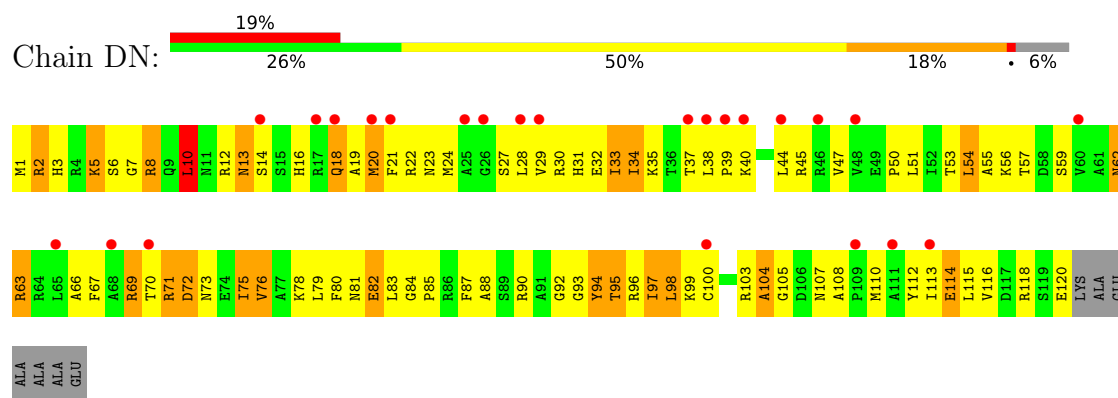
- Molecule 36: 50S ribosomal protein L16



- Molecule 37: 50S ribosomal protein L17



- Molecule 37: 50S ribosomal protein L17



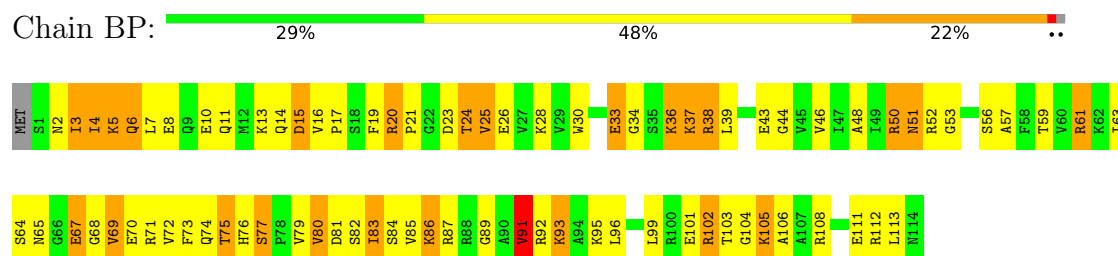
- Molecule 38: 50S ribosomal protein L18



- Molecule 38: 50S ribosomal protein L18

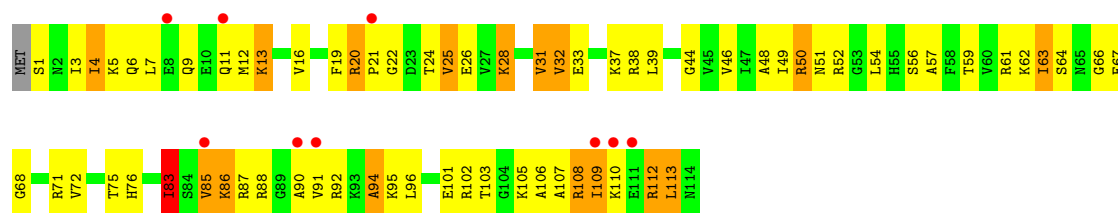


- Molecule 39: 50S ribosomal protein L19



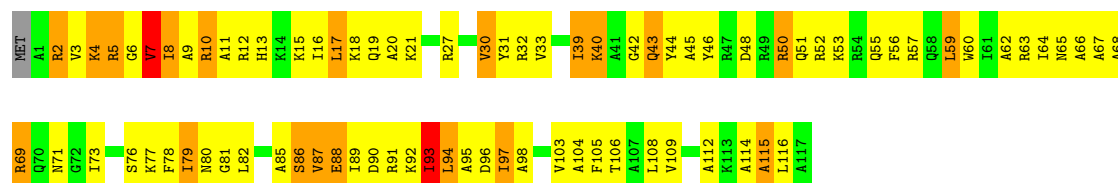
- Molecule 39: 50S ribosomal protein L19





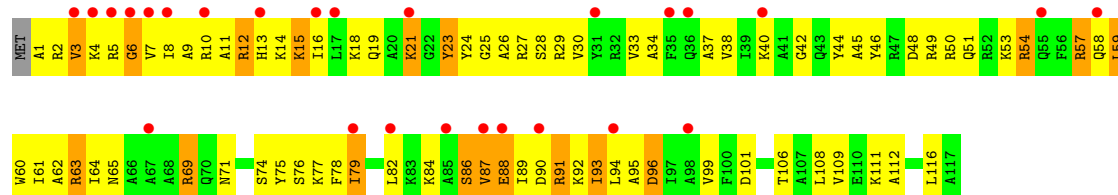
• Molecule 40: 50S ribosomal protein L20

Chain BQ: 30% 51% 17% ..



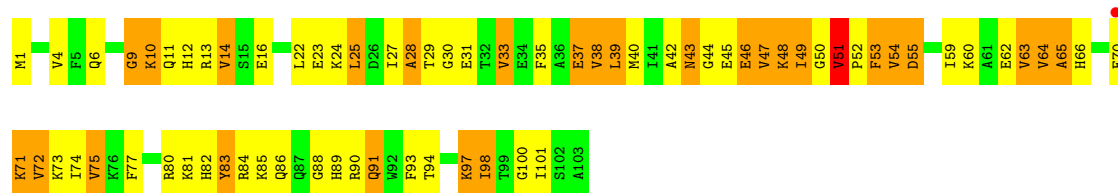
• Molecule 40: 50S ribosomal protein L20

Chain DQ: 22% 31% 53% 15% .



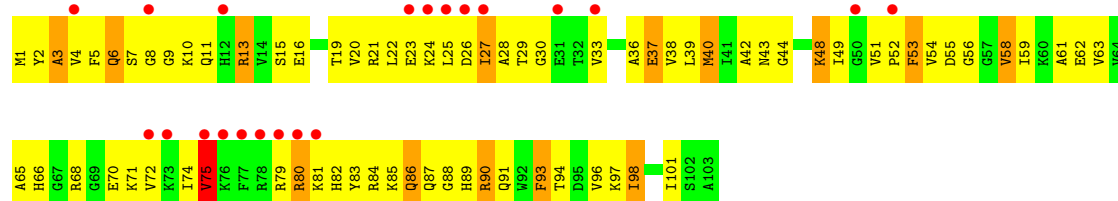
• Molecule 41: 50S ribosomal protein L21

Chain BR: 32% 41% 26% .

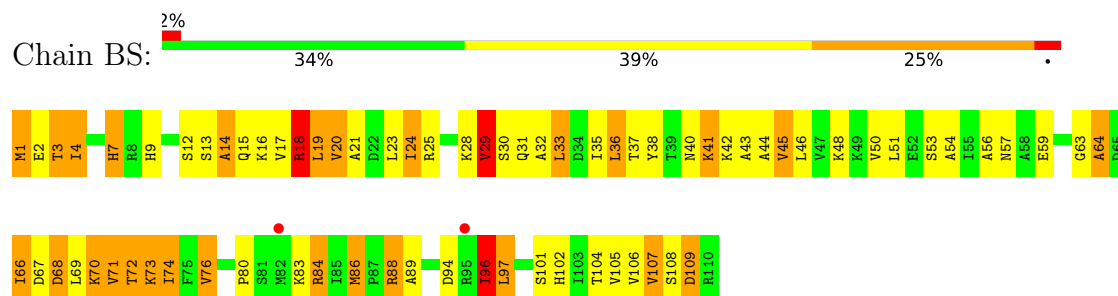


• Molecule 41: 50S ribosomal protein L21

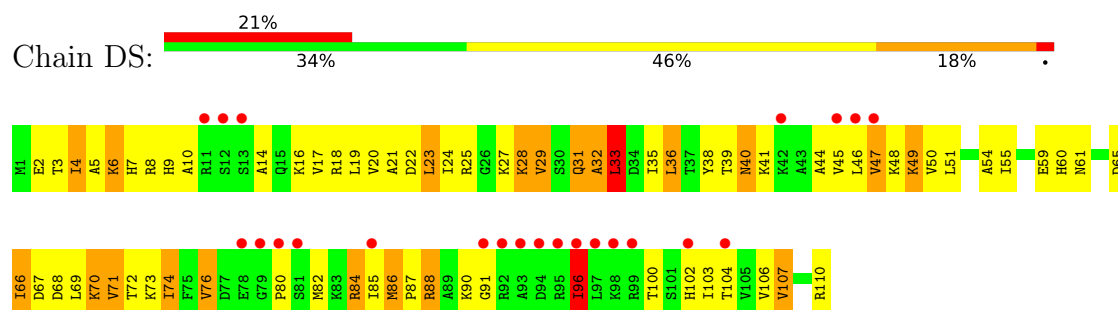
Chain DR: 20% 27% 58% 14% .



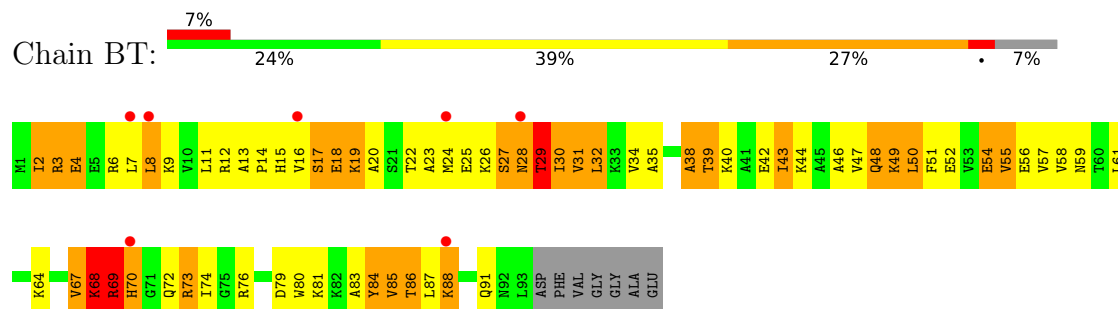
- Molecule 42: 50S ribosomal protein L22



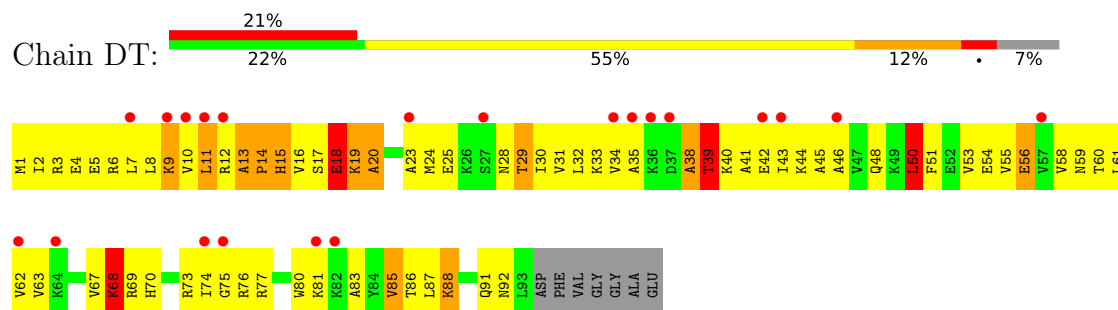
- Molecule 42: 50S ribosomal protein L22



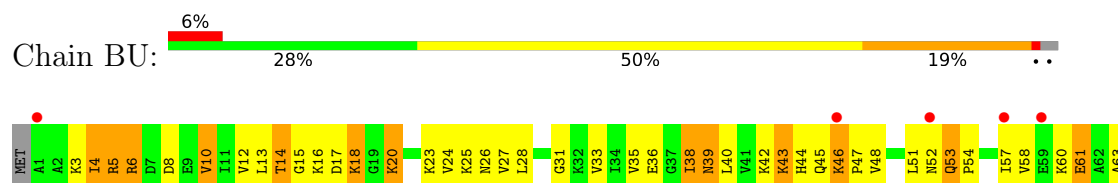
- Molecule 43: 50S ribosomal protein L23



- Molecule 43: 50S ribosomal protein L23

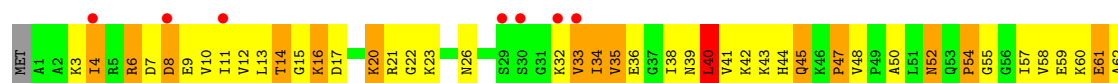


- Molecule 44: 50S ribosomal protein L24

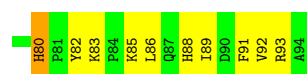
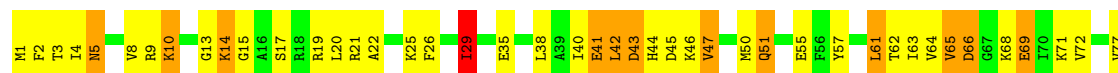




- Molecule 44: 50S ribosomal protein L24



- Molecule 45: 50S ribosomal protein L25



- Molecule 45: 50S ribosomal protein L25

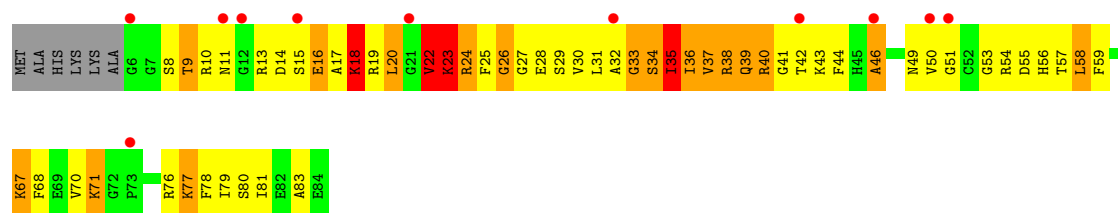


- Molecule 46: 50S ribosomal protein L27

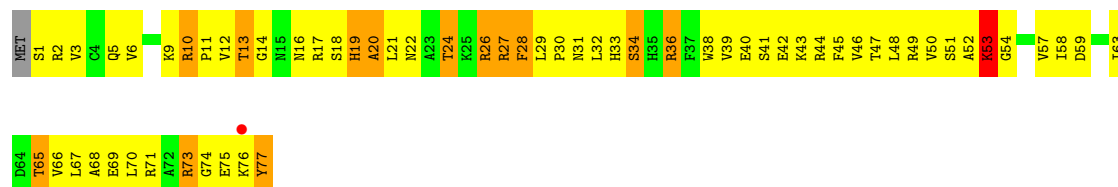


- Molecule 46: 50S ribosomal protein L27

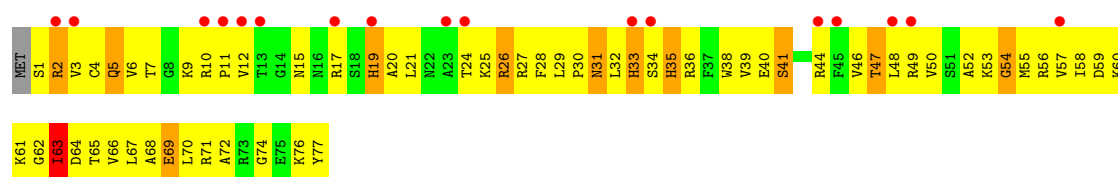




• Molecule 47: 50S ribosomal protein L28



• Molecule 47: 50S ribosomal protein L28



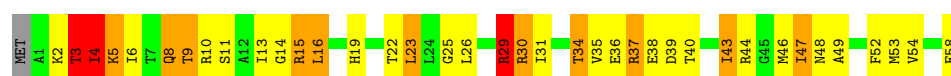
• Molecule 48: 50S ribosomal protein L29



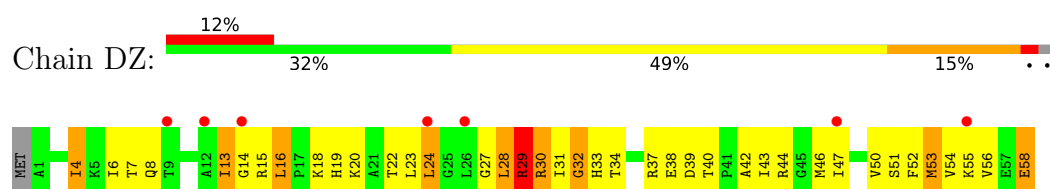
• Molecule 48: 50S ribosomal protein L29



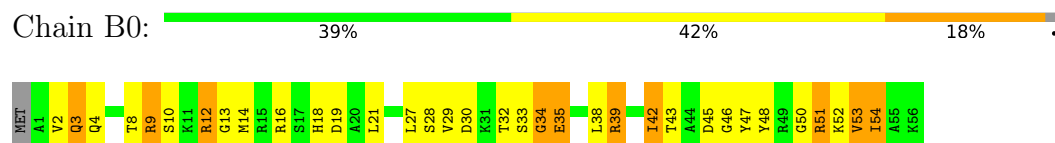
• Molecule 49: 50S ribosomal protein L30



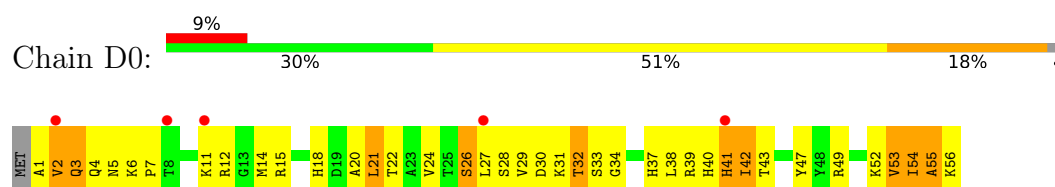
• Molecule 49: 50S ribosomal protein L30



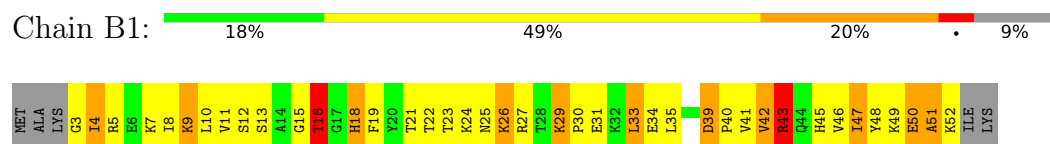
- Molecule 50: 50S ribosomal protein L32



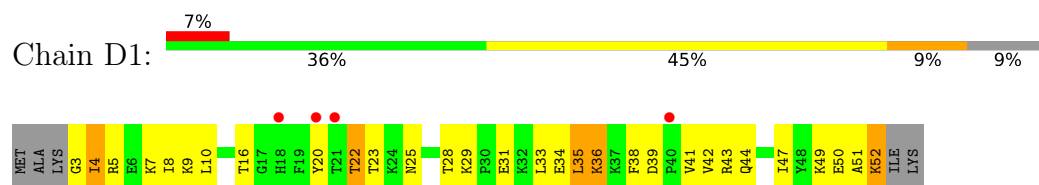
- Molecule 50: 50S ribosomal protein L32



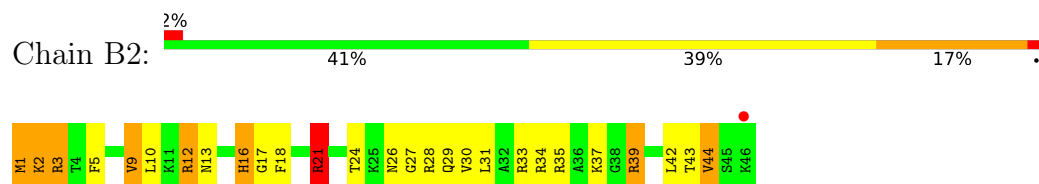
- Molecule 51: 50S ribosomal protein L33



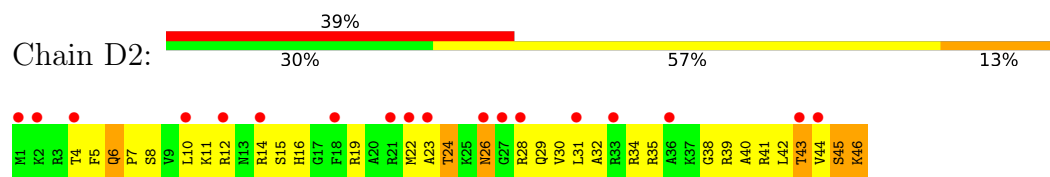
- Molecule 51: 50S ribosomal protein L33



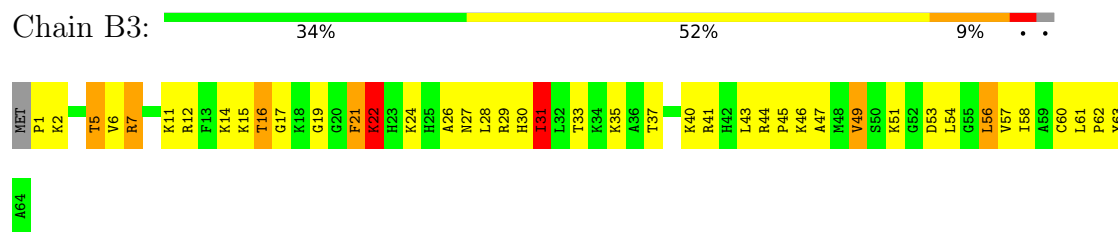
- Molecule 52: 50S ribosomal protein L34



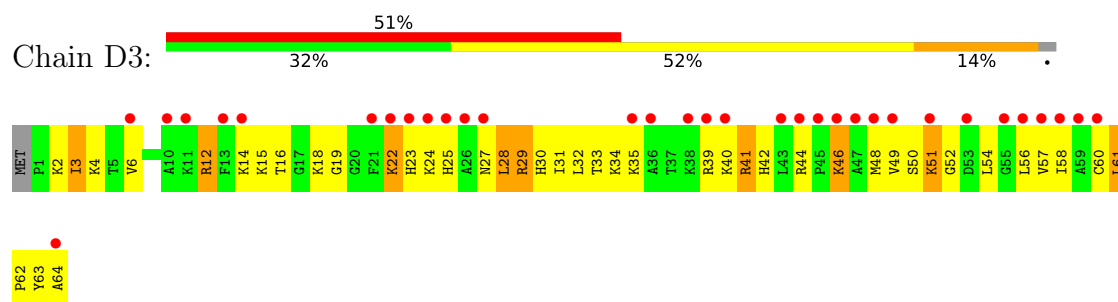
- Molecule 52: 50S ribosomal protein L34



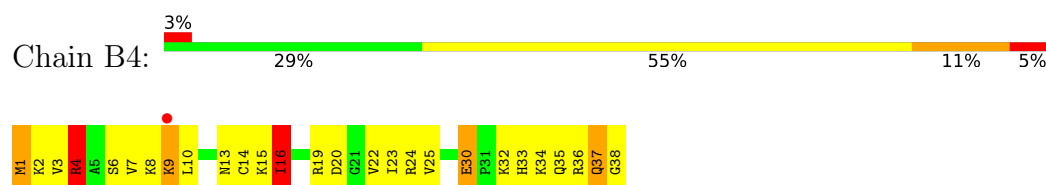
- Molecule 53: 50S ribosomal protein L35



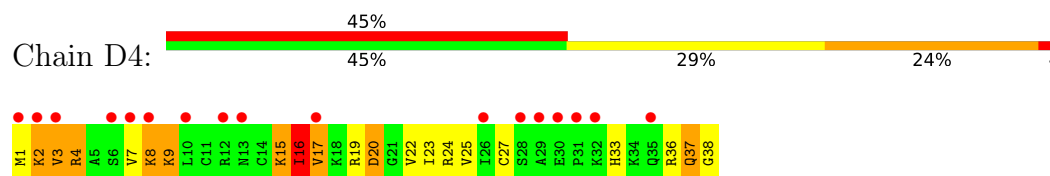
- Molecule 53: 50S ribosomal protein L35



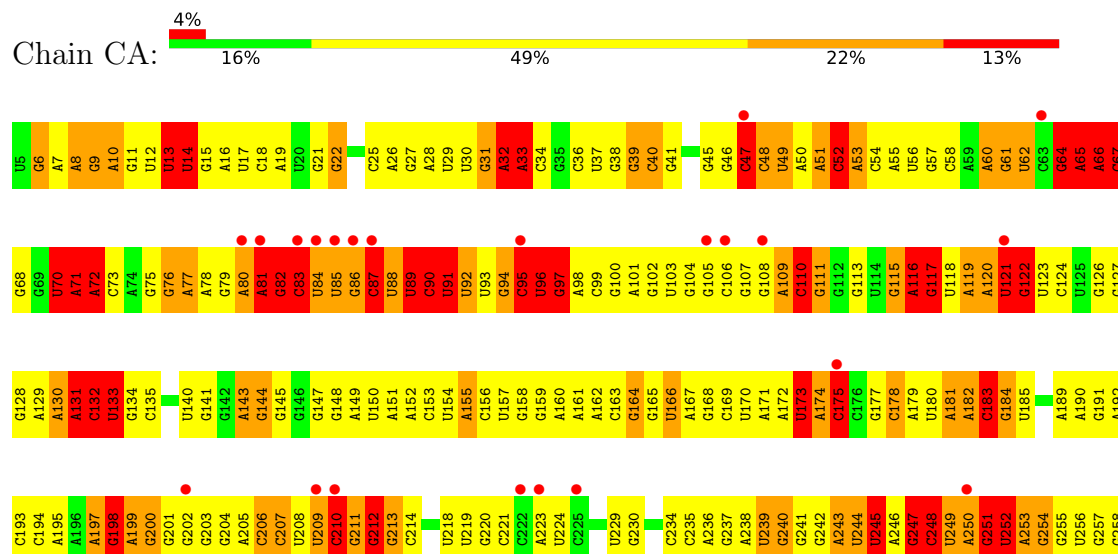
- Molecule 54: 50S ribosomal protein L36



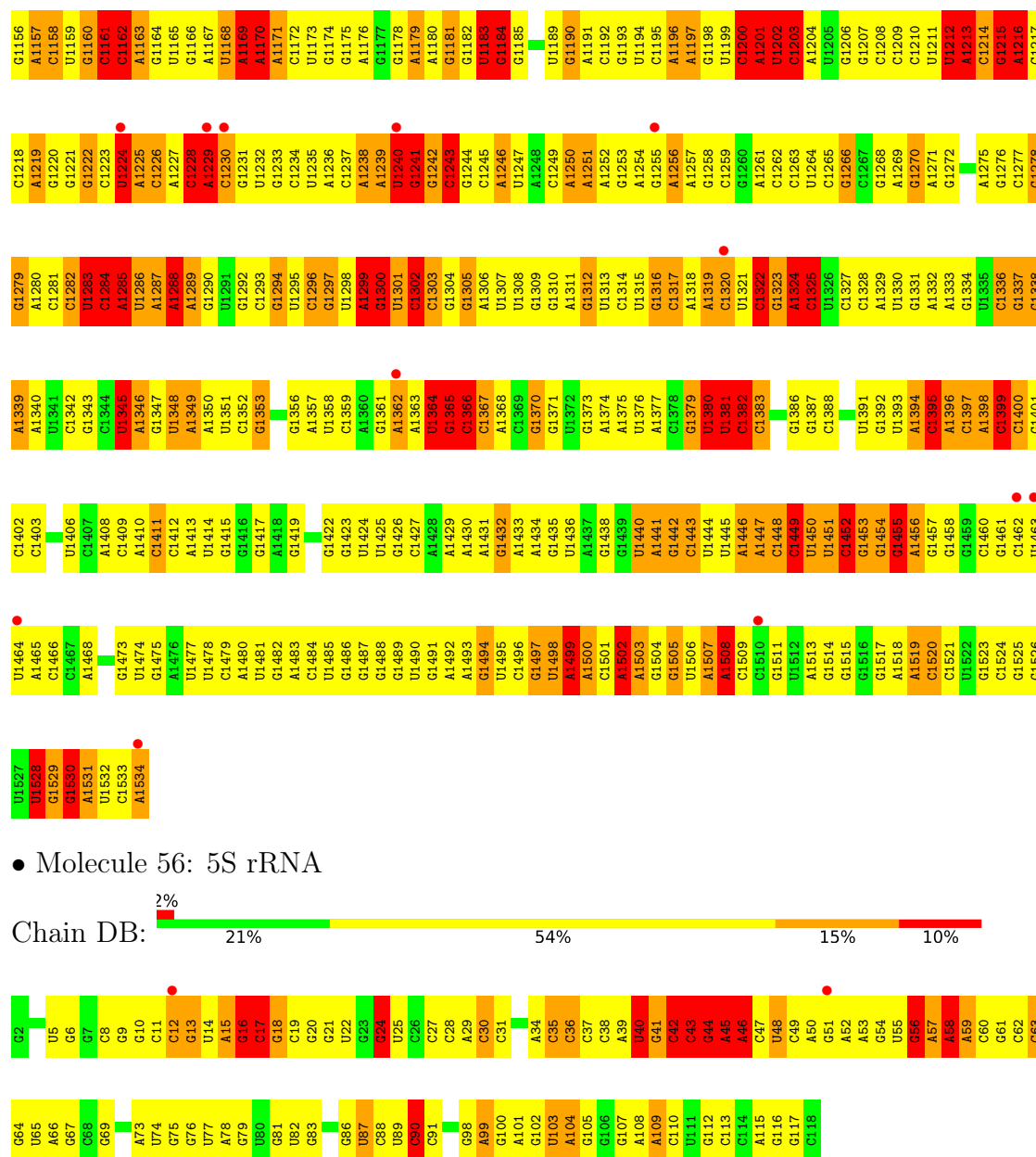
- Molecule 54: 50S ribosomal protein L36



- Molecule 55: 16S rRNA







4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.95Å 433.08Å 624.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.44 – 3.71 73.44 – 3.71	Depositor EDS
% Data completeness (in resolution range)	75.7 (73.44-3.71) 75.7 (73.44-3.71)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 3.67Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.227 , 0.268 0.235 , 0.275	Depositor DCC
R_{free} test set	9161 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å ²)	109.1	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 87.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	286150	wwPDB-VP
Average B, all atoms (Å ²)	163.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% 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: ZN, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	AB	0.34	0/1735	0.76	2/2338 (0.1%)
1	CB	0.35	0/1735	0.84	1/2338 (0.0%)
2	AC	0.37	0/1651	0.80	3/2225 (0.1%)
2	CC	0.36	0/1651	0.82	1/2225 (0.0%)
3	AD	0.35	0/1665	0.78	0/2227
3	CD	0.38	0/1665	0.83	5/2227 (0.2%)
4	AE	0.44	0/1118	0.89	5/1504 (0.3%)
4	CE	0.40	0/1118	0.87	0/1504
5	AF	0.35	0/835	0.77	0/1128
5	CF	0.35	0/835	0.76	0/1128
6	AG	0.33	0/1195	0.74	0/1602
6	CG	0.35	0/1187	0.85	1/1591 (0.1%)
7	AH	0.34	0/989	0.88	1/1326 (0.1%)
7	CH	0.33	0/989	0.84	2/1326 (0.2%)
8	AI	0.31	0/1034	0.77	2/1375 (0.1%)
8	CI	0.33	0/1034	0.83	0/1375
9	AJ	0.36	0/796	0.87	4/1077 (0.4%)
9	CJ	0.34	0/796	0.80	2/1077 (0.2%)
10	AK	0.36	0/893	0.86	3/1205 (0.2%)
10	CK	0.37	0/893	0.83	0/1205
11	AL	0.43	0/969	0.92	1/1300 (0.1%)
11	CL	0.39	0/969	0.85	1/1300 (0.1%)
12	AM	0.51	0/892	0.93	2/1193 (0.2%)
12	CM	0.49	1/884 (0.1%)	0.86	2/1181 (0.2%)
13	AN	0.35	0/785	0.87	4/1043 (0.4%)
13	CN	0.33	0/780	0.82	2/1036 (0.2%)
14	AO	0.34	0/722	0.83	2/964 (0.2%)
14	CO	0.32	0/722	0.83	2/964 (0.2%)
15	AP	0.37	0/659	0.83	3/884 (0.3%)
15	CP	0.35	0/648	0.84	1/870 (0.1%)
16	AQ	0.41	0/657	0.82	0/881
16	CQ	0.35	0/657	0.76	0/881

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AR	0.34	0/462	0.84	0/621
17	CR	0.37	0/462	0.87	2/621 (0.3%)
18	AS	0.31	0/652	0.75	0/877
18	CS	0.30	0/652	0.80	1/877 (0.1%)
19	AT	0.37	0/671	0.89	1/888 (0.1%)
19	CT	0.32	0/671	0.85	3/888 (0.3%)
20	AU	0.33	0/430	0.83	1/570 (0.2%)
20	CU	0.36	0/430	0.84	0/570
21	AA	0.36	1/36834 (0.0%)	1.03	309/57462 (0.5%)
22	AV	0.37	0/408	0.65	0/634
22	AX	0.35	0/408	0.64	0/634
22	CV	0.36	0/408	0.73	1/634 (0.2%)
22	CX	0.30	0/408	0.54	0/634
23	AW	0.69	1/131 (0.8%)	1.54	4/200 (2.0%)
23	CW	0.57	0/131	1.52	4/200 (2.0%)
24	BA	0.45	3/68626 (0.0%)	1.18	814/107056 (0.8%)
24	DA	0.36	2/68314 (0.0%)	1.05	614/106569 (0.6%)
25	BB	0.41	0/2828	1.21	37/4410 (0.8%)
26	BC	0.59	0/2121	1.09	11/2852 (0.4%)
26	DC	0.43	0/2121	0.92	4/2852 (0.1%)
27	BD	0.67	0/1586	1.09	4/2134 (0.2%)
27	DD	0.41	0/1586	0.88	3/2134 (0.1%)
28	BE	0.56	0/1571	1.02	6/2113 (0.3%)
28	DE	0.33	0/1571	0.81	2/2113 (0.1%)
29	BF	0.51	0/1434	0.91	2/1926 (0.1%)
29	DF	0.48	0/1444	0.93	9/1937 (0.5%)
30	BG	0.58	0/1343	1.03	9/1816 (0.5%)
30	DG	0.32	0/1343	0.83	6/1816 (0.3%)
31	BH	0.92	6/1122 (0.5%)	1.22	11/1515 (0.7%)
31	DH	0.69	4/1122 (0.4%)	0.99	9/1515 (0.6%)
32	BI	0.36	0/1046	0.91	4/1410 (0.3%)
32	DI	0.34	0/1046	0.80	1/1410 (0.1%)
33	BJ	0.71	0/1152	1.12	5/1551 (0.3%)
33	DJ	0.37	0/1152	0.89	3/1551 (0.2%)
34	BK	0.73	0/947	1.16	7/1268 (0.6%)
34	DK	0.41	0/947	0.92	4/1268 (0.3%)
35	BL	0.57	0/1054	1.16	5/1403 (0.4%)
35	DL	0.35	0/1054	0.79	1/1403 (0.1%)
36	BM	0.68	0/1093	1.24	10/1460 (0.7%)
36	DM	0.39	0/1093	0.81	2/1460 (0.1%)
37	BN	0.73	0/973	1.13	6/1301 (0.5%)
37	DN	0.36	0/973	0.83	0/1301
38	BO	0.56	0/902	0.90	1/1209 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DO	0.32	0/902	0.78	0/1209
39	BP	0.64	0/929	1.11	4/1242 (0.3%)
39	DP	0.36	0/929	0.80	1/1242 (0.1%)
40	BQ	0.78	0/960	1.02	4/1278 (0.3%)
40	DQ	0.36	0/960	0.83	1/1278 (0.1%)
41	BR	0.69	0/829	1.22	6/1107 (0.5%)
41	DR	0.34	0/829	0.73	0/1107
42	BS	0.70	0/864	1.09	3/1156 (0.3%)
42	DS	0.41	0/864	0.83	0/1156
43	BT	0.62	0/744	1.03	3/994 (0.3%)
43	DT	0.33	0/744	0.80	2/994 (0.2%)
44	BU	0.54	0/787	1.05	6/1051 (0.6%)
44	DU	0.34	0/787	0.85	0/1051
45	BV	0.60	0/766	1.04	5/1025 (0.5%)
45	DV	0.42	0/766	0.85	2/1025 (0.2%)
46	BW	0.65	0/603	1.14	4/797 (0.5%)
46	DW	0.32	0/603	0.69	0/797
47	BX	0.56	0/635	0.96	2/848 (0.2%)
47	DX	0.40	0/635	0.90	3/848 (0.4%)
48	BY	0.53	0/510	0.96	2/677 (0.3%)
48	DY	0.29	0/510	0.78	0/677
49	BZ	0.76	0/453	1.13	4/605 (0.7%)
49	DZ	0.37	0/453	0.79	0/605
50	B0	0.59	0/450	1.00	0/599
50	D0	0.34	0/450	0.84	0/599
51	B1	0.49	0/416	0.98	2/554 (0.4%)
51	D1	0.35	0/416	0.80	1/554 (0.2%)
52	B2	0.64	0/380	1.11	2/498 (0.4%)
52	D2	0.36	0/380	0.98	2/498 (0.4%)
53	B3	0.64	0/513	1.11	4/676 (0.6%)
53	D3	0.36	0/513	0.75	0/676
54	B4	0.68	0/303	1.16	3/397 (0.8%)
54	D4	0.48	0/303	0.77	0/397
55	CA	0.35	0/36762	1.04	326/57350 (0.6%)
56	DB	0.35	0/2803	0.92	16/4371 (0.4%)
All	All	0.41	18/308631 (0.0%)	1.04	2376/461501 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
12	AM	0	1
27	BD	0	1
31	BH	0	2
31	DH	0	3
37	BN	0	1
All	All	0	8

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	BH	48	GLU	CA-C	-13.69	1.35	1.52
31	BH	48	GLU	C-O	12.37	1.41	1.24
31	BH	49	ALA	N-CA	10.50	1.59	1.46
31	DH	49	ALA	CA-CB	-10.39	1.35	1.53
31	BH	48	GLU	N-CA	-7.70	1.38	1.46

The worst 5 of 2376 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	BH	49	ALA	N-CA-C	-17.08	90.56	111.40
31	BH	48	GLU	CA-C-O	-15.36	103.26	119.08
24	BA	790	U	P-O3'-C3'	-13.23	100.36	120.20
24	BA	2347	C	N1-C1'-C2'	-13.22	92.17	112.00
24	BA	1145	C	P-O5'-C5'	-12.72	101.82	120.90

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	AM	70	ARG	Peptide
27	BD	10	GLY	Peptide
31	BH	48	GLU	Mainchain
31	BH	49	ALA	Mainchain
37	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	264	0
1	CB	1704	0	1732	217	0
2	AC	1624	0	1699	145	0
2	CC	1624	0	1699	157	0
3	AD	1643	0	1710	145	0
3	CD	1643	0	1710	158	0
4	AE	1105	0	1148	205	0
4	CE	1105	0	1148	135	0
5	AF	817	0	808	91	0
5	CF	817	0	808	80	0
6	AG	1181	0	1240	107	0
6	CG	1174	0	1230	161	0
7	AH	979	0	1034	117	0
7	CH	979	0	1034	100	0
8	AI	1022	0	1070	127	0
8	CI	1022	0	1070	109	0
9	AJ	786	0	828	72	0
9	CJ	786	0	828	113	0
10	AK	877	0	887	102	0
10	CK	877	0	887	91	0
11	AL	955	0	1019	101	0
11	CL	955	0	1019	102	0
12	AM	883	0	944	75	0
12	CM	876	0	937	126	0
13	AN	774	0	827	77	0
13	CN	769	0	822	88	0
14	AO	714	0	737	52	0
14	CO	714	0	737	47	0
15	AP	649	0	666	68	0
15	CP	638	0	656	61	0
16	AQ	648	0	691	73	0
16	CQ	648	0	691	63	0
17	AR	455	0	478	36	0
17	CR	455	0	478	47	0
18	AS	637	0	665	47	0
18	CS	637	0	665	82	0
19	AT	665	0	714	62	0
19	CT	665	0	714	68	0
20	AU	425	0	449	65	0
20	CU	425	0	449	72	0
21	AA	32895	0	16553	1797	0
22	AV	365	0	185	24	0
22	AX	365	0	185	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	CV	365	0	185	26	0
22	CX	365	0	185	11	0
23	AW	120	0	61	8	0
23	CW	120	0	61	4	0
24	BA	61274	0	30819	3129	0
24	DA	60995	0	30679	3830	0
25	BB	2529	0	1281	112	0
26	BC	2082	0	2157	237	0
26	DC	2082	0	2157	243	0
27	BD	1565	0	1616	207	0
27	DD	1565	0	1616	172	0
28	BE	1552	0	1619	165	0
28	DE	1552	0	1619	182	0
29	BF	1410	0	1447	153	0
29	DF	1420	0	1460	193	0
30	BG	1323	0	1374	153	0
30	DG	1323	0	1374	123	0
31	BH	1111	0	1148	115	0
31	DH	1111	0	1148	105	0
32	BI	1032	0	1088	121	0
32	DI	1032	0	1088	75	0
33	BJ	1129	0	1162	169	0
33	DJ	1129	0	1162	132	0
34	BK	938	0	1012	107	0
34	DK	938	0	1012	115	0
35	BL	1045	0	1117	135	0
35	DL	1045	0	1117	133	0
36	BM	1074	0	1157	135	0
36	DM	1074	0	1157	103	0
37	BN	960	0	1000	112	0
37	DN	960	0	1000	113	0
38	BO	892	0	923	84	0
38	DO	892	0	923	94	0
39	BP	917	0	965	124	0
39	DP	917	0	965	87	0
40	BQ	947	0	1022	153	0
40	DQ	947	0	1022	129	0
41	BR	816	0	839	108	0
41	DR	816	0	839	94	0
42	BS	857	0	922	96	0
42	DS	857	0	922	90	0
43	BT	738	0	807	106	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	DT	738	0	807	102	0
44	BU	779	0	834	65	0
44	DU	779	0	834	94	0
45	BV	753	0	780	58	0
45	DV	753	0	780	101	0
46	BW	596	0	610	182	0
46	DW	596	0	610	105	0
47	BX	625	0	655	70	0
47	DX	625	0	655	80	0
48	BY	509	0	543	50	0
48	DY	509	0	543	58	0
49	BZ	449	0	491	42	0
49	DZ	449	0	491	44	0
50	B0	444	0	461	38	0
50	D0	444	0	461	64	0
51	B1	409	0	440	46	0
51	D1	409	0	440	36	0
52	B2	377	0	418	30	0
52	D2	377	0	418	44	0
53	B3	504	0	574	42	0
53	D3	504	0	574	52	0
54	B4	302	0	340	40	0
54	D4	302	0	340	28	0
55	CA	32831	0	16521	1991	0
56	DB	2507	0	1270	159	0
57	AA	43	0	0	0	0
57	BA	136	0	0	0	0
57	BB	4	0	0	0	0
57	BD	1	0	0	0	0
57	CA	42	0	0	0	0
57	D4	1	0	0	0	0
57	DA	132	0	0	0	0
57	DB	1	0	0	0	0
57	DC	2	0	0	0	0
57	DJ	1	0	0	0	0
58	B4	1	0	0	0	0
58	D4	1	0	0	0	0
59	AA	196	0	0	7	0
59	AE	1	0	0	0	0
59	AL	3	0	0	0	0
59	AN	6	0	0	1	0
59	AT	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	AU	1	0	0	0	0
59	B2	1	0	0	0	0
59	B3	3	0	0	0	0
59	B4	2	0	0	0	0
59	BA	615	0	0	21	0
59	BB	20	0	0	1	0
59	BC	8	0	0	1	0
59	BD	3	0	0	4	0
59	BE	1	0	0	0	0
59	BL	3	0	0	0	0
59	BN	3	0	0	0	0
59	BT	1	0	0	1	0
59	CA	195	0	0	6	0
59	CE	4	0	0	0	0
59	CI	1	0	0	0	0
59	CL	1	0	0	0	0
59	CN	2	0	0	0	0
59	CT	2	0	0	0	0
59	CU	2	0	0	0	0
59	D2	1	0	0	0	0
59	D3	1	0	0	0	0
59	D4	5	0	0	0	0
59	DA	600	0	0	17	0
59	DB	4	0	0	0	0
59	DC	12	0	0	0	0
59	DD	2	0	0	0	0
59	DE	3	0	0	0	0
59	DJ	3	0	0	0	0
59	DL	6	0	0	0	0
59	DN	2	0	0	1	0
59	DT	2	0	0	0	0
59	DU	1	0	0	0	0
59	DV	1	0	0	0	0
All	All	286150	0	191700	19690	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 41.

The worst 5 of 19690 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)
12:AM:67:ASP:O	12:AM:70:ARG:HD2	1.23	1.31
55:CA:1213:A:O2'	55:CA:1214:C:H5'	1.29	1.25
24:DA:604:G:O2'	24:DA:605:G:H5'	1.40	1.19
40:BQ:63:ARG:NH1	40:BQ:96:ASP:HA	1.56	1.18
24:DA:297:G:H5''	44:DU:84:PHE:HB2	1.26	1.18

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AB	216/241 (90%)	119 (55%)	69 (32%)	28 (13%)	0	3
1	CB	216/241 (90%)	144 (67%)	50 (23%)	22 (10%)	0	6
2	AC	204/233 (88%)	140 (69%)	48 (24%)	16 (8%)	1	10
2	CC	204/233 (88%)	136 (67%)	52 (26%)	16 (8%)	1	10
3	AD	203/206 (98%)	143 (70%)	43 (21%)	17 (8%)	0	9
3	CD	203/206 (98%)	136 (67%)	46 (23%)	21 (10%)	0	6
4	AE	148/167 (89%)	105 (71%)	27 (18%)	16 (11%)	0	5
4	CE	148/167 (89%)	100 (68%)	34 (23%)	14 (10%)	0	7
5	AF	98/135 (73%)	68 (69%)	22 (22%)	8 (8%)	0	9
5	CF	98/135 (73%)	65 (66%)	27 (28%)	6 (6%)	1	14
6	AG	149/179 (83%)	103 (69%)	36 (24%)	10 (7%)	1	13
6	CG	148/179 (83%)	84 (57%)	44 (30%)	20 (14%)	0	3
7	AH	127/130 (98%)	90 (71%)	27 (21%)	10 (8%)	1	10
7	CH	127/130 (98%)	88 (69%)	30 (24%)	9 (7%)	1	12
8	AI	125/130 (96%)	81 (65%)	32 (26%)	12 (10%)	0	7
8	CI	125/130 (96%)	88 (70%)	33 (26%)	4 (3%)	3	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	AJ	96/103 (93%)	69 (72%)	16 (17%)	11 (12%)	0	4
9	CJ	96/103 (93%)	62 (65%)	22 (23%)	12 (12%)	0	4
10	AK	115/129 (89%)	84 (73%)	22 (19%)	9 (8%)	1	10
10	CK	115/129 (89%)	86 (75%)	19 (16%)	10 (9%)	0	8
11	AL	121/124 (98%)	82 (68%)	27 (22%)	12 (10%)	0	6
11	CL	121/124 (98%)	86 (71%)	26 (22%)	9 (7%)	1	11
12	AM	112/118 (95%)	89 (80%)	16 (14%)	7 (6%)	1	14
12	CM	111/118 (94%)	71 (64%)	28 (25%)	12 (11%)	0	5
13	AN	92/101 (91%)	63 (68%)	18 (20%)	11 (12%)	0	4
13	CN	91/101 (90%)	62 (68%)	24 (26%)	5 (6%)	1	16
14	AO	86/89 (97%)	64 (74%)	20 (23%)	2 (2%)	5	30
14	CO	86/89 (97%)	67 (78%)	19 (22%)	0	100	100
15	AP	80/82 (98%)	52 (65%)	22 (28%)	6 (8%)	1	11
15	CP	78/82 (95%)	52 (67%)	20 (26%)	6 (8%)	1	10
16	AQ	78/84 (93%)	47 (60%)	20 (26%)	11 (14%)	0	3
16	CQ	78/84 (93%)	57 (73%)	16 (20%)	5 (6%)	1	14
17	AR	53/75 (71%)	39 (74%)	11 (21%)	3 (6%)	1	15
17	CR	53/75 (71%)	39 (74%)	11 (21%)	3 (6%)	1	15
18	AS	77/92 (84%)	61 (79%)	13 (17%)	3 (4%)	2	21
18	CS	77/92 (84%)	55 (71%)	20 (26%)	2 (3%)	4	27
19	AT	83/87 (95%)	63 (76%)	14 (17%)	6 (7%)	1	12
19	CT	83/87 (95%)	59 (71%)	21 (25%)	3 (4%)	2	23
20	AU	49/71 (69%)	26 (53%)	16 (33%)	7 (14%)	0	3
20	CU	49/71 (69%)	23 (47%)	17 (35%)	9 (18%)	0	1
26	BC	269/273 (98%)	192 (71%)	48 (18%)	29 (11%)	0	5
26	DC	269/273 (98%)	169 (63%)	73 (27%)	27 (10%)	0	6
27	BD	207/209 (99%)	141 (68%)	35 (17%)	31 (15%)	0	2
27	DD	207/209 (99%)	129 (62%)	48 (23%)	30 (14%)	0	3
28	BE	199/201 (99%)	138 (69%)	41 (21%)	20 (10%)	0	6
28	DE	199/201 (99%)	129 (65%)	49 (25%)	21 (11%)	0	5
29	BF	175/179 (98%)	133 (76%)	26 (15%)	16 (9%)	0	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	DF	176/179 (98%)	94 (53%)	43 (24%)	39 (22%)	0	0
30	BG	174/177 (98%)	114 (66%)	34 (20%)	26 (15%)	0	3
30	DG	174/177 (98%)	109 (63%)	36 (21%)	29 (17%)	0	2
31	BH	147/149 (99%)	63 (43%)	53 (36%)	31 (21%)	0	1
31	DH	147/149 (99%)	78 (53%)	48 (33%)	21 (14%)	0	3
32	BI	139/142 (98%)	84 (60%)	42 (30%)	13 (9%)	0	7
32	DI	139/142 (98%)	81 (58%)	39 (28%)	19 (14%)	0	3
33	BJ	140/142 (99%)	100 (71%)	22 (16%)	18 (13%)	0	3
33	DJ	140/142 (99%)	95 (68%)	31 (22%)	14 (10%)	0	6
34	BK	120/123 (98%)	86 (72%)	17 (14%)	17 (14%)	0	3
34	DK	120/123 (98%)	79 (66%)	22 (18%)	19 (16%)	0	2
35	BL	141/144 (98%)	106 (75%)	23 (16%)	12 (8%)	0	8
35	DL	141/144 (98%)	80 (57%)	42 (30%)	19 (14%)	0	3
36	BM	134/136 (98%)	95 (71%)	16 (12%)	23 (17%)	0	2
36	DM	134/136 (98%)	89 (66%)	32 (24%)	13 (10%)	0	7
37	BN	118/127 (93%)	85 (72%)	23 (20%)	10 (8%)	0	8
37	DN	118/127 (93%)	73 (62%)	32 (27%)	13 (11%)	0	5
38	BO	114/117 (97%)	84 (74%)	20 (18%)	10 (9%)	0	8
38	DO	114/117 (97%)	80 (70%)	28 (25%)	6 (5%)	1	17
39	BP	112/115 (97%)	74 (66%)	23 (20%)	15 (13%)	0	3
39	DP	112/115 (97%)	67 (60%)	30 (27%)	15 (13%)	0	3
40	BQ	115/118 (98%)	85 (74%)	23 (20%)	7 (6%)	1	14
40	DQ	115/118 (98%)	85 (74%)	22 (19%)	8 (7%)	1	12
41	BR	101/103 (98%)	75 (74%)	14 (14%)	12 (12%)	0	4
41	DR	101/103 (98%)	71 (70%)	20 (20%)	10 (10%)	0	6
42	BS	108/110 (98%)	81 (75%)	20 (18%)	7 (6%)	1	14
42	DS	108/110 (98%)	80 (74%)	18 (17%)	10 (9%)	0	8
43	BT	91/100 (91%)	55 (60%)	20 (22%)	16 (18%)	0	1
43	DT	91/100 (91%)	47 (52%)	30 (33%)	14 (15%)	0	2
44	BU	100/104 (96%)	68 (68%)	16 (16%)	16 (16%)	0	2
44	DU	100/104 (96%)	49 (49%)	29 (29%)	22 (22%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	BV	92/94 (98%)	76 (83%)	15 (16%)	1 (1%)	11	41
45	DV	92/94 (98%)	59 (64%)	25 (27%)	8 (9%)	0	8
46	BW	77/85 (91%)	32 (42%)	18 (23%)	27 (35%)	0	0
46	DW	77/85 (91%)	34 (44%)	25 (32%)	18 (23%)	0	0
47	BX	75/78 (96%)	58 (77%)	12 (16%)	5 (7%)	1	13
47	DX	75/78 (96%)	49 (65%)	19 (25%)	7 (9%)	0	8
48	BY	61/63 (97%)	39 (64%)	15 (25%)	7 (12%)	0	4
48	DY	61/63 (97%)	45 (74%)	11 (18%)	5 (8%)	0	9
49	BZ	56/59 (95%)	43 (77%)	10 (18%)	3 (5%)	1	16
49	DZ	56/59 (95%)	35 (62%)	14 (25%)	7 (12%)	0	4
50	B0	54/57 (95%)	39 (72%)	8 (15%)	7 (13%)	0	3
50	D0	54/57 (95%)	39 (72%)	8 (15%)	7 (13%)	0	3
51	B1	48/55 (87%)	32 (67%)	9 (19%)	7 (15%)	0	3
51	D1	48/55 (87%)	37 (77%)	7 (15%)	4 (8%)	0	9
52	B2	44/46 (96%)	36 (82%)	6 (14%)	2 (4%)	2	18
52	D2	44/46 (96%)	30 (68%)	9 (20%)	5 (11%)	0	4
53	B3	62/65 (95%)	50 (81%)	10 (16%)	2 (3%)	3	25
53	D3	62/65 (95%)	42 (68%)	15 (24%)	5 (8%)	1	9
54	B4	36/38 (95%)	27 (75%)	6 (17%)	3 (8%)	0	9
54	D4	36/38 (95%)	22 (61%)	8 (22%)	6 (17%)	0	2
All	All	11238/11970 (94%)	7515 (67%)	2516 (22%)	1207 (11%)	0	5

5 of 1207 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AB	20	ARG
1	AB	22	TRP
1	AB	37	VAL
1	AB	71	THR
1	AB	125	PHE

5.3.2 Protein sidechains ⓘ

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AB	180/199 (90%)	150 (83%)	30 (17%)	2	14
1	CB	180/199 (90%)	161 (89%)	19 (11%)	6	27
2	AC	170/190 (90%)	147 (86%)	23 (14%)	4	20
2	CC	170/190 (90%)	147 (86%)	23 (14%)	4	20
3	AD	172/173 (99%)	151 (88%)	21 (12%)	5	22
3	CD	172/173 (99%)	147 (86%)	25 (14%)	3	17
4	AE	113/126 (90%)	93 (82%)	20 (18%)	2	12
4	CE	113/126 (90%)	96 (85%)	17 (15%)	3	16
5	AF	87/116 (75%)	76 (87%)	11 (13%)	4	21
5	CF	87/116 (75%)	76 (87%)	11 (13%)	4	21
6	AG	124/147 (84%)	114 (92%)	10 (8%)	11	36
6	CG	123/147 (84%)	93 (76%)	30 (24%)	1	5
7	AH	104/105 (99%)	91 (88%)	13 (12%)	4	21
7	CH	104/105 (99%)	92 (88%)	12 (12%)	5	24
8	AI	105/107 (98%)	92 (88%)	13 (12%)	4	21
8	CI	105/107 (98%)	92 (88%)	13 (12%)	4	21
9	AJ	86/90 (96%)	75 (87%)	11 (13%)	4	21
9	CJ	86/90 (96%)	75 (87%)	11 (13%)	4	21
10	AK	90/99 (91%)	80 (89%)	10 (11%)	6	25
10	CK	90/99 (91%)	82 (91%)	8 (9%)	9	33
11	AL	103/104 (99%)	85 (82%)	18 (18%)	2	12
11	CL	103/104 (99%)	92 (89%)	11 (11%)	6	27
12	AM	92/96 (96%)	84 (91%)	8 (9%)	9	34
12	CM	91/96 (95%)	75 (82%)	16 (18%)	2	12
13	AN	79/84 (94%)	72 (91%)	7 (9%)	9	33
13	CN	79/84 (94%)	68 (86%)	11 (14%)	3	18
14	AO	76/77 (99%)	73 (96%)	3 (4%)	28	52
14	CO	76/77 (99%)	71 (93%)	5 (7%)	15	42
15	AP	65/65 (100%)	58 (89%)	7 (11%)	6	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	CP	65/65 (100%)	56 (86%)	9 (14%)	3	19
16	AQ	74/78 (95%)	60 (81%)	14 (19%)	1	10
16	CQ	74/78 (95%)	62 (84%)	12 (16%)	2	14
17	AR	48/65 (74%)	45 (94%)	3 (6%)	16	43
17	CR	48/65 (74%)	44 (92%)	4 (8%)	10	35
18	AS	70/79 (89%)	63 (90%)	7 (10%)	7	29
18	CS	70/79 (89%)	60 (86%)	10 (14%)	3	18
19	AT	65/66 (98%)	55 (85%)	10 (15%)	2	16
19	CT	65/66 (98%)	56 (86%)	9 (14%)	3	19
20	AU	44/61 (72%)	38 (86%)	6 (14%)	3	19
20	CU	44/61 (72%)	36 (82%)	8 (18%)	2	11
26	BC	216/218 (99%)	173 (80%)	43 (20%)	1	9
26	DC	216/218 (99%)	191 (88%)	25 (12%)	5	24
27	BD	164/164 (100%)	133 (81%)	31 (19%)	1	10
27	DD	164/164 (100%)	139 (85%)	25 (15%)	3	16
28	BE	165/165 (100%)	127 (77%)	38 (23%)	1	6
28	DE	165/165 (100%)	147 (89%)	18 (11%)	6	26
29	BF	148/150 (99%)	126 (85%)	22 (15%)	3	16
29	DF	149/150 (99%)	118 (79%)	31 (21%)	1	8
30	BG	137/138 (99%)	106 (77%)	31 (23%)	1	6
30	DG	137/138 (99%)	117 (85%)	20 (15%)	3	17
31	BH	114/114 (100%)	96 (84%)	18 (16%)	2	15
31	DH	114/114 (100%)	99 (87%)	15 (13%)	4	20
32	BI	109/110 (99%)	96 (88%)	13 (12%)	5	23
32	DI	109/110 (99%)	100 (92%)	9 (8%)	10	35
33	BJ	116/116 (100%)	88 (76%)	28 (24%)	1	5
33	DJ	116/116 (100%)	97 (84%)	19 (16%)	2	14
34	BK	103/104 (99%)	76 (74%)	27 (26%)	0	4
34	DK	103/104 (99%)	83 (81%)	20 (19%)	1	9
35	BL	102/103 (99%)	75 (74%)	27 (26%)	0	4
35	DL	102/103 (99%)	89 (87%)	13 (13%)	4	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	BM	109/109 (100%)	86 (79%)	23 (21%)	1	7
36	DM	109/109 (100%)	96 (88%)	13 (12%)	5	23
37	BN	100/103 (97%)	79 (79%)	21 (21%)	1	7
37	DN	100/103 (97%)	81 (81%)	19 (19%)	1	10
38	BO	86/87 (99%)	63 (73%)	23 (27%)	0	4
38	DO	86/87 (99%)	77 (90%)	9 (10%)	6	28
39	BP	99/100 (99%)	80 (81%)	19 (19%)	1	9
39	DP	99/100 (99%)	91 (92%)	8 (8%)	11	36
40	BQ	89/90 (99%)	73 (82%)	16 (18%)	2	12
40	DQ	89/90 (99%)	77 (86%)	12 (14%)	4	20
41	BR	84/84 (100%)	66 (79%)	18 (21%)	1	7
41	DR	84/84 (100%)	74 (88%)	10 (12%)	5	23
42	BS	93/93 (100%)	63 (68%)	30 (32%)	0	1
42	DS	93/93 (100%)	73 (78%)	20 (22%)	1	7
43	BT	80/84 (95%)	62 (78%)	18 (22%)	1	6
43	DT	80/84 (95%)	74 (92%)	6 (8%)	12	39
44	BU	83/85 (98%)	67 (81%)	16 (19%)	1	9
44	DU	83/85 (98%)	69 (83%)	14 (17%)	2	13
45	BV	78/78 (100%)	60 (77%)	18 (23%)	1	6
45	DV	78/78 (100%)	68 (87%)	10 (13%)	4	21
46	BW	59/63 (94%)	44 (75%)	15 (25%)	0	4
46	DW	59/63 (94%)	46 (78%)	13 (22%)	1	7
47	BX	67/68 (98%)	54 (81%)	13 (19%)	1	9
47	DX	67/68 (98%)	59 (88%)	8 (12%)	5	23
48	BY	55/55 (100%)	42 (76%)	13 (24%)	1	6
48	DY	55/55 (100%)	51 (93%)	4 (7%)	13	39
49	BZ	48/49 (98%)	34 (71%)	14 (29%)	0	2
49	DZ	48/49 (98%)	40 (83%)	8 (17%)	2	14
50	B0	47/48 (98%)	42 (89%)	5 (11%)	6	27
50	D0	47/48 (98%)	42 (89%)	5 (11%)	6	27
51	B1	45/49 (92%)	34 (76%)	11 (24%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	D1	45/49 (92%)	41 (91%)	4 (9%)	9	33
52	B2	38/38 (100%)	31 (82%)	7 (18%)	1	11
52	D2	38/38 (100%)	34 (90%)	4 (10%)	6	28
53	B3	51/52 (98%)	44 (86%)	7 (14%)	3	19
53	D3	51/52 (98%)	42 (82%)	9 (18%)	2	12
54	B4	34/34 (100%)	29 (85%)	5 (15%)	3	17
54	D4	34/34 (100%)	29 (85%)	5 (15%)	3	17
All	All	9331/9756 (96%)	7876 (84%)	1455 (16%)	2	15

5 of 1455 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	CG	67	ASN
28	DE	166	LYS
8	CI	20	ILE
6	CG	66	GLU
16	CQ	51	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 343 such sidechains are listed below:

Mol	Chain	Res	Type
11	CL	95	HIS
34	DK	89	ASN
13	CN	70	HIS
27	DD	185	ASN
39	DP	65	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1532/1533 (99%)	478 (31%)	230 (15%)
22	AV	17/17 (100%)	3 (17%)	1 (5%)
22	AX	17/17 (100%)	2 (11%)	1 (5%)
22	CV	17/17 (100%)	3 (17%)	1 (5%)
22	CX	16/17 (94%)	2 (12%)	0
23	AW	5/6 (83%)	3 (60%)	1 (20%)
23	CW	5/6 (83%)	2 (40%)	1 (20%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
24	BA	2850/2903 (98%)	981 (34%)	497 (17%)
24	DA	2838/2903 (97%)	1054 (37%)	505 (17%)
25	BB	117/118 (99%)	37 (31%)	22 (18%)
55	CA	1529/1530 (99%)	530 (34%)	245 (16%)
56	DB	116/117 (99%)	30 (25%)	13 (11%)
All	All	9059/9184 (98%)	3125 (34%)	1517 (16%)

5 of 3125 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	5	U
21	AA	6	G
21	AA	7	A
21	AA	9	G
21	AA	10	A

5 of 1517 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
55	CA	1053	G
24	DA	778	G
55	CA	1213	A
55	CA	1051	C
24	DA	223	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [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%)	0.96	34 (15%) 5 7	170, 274, 284, 290	0
1	CB	218/241 (90%)	0.41	9 (4%) 41 26	159, 222, 233, 241	0
2	AC	206/233 (88%)	-0.18	0 100 100	133, 162, 187, 202	0
2	CC	206/233 (88%)	0.19	1 (0%) 87 69	140, 172, 212, 228	0
3	AD	205/206 (99%)	0.13	4 (1%) 65 41	122, 157, 195, 218	0
3	CD	205/206 (99%)	0.23	6 (2%) 53 34	112, 131, 152, 165	0
4	AE	150/167 (89%)	1.74	49 (32%) 1 1	108, 211, 223, 227	0
4	CE	150/167 (89%)	0.65	13 (8%) 16 14	100, 156, 171, 176	0
5	AF	100/135 (74%)	0.15	2 (2%) 65 41	197, 229, 250, 260	0
5	CF	100/135 (74%)	0.15	3 (3%) 52 33	164, 186, 203, 209	0
6	AG	151/179 (84%)	0.11	5 (3%) 49 31	158, 192, 220, 237	0
6	CG	150/179 (83%)	0.75	16 (10%) 11 12	142, 194, 228, 244	0
7	AH	129/130 (99%)	-0.02	0 100 100	127, 155, 181, 193	0
7	CH	129/130 (99%)	0.17	1 (0%) 82 60	152, 177, 195, 203	0
8	AI	127/130 (97%)	0.53	8 (6%) 26 18	142, 193, 220, 233	0
8	CI	127/130 (97%)	0.69	12 (9%) 14 13	155, 195, 223, 232	0
9	AJ	98/103 (95%)	0.48	6 (6%) 27 19	135, 181, 216, 239	0
9	CJ	98/103 (95%)	0.50	5 (5%) 33 22	155, 196, 230, 240	0
10	AK	117/129 (90%)	-0.09	1 (0%) 81 58	132, 195, 243, 254	0
10	CK	117/129 (90%)	0.11	2 (1%) 69 43	125, 155, 181, 196	0
11	AL	123/124 (99%)	0.23	5 (4%) 41 26	89, 106, 131, 150	0
11	CL	123/124 (99%)	0.48	6 (4%) 35 23	117, 139, 155, 161	0
12	AM	114/118 (96%)	0.21	2 (1%) 67 43	157, 219, 252, 264	0
12	CM	113/118 (95%)	0.60	8 (7%) 22 16	195, 269, 309, 322	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AN	96/101 (95%)	0.59	6 (6%) 26 18	142, 165, 217, 227	0
13	CN	95/101 (94%)	0.81	8 (8%) 17 14	155, 207, 265, 284	0
14	AO	88/89 (98%)	-0.01	1 (1%) 78 54	138, 168, 199, 219	0
14	CO	88/89 (98%)	0.21	4 (4%) 38 24	142, 174, 193, 201	0
15	AP	82/82 (100%)	0.17	1 (1%) 76 51	117, 144, 178, 192	0
15	CP	80/82 (97%)	0.63	4 (5%) 34 22	151, 180, 203, 207	0
16	AQ	80/84 (95%)	0.32	3 (3%) 44 28	90, 113, 135, 144	0
16	CQ	80/84 (95%)	0.19	0 100 100	99, 123, 145, 163	0
17	AR	55/75 (73%)	0.11	1 (1%) 67 43	175, 198, 219, 234	0
17	CR	55/75 (73%)	0.01	0 100 100	148, 165, 180, 187	0
18	AS	79/92 (85%)	0.23	2 (2%) 58 37	171, 203, 244, 257	0
18	CS	79/92 (85%)	0.56	8 (10%) 12 13	223, 265, 319, 334	0
19	AT	85/87 (97%)	0.22	3 (3%) 47 30	114, 141, 164, 180	0
19	CT	85/87 (97%)	0.92	13 (15%) 5 7	194, 242, 275, 283	0
20	AU	51/71 (71%)	0.65	5 (9%) 13 13	133, 168, 248, 252	0
20	CU	51/71 (71%)	0.43	6 (11%) 9 10	126, 150, 183, 193	0
21	AA	1533/1533 (100%)	-0.17	34 (2%) 62 40	76, 150, 233, 282	0
22	AV	17/17 (100%)	0.26	0 100 100	142, 154, 182, 203	0
22	AX	17/17 (100%)	-0.39	0 100 100	139, 144, 186, 195	0
22	CV	17/17 (100%)	0.23	1 (5%) 28 19	158, 162, 193, 208	0
22	CX	17/17 (100%)	0.35	0 100 100	187, 193, 221, 222	0
23	AW	6/6 (100%)	0.63	0 100 100	136, 138, 143, 152	0
23	CW	6/6 (100%)	0.63	1 (16%) 4 6	160, 160, 168, 179	0
24	BA	2854/2903 (98%)	-0.39	47 (1%) 70 45	52, 81, 194, 355	0
24	DA	2841/2903 (97%)	0.75	242 (8%) 16 14	132, 200, 303, 402	0
25	BB	118/118 (100%)	-0.39	0 100 100	66, 101, 133, 171	0
26	BC	271/273 (99%)	0.18	8 (2%) 52 33	60, 99, 129, 161	0
26	DC	271/273 (99%)	0.92	40 (14%) 5 7	133, 157, 179, 190	0
27	BD	209/209 (100%)	-0.09	0 100 100	55, 75, 114, 129	0
27	DD	209/209 (100%)	1.00	36 (17%) 4 5	147, 200, 232, 242	0
28	BE	201/201 (100%)	-0.14	0 100 100	56, 96, 129, 157	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DE	201/201 (100%)	1.08	44 (21%) 2 3	154, 282, 335, 351	0
29	BF	177/179 (98%)	0.28	4 (2%) 61 38	120, 166, 201, 215	0
29	DF	178/179 (99%)	0.32	6 (3%) 48 30	307, 314, 321, 323	0
30	BG	176/177 (99%)	-0.08	1 (0%) 85 66	83, 108, 134, 152	0
30	DG	176/177 (99%)	0.40	8 (4%) 38 24	186, 221, 245, 259	0
31	BH	149/149 (100%)	0.42	6 (4%) 42 27	110, 239, 259, 264	0
31	DH	149/149 (100%)	0.82	18 (12%) 8 10	186, 240, 256, 260	0
32	BI	141/142 (99%)	0.63	7 (4%) 34 22	243, 307, 359, 366	0
32	DI	141/142 (99%)	0.44	5 (3%) 47 30	367, 394, 412, 419	0
33	BJ	142/142 (100%)	-0.07	0 100 100	59, 76, 102, 132	0
33	DJ	142/142 (100%)	0.82	21 (14%) 5 7	161, 201, 223, 233	0
34	BK	122/123 (99%)	-0.09	4 (3%) 49 31	55, 73, 113, 169	0
34	DK	122/123 (99%)	0.34	5 (4%) 41 26	151, 171, 189, 198	0
35	BL	143/144 (99%)	0.14	4 (2%) 55 34	55, 93, 124, 136	0
35	DL	143/144 (99%)	1.38	38 (26%) 1 2	166, 240, 288, 297	0
36	BM	136/136 (100%)	-0.10	0 100 100	58, 81, 111, 138	0
36	DM	136/136 (100%)	0.59	9 (6%) 24 18	144, 181, 210, 232	0
37	BN	120/127 (94%)	-0.05	1 (0%) 82 60	61, 76, 96, 141	0
37	DN	120/127 (94%)	1.13	24 (20%) 3 4	183, 222, 252, 266	0
38	BO	116/117 (99%)	0.01	0 100 100	96, 105, 123, 147	0
38	DO	116/117 (99%)	0.64	6 (5%) 33 22	286, 293, 297, 303	0
39	BP	114/115 (99%)	-0.25	0 100 100	64, 81, 119, 134	0
39	DP	114/115 (99%)	0.72	9 (7%) 18 15	179, 203, 220, 230	0
40	BQ	117/118 (99%)	-0.08	0 100 100	56, 77, 99, 120	0
40	DQ	117/118 (99%)	1.31	26 (22%) 2 3	184, 211, 240, 247	0
41	BR	103/103 (100%)	0.01	1 (0%) 79 55	55, 87, 114, 131	0
41	DR	103/103 (100%)	1.05	21 (20%) 3 3	173, 249, 271, 277	0
42	BS	110/110 (100%)	-0.17	2 (1%) 67 43	55, 70, 105, 159	0
42	DS	110/110 (100%)	1.23	23 (20%) 2 3	159, 223, 269, 278	0
43	BT	93/100 (93%)	0.59	7 (7%) 20 15	65, 105, 142, 151	0
43	DT	93/100 (93%)	1.11	21 (22%) 2 3	206, 253, 285, 294	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BU	102/104 (98%)	0.36	6 (5%) 28 19	89, 114, 136, 158	0
44	DU	102/104 (98%)	1.13	14 (13%) 6 8	272, 312, 355, 358	0
45	BV	94/94 (100%)	-0.16	0 100 100	71, 90, 116, 126	0
45	DV	94/94 (100%)	0.53	5 (5%) 32 22	228, 241, 252, 254	0
46	BW	79/85 (92%)	0.56	9 (11%) 10 11	68, 86, 136, 156	0
46	DW	79/85 (92%)	0.92	11 (13%) 6 8	156, 216, 233, 252	0
47	BX	77/78 (98%)	0.13	1 (1%) 75 50	65, 101, 124, 137	0
47	DX	77/78 (98%)	1.35	17 (22%) 2 3	157, 185, 209, 224	0
48	BY	63/63 (100%)	0.13	2 (3%) 50 32	101, 123, 149, 159	0
48	DY	63/63 (100%)	1.42	15 (23%) 2 2	264, 288, 316, 329	0
49	BZ	58/59 (98%)	0.06	0 100 100	64, 74, 111, 141	0
49	DZ	58/59 (98%)	1.05	7 (12%) 8 10	188, 215, 238, 248	0
50	B0	56/57 (98%)	-0.31	0 100 100	54, 77, 113, 132	0
50	D0	56/57 (98%)	0.82	5 (8%) 15 14	157, 230, 260, 265	0
51	B1	50/55 (90%)	-0.12	0 100 100	76, 100, 118, 132	0
51	D1	50/55 (90%)	0.58	4 (8%) 18 14	174, 207, 228, 238	0
52	B2	46/46 (100%)	0.07	1 (2%) 62 40	62, 75, 103, 137	0
52	D2	46/46 (100%)	1.71	18 (39%) 1 1	155, 182, 198, 202	0
53	B3	64/65 (98%)	0.13	0 100 100	58, 73, 96, 120	0
53	D3	64/65 (98%)	2.15	33 (51%) 0 1	180, 194, 211, 215	0
54	B4	38/38 (100%)	0.22	1 (2%) 57 36	69, 84, 110, 120	0
54	D4	38/38 (100%)	2.09	17 (44%) 0 1	171, 187, 198, 203	0
55	CA	1530/1530 (100%)	0.31	56 (3%) 45 29	109, 171, 272, 362	0
56	DB	117/117 (100%)	0.55	2 (1%) 69 43	219, 294, 300, 302	0
All	All	20511/21154 (96%)	0.31	1217 (5%) 28 19	52, 166, 293, 419	0

The worst 5 of 1217 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	AE	114	LEU	10.5
8	CI	129	ARG	8.2
11	CL	123	ALA	8.0
47	DX	19	HIS	7.8
48	DY	13	GLU	7.6

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	CA	1636	1/1	-0.21	0.72	120,120,120,120	0
57	MG	DA	3020	1/1	-0.03	0.32	229,229,229,229	0
57	MG	DA	3128	1/1	0.02	0.43	132,132,132,132	0
57	MG	DA	3058	1/1	0.14	0.43	162,162,162,162	0
57	MG	DA	3060	1/1	0.20	0.73	132,132,132,132	0
57	MG	BA	3131	1/1	0.23	0.54	68,68,68,68	0
57	MG	DA	3074	1/1	0.24	0.37	187,187,187,187	0
57	MG	DA	3072	1/1	0.25	0.18	182,182,182,182	0
57	MG	DA	3129	1/1	0.26	0.64	132,132,132,132	0
57	MG	DA	3063	1/1	0.28	0.79	157,157,157,157	0
57	MG	CA	1640	1/1	0.29	0.39	118,118,118,118	0
57	MG	DA	3003	1/1	0.30	0.21	229,229,229,229	0
57	MG	BA	3058	1/1	0.33	0.45	63,63,63,63	0
57	MG	DA	3002	1/1	0.38	0.34	212,212,212,212	0
57	MG	CA	1617	1/1	0.38	0.10	183,183,183,183	0
57	MG	CA	1619	1/1	0.39	0.32	135,135,135,135	0
57	MG	DA	3015	1/1	0.43	0.28	164,164,164,164	0
57	MG	DA	3094	1/1	0.43	0.17	173,173,173,173	0
57	MG	D4	101	1/1	0.44	0.35	183,183,183,183	0
57	MG	CA	1627	1/1	0.47	0.20	136,136,136,136	0
57	MG	DA	3092	1/1	0.47	0.14	198,198,198,198	0
57	MG	DA	3013	1/1	0.47	0.17	165,165,165,165	0
57	MG	BA	3124	1/1	0.48	0.60	59,59,59,59	0
57	MG	AA	1627	1/1	0.48	0.47	142,142,142,142	0
57	MG	CA	1610	1/1	0.48	0.15	181,181,181,181	0
57	MG	BA	3062	1/1	0.48	0.52	55,55,55,55	0
57	MG	DA	3059	1/1	0.48	0.19	136,136,136,136	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3070	1/1	0.48	0.15	158,158,158,158	0
57	MG	DA	3005	1/1	0.48	0.24	197,197,197,197	0
57	MG	CA	1614	1/1	0.51	0.29	146,146,146,146	0
57	MG	DA	3132	1/1	0.52	0.15	198,198,198,198	0
57	MG	DA	3030	1/1	0.52	0.21	164,164,164,164	0
57	MG	DA	3045	1/1	0.53	0.16	188,188,188,188	0
57	MG	DA	3078	1/1	0.53	0.34	144,144,144,144	0
57	MG	DA	3082	1/1	0.53	0.14	220,220,220,220	0
57	MG	DA	3069	1/1	0.55	0.24	139,139,139,139	0
57	MG	DA	3016	1/1	0.56	0.23	175,175,175,175	0
57	MG	AA	1630	1/1	0.57	0.26	99,99,99,99	0
57	MG	DA	3007	1/1	0.59	0.14	250,250,250,250	0
57	MG	CA	1625	1/1	0.59	0.21	127,127,127,127	0
57	MG	DA	3042	1/1	0.59	0.12	179,179,179,179	0
57	MG	DA	3108	1/1	0.59	0.19	172,172,172,172	0
57	MG	DA	3022	1/1	0.61	0.20	152,152,152,152	0
57	MG	AA	1641	1/1	0.62	0.30	108,108,108,108	0
57	MG	CA	1628	1/1	0.62	0.39	99,99,99,99	0
57	MG	CA	1602	1/1	0.63	0.13	177,177,177,177	0
57	MG	DA	3091	1/1	0.63	0.20	174,174,174,174	0
57	MG	CA	1629	1/1	0.63	0.13	157,157,157,157	0
57	MG	AA	1607	1/1	0.64	0.19	113,113,113,113	0
57	MG	DA	3109	1/1	0.65	0.21	145,145,145,145	0
57	MG	DA	3039	1/1	0.66	0.11	186,186,186,186	0
57	MG	DA	3111	1/1	0.67	0.11	160,160,160,160	0
57	MG	DA	3123	1/1	0.67	0.17	225,225,225,225	0
57	MG	DC	301	1/1	0.67	0.09	135,135,135,135	0
57	MG	DA	3075	1/1	0.67	0.25	155,155,155,155	0
57	MG	DA	3006	1/1	0.68	0.09	296,296,296,296	0
57	MG	CA	1603	1/1	0.68	0.19	141,141,141,141	0
57	MG	DA	3097	1/1	0.68	0.18	156,156,156,156	0
57	MG	DA	3064	1/1	0.68	0.10	157,157,157,157	0
57	MG	DA	3036	1/1	0.68	0.22	212,212,212,212	0
57	MG	DJ	201	1/1	0.68	0.11	183,183,183,183	0
57	MG	AA	1619	1/1	0.68	0.22	162,162,162,162	0
57	MG	AA	1637	1/1	0.70	0.21	118,118,118,118	0
57	MG	DA	3018	1/1	0.70	0.18	248,248,248,248	0
57	MG	DA	3026	1/1	0.70	0.23	160,160,160,160	0
57	MG	DA	3076	1/1	0.71	0.30	145,145,145,145	0
57	MG	DA	3106	1/1	0.71	0.17	228,228,228,228	0
57	MG	DA	3011	1/1	0.72	0.24	184,184,184,184	0
57	MG	DA	3049	1/1	0.72	0.08	249,249,249,249	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3057	1/1	0.72	0.23	133,133,133,133	0
57	MG	DA	3019	1/1	0.72	0.16	245,245,245,245	0
57	MG	BA	3035	1/1	0.72	0.28	72,72,72,72	0
57	MG	DA	3014	1/1	0.73	0.14	162,162,162,162	0
57	MG	CA	1620	1/1	0.73	0.17	150,150,150,150	0
57	MG	DA	3096	1/1	0.74	0.13	190,190,190,190	0
57	MG	BA	3075	1/1	0.74	0.28	58,58,58,58	0
57	MG	DA	3083	1/1	0.74	0.07	303,303,303,303	0
57	MG	AA	1617	1/1	0.74	0.20	150,150,150,150	0
57	MG	DA	3071	1/1	0.74	0.15	184,184,184,184	0
57	MG	DA	3110	1/1	0.74	0.10	219,219,219,219	0
57	MG	AA	1636	1/1	0.74	0.13	154,154,154,154	0
57	MG	AA	1621	1/1	0.75	0.16	80,80,80,80	0
57	MG	DA	3098	1/1	0.75	0.11	170,170,170,170	0
57	MG	DA	3062	1/1	0.76	0.24	160,160,160,160	0
57	MG	DA	3010	1/1	0.76	0.16	210,210,210,210	0
57	MG	DA	3125	1/1	0.76	0.12	187,187,187,187	0
57	MG	CA	1601	1/1	0.77	0.12	224,224,224,224	0
57	MG	AA	1624	1/1	0.77	0.10	131,131,131,131	0
57	MG	DA	3073	1/1	0.77	0.10	312,312,312,312	0
57	MG	CA	1622	1/1	0.77	0.11	216,216,216,216	0
57	MG	DA	3095	1/1	0.78	0.10	152,152,152,152	0
57	MG	BA	3004	1/1	0.79	0.18	86,86,86,86	0
57	MG	CA	1607	1/1	0.79	0.10	134,134,134,134	0
57	MG	DA	3038	1/1	0.79	0.13	197,197,197,197	0
57	MG	DA	3028	1/1	0.79	0.14	165,165,165,165	0
57	MG	DA	3084	1/1	0.79	0.17	214,214,214,214	0
57	MG	DA	3131	1/1	0.80	0.21	181,181,181,181	0
57	MG	BA	3061	1/1	0.80	0.32	56,56,56,56	0
57	MG	DA	3100	1/1	0.80	0.12	150,150,150,150	0
57	MG	DA	3027	1/1	0.80	0.10	171,171,171,171	0
57	MG	DA	3107	1/1	0.80	0.12	137,137,137,137	0
57	MG	BA	3098	1/1	0.81	0.30	72,72,72,72	0
57	MG	DA	3088	1/1	0.81	0.10	180,180,180,180	0
57	MG	DA	3043	1/1	0.81	0.08	208,208,208,208	0
57	MG	DA	3029	1/1	0.81	0.16	179,179,179,179	0
57	MG	BB	201	1/1	0.81	0.30	118,118,118,118	0
57	MG	BA	3112	1/1	0.81	0.12	64,64,64,64	0
57	MG	BA	3115	1/1	0.81	0.31	65,65,65,65	0
57	MG	BA	3028	1/1	0.81	0.26	57,57,57,57	0
57	MG	DA	3113	1/1	0.81	0.10	182,182,182,182	0
57	MG	AA	1628	1/1	0.82	0.10	134,134,134,134	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3044	1/1	0.82	0.15	210,210,210,210	0
57	MG	BA	3093	1/1	0.82	0.17	104,104,104,104	0
57	MG	DA	3114	1/1	0.82	0.16	135,135,135,135	0
57	MG	DA	3121	1/1	0.82	0.20	206,206,206,206	0
57	MG	AA	1625	1/1	0.82	0.19	114,114,114,114	0
57	MG	BA	3015	1/1	0.82	0.40	55,55,55,55	0
57	MG	CA	1606	1/1	0.83	0.09	124,124,124,124	0
57	MG	CA	1637	1/1	0.83	0.17	112,112,112,112	0
57	MG	BA	3136	1/1	0.83	0.38	64,64,64,64	0
57	MG	CA	1615	1/1	0.83	0.10	156,156,156,156	0
57	MG	DB	201	1/1	0.83	0.14	224,224,224,224	0
57	MG	DA	3079	1/1	0.83	0.11	148,148,148,148	0
57	MG	CA	1616	1/1	0.83	0.18	199,199,199,199	0
57	MG	DA	3048	1/1	0.83	0.10	203,203,203,203	0
57	MG	DA	3130	1/1	0.84	0.12	170,170,170,170	0
57	MG	DA	3118	1/1	0.84	0.17	181,181,181,181	0
57	MG	DA	3093	1/1	0.84	0.16	208,208,208,208	0
57	MG	BA	3030	1/1	0.84	0.32	58,58,58,58	0
57	MG	DA	3017	1/1	0.84	0.13	187,187,187,187	0
57	MG	BA	3133	1/1	0.84	0.38	73,73,73,73	0
57	MG	DA	3047	1/1	0.84	0.18	208,208,208,208	0
57	MG	CA	1613	1/1	0.85	0.10	121,121,121,121	0
57	MG	AA	1616	1/1	0.85	0.20	161,161,161,161	0
57	MG	AA	1620	1/1	0.85	0.09	186,186,186,186	0
57	MG	CA	1608	1/1	0.85	0.11	121,121,121,121	0
57	MG	AA	1604	1/1	0.85	0.07	157,157,157,157	0
57	MG	DA	3001	1/1	0.85	0.15	206,206,206,206	0
57	MG	DA	3103	1/1	0.85	0.12	150,150,150,150	0
57	MG	DA	3033	1/1	0.86	0.11	162,162,162,162	0
57	MG	DA	3086	1/1	0.86	0.10	196,196,196,196	0
57	MG	CA	1623	1/1	0.86	0.16	123,123,123,123	0
57	MG	BA	3060	1/1	0.86	0.31	56,56,56,56	0
57	MG	AA	1610	1/1	0.86	0.10	155,155,155,155	0
57	MG	AA	1629	1/1	0.86	0.16	161,161,161,161	0
57	MG	DA	3052	1/1	0.86	0.09	144,144,144,144	0
57	MG	DA	3068	1/1	0.86	0.18	143,143,143,143	0
57	MG	DA	3080	1/1	0.86	0.10	134,134,134,134	0
57	MG	DA	3054	1/1	0.86	0.11	155,155,155,155	0
57	MG	DA	3117	1/1	0.86	0.15	170,170,170,170	0
57	MG	CA	1611	1/1	0.86	0.12	132,132,132,132	0
57	MG	DA	3037	1/1	0.87	0.12	204,204,204,204	0
57	MG	DA	3085	1/1	0.87	0.11	167,167,167,167	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	CA	1612	1/1	0.87	0.09	124,124,124,124	0
57	MG	DA	3055	1/1	0.87	0.07	136,136,136,136	0
57	MG	DA	3056	1/1	0.87	0.12	141,141,141,141	0
57	MG	BA	3007	1/1	0.87	0.14	111,111,111,111	0
57	MG	CA	1632	1/1	0.87	0.11	210,210,210,210	0
57	MG	CA	1642	1/1	0.87	0.07	170,170,170,170	0
57	MG	DA	3051	1/1	0.87	0.09	160,160,160,160	0
57	MG	CA	1634	1/1	0.88	0.07	153,153,153,153	0
57	MG	DA	3101	1/1	0.88	0.10	155,155,155,155	0
57	MG	AA	1602	1/1	0.88	0.24	97,97,97,97	0
57	MG	CA	1630	1/1	0.88	0.20	99,99,99,99	0
57	MG	AA	1611	1/1	0.88	0.14	126,126,126,126	0
57	MG	BA	3014	1/1	0.89	0.29	55,55,55,55	0
57	MG	BA	3046	1/1	0.89	0.11	77,77,77,77	0
57	MG	BA	3113	1/1	0.89	0.10	54,54,54,54	0
57	MG	BA	3088	1/1	0.89	0.15	77,77,77,77	0
57	MG	DC	302	1/1	0.89	0.11	140,140,140,140	0
57	MG	DA	3099	1/1	0.89	0.07	211,211,211,211	0
57	MG	AA	1614	1/1	0.89	0.08	150,150,150,150	0
57	MG	AA	1609	1/1	0.90	0.09	118,118,118,118	0
57	MG	DA	3065	1/1	0.90	0.08	152,152,152,152	0
57	MG	BA	3092	1/1	0.90	0.08	127,127,127,127	0
57	MG	DA	3025	1/1	0.90	0.08	135,135,135,135	0
57	MG	DA	3009	1/1	0.90	0.18	199,199,199,199	0
57	MG	DA	3034	1/1	0.90	0.14	158,158,158,158	0
57	MG	DA	3061	1/1	0.90	0.09	134,134,134,134	0
57	MG	DA	3035	1/1	0.90	0.11	155,155,155,155	0
57	MG	BA	3056	1/1	0.90	0.25	64,64,64,64	0
57	MG	BA	3019	1/1	0.91	0.09	86,86,86,86	0
57	MG	DA	3127	1/1	0.91	0.24	138,138,138,138	0
57	MG	BA	3003	1/1	0.91	0.09	90,90,90,90	0
57	MG	CA	1631	1/1	0.91	0.09	130,130,130,130	0
57	MG	BA	3011	1/1	0.91	0.28	62,62,62,62	0
57	MG	DA	3087	1/1	0.91	0.06	208,208,208,208	0
57	MG	DA	3004	1/1	0.91	0.16	206,206,206,206	0
57	MG	DA	3115	1/1	0.91	0.07	154,154,154,154	0
57	MG	DA	3067	1/1	0.91	0.08	147,147,147,147	0
57	MG	DA	3023	1/1	0.91	0.11	148,148,148,148	0
57	MG	DA	3032	1/1	0.91	0.10	161,161,161,161	0
57	MG	DA	3040	1/1	0.91	0.09	171,171,171,171	0
57	MG	DA	3046	1/1	0.92	0.12	172,172,172,172	0
57	MG	DA	3012	1/1	0.92	0.15	168,168,168,168	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	AA	1631	1/1	0.92	0.17	114,114,114,114	0
57	MG	AA	1615	1/1	0.92	0.06	153,153,153,153	0
57	MG	DA	3050	1/1	0.92	0.07	180,180,180,180	0
57	MG	CA	1609	1/1	0.92	0.07	131,131,131,131	0
57	MG	AA	1601	1/1	0.92	0.07	133,133,133,133	0
57	MG	BA	3005	1/1	0.92	0.09	91,91,91,91	0
57	MG	BA	3099	1/1	0.92	0.11	58,58,58,58	0
57	MG	BB	202	1/1	0.92	0.10	127,127,127,127	0
57	MG	BD	301	1/1	0.92	0.14	55,55,55,55	0
57	MG	BA	3101	1/1	0.92	0.15	54,54,54,54	0
57	MG	BA	3077	1/1	0.92	0.15	63,63,63,63	0
57	MG	DA	3102	1/1	0.92	0.07	141,141,141,141	0
57	MG	DA	3081	1/1	0.92	0.08	182,182,182,182	0
57	MG	DA	3041	1/1	0.92	0.10	176,176,176,176	0
57	MG	DA	3008	1/1	0.92	0.06	198,198,198,198	0
57	MG	BA	3081	1/1	0.92	0.14	56,56,56,56	0
57	MG	CA	1635	1/1	0.92	0.07	142,142,142,142	0
57	MG	BA	3085	1/1	0.92	0.37	59,59,59,59	0
57	MG	BA	3079	1/1	0.93	0.07	110,110,110,110	0
57	MG	BA	3114	1/1	0.93	0.07	88,88,88,88	0
57	MG	BA	3051	1/1	0.93	0.15	57,57,57,57	0
57	MG	BA	3119	1/1	0.93	0.28	68,68,68,68	0
57	MG	BA	3123	1/1	0.93	0.07	79,79,79,79	0
57	MG	CA	1604	1/1	0.93	0.06	117,117,117,117	0
57	MG	DA	3053	1/1	0.93	0.12	144,144,144,144	0
57	MG	BA	3095	1/1	0.93	0.10	92,92,92,92	0
57	MG	AA	1608	1/1	0.93	0.13	105,105,105,105	0
57	MG	DA	3089	1/1	0.93	0.11	179,179,179,179	0
57	MG	BA	3086	1/1	0.93	0.09	60,60,60,60	0
57	MG	CA	1638	1/1	0.93	0.08	226,226,226,226	0
57	MG	CA	1639	1/1	0.93	0.04	266,266,266,266	0
57	MG	BA	3135	1/1	0.93	0.32	60,60,60,60	0
57	MG	BA	3032	1/1	0.93	0.10	57,57,57,57	0
57	MG	BA	3089	1/1	0.93	0.19	66,66,66,66	0
57	MG	BA	3071	1/1	0.94	0.30	55,55,55,55	0
57	MG	BA	3044	1/1	0.94	0.07	88,88,88,88	0
57	MG	DA	3066	1/1	0.94	0.08	150,150,150,150	0
57	MG	DA	3119	1/1	0.94	0.07	147,147,147,147	0
57	MG	CA	1621	1/1	0.94	0.08	115,115,115,115	0
57	MG	DA	3024	1/1	0.94	0.07	162,162,162,162	0
57	MG	DA	3124	1/1	0.94	0.18	168,168,168,168	0
57	MG	BA	3002	1/1	0.94	0.35	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	AA	1633	1/1	0.94	0.08	128,128,128,128	0
57	MG	DA	3105	1/1	0.94	0.06	159,159,159,159	0
57	MG	BA	3080	1/1	0.94	0.10	93,93,93,93	0
57	MG	BA	3107	1/1	0.94	0.09	67,67,67,67	0
57	MG	AA	1635	1/1	0.94	0.07	148,148,148,148	0
57	MG	BA	3026	1/1	0.94	0.33	59,59,59,59	0
57	MG	AA	1603	1/1	0.94	0.07	93,93,93,93	0
57	MG	AA	1613	1/1	0.94	0.10	95,95,95,95	0
57	MG	DA	3112	1/1	0.94	0.07	143,143,143,143	0
57	MG	BA	3009	1/1	0.94	0.07	61,61,61,61	0
57	MG	AA	1632	1/1	0.94	0.09	117,117,117,117	0
57	MG	BA	3048	1/1	0.95	0.15	91,91,91,91	0
57	MG	BB	204	1/1	0.95	0.07	74,74,74,74	0
57	MG	DA	3077	1/1	0.95	0.07	162,162,162,162	0
57	MG	AA	1634	1/1	0.95	0.05	121,121,121,121	0
57	MG	DA	3126	1/1	0.95	0.12	199,199,199,199	0
57	MG	BA	3076	1/1	0.95	0.07	62,62,62,62	0
57	MG	BA	3021	1/1	0.95	0.23	59,59,59,59	0
57	MG	CA	1641	1/1	0.95	0.08	151,151,151,151	0
57	MG	BA	3022	1/1	0.95	0.15	55,55,55,55	0
57	MG	BA	3037	1/1	0.95	0.26	58,58,58,58	0
57	MG	AA	1639	1/1	0.95	0.07	143,143,143,143	0
57	MG	BA	3016	1/1	0.95	0.27	56,56,56,56	0
57	MG	DA	3116	1/1	0.95	0.08	133,133,133,133	0
57	MG	CA	1633	1/1	0.95	0.09	123,123,123,123	0
57	MG	BA	3066	1/1	0.95	0.10	61,61,61,61	0
57	MG	BA	3047	1/1	0.95	0.09	78,78,78,78	0
57	MG	BA	3072	1/1	0.96	0.30	55,55,55,55	0
57	MG	AA	1638	1/1	0.96	0.10	107,107,107,107	0
57	MG	AA	1612	1/1	0.96	0.06	106,106,106,106	0
57	MG	AA	1623	1/1	0.96	0.07	129,129,129,129	0
57	MG	BA	3064	1/1	0.96	0.10	55,55,55,55	0
57	MG	BA	3045	1/1	0.96	0.21	80,80,80,80	0
57	MG	DA	3120	1/1	0.96	0.11	159,159,159,159	0
57	MG	CA	1624	1/1	0.96	0.15	99,99,99,99	0
57	MG	DA	3122	1/1	0.96	0.13	146,146,146,146	0
57	MG	BA	3127	1/1	0.96	0.09	57,57,57,57	0
57	MG	CA	1626	1/1	0.96	0.16	139,139,139,139	0
57	MG	BA	3128	1/1	0.96	0.06	64,64,64,64	0
57	MG	BA	3068	1/1	0.96	0.08	65,65,65,65	0
57	MG	BA	3132	1/1	0.96	0.25	61,61,61,61	0
57	MG	DA	3104	1/1	0.96	0.12	142,142,142,142	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3083	1/1	0.96	0.11	59,59,59,59	0
57	MG	BA	3103	1/1	0.96	0.10	81,81,81,81	0
57	MG	BA	3105	1/1	0.96	0.07	55,55,55,55	0
57	MG	AA	1606	1/1	0.96	0.06	119,119,119,119	0
57	MG	BA	3111	1/1	0.96	0.12	55,55,55,55	0
57	MG	BA	3059	1/1	0.96	0.13	69,69,69,69	0
57	MG	DA	3031	1/1	0.96	0.05	159,159,159,159	0
57	MG	DA	3090	1/1	0.96	0.05	200,200,200,200	0
57	MG	DA	3070	1/1	0.96	0.04	147,147,147,147	0
57	MG	BA	3109	1/1	0.97	0.07	60,60,60,60	0
57	MG	BA	3110	1/1	0.97	0.06	61,61,61,61	0
57	MG	AA	1605	1/1	0.97	0.10	124,124,124,124	0
57	MG	BA	3057	1/1	0.97	0.26	61,61,61,61	0
57	MG	CA	1618	1/1	0.97	0.09	148,148,148,148	0
57	MG	BA	3010	1/1	0.97	0.05	64,64,64,64	0
57	MG	BA	3090	1/1	0.97	0.07	63,63,63,63	0
57	MG	BA	3074	1/1	0.97	0.13	54,54,54,54	0
57	MG	AA	1618	1/1	0.97	0.06	131,131,131,131	0
57	MG	DA	3021	1/1	0.97	0.21	151,151,151,151	0
57	MG	BA	3122	1/1	0.97	0.06	57,57,57,57	0
57	MG	AA	1643	1/1	0.97	0.04	101,101,101,101	0
57	MG	CA	1605	1/1	0.97	0.05	115,115,115,115	0
57	MG	AA	1626	1/1	0.97	0.14	136,136,136,136	0
57	MG	BA	3125	1/1	0.97	0.11	58,58,58,58	0
57	MG	BA	3126	1/1	0.97	0.07	70,70,70,70	0
57	MG	BA	3049	1/1	0.97	0.07	61,61,61,61	0
57	MG	BA	3042	1/1	0.97	0.05	68,68,68,68	0
57	MG	BA	3052	1/1	0.97	0.04	54,54,54,54	0
57	MG	BA	3053	1/1	0.97	0.10	57,57,57,57	0
57	MG	BA	3069	1/1	0.97	0.05	65,65,65,65	0
57	MG	BA	3102	1/1	0.98	0.17	57,57,57,57	0
57	MG	BA	3006	1/1	0.98	0.04	101,101,101,101	0
57	MG	BA	3104	1/1	0.98	0.06	55,55,55,55	0
57	MG	BA	3039	1/1	0.98	0.06	57,57,57,57	0
57	MG	BA	3040	1/1	0.98	0.08	58,58,58,58	0
57	MG	AA	1622	1/1	0.98	0.05	113,113,113,113	0
57	MG	BA	3087	1/1	0.98	0.05	61,61,61,61	0
57	MG	BA	3043	1/1	0.98	0.07	68,68,68,68	0
57	MG	AA	1642	1/1	0.98	0.09	90,90,90,90	0
57	MG	AA	1640	1/1	0.98	0.04	160,160,160,160	0
57	MG	BA	3091	1/1	0.98	0.05	88,88,88,88	0
57	MG	BA	3020	1/1	0.98	0.22	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3118	1/1	0.98	0.06	60,60,60,60	0
57	MG	BA	3034	1/1	0.98	0.04	57,57,57,57	0
57	MG	BA	3121	1/1	0.98	0.10	64,64,64,64	0
57	MG	BA	3094	1/1	0.98	0.05	92,92,92,92	0
57	MG	BA	3001	1/1	0.98	0.12	61,61,61,61	0
57	MG	BA	3078	1/1	0.98	0.04	100,100,100,100	0
57	MG	BA	3063	1/1	0.98	0.09	54,54,54,54	0
57	MG	BA	3100	1/1	0.98	0.05	74,74,74,74	0
57	MG	BA	3036	1/1	0.98	0.04	65,65,65,65	0
58	ZN	D4	102	1/1	0.98	0.14	99,99,99,99	0
57	MG	BA	3054	1/1	0.99	0.03	62,62,62,62	0
57	MG	BA	3134	1/1	0.99	0.04	55,55,55,55	0
57	MG	BA	3055	1/1	0.99	0.07	62,62,62,62	0
57	MG	BA	3033	1/1	0.99	0.06	56,56,56,56	0
57	MG	BA	3024	1/1	0.99	0.05	60,60,60,60	0
57	MG	BA	3025	1/1	0.99	0.03	59,59,59,59	0
57	MG	BB	203	1/1	0.99	0.04	69,69,69,69	0
57	MG	BA	3012	1/1	0.99	0.04	54,54,54,54	0
57	MG	BA	3008	1/1	0.99	0.04	59,59,59,59	0
57	MG	BA	3038	1/1	0.99	0.03	59,59,59,59	0
57	MG	BA	3116	1/1	0.99	0.09	55,55,55,55	0
57	MG	BA	3117	1/1	0.99	0.04	67,67,67,67	0
57	MG	BA	3029	1/1	0.99	0.06	54,54,54,54	0
57	MG	BA	3096	1/1	0.99	0.17	61,61,61,61	0
57	MG	BA	3120	1/1	0.99	0.04	59,59,59,59	0
57	MG	BA	3097	1/1	0.99	0.06	65,65,65,65	0
57	MG	BA	3050	1/1	0.99	0.05	56,56,56,56	0
57	MG	BA	3017	1/1	0.99	0.03	56,56,56,56	0
57	MG	BA	3065	1/1	0.99	0.08	55,55,55,55	0
57	MG	BA	3082	1/1	0.99	0.04	55,55,55,55	0
57	MG	BA	3041	1/1	0.99	0.06	60,60,60,60	0
57	MG	BA	3084	1/1	0.99	0.18	61,61,61,61	0
57	MG	BA	3067	1/1	0.99	0.05	57,57,57,57	0
57	MG	BA	3129	1/1	0.99	0.04	55,55,55,55	0
57	MG	BA	3130	1/1	0.99	0.09	68,68,68,68	0
57	MG	BA	3018	1/1	0.99	0.03	80,80,80,80	0
58	ZN	B4	101	1/1	0.99	0.02	99,99,99,99	0
57	MG	BA	3106	1/1	0.99	0.05	58,58,58,58	0
57	MG	BA	3023	1/1	1.00	0.05	59,59,59,59	0
57	MG	BA	3108	1/1	1.00	0.09	58,58,58,58	0
57	MG	BA	3073	1/1	1.00	0.03	61,61,61,61	0
57	MG	BA	3013	1/1	1.00	0.05	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3027	1/1	1.00	0.09	59,59,59,59	0
57	MG	BA	3031	1/1	1.00	0.08	59,59,59,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.