



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 03:20 am BST

PDB ID : 4V6E
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

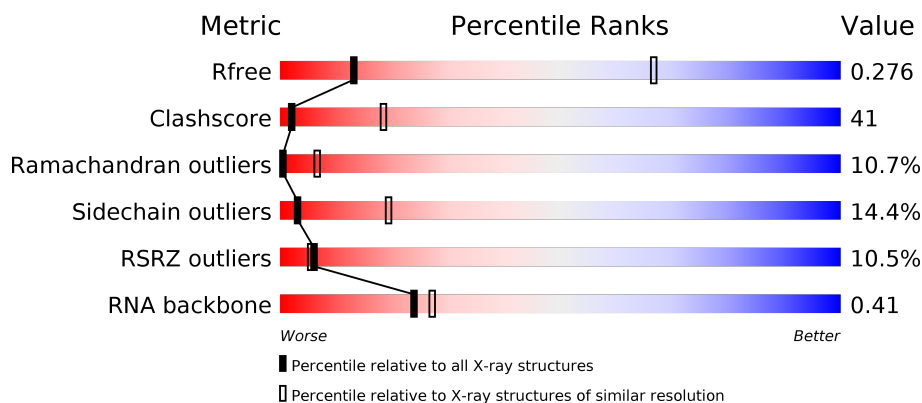
1 Overall quality at a glance

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}	130704	1089 (3.90-3.54)
Clashscore	141614	1012 (3.88-3.56)
Ramachandran outliers	138981	1114 (3.90-3.54)
Sidechain outliers	138945	1110 (3.90-3.54)
RSRZ outliers	127900	1020 (3.90-3.54)
RNA backbone	3102	1027 (4.40-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AB	241	<div> <div>34%</div> <div> <div>19%</div> <div>53%</div> <div>17%</div> <div>•</div> <div>10%</div> </div> </div>
1	CB	241	<div> <div>15%</div> <div> <div>22%</div> <div>55%</div> <div>12%</div> <div>•</div> <div>10%</div> </div> </div>
2	AC	233	<div> <div>5%</div> <div> <div>33%</div> <div>43%</div> <div>12%</div> <div>12%</div> </div> </div>
2	CC	233	<div> <div>7%</div> <div> <div>30%</div> <div>45%</div> <div>12%</div> <div>12%</div> </div> </div>

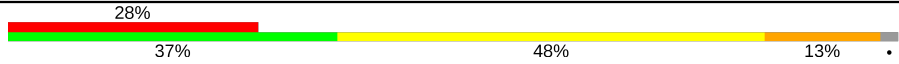
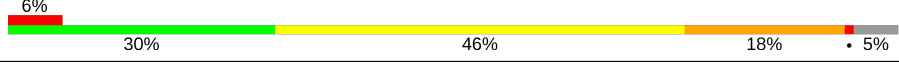
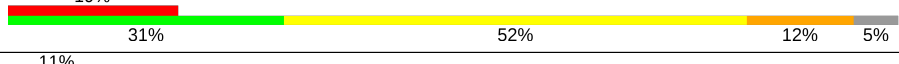
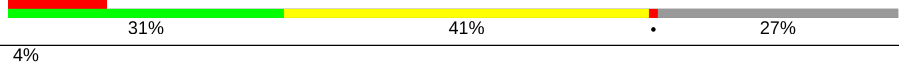
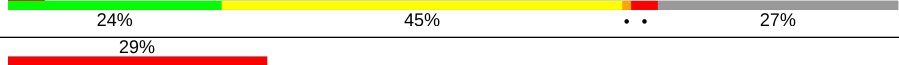
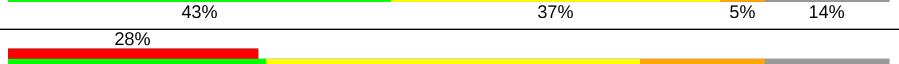
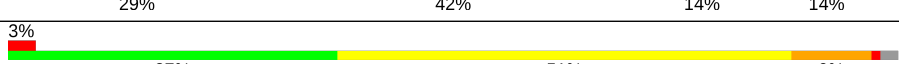
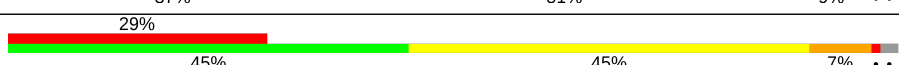
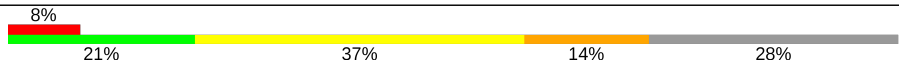

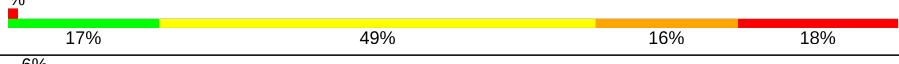
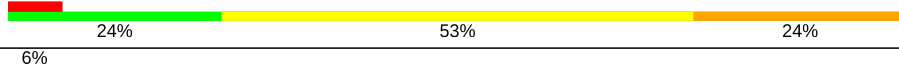
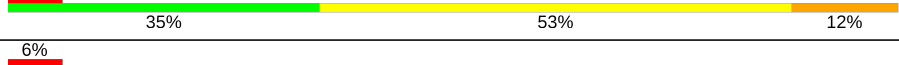
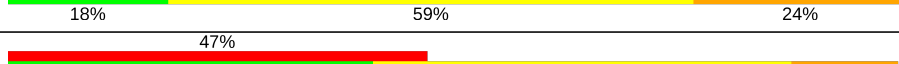

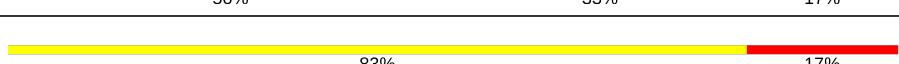
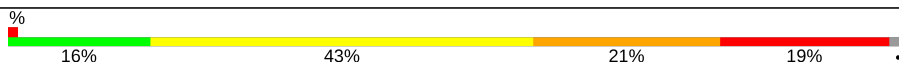

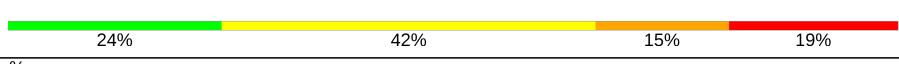






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Mol	Chain	Length	Quality of chain
3	AD	206	
3	CD	206	
4	AE	167	
4	CE	167	
5	AF	135	
5	CF	135	
6	AG	179	
6	CG	179	
7	AH	130	
7	CH	130	
8	AI	130	
8	CI	130	
9	AJ	103	
9	CJ	103	
10	AK	129	
10	CK	129	
11	AL	124	
11	CL	124	
12	AM	118	
12	CM	118	
13	AN	101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

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Mol	Chain	Length	Quality of chain
15	CP	82	
16	AQ	84	
16	CQ	84	
17	AR	75	
17	CR	75	
18	AS	92	
18	CS	92	
19	AT	87	
19	CT	87	
20	AU	71	
20	CU	71	
21	AA	1533	
22	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% 53% 18% .
28	DE	201	 23% 34% 52% 13% .
29	BF	179	 18% 35% 47% 16% ..
29	DF	179	 42% 27% 46% 23% ..
30	BG	177	 2% 35% 41% 21% ..
30	DG	177	 31% 36% 45% 18% ..
31	BH	149	 38% 33% 42% 21% .
31	DH	149	 28% 37% 40% 19% .
32	BI	142	 42% 34% 49% 15% ..
32	DI	142	 61% 42% 46% 10% ..
33	BJ	142	 20% 58% 18% .
33	DJ	142	 25% 32% 55% 11% .
34	BK	123	 27% 52% 18% ..
34	DK	123	 29% 28% 46% 24% ..
35	BL	144	 35% 48% 15% ..
35	DL	144	 26% 32% 49% 17% ..
36	BM	136	 27% 49% 22% .
36	DM	136	 40% 35% 54% 11% .
37	BN	127	 31% 46% 17% . 6%
37	DN	127	 41% 28% 50% 16% . 6%
38	BO	117	 30% 54% 15% ..
38	DO	117	 48% 35% 56% 8% ..
39	BP	115	 31% 46% 21% ..
39	DP	115	 29% 41% 43% 14% ..
40	BQ	118	 31% 50% 18% .

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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	1619	-	-	-	X
57	MG	AA	1637	-	-	-	X
57	MG	BA	3115	-	-	-	X
57	MG	CA	1614	-	-	-	X
57	MG	CA	1619	-	-	-	X
57	MG	CA	1620	-	-	-	X
57	MG	D4	101	-	-	-	X
57	MG	DA	3002	-	-	-	X
57	MG	DA	3003	-	-	-	X
57	MG	DA	3005	-	-	-	X
57	MG	DA	3015	-	-	-	X
57	MG	DA	3016	-	-	-	X
57	MG	DA	3020	-	-	-	X
57	MG	DA	3022	-	-	-	X
57	MG	DA	3029	-	-	-	X
57	MG	DA	3038	-	-	-	X
57	MG	DA	3041	-	-	-	X
57	MG	DA	3058	-	-	-	X
57	MG	DA	3060	-	-	-	X
57	MG	DA	3063	-	-	-	X
57	MG	DA	3064	-	-	-	X
57	MG	DA	3069	-	-	-	X
57	MG	DA	3072	-	-	-	X
57	MG	DA	3075	-	-	-	X
57	MG	DA	3078	-	-	-	X
57	MG	DA	3082	-	-	-	X
57	MG	DA	3094	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	DA	3108	-	-	-	X
57	MG	DA	3109	-	-	-	X
57	MG	DA	3121	-	-	-	X
57	MG	DA	3128	-	-	-	X
57	MG	DA	3129	-	-	-	X
57	MG	DJ	201	-	-	-	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	S	0	0	0
			892	552	178	162				
38	DO	116	Total	C	N	O	S	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	S	0	0	0
			947	604	192	151				
40	DQ	117	Total	C	N	O	S	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 (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	BB	4	Total	Mg	0	0
			4	4		
57	BA	136	Total	Mg	0	0
			136	136		
57	CA	42	Total	Mg	0	0
			42	42		
57	DJ	1	Total	Mg	0	0
			1	1		
57	BD	1	Total	Mg	0	0
			1	1		
57	AA	43	Total	Mg	0	0
			43	43		
57	D4	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	DA	132	Total 132	Mg 132	0	0
57	DC	2	Total 2	Mg 2	0	0
57	DB	1	Total 1	Mg 1	0	0

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 59 is water.

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

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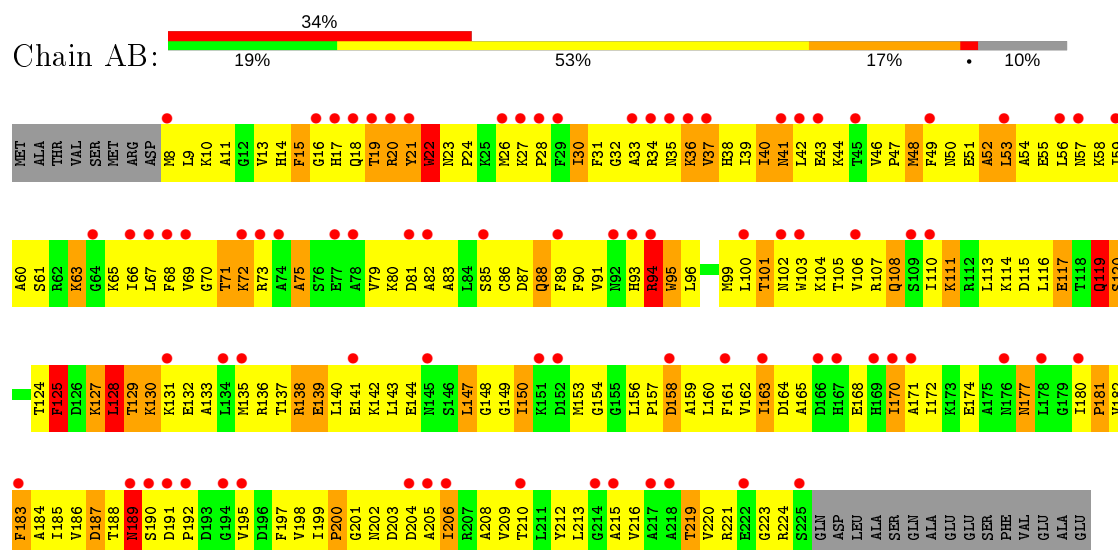
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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59	DV	1	Total 1	O 1	0	0
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59	D3	1	Total 1	O 1	0	0
59	D4	5	Total 5	O 5	0	0

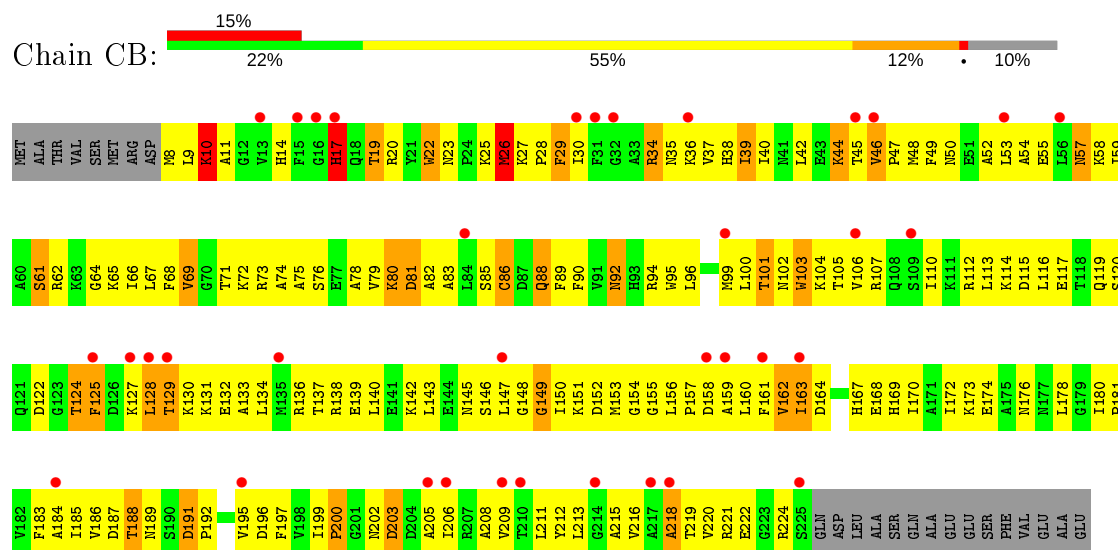
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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

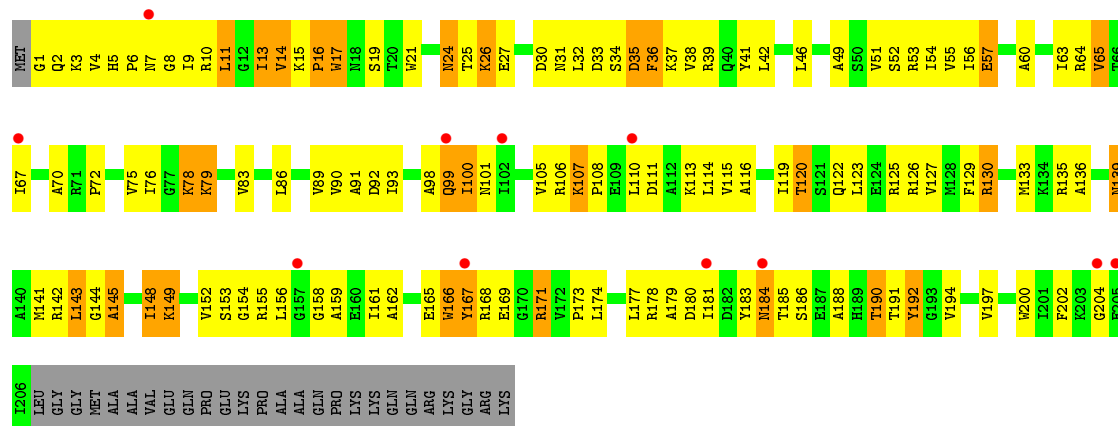


• Molecule 1: 30S ribosomal protein S2

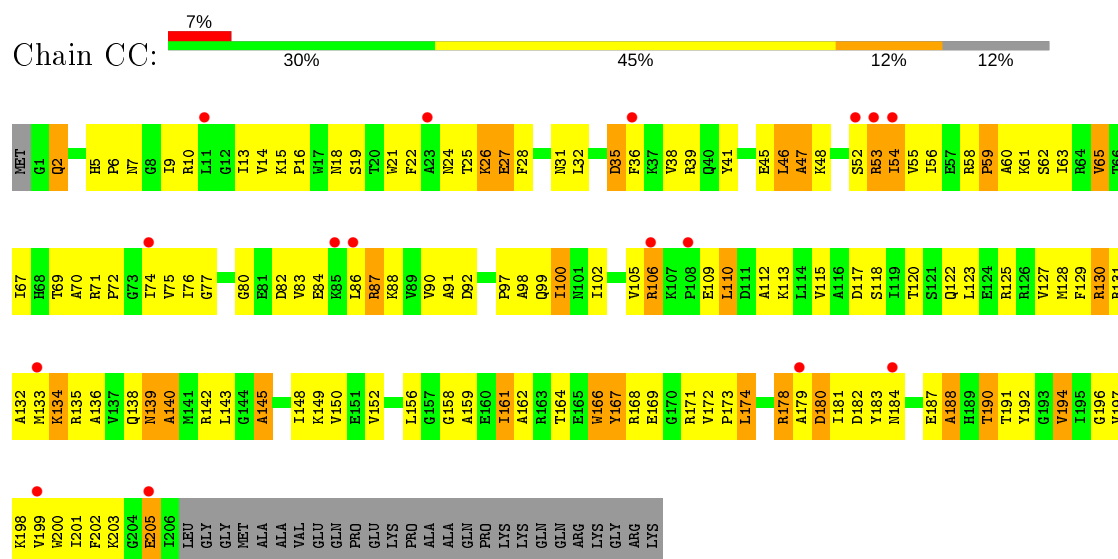


• Molecule 2: 30S ribosomal protein S3

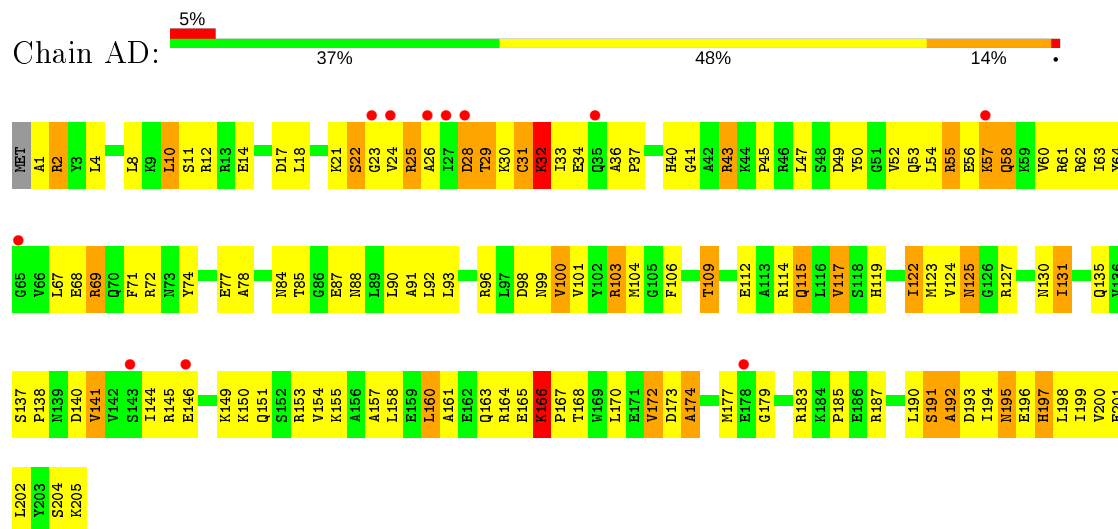




- Molecule 2: 30S ribosomal protein S3

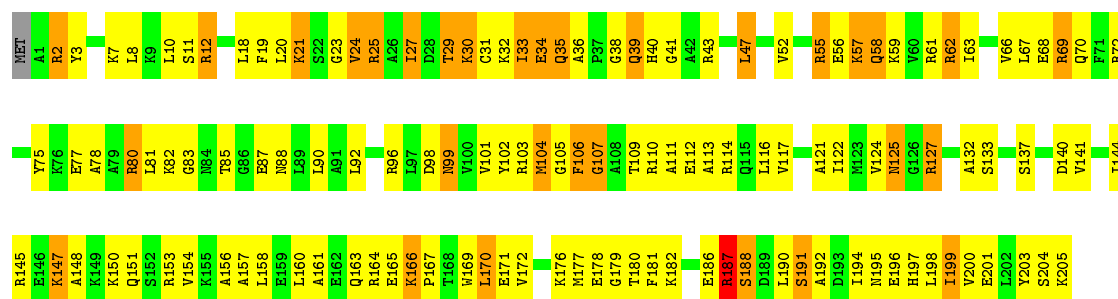


- Molecule 3: 30S ribosomal protein S4



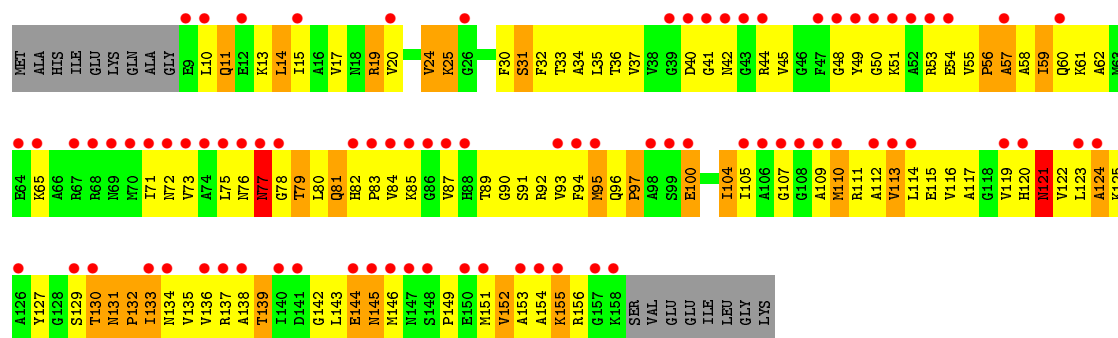
- Molecule 3: 30S ribosomal protein S4

Chain CD: 



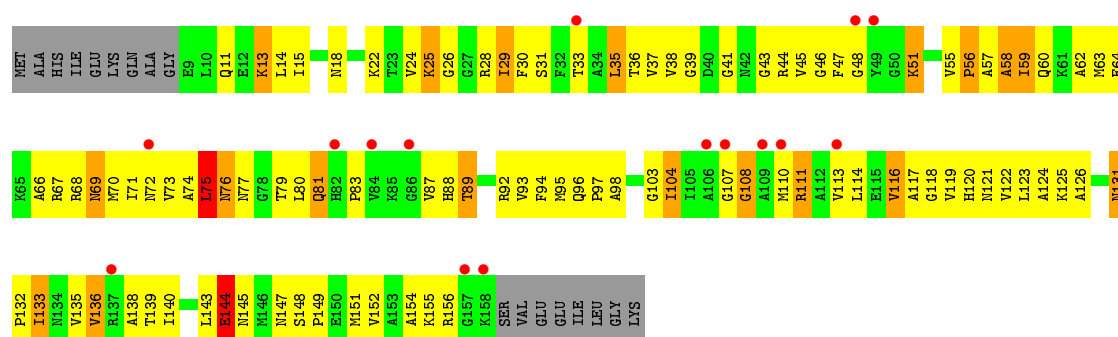
• Molecule 4: 30S ribosomal protein S5

Chain AE: 




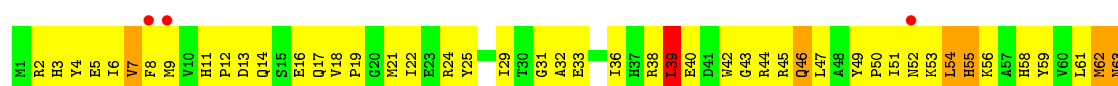
• Molecule 4: 30S ribosomal protein S5

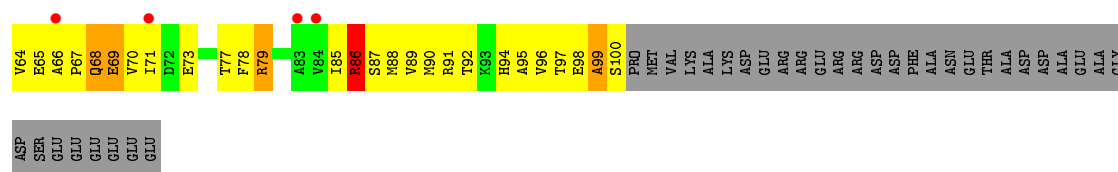
Chain CE: 



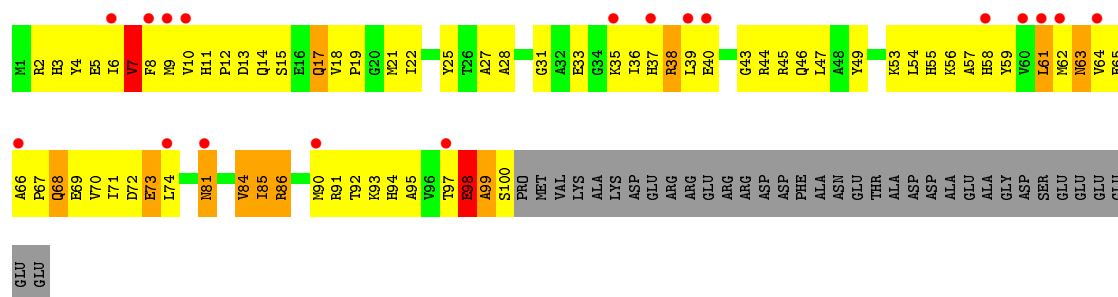
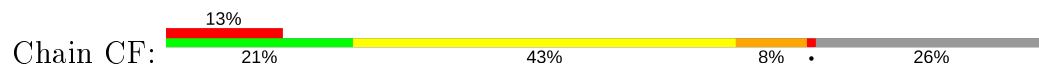
• Molecule 5: 30S ribosomal protein S6

Chain AF: 

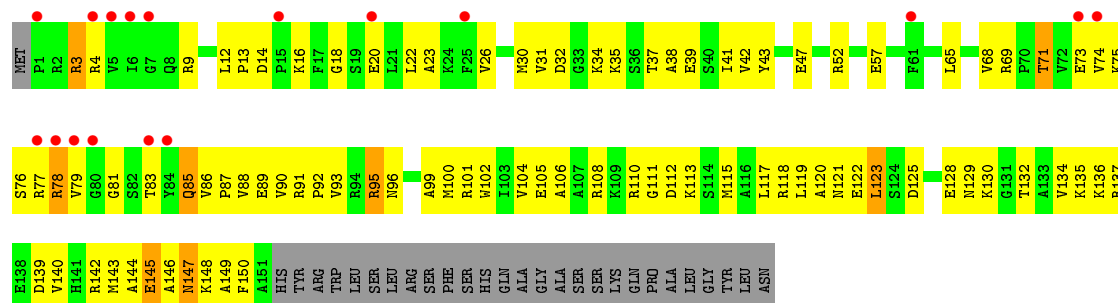




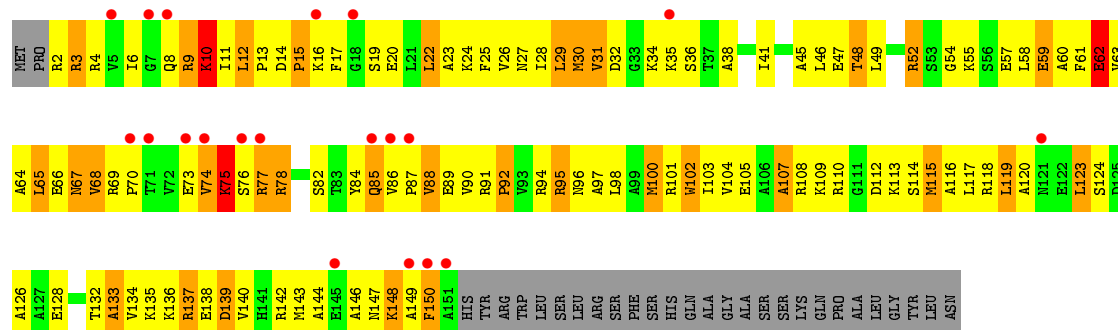
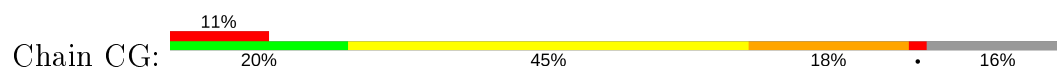
- Molecule 5: 30S ribosomal protein S6



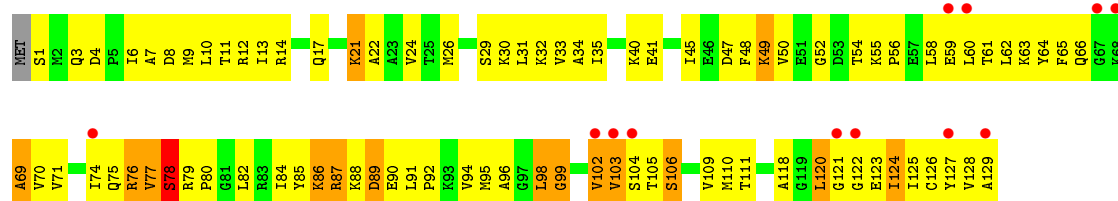
- Molecule 6: 30S ribosomal protein S7



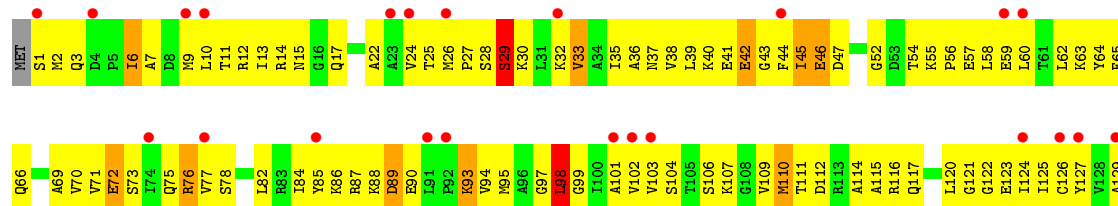
- Molecule 6: 30S ribosomal protein S7



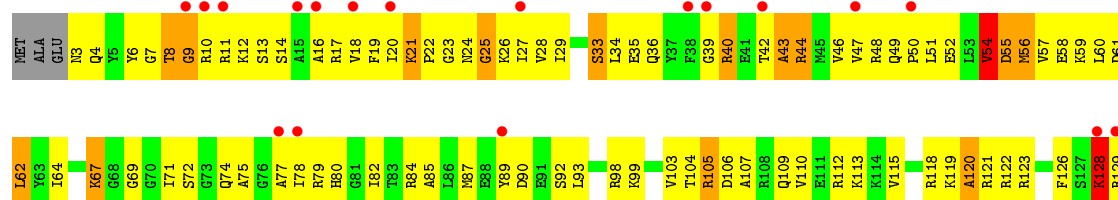
- Molecule 7: 30S ribosomal protein S8



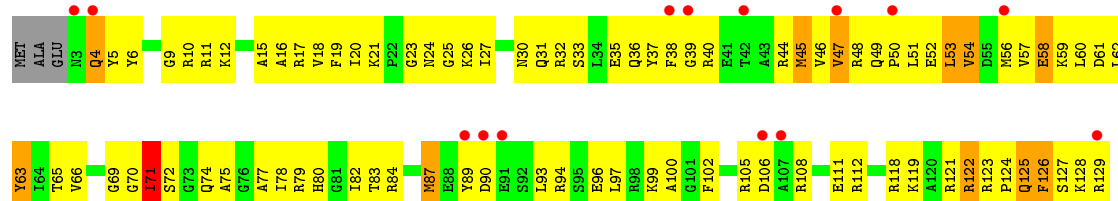
- Molecule 7: 30S ribosomal protein S8



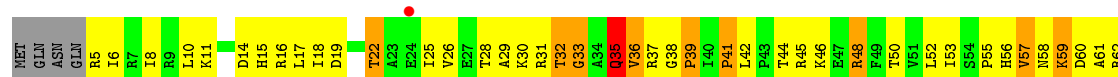
- Molecule 8: 30S ribosomal protein S9



- Molecule 8: 30S ribosomal protein S9

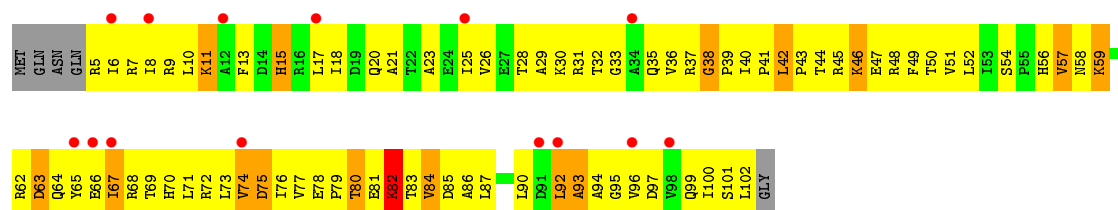


- Molecule 9: 30S ribosomal protein S10

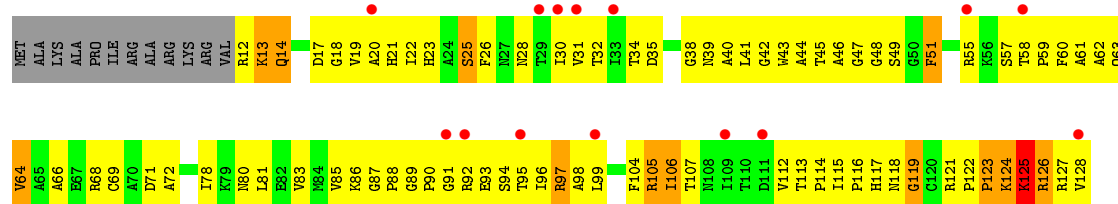




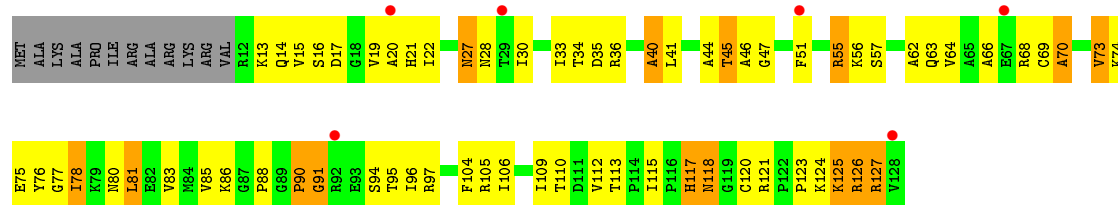
• Molecule 9: 30S ribosomal protein S10



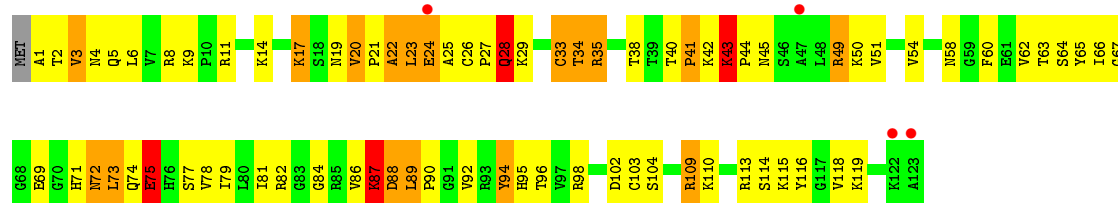
• Molecule 10: 30S ribosomal protein S11



• Molecule 10: 30S ribosomal protein S11

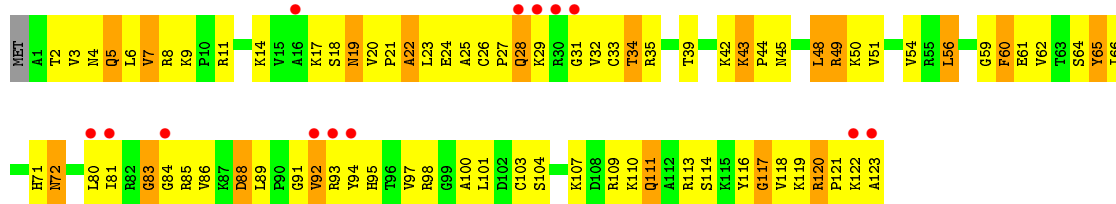


• Molecule 11: 30S ribosomal protein S12

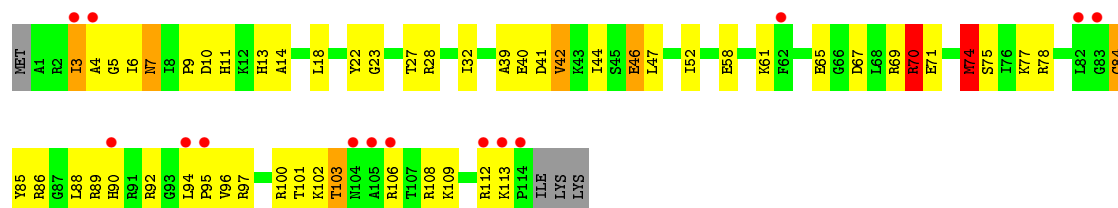


• Molecule 11: 30S ribosomal protein S12

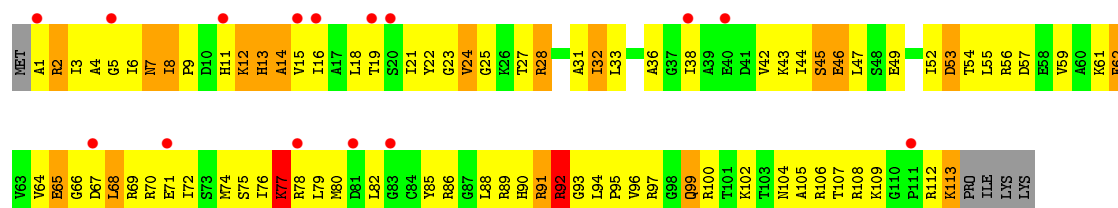




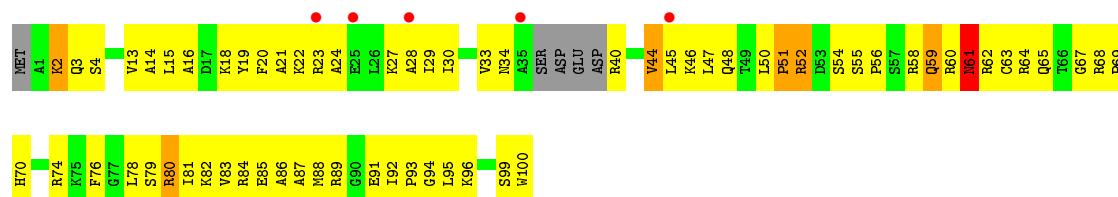
• Molecule 12: 30S ribosomal protein S13



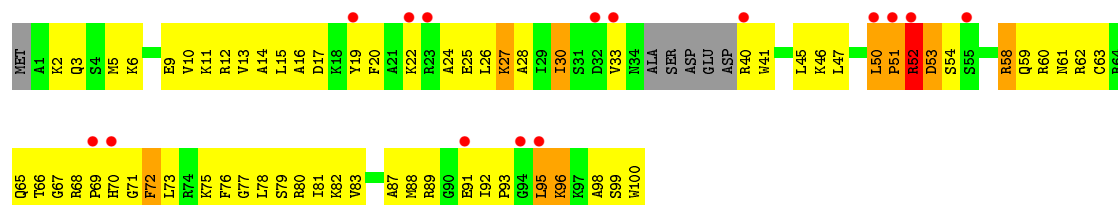
• Molecule 12: 30S ribosomal protein S13



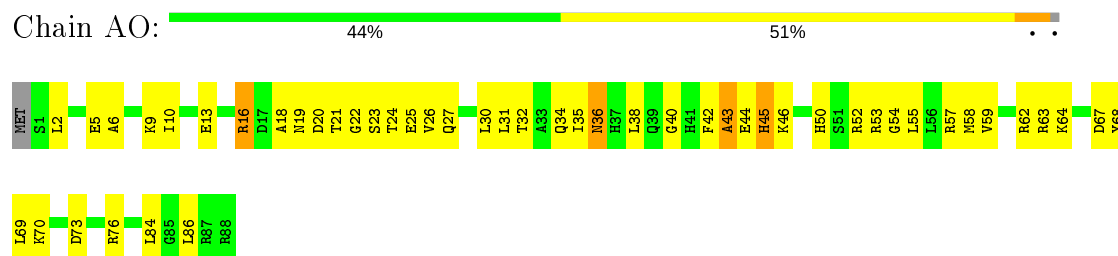
• Molecule 13: 30S ribosomal protein S14



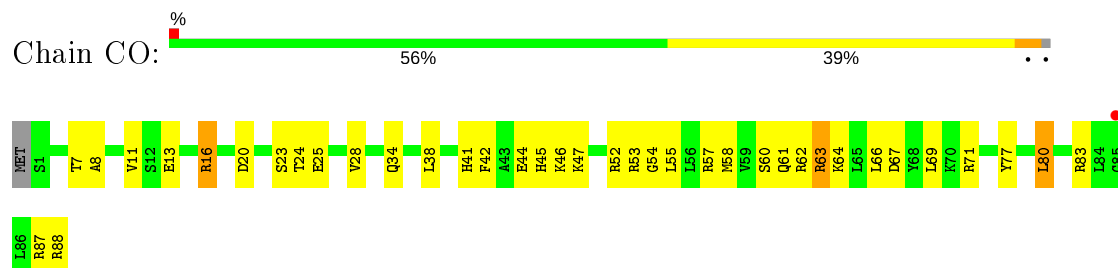
• Molecule 13: 30S ribosomal protein S14



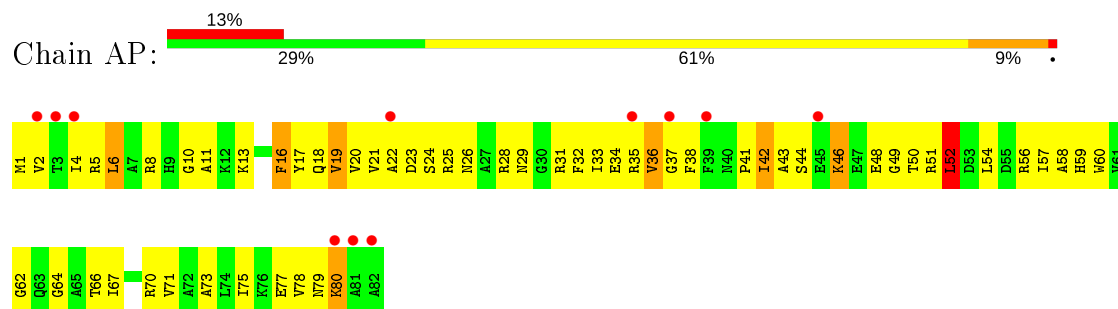
- Molecule 14: 30S ribosomal protein S15



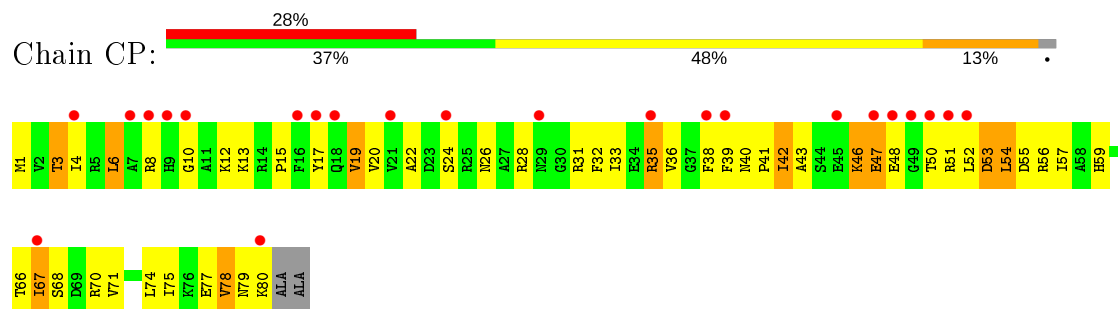
- Molecule 14: 30S ribosomal protein S15



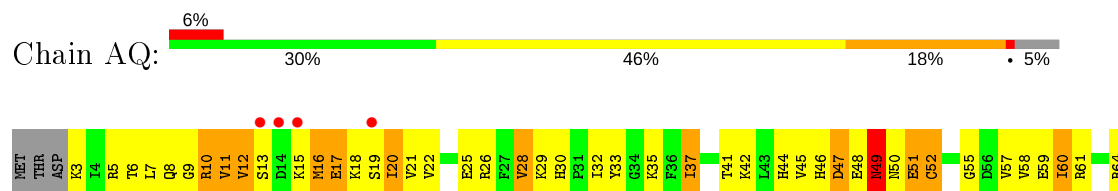
- Molecule 15: 30S ribosomal protein S16



- Molecule 15: 30S ribosomal protein S16

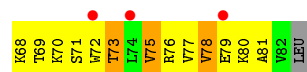


- Molecule 16: 30S ribosomal protein S17

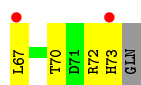
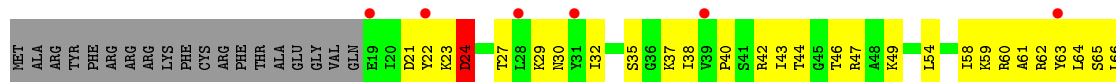




- Molecule 16: 30S ribosomal protein S17



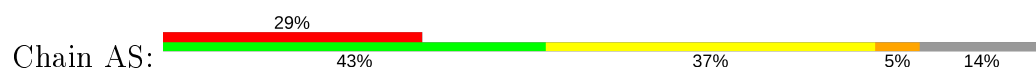
- Molecule 17: 30S ribosomal protein S18



- Molecule 17: 30S ribosomal protein S18

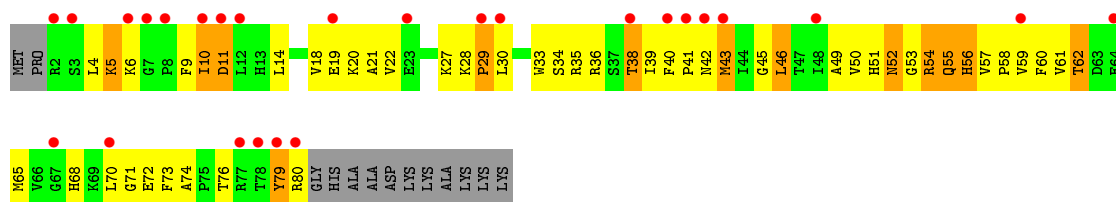


- Molecule 18: 30S ribosomal protein S19



- Molecule 18: 30S ribosomal protein S19





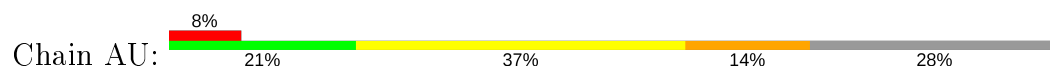
• Molecule 19: 30S ribosomal protein S20



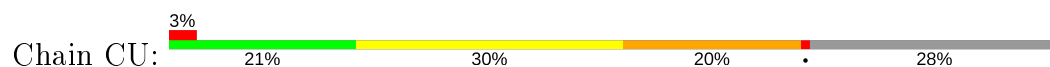
• Molecule 19: 30S ribosomal protein S20



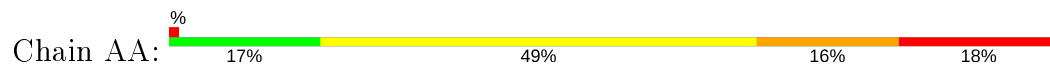
• Molecule 20: 30S ribosomal protein S21



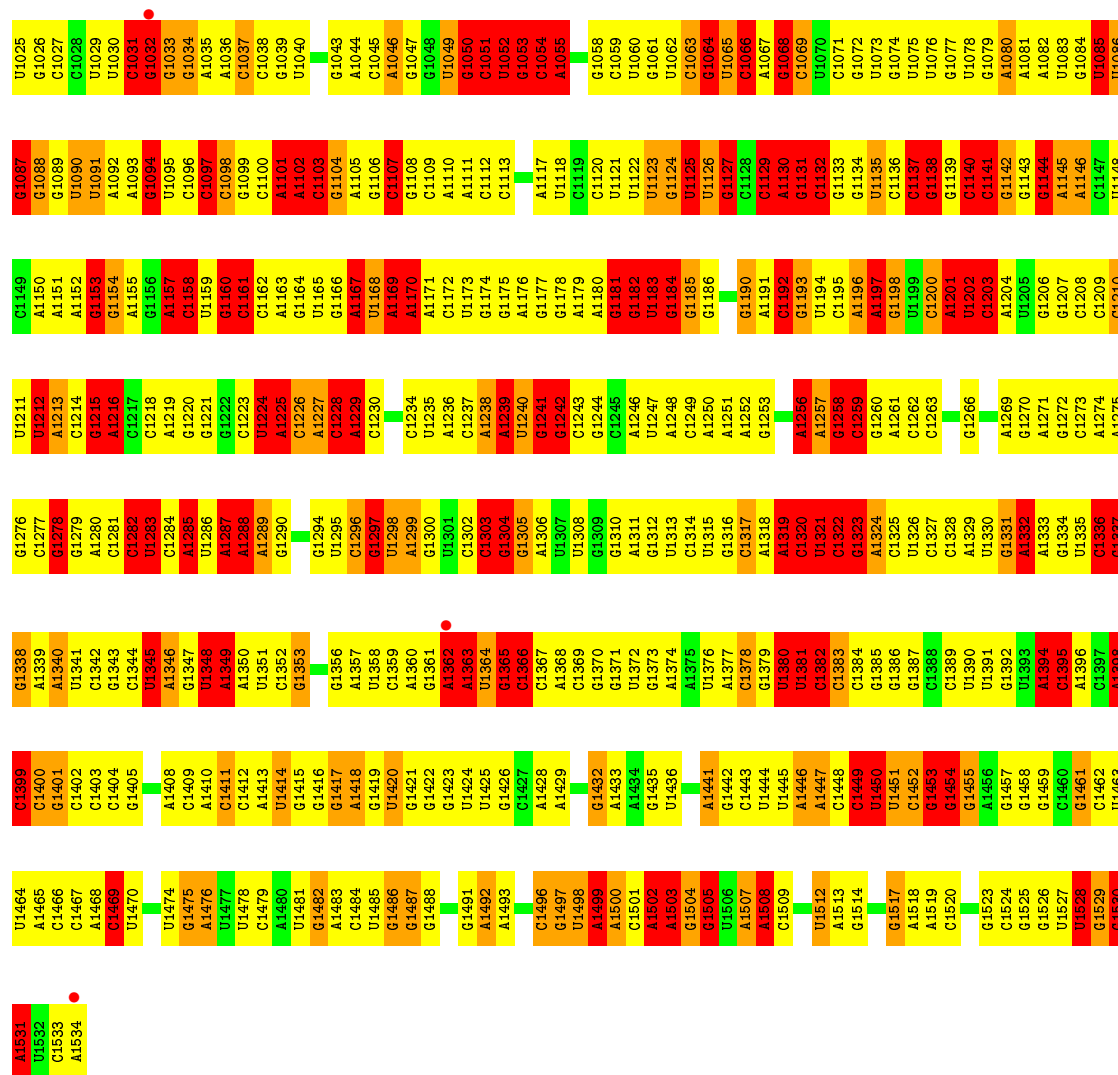
• Molecule 20: 30S ribosomal protein S21

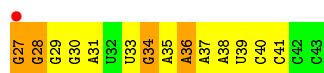


• Molecule 21: 16S rRNA

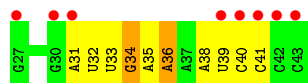
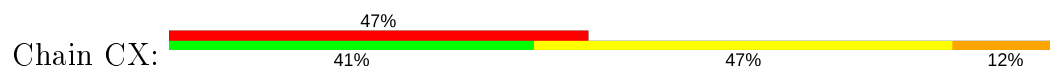


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A958	G895	U828	G765	G703	U638	U571	C511	G449	A383	C316	U252	A189	G126	A3
A959	G896	G829	A766	A704	G839	A572	U512	G450	G384	U317	A253	A190	G127	U4
U960	C937	G830	A767	G705	A640	A573	C513	G451	C385	G318	G254	G191	G128	U5
U961	G897	A831	A768	A706	U641	A574	G514	A452	C386	G319	G255	A192	A129	G6
G962	G898	G832	G769	G707	A642	G575	G515	G453	U387	A320	U256	C193	A130	A7
G963	A900	G833	C770	C708	C643	C576	U516	G454	G388	A321		C194	A131	A8
A964	G901	U834		U709	U644	C577	C517	G455	A389			A195	A132	G9
U965	G902	U835	G774	G710	G645	C578	C518	A456	U390	G324	G260	A196	U133	G10
G966	G903		G775	G711	G646		G391			A325	U261	A197	G134	G11
A968						C580	A520	U458		G326	A262	G198	C135	U12
A969	U904	G838	G778	G713	G650	G581	G521	A459	G394	A327	A263	A199	G138	U13
	A908	C840	C779	G714	C851	C582	C522	A460	C395	C328	G264	G200	U14	U14
A909		U852	A780	A715	U852	A583	A523	A461	C396	A329	G265	G201	A139	G15
C910	A910	U853	A781	A716	U853		G524	A462	C397	C330	G266	G202	U140	A16
U911	U911	U843	A782	U717	G654	C586	C525	U463	U398	C331	A267	G203	G141	U17
A912	C912	G844	A783	A718	A855	G587	C526	U464		G332	U268	G204	G142	C18
A975	A913	A845	A784	C719	G856	G588	G527	A465	C401	U333	C269	A205	A143	A19
G976	A914	G846	G785	C720	U657	U589	C528	A466	G402	C334	A270	C206	G144	U20
A977	A915	G847	G786	G721	C658	U590	G529	U467	G403	C335	C271	C207	G145	G21
A978	U916	C848	A787	G722			G530	A468		A336	C272	U208	G146	G22
C979	G917	G849	U788	U723	U662	U594	U531	C469	G406	G337	U273	U209	G147	C23
C980	A918		U789	G724	A663	A595	A532	C470	U407	A338	A274	G211	G148	U24
U981	A919	G852	A790	G725	G664	A596	A533	U471	A408	C339	G275	G212		C25
U982	U920	C853	G791	C726	A665	G597	U534	U472	U409	U340	G276	G213	A151	A26
A983	U921	U854	G792	G727	G666	U598	A535	U473	G410	C341	C277	G214		
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U986	C924	C857	G795	G731	G669	G601	G538		G413	A344	C280	U216	C156	G31
G987	G925	G858	C796	G732	G670	A602	A539	U479	A414	C345	C281	U217	U157	A32
G988	G926	G859	C797	G733	G671	U603	G540	U480	A415	G346	A282	U218	G158	A33
	G927	A860	U798	G734	U672	G604	G541	A481	G416	G347	U283	U219	G159	C34
					A673		G542	A482	G417	G348	C284	G220	A160	C35
U991	G928		G799	G735	A675	U605	G543	A483	U420	A349	C285		A161	G36
U992	G929	C866	U800	G736	G674	G606	U543	C484	G418	G350		A223	A162	U37
G993	C930	G867	G801	C737	A675	A607	G544	G484	C419			G224	G163	G38
A994	C931	C868	A802	C738	A676	A608	C545	U485	G425	C351	G289	G225	G164	G39
		G869	G803	C739	U677	A609	A546	U486	U421	C352	C290	G226	G165	C40
		U870	U804	U740	U678	U610	A547	A487	C422	A353	U291	G227	G166	C41
							G548	C488	G423	G354		A228	A167	G42
G995	C936	A871	C805	G741	C679		C549	C489	G424	C355	U294	U229	G168	C43
U997	A937	A872	C806	G742	C880	C613	G550	G490	G425	A356	U296	G230	G169	A44
		G873	A807	C737	A675	G614	G551	G491	U426		G297	U231	U170	A45
A998	A938	G874	C808	C744	G682	G615	U551	C492	G427	G360		G232	A171	G46
G999	G939	U875	G809	G745	G683	G616	U552	A493	G428		A298	G233	A172	C47
	C940	C876	C810	A746	U684		A553	G494	U429	A364	G299	C234	U173	C48
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A1004	G942	A878	G812	G748	U686		U555	A496	A431	A366	G301	C236	C175	A50
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G1006	G944	C880	A814	C750	G688	C823	G557	G497	G434	G368	G303	G237	G177	C52
U1007		G881	A815	U751	C689	G624	G558	A498	U435	U369	U304		G178	A53
U1008	G945		A816	G752	A559	U625	A559	A499	A436	C370	G305	G240	C179	C54
	A946		C817	A753	A560	G626	A560	G500	C436	A371	A306		A179	
G1010	G947		G818	C754	U561	G627	U561	C501	U437	C372	A243		U180	G57
A1015	C948	G885	U819	C755	G628	G628	A502	A502	U438	A373	C308	U244	A181	C58
U1017	A949	G886	A820	G756	A629	G629	C503	G503	U439	A374	A309	U245	A182	C59
	G951	G887	G821	U757	A630	G631	C504	G504	C440	U375	G310	G247	A120	A60
		G888	U822		A695	C631	G505	G505	A441	G376	C311	C248	C183	A59
G1020	U952	A889					U565	G506			C312	U249	G184	A61
A1021	G953	G890	C823	G760	U697	U632	G566	G507	G445	G380	A313	C249	U185	A62
G954		A892	A825	U761	G700	G633	G567	U508	G446	C381	C314		G187	C63
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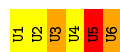
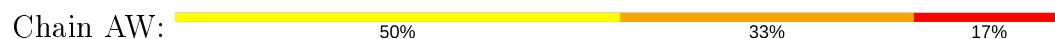




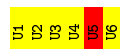
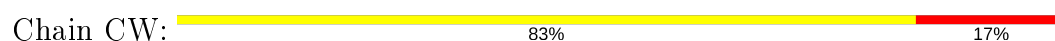
- Molecule 22: P-site tRNA ASL fragment



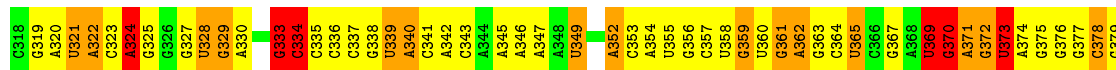
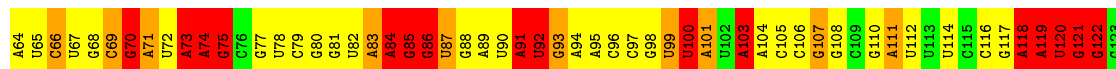
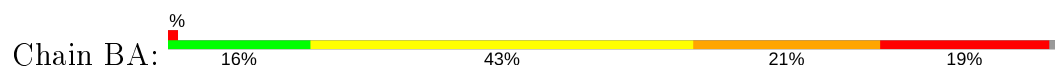
- Molecule 23: messenger RNA



- Molecule 23: messenger RNA

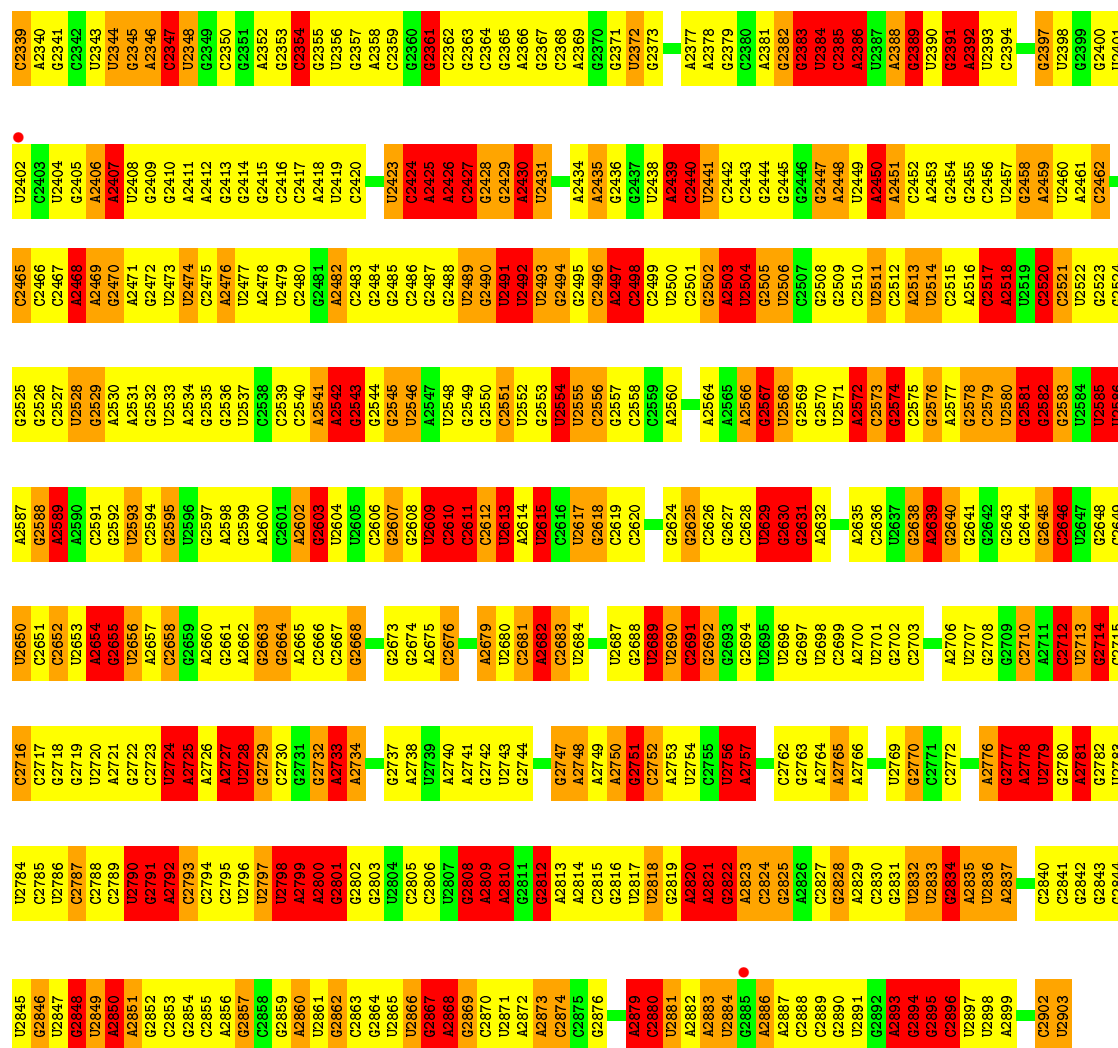


- Molecule 24: 23S rRNA

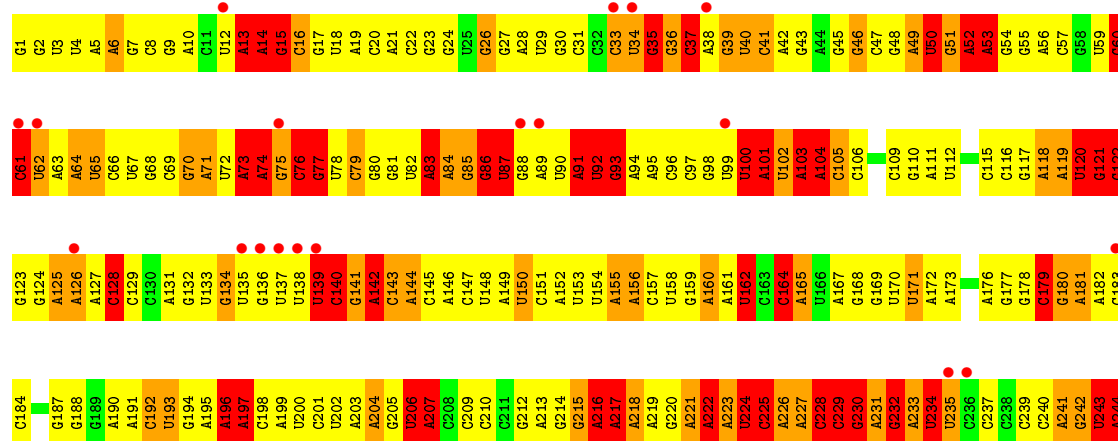
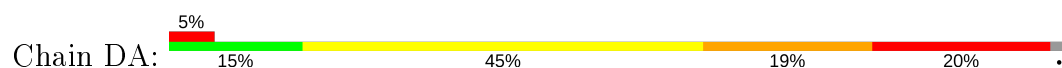


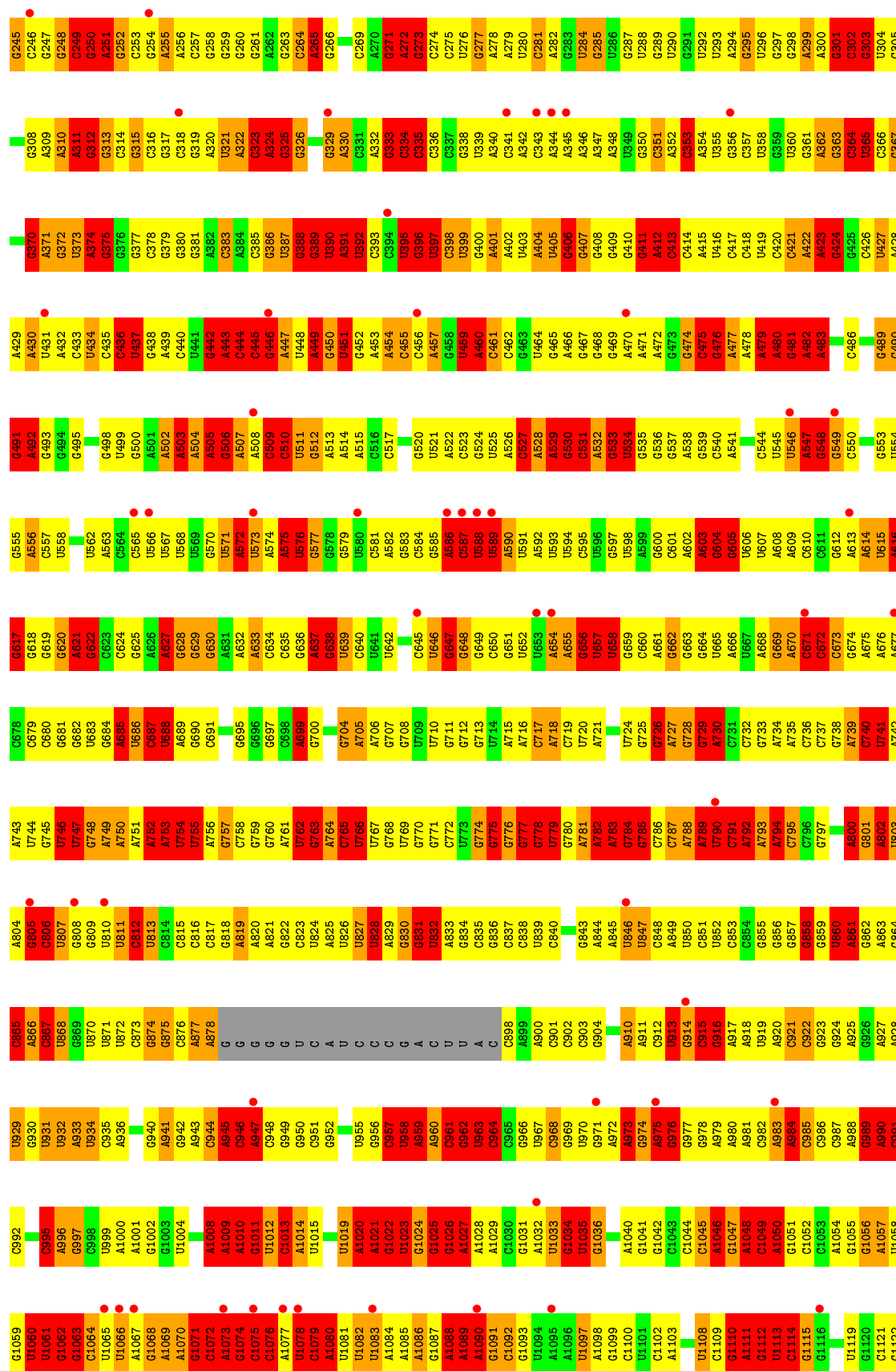


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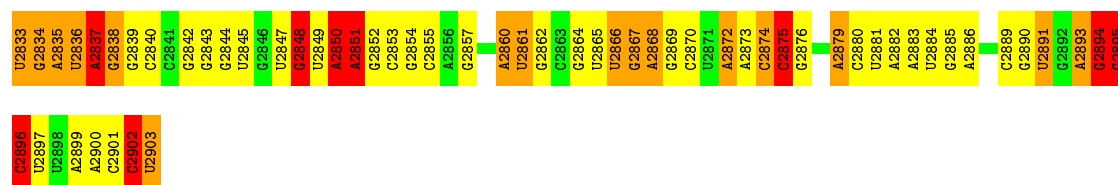
• Molecule 24: 23S rRNA





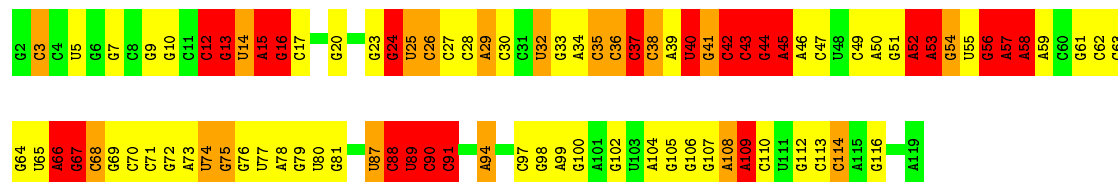
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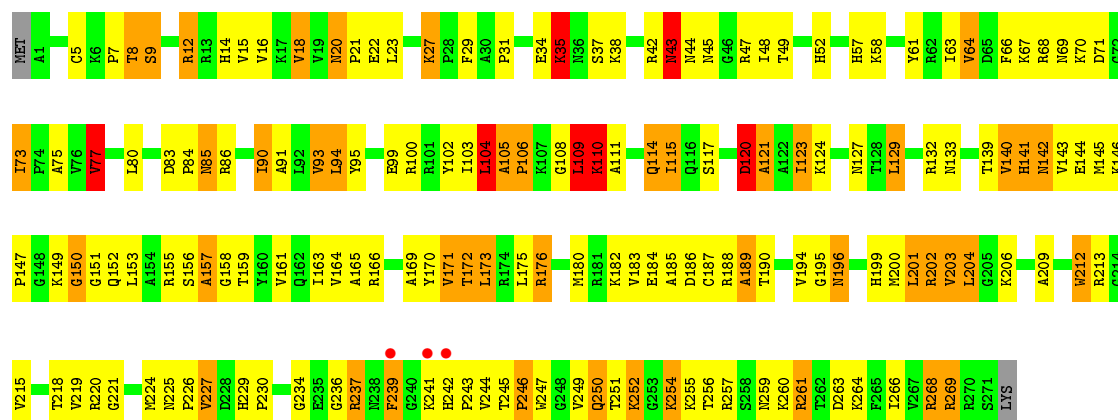
• Molecule 25: 5S rRNA

Chain BB: 24% 42% 15% 19%



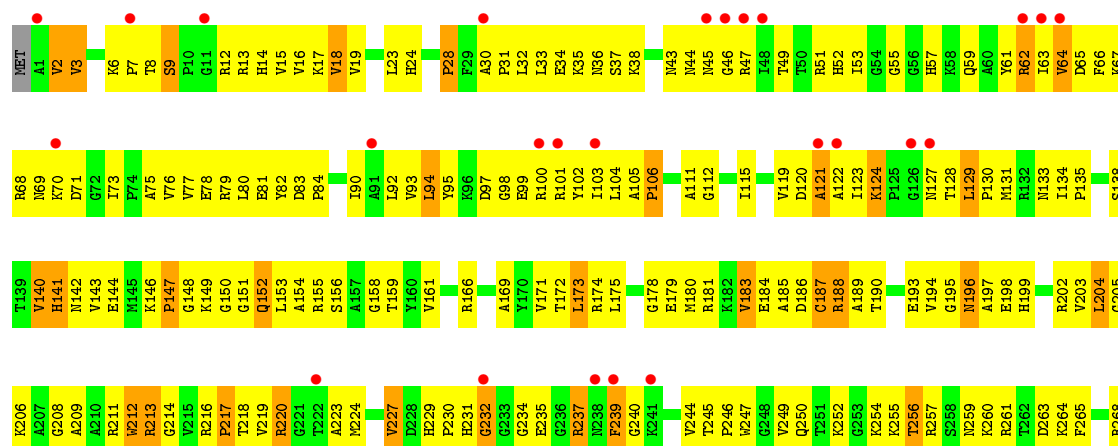
• Molecule 26: 50S ribosomal protein L2

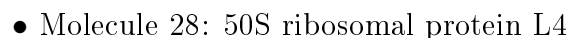
Chain BC: 38% 42% 16%

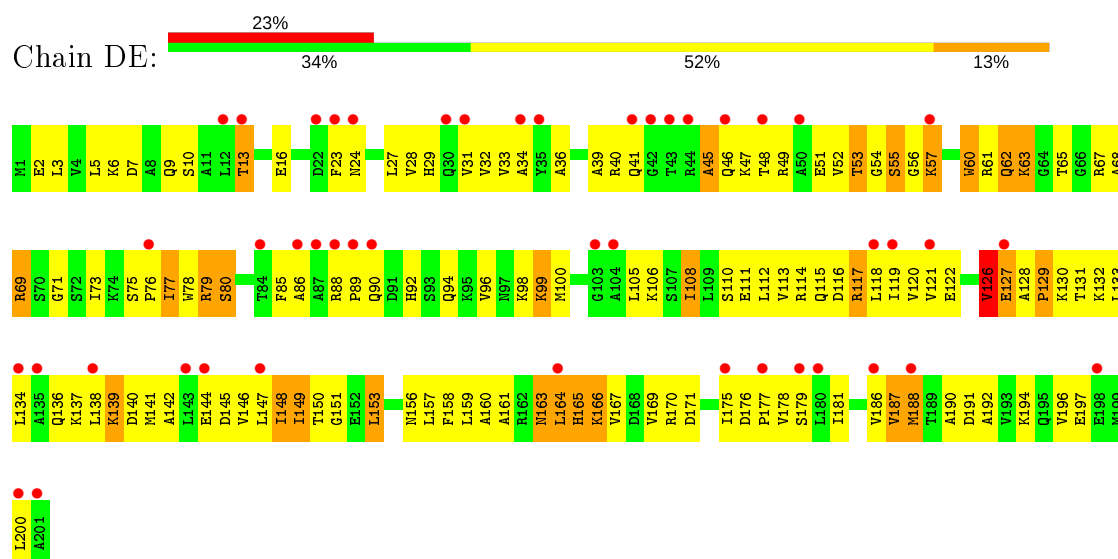


• Molecule 26: 50S ribosomal protein L2

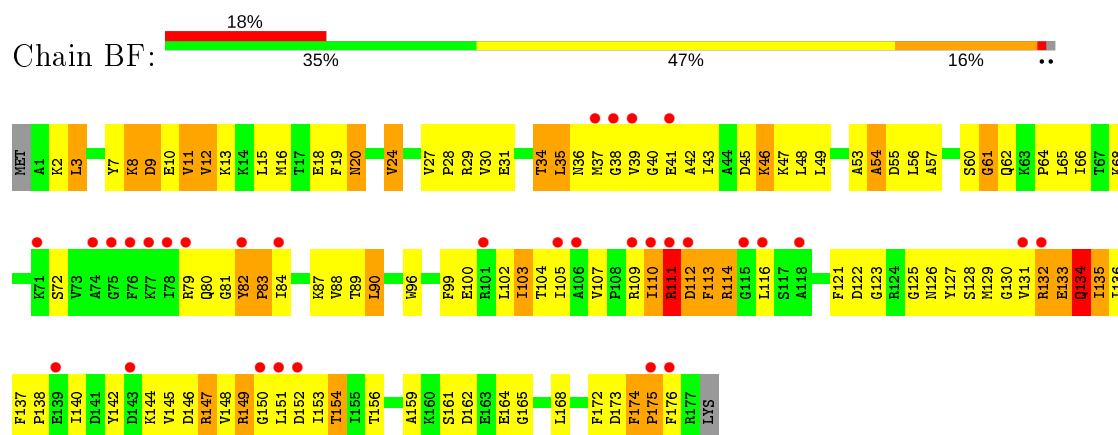
Chain DC: 9% 32% 56% 11%



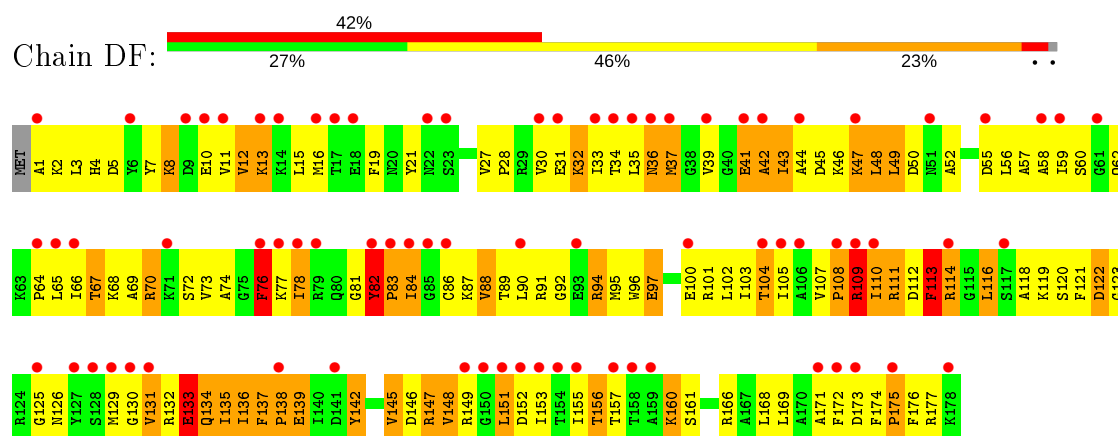


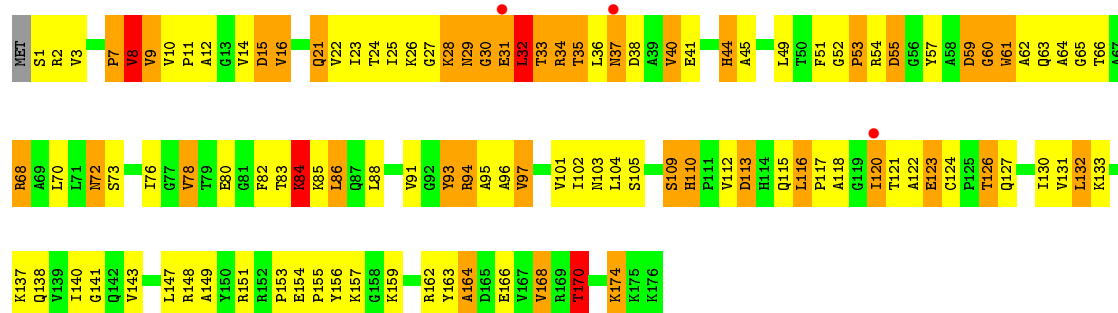


• Molecule 29: 50S ribosomal protein L5

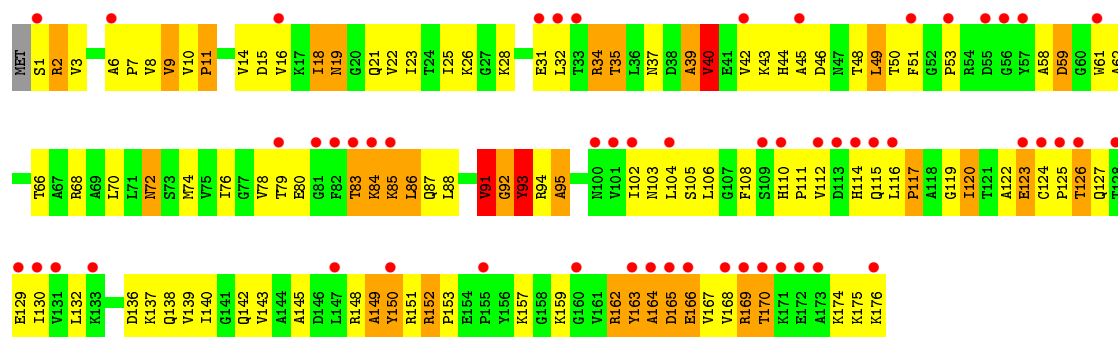


• Molecule 29: 50S ribosomal protein L5

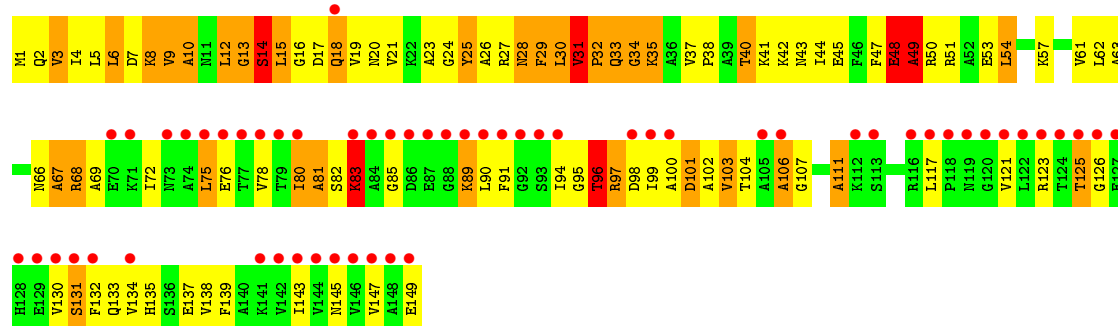




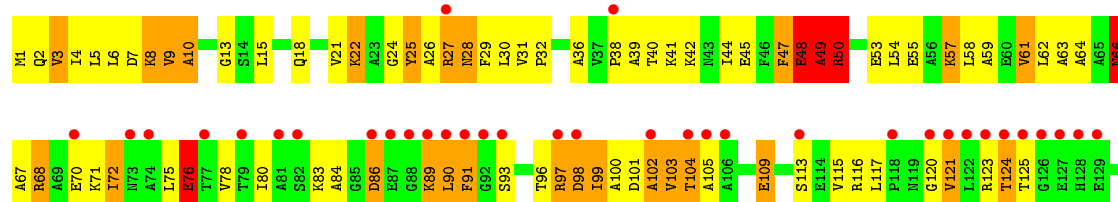
• Molecule 30: 50S ribosomal protein L6

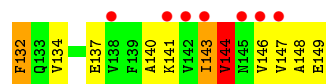


• Molecule 31: 50S ribosomal protein L9

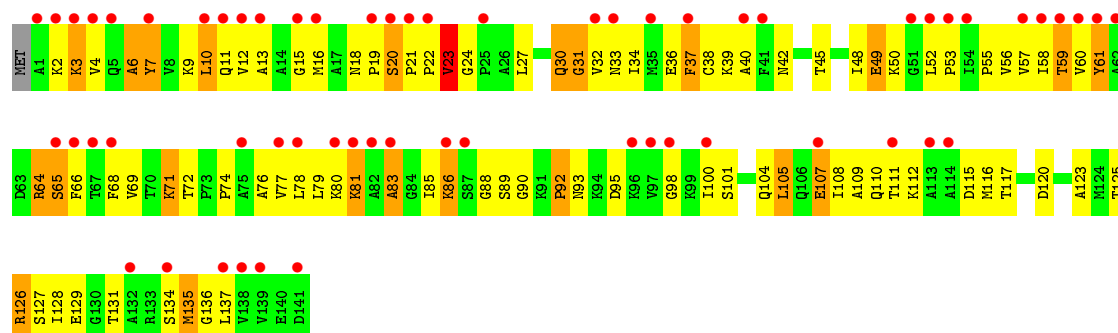
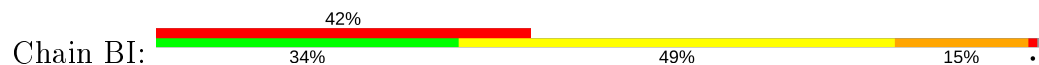


• Molecule 31: 50S ribosomal protein L9

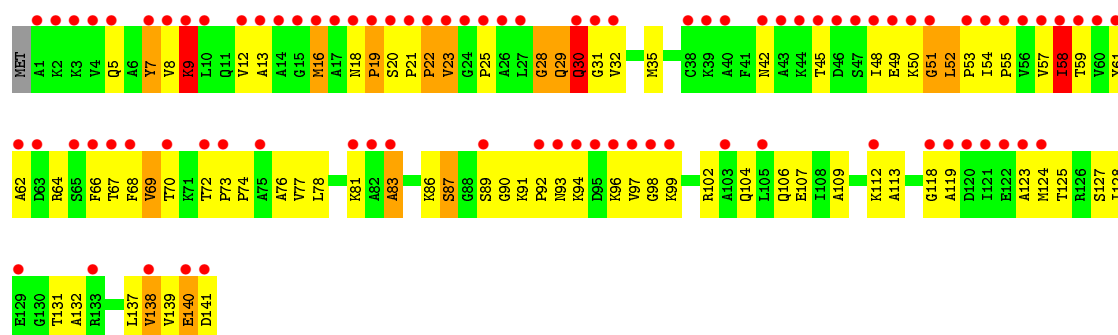
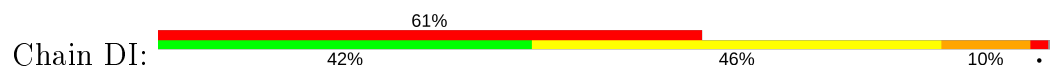




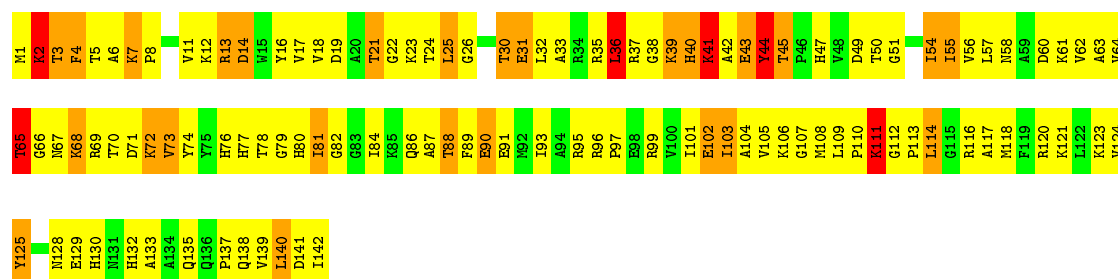
- Molecule 32: 50S ribosomal protein L11



- Molecule 32: 50S ribosomal protein L11

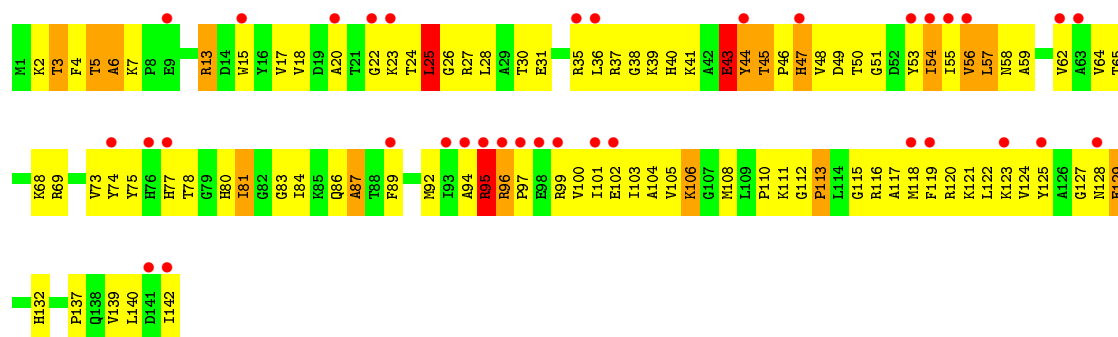


- Molecule 33: 50S ribosomal protein L13

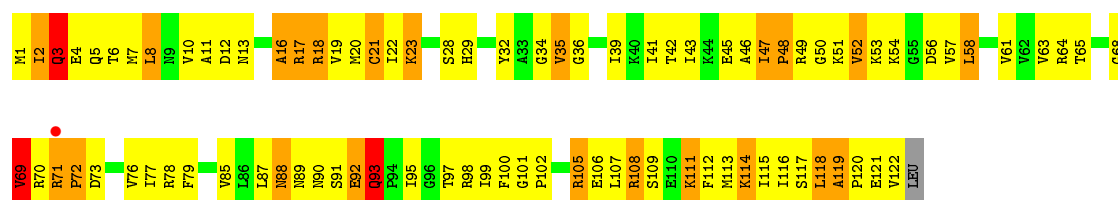


- Molecule 33: 50S ribosomal protein L13

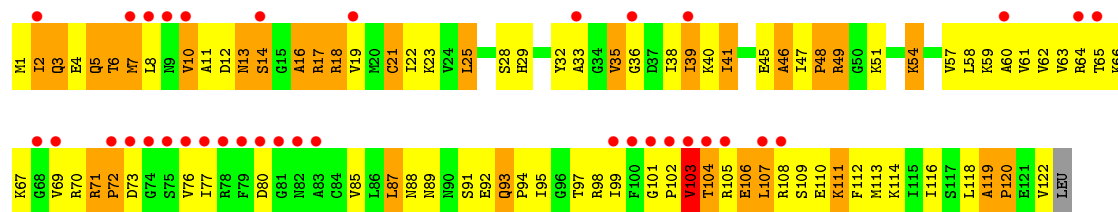




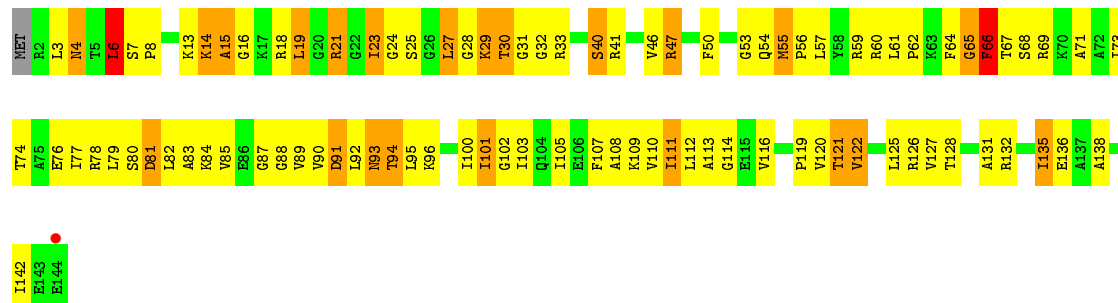
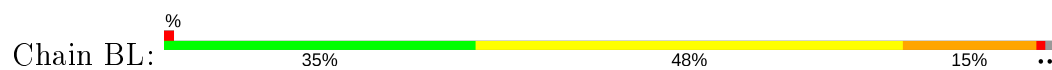
• Molecule 34: 50S ribosomal protein L14



• Molecule 34: 50S ribosomal protein L14

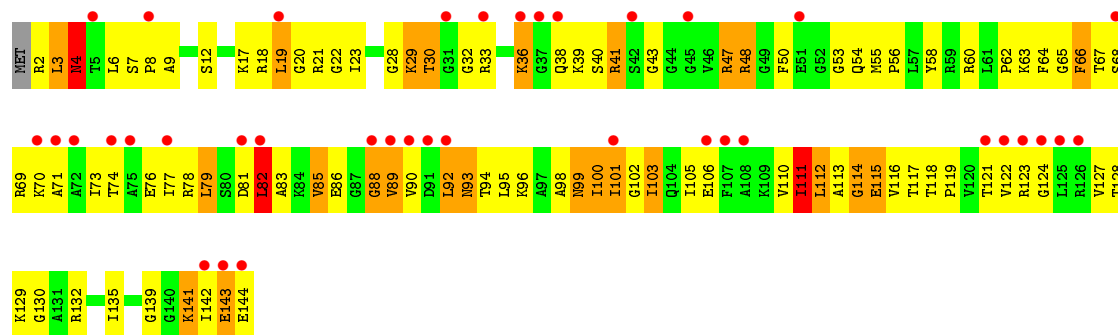


• Molecule 35: 50S ribosomal protein L15

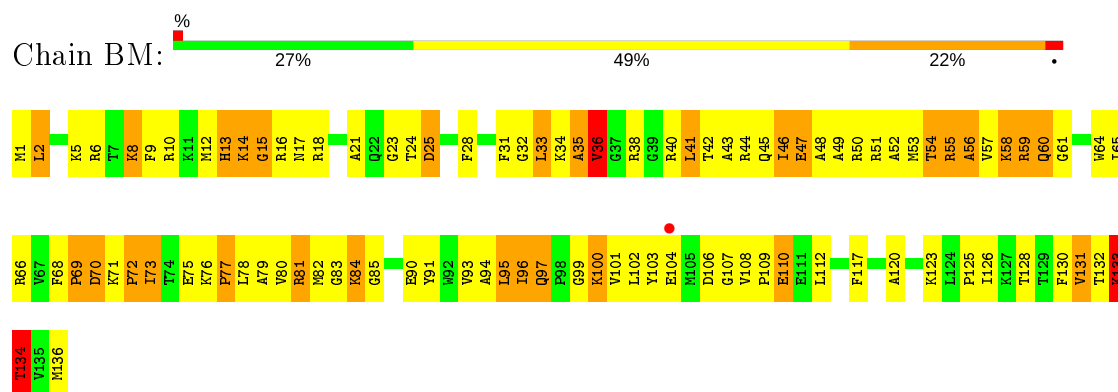


• Molecule 35: 50S ribosomal protein L15

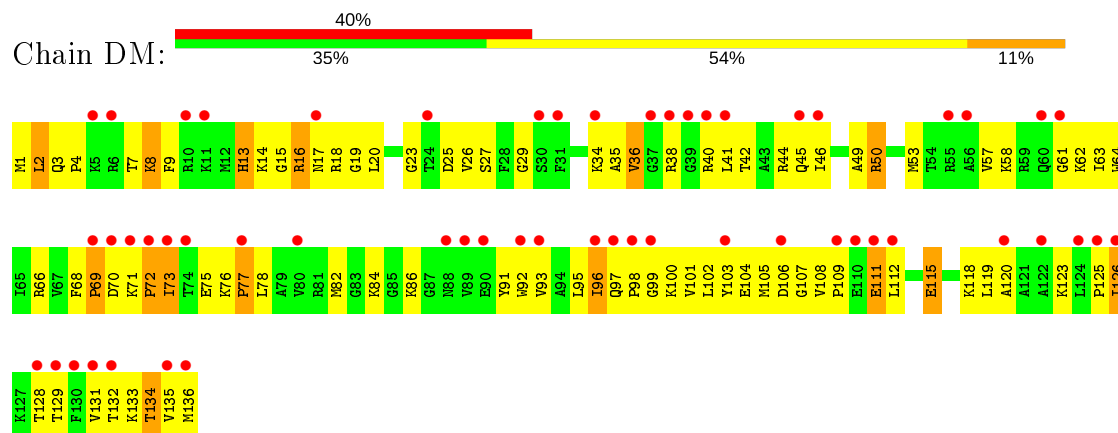




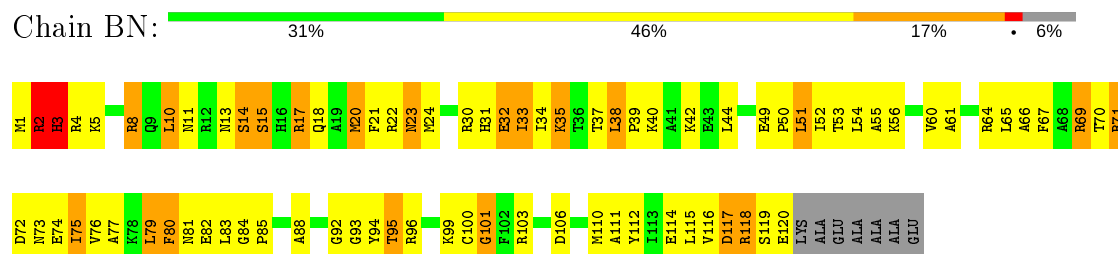
• Molecule 36: 50S ribosomal protein L16



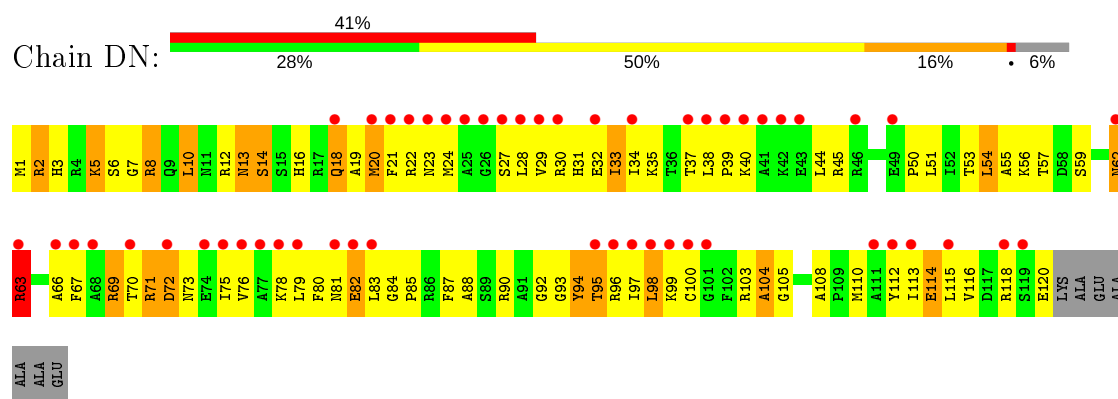
• Molecule 36: 50S ribosomal protein L16



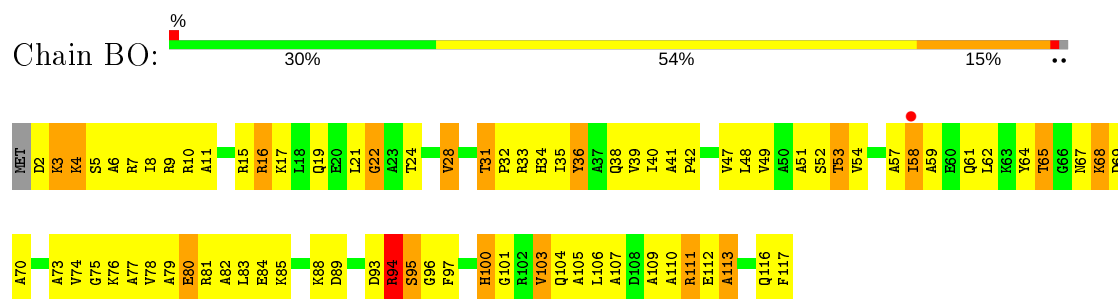
• Molecule 37: 50S ribosomal protein L17



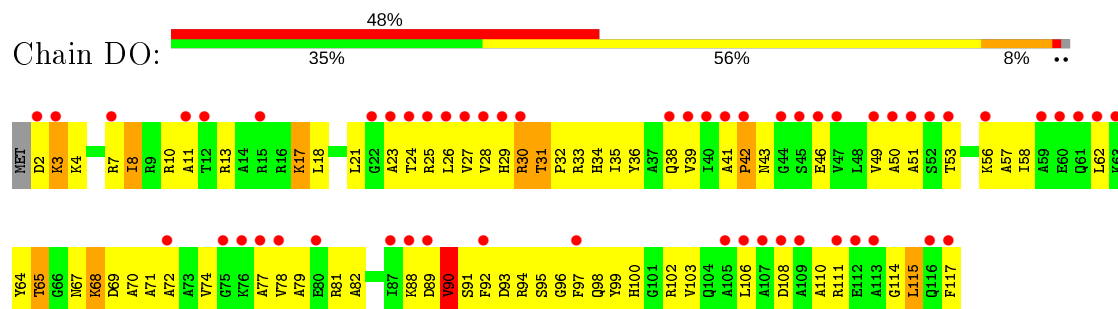
• Molecule 37: 50S ribosomal protein L17



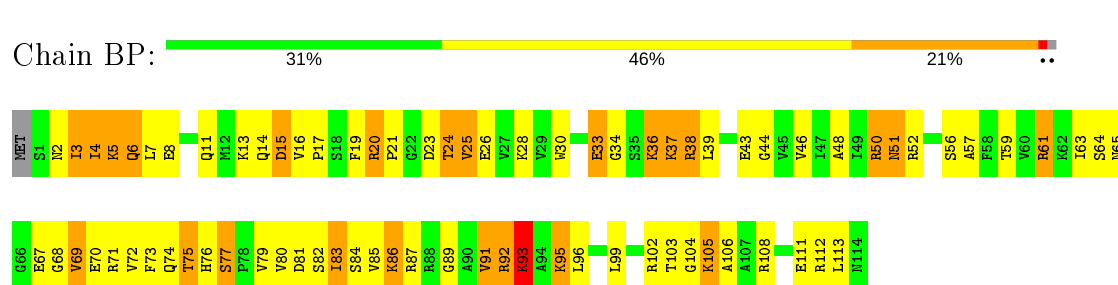
- Molecule 38: 50S ribosomal protein L18



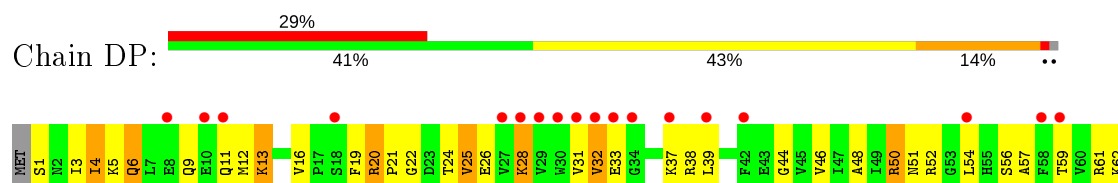
- Molecule 38: 50S ribosomal protein L18



- Molecule 39: 50S ribosomal protein L19

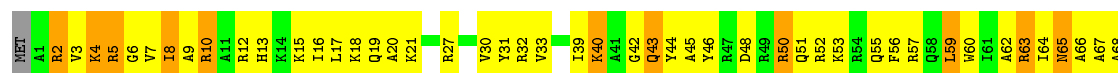
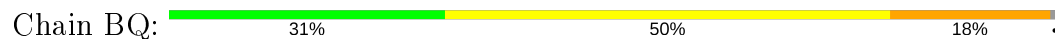


- Molecule 39: 50S ribosomal protein L19

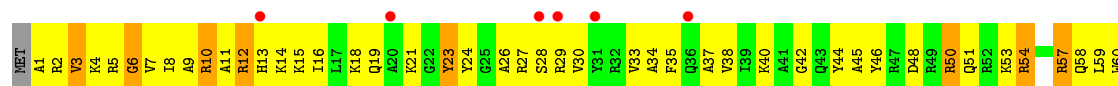




- Molecule 40: 50S ribosomal protein L20



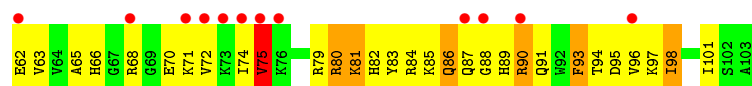
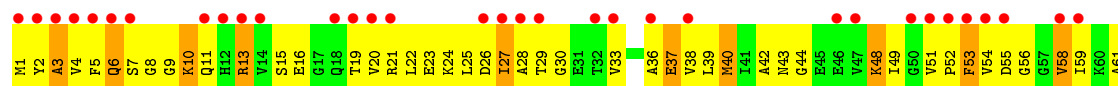
- Molecule 40: 50S ribosomal protein L20



- Molecule 41: 50S ribosomal protein L21

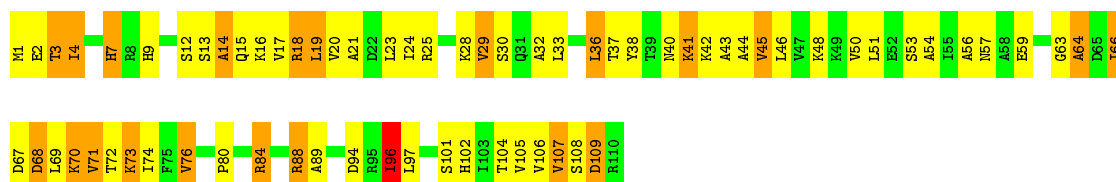


- Molecule 41: 50S ribosomal protein L21

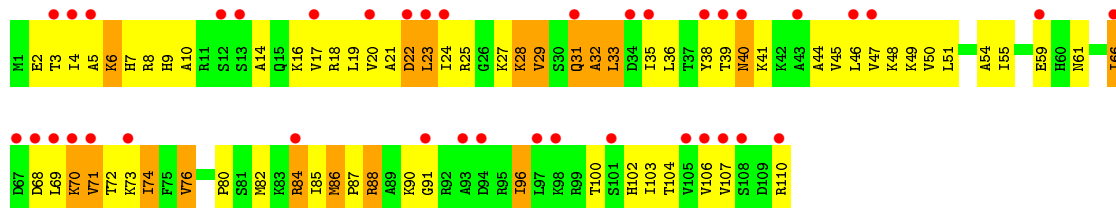


- Molecule 42: 50S ribosomal protein L22

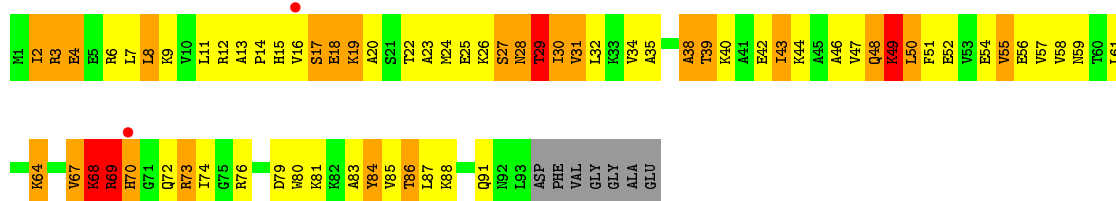
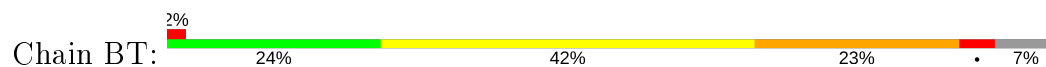




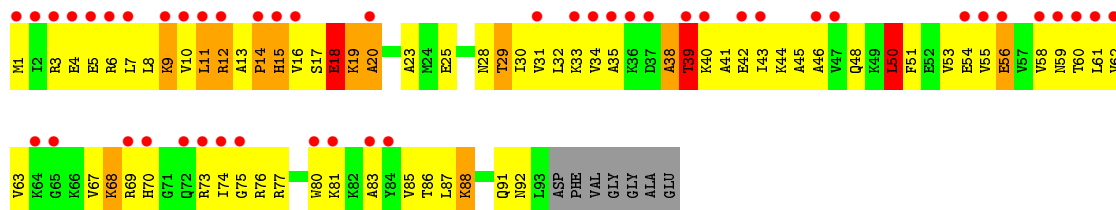
• Molecule 42: 50S ribosomal protein L22



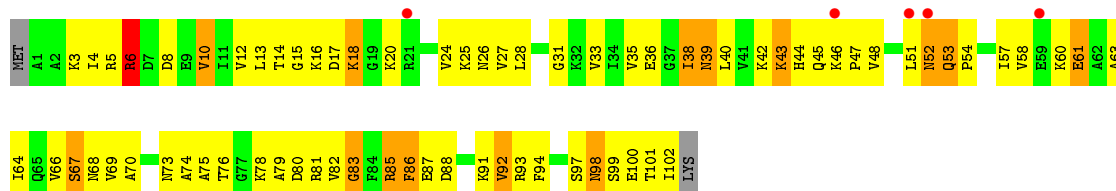
• Molecule 43: 50S ribosomal protein L23



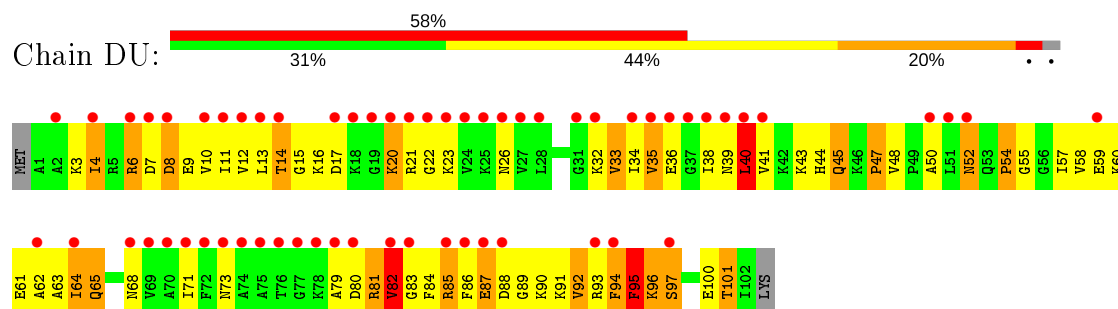
• Molecule 43: 50S ribosomal protein L23



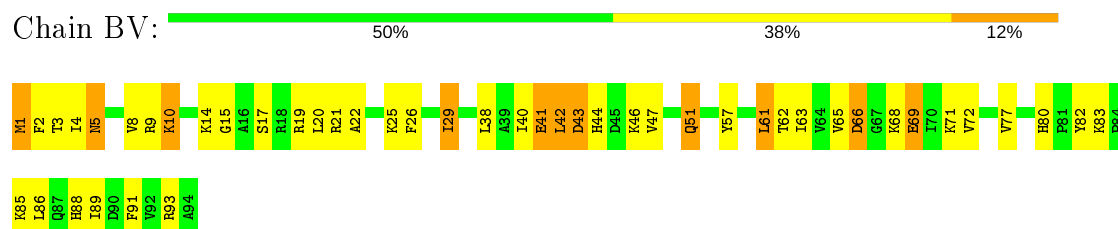
• Molecule 44: 50S ribosomal protein L24



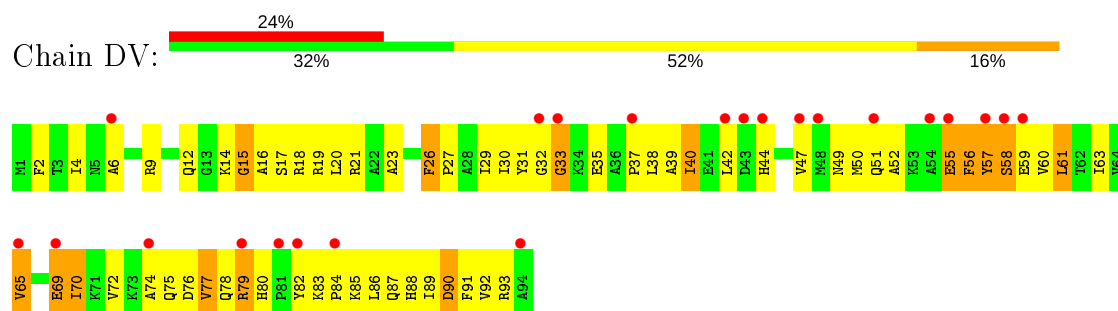
- Molecule 44: 50S ribosomal protein L24



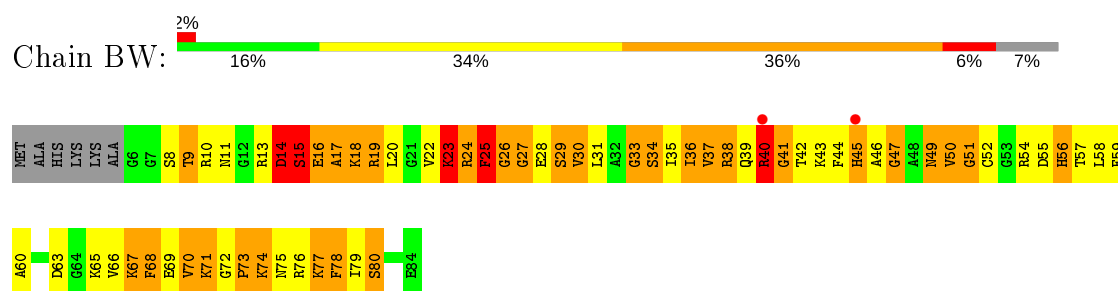
- Molecule 45: 50S ribosomal protein L25



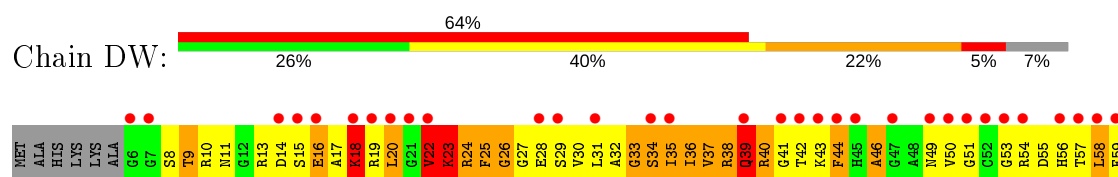
- Molecule 45: 50S ribosomal protein L25

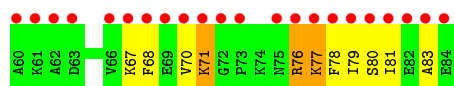


- Molecule 46: 50S ribosomal protein L27



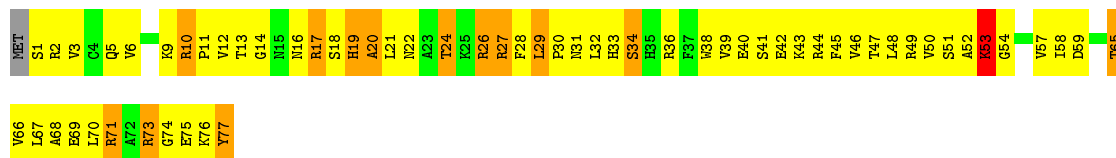
- Molecule 46: 50S ribosomal protein L27





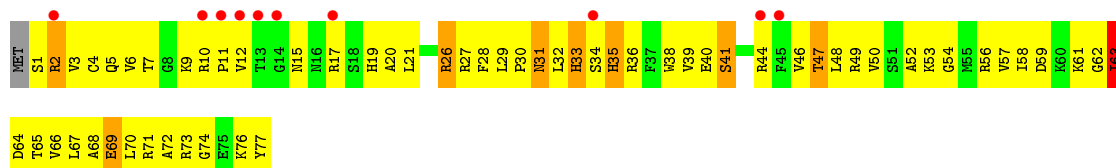
- Molecule 47: 50S ribosomal protein L28

Chain BX: 21% 60% 17% ..



- Molecule 47: 50S ribosomal protein L28

Chain DX: 13% 22% 65% 10% ..



- Molecule 48: 50S ribosomal protein L29

Chain BY: 5% 40% 43% 13% 5%



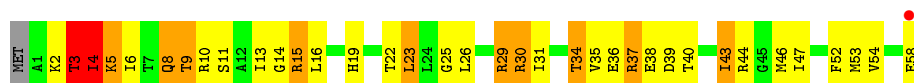
- Molecule 48: 50S ribosomal protein L29

Chain DY: 25% 38% 52% 10%



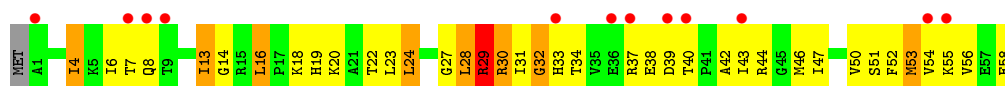
- Molecule 49: 50S ribosomal protein L30

Chain BZ: 2% 37% 41% 17% ..

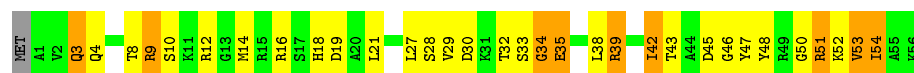


- Molecule 49: 50S ribosomal protein L30

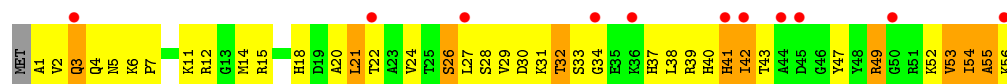
Chain DZ: 20% 34% 49% 14% ..



- Molecule 50: 50S ribosomal protein L32



- Molecule 50: 50S ribosomal protein L32



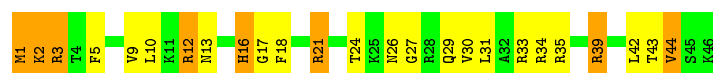
- Molecule 51: 50S ribosomal protein L33



- Molecule 51: 50S ribosomal protein L33



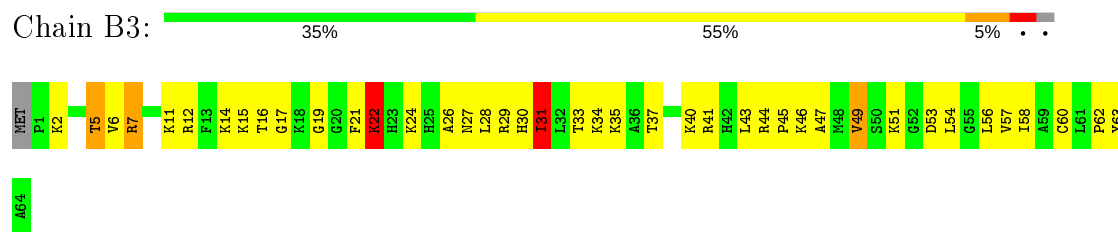
- Molecule 52: 50S ribosomal protein L34



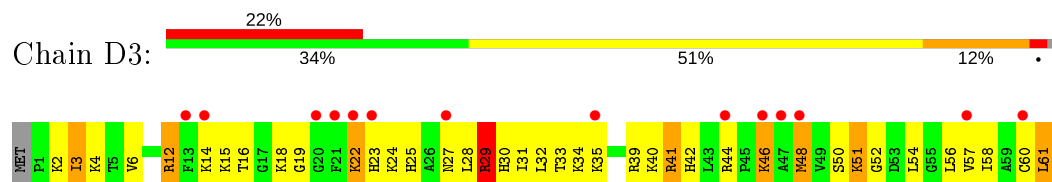
- Molecule 52: 50S ribosomal protein L34



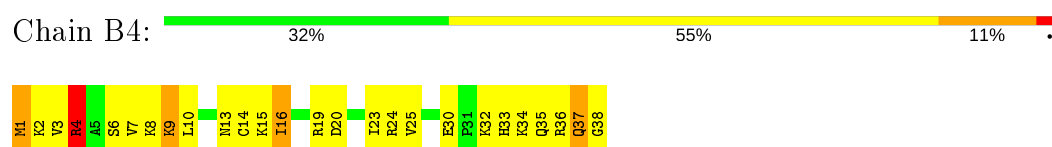
- Molecule 53: 50S ribosomal protein L35



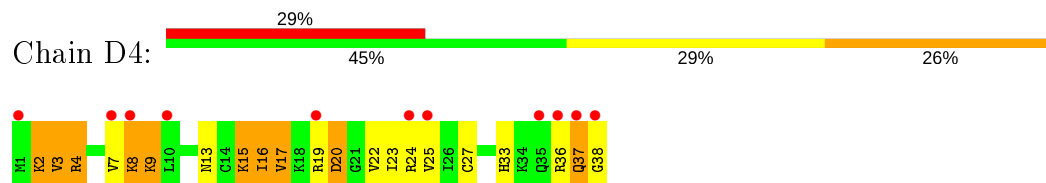
- Molecule 53: 50S ribosomal protein L35



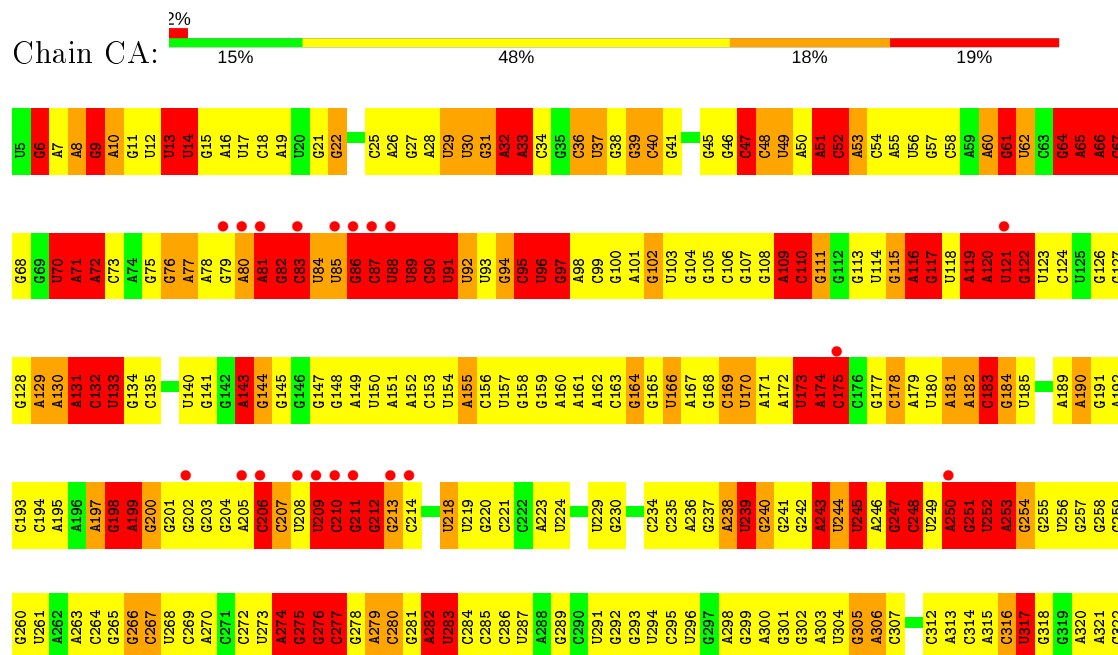
- Molecule 54: 50S ribosomal protein L36



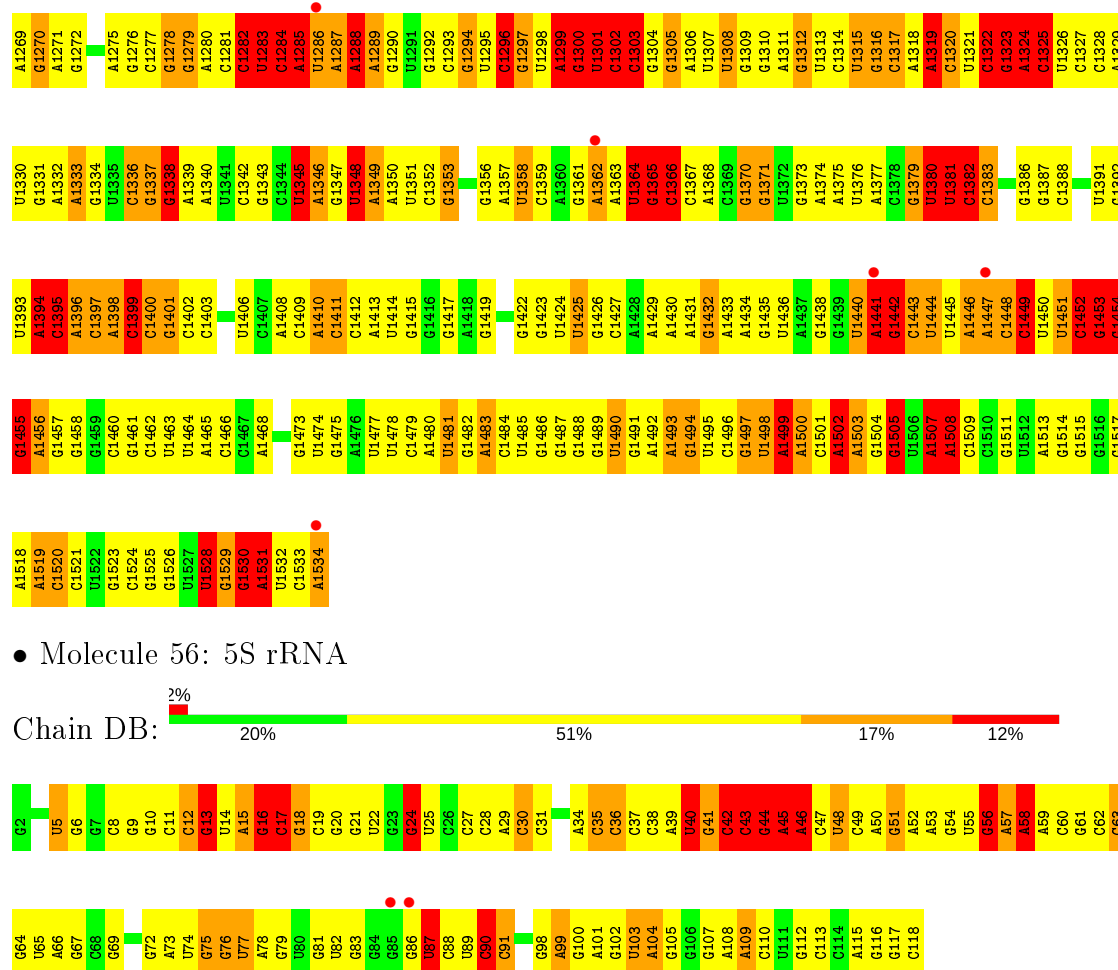
- Molecule 54: 50S ribosomal protein L36



- Molecule 55: 16S rRNA



C1209	C1210	U1211	U1212	A1213	A1214	G1215	G1216	A1217	A1218	A1219	G1220	G1221	C1222	C1223	C1224	A1225	A1226	C1227	C1228	A1229	U1230	C1231	U1232	C1233	C1234	U1235	A1236	C1237	A1238	C1239	U1240	C1241	A1242	U1243	C1244	C1245	A1246	U1247	U1248	C1249	A1250	A1251	C1252	C1253	U1254	C1255	A1256	C1257	U1258	C1259	A1260	C1261	C1262	C1263	A1264	U1265	C1266	C1267																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
U1083	G1084	U1085	U1086	G1087	G1088	G1089	U1090	U1091	A1092	A1093	G1094	U1095	C1096	C1097	C1098	G1099	C1100	A1101	A1102	C1103	G1104	G1105	G1106	G1107	G1108	C1109	G1110	C1111	C1112	U1113	U1114	U1115	U1116	U1117	U1118	C1119	C1120	U1121	U1122	U1123	U1124	U1125	U1126	U1127	C1128	C1129	A1129	C1130	G1131	C1132	G1133	C1134	U1135	C1136	C1137	U1138	G1139	C1140	C1141	C1142	G1143	U1144	C1145	A1146																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
C1147	U1021	U1022	U1023	U1024	U1025	U1026	U1029	U1030	U1031	C1032	G1033	U1034	U1035	C1036	C1037	C1038	C1039	U1040	U1041	A1042	C1043	A1044	C1045	C1046	C1047	U1048	U1049	C1050	C1051	U1052	U1053	C1054	C1055	U1056	C1057	U1058	C1059	U1060	G1061	U1062	C1063	U1064	U1065	C1066	A1067	U1068	C1069	U1070	U1071	C1072	U1073	U1074	U1075	U1076	U1077	U1078	C1079	A1080	U1081	U1082																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
A959	U960	U961	C962	U965	U966	U967	U968	U969	C970	C971	C972	U973	U974	U975	U976	U977	U978	U979	U980	U981	U982	U983	U984	U985	U986	U987	U988	U989	U990	U991	U992	U993	U994	C995	U996	U997	U998	U999	U1000	C1001	C1002	U1003	U1004	C1005	U1006	U1007	U1008	U1009	U1010	C1011	A1012	C1013	C1014	C1015	U1016	U1017	U1018	U1019	U1020																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
U891	A892	C893	C894	C895	C896	C897	C898	A900	A901	A902	A903	A904	A905	A906	A907	A908	A909	C910	U911	C912	A913	A914	A915	U916	U917	U918	U919	U920	U921	U922	A923	C924	U925	U926	U927	U928	U929	C930	C931	U932	C933	C934	A935	C936	C937	U938	U939	U940	U941	U942	U943	U944	U945	U946	U947	U948	U949	U950	U951	U952	U953	U954	U955	U956	U957	U958	U959																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
A704	C705	A706	U707	C708	U709	U710	U711	U712	U713	U714	A715	A716	U717	U718	U719	A720	U721	U722	U723	U724	U725	C726	U727	A728	U729	C730	U731	C732	U733	U734	C735	U736	U737	U738	U739	U740	C741	U742	A743	C744	U745	U746	U747	U748	U749	U750	U751	U752	A753	U754	U755	U756	U757	U758	U759	U760	U761	U762	U763	U764	U765	U766	U767	U768	U769	U770	U771	U772	U773	U774	U775	U776	U777	U778	U779	U780	U781	U782	U783	U784	U785	U786	U787	U788	U789	U790	U791	U792	U793	U794	U795	U796	U797	U798	U799	U800	U801	U802	U803	U804	U805	U806	U807	U808	U809	U810	U811	U812	U813	U814	U815	U816	U817	U818	U819	U820	U821	U822	U823	U824	U825	U826	U827	U828	U829	U830	U831	U832	U833	U834	U835	U836	U837	U838	U839	U840	U841	U842	U843	U844	U845	U846	U847	U848	U849	U850	U851	U852	U853	U854	U855	U856	U857	U858	U859	U860	U861	U862	U863	U864	U865	U866	U867	U868	U869	U870	U871	U872	U873	U874	U875	U876	U877	U878	U879	U880	U881	U882	U883	U884	U885	U886	U887	U888	U889	U890	U891	U892	U893	U894	U895	U896	U897	U898	U899	U900	U901	U902	U903	U904	U905	U906	U907	U908	U909	U910	U911	U912	U913	U914	U915	U916	U917	U918	U919	U920	U921	U922	U923	U924	U925	U926	U927	U928	U929	U930	U931	U932	U933	U934	U935	U936	U937	U938	U939	U940	U941	U942	U943	U944	U945	U946	U947	U948	U949	U950	U951	U952	U953	U954	U955	U956	U957	U958	U959	U960	U961	U962	U963	U964	U965	U966	U967	U968	U969	U970	U971	U972	U973	U974	U975	U976	U977	U978	U979	U980	U981	U982	U983	U984	U985	U986	U987	U988	U989	U990	U991	U992	U993	U994	U995	U996	U997	U998	U999	U1000	U1001	U1002	U1003	U1004	U1005	U1006	U1007	U1008	U1009	U1010	U1011	U1012	U1013	U1014	U1015	U1016	U1017	U1018	U1019	U1020	U1021	U1022	U1023	U1024	U1025	U1026	U1027	U1028	U1029	U1030	U1031	U1032	U1033	U1034	U1035	U1036	U1037	U1038	U1039	U1040	U1041	U1042	U1043	U1044	U1045	U1046	U1047	U1048	U1049	U1050	U1051	U1052	U1053	U1054	U1055	U1056	U1057	U1058	U1059	U1060	U1061	U1062	U1063	U1064	U1065	U1066	U1067	U1068	U1069	U1070	U1071	U1072	U1073	U1074	U1075	U1076	U1077	U1078	U1079	U1080	U1081	U1082	U1083	U1084	U1085	U1086	U1087	U1088	U1089	U1090	U1091	U1092	U1093	U1094	U1095	U1096	U1097	U1098	U1099	U1100	U1101	U1102	U1103	U1104	U1105	U1106	U1107	U1108	U1109	U1110	U1111	U1112	U1113	U1114	U1115	U1116	U1117	U1118	U1119	U1120	U1121	U1122	U1123	U1124	U1125	U1126	U1127	U1128	U1129	U1130	U1131	U1132	U1133	U1134	U1135	U1136	U1137	U1138	U1139	U1140	U1141	U1142	U1143	U1144	U1145	U1146	U1147	U1148	U1149	U1150	U1151	U1152	U1153	U1154	U1155	U1156	U1157	U1158	U1159	U1160	U1161	U1162	U1163	U1164	U1165	U1166	U1167	U1168	U1169	U1170	U1171	U1172	U1173	U1174	U1175	U1176	U1177	U1178	U1179	U1180	U1181	U1182	U1183	U1184	U1185	U1186	U1187	U1188	U1189	U1190	U1191	U1192	U1193	U1194	U1195	U1196	U1197	U1198	U1199	U1200	U1201	U1202	U1203	U1204	U1205	U1206	U1207	U1208	U1209	U1210	U1211	U1212	U1213	U1214	U1215	U1216	U1217	U1218	U1219	U1220	U1221	U1222	U1223	U1224	U1225	U1226	U1227	U1228	U1229	U1230	U1231	U1232	U1233	U1234	U1235	U1236	U1237	U1238	U1239	U1240	U1241	U1242	U1243	U1244	U1245	U1246	U1247	U1248	U1249	U1250	U1251	U1252	U1253	U1254	U1255	U1256	U1257	U1258	U1259	U1260	U1261	U1262	U1263	U1264	U1265	U1266	U1267	U1268	U1269	U1270	U1271	U1272	U1273	U1274	U1275	U1276	U1277	U1278	U1279	U1280	U1281	U1282	U1283	U1284	U1285	U1286	U1287	U1288	U1289	U1290	U1291	U1292	U1293	U1294	U1295	U1296	U1297	U1298	U1299	U1300	U1301	U1302	U1303	U1304	U1305	U1306	U1307	U1308	U1309	U1310	U1311	U1312	U1313	U1314	U1315	U1316	U1317	U1318	U1319	U1320	U1321	U1322	U1323	U1324	U1325	U1326	U1327	U1328	U1329	U1330	U1331	U1332	U1333	U1334	U1335	U1336	U1337	U1338	U1339	U1340	U1341	U1342	U1343	U1344	U1345	U1346	U1347	U1348	U1349	U1350	U1351	U1352	U1353	U1354	U1355	U1356	U1357	U1358	U1359	U1360	U1361	U1362	U1363	U1364	U1365	U1366	U1367	U1368	U1369	U1370	U1371	U1372	U1373	U1374	U1375	U1376	U1377	U1378	U1379	U1380	U1381	U1382	U1383	U1384	U1385	U1386	U1387	U1388	U1389	U1390	U1391	U1392	U1393	U1394	U1395	U1396	U1397	U1398	U1399	U1400	U1401	U1402	U1403	U1404	U1405	U1406	U1407	U1408	U1409	U1410	U1411	U1412	U1413	U1414	U1415	U1416	U1417	U1418	U1419	U1420	U1421	U1422	U1423	U1424	U1425	U1426	U1427	U1428	U1429	U1430	U1431	U1432	U1433	U1434	U1435	U1436	U1437	U1438	U1439	U1440	U1441	U1442	U1443	U1444	U1445	U1446	U1447	U1448	U1449	U1450	U1451	U1452	U1453	U1454	U1455	U1456	U1457	U1458	U1459	U1460	U1461	U1462	U1463	U1464	U1465	U1466	U1467	U1468	U1469	U1470	U1471	U1472	U1473	U1474	U1475	U1476	U1477	U1478	U1479	U1480	U1481	U1482	U1483	U1484	U1485	U1486	U1487	U1488	U1489	U1490	U1491	U1492	U1493	U1494	U1495	U1496	U1497	U1498	U1499	U1500	U1501	U1502	U1503	U1504	U1505	U1506	U1507	U1508	U1509	U1510	U1511	U1512	U1513	U1514	U1515	U1516	U1517	U1518	U1519	U1520	U1521	U1522	U1523	U1524	U1525	U1526	U1527	U1528	U1529	U1530	U1531	U1532	U1533	U1534	U1535	U1536	U1537	U1538	U1539	U1540	U1541	U1542	U1543	U1544	U1545	U1546	U1547	U1548	U1549	U1550	U1551	U1552	U1553	U1554	U1555	U1556	U1557	U1558	U1559	U1560	U1561	U1562	U1563	U1564	U1565	U1566	U1567	U1568	U1569	U1570	U1571	U1572	U1573	U1574	U1575	U1576	U1577	U1578	U1579	U1580	U1581	U1582	U1583	U1584	U1585	U1586	U1587	U1588	U1589	U1590	U1591	U1592	U1593	U1594	U1595	U1596	U1597	U1598	U1599	U1600	U1601	U1602	U1603	U1604	U1605	U1606	U1607	U1608	U1609	U1610	U1611	U1612	U1613	U1614	U1615	U1616	U1617	U1618	U1619	U1620	U1621	U1622	U1623	U1624	U1625	U1626	U1627	U1628	U1629	U1630	U1631	U1632	U1633	U1634	U1635	U1636	U1637	U1638	U1639	U1640	U1641	U1642	U1643	U1644	U1645	U1646	U1647	U1648	U1649	U1650	U1651	U1652	U1653	U1654	U1655	U1656	U1657	U1658	U1659	U1660	U1661	U1662	U1663	U1664	U1665	U1666	U1667	U1668	U1669	U1670	U1671	U1672	U1673	U1674	U1675	U1676	U1677	U1678	U1679	U1680	U1681	U1682	U1683	U1684



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 , 0.276	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)	0.23 , 85.5	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	0.92	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	0.25	0/1735	0.47	0/2338
1	CB	0.25	0/1735	0.46	0/2338
2	AC	0.27	0/1651	0.48	0/2225
2	CC	0.26	0/1651	0.47	0/2225
3	AD	0.27	0/1665	0.48	0/2227
3	CD	0.30	0/1665	0.50	0/2227
4	AE	0.30	0/1118	0.54	0/1504
4	CE	0.29	0/1118	0.53	0/1504
5	AF	0.26	0/835	0.46	0/1128
5	CF	0.26	0/835	0.46	0/1128
6	AG	0.25	0/1195	0.43	0/1602
6	CG	0.27	0/1187	0.50	0/1591
7	AH	0.27	0/989	0.50	0/1326
7	CH	0.25	0/989	0.47	0/1326
8	AI	0.24	0/1034	0.45	0/1375
8	CI	0.25	0/1034	0.47	0/1375
9	AJ	0.25	0/796	0.48	0/1077
9	CJ	0.24	0/796	0.47	0/1077
10	AK	0.26	0/893	0.48	0/1205
10	CK	0.26	0/893	0.50	0/1205
11	AL	0.33	0/969	0.62	0/1300
11	CL	0.31	0/969	0.53	0/1300
12	AM	0.36	0/892	0.64	3/1193 (0.3%)
12	CM	0.38	0/884	0.53	0/1181
13	AN	0.26	0/785	0.48	0/1043
13	CN	0.25	0/780	0.43	0/1036
14	AO	0.26	0/722	0.48	0/964
14	CO	0.24	0/722	0.46	0/964
15	AP	0.27	0/659	0.46	0/884
15	CP	0.27	0/648	0.47	0/870
16	AQ	0.33	0/657	0.55	0/881
16	CQ	0.26	0/657	0.46	0/881

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AR	0.25	0/462	0.48	0/621
17	CR	0.27	0/462	0.49	0/621
18	AS	0.24	0/652	0.43	0/877
18	CS	0.23	0/652	0.46	0/877
19	AT	0.29	0/671	0.51	0/888
19	CT	0.24	0/671	0.44	0/888
20	AU	0.27	0/430	0.46	0/570
20	CU	0.29	0/430	0.54	0/570
21	AA	0.55	1/36834 (0.0%)	1.44	678/57462 (1.2%)
22	AV	0.59	0/408	1.14	1/634 (0.2%)
22	AX	0.52	0/408	1.04	0/634
22	CV	0.56	0/408	1.14	0/634
22	CX	0.41	0/408	0.82	0/634
23	AW	0.88	0/131	1.88	5/200 (2.5%)
23	CW	0.73	0/131	1.93	7/200 (3.5%)
24	BA	0.76	12/68626 (0.0%)	1.69	1758/107056 (1.6%)
24	DA	0.53	1/68314 (0.0%)	1.46	1365/106569 (1.3%)
25	BB	0.66	0/2828	1.67	74/4410 (1.7%)
26	BC	0.45	0/2121	0.72	1/2852 (0.0%)
26	DC	0.33	0/2121	0.54	0/2852
27	BD	0.50	0/1586	0.75	1/2134 (0.0%)
27	DD	0.31	0/1586	0.55	0/2134
28	BE	0.44	0/1571	0.67	0/2113
28	DE	0.25	0/1571	0.47	0/2113
29	BF	0.41	0/1434	0.68	3/1926 (0.2%)
29	DF	0.35	0/1444	0.73	5/1937 (0.3%)
30	BG	0.43	0/1343	0.65	0/1816
30	DG	0.23	0/1343	0.46	0/1816
31	BH	0.70	6/1122 (0.5%)	0.83	6/1515 (0.4%)
31	DH	0.53	3/1122 (0.3%)	0.67	3/1515 (0.2%)
32	BI	0.24	0/1046	0.50	0/1410
32	DI	0.23	0/1046	0.44	0/1410
33	BJ	0.55	0/1152	0.75	0/1551
33	DJ	0.28	0/1152	0.55	0/1551
34	BK	0.55	0/947	0.83	0/1268
34	DK	0.31	0/947	0.54	0/1268
35	BL	0.42	0/1054	0.77	1/1403 (0.1%)
35	DL	0.27	0/1054	0.51	0/1403
36	BM	0.51	0/1093	0.77	1/1460 (0.1%)
36	DM	0.31	0/1093	0.48	0/1460
37	BN	0.55	0/973	0.79	0/1301
37	DN	0.27	0/973	0.49	0/1301
38	BO	0.42	0/902	0.63	0/1209

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DO	0.24	0/902	0.44	0/1209
39	BP	0.51	0/929	0.77	0/1242
39	DP	0.28	0/929	0.49	0/1242
40	BQ	0.60	0/960	0.71	0/1278
40	DQ	0.28	0/960	0.46	0/1278
41	BR	0.56	0/829	0.85	1/1107 (0.1%)
41	DR	0.28	0/829	0.50	0/1107
42	BS	0.50	0/864	0.75	0/1156
42	DS	0.29	0/864	0.54	0/1156
43	BT	0.48	0/744	0.70	0/994
43	DT	0.25	0/744	0.49	0/994
44	BU	0.41	0/787	0.70	0/1051
44	DU	0.25	0/787	0.47	0/1051
45	BV	0.48	0/766	0.66	0/1025
45	DV	0.38	0/766	0.54	0/1025
46	BW	0.51	0/603	0.76	0/797
46	DW	0.26	0/603	0.47	0/797
47	BX	0.42	0/635	0.67	0/848
47	DX	0.30	0/635	0.55	0/848
48	BY	0.40	0/510	0.66	0/677
48	DY	0.23	0/510	0.44	0/677
49	BZ	0.52	0/453	0.77	0/605
49	DZ	0.28	0/453	0.51	0/605
50	B0	0.45	0/450	0.79	0/599
50	D0	0.28	0/450	0.51	0/599
51	B1	0.40	0/416	0.63	0/554
51	D1	0.28	0/416	0.46	0/554
52	B2	0.47	0/380	0.73	0/498
52	D2	0.28	0/380	0.55	0/498
53	B3	0.51	0/513	0.76	0/676
53	D3	0.26	0/513	0.51	0/676
54	B4	0.47	0/303	0.76	0/397
54	D4	0.30	0/303	0.49	0/397
55	CA	0.53	0/36762	1.45	712/57350 (1.2%)
56	DB	0.52	0/2803	1.35	52/4371 (1.2%)
All	All	0.55	23/308631 (0.0%)	1.35	4677/461501 (1.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
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 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BA	1142	A	N9-C4	-13.92	1.29	1.37
31	BH	48	GLU	C-O	9.51	1.41	1.23
24	BA	2451	A	C8-N7	9.03	1.37	1.31
31	DH	49	ALA	CA-CB	-7.88	1.35	1.52
31	BH	48	GLU	CA-CB	6.93	1.69	1.53

The worst 5 of 4677 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BA	2447	G	C6-N1-C2	-22.51	111.59	125.10
24	BA	2451	A	C5-N7-C8	-17.23	95.28	103.90
24	BA	2347	C	N1-C1'-C2'	-16.79	92.17	114.00
24	BA	790	U	P-O3'-C3'	-16.12	100.36	119.70
25	BB	88	C	O4'-C1'-N1	-15.24	96.01	108.20

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	253	0
1	CB	1704	0	1732	203	0
2	AC	1624	0	1699	133	0
2	CC	1624	0	1699	149	0
3	AD	1643	0	1710	139	0
3	CD	1643	0	1710	139	0
4	AE	1105	0	1148	196	0
4	CE	1105	0	1148	127	0
5	AF	817	0	808	91	0
5	CF	817	0	808	76	0
6	AG	1181	0	1240	100	0
6	CG	1174	0	1230	154	0
7	AH	979	0	1034	107	0
7	CH	979	0	1034	95	0
8	AI	1022	0	1070	122	0
8	CI	1022	0	1070	108	0
9	AJ	786	0	828	69	0
9	CJ	786	0	828	114	0
10	AK	877	0	887	103	0
10	CK	877	0	887	82	0
11	AL	955	0	1019	97	0
11	CL	955	0	1019	101	0
12	AM	883	0	944	69	0
12	CM	876	0	937	123	0
13	AN	774	0	827	72	0
13	CN	769	0	822	83	0
14	AO	714	0	737	50	0
14	CO	714	0	737	40	0
15	AP	649	0	666	63	0
15	CP	638	0	656	56	0
16	AQ	648	0	691	70	0
16	CQ	648	0	691	59	0
17	AR	455	0	478	36	0
17	CR	455	0	478	41	0
18	AS	637	0	665	42	0
18	CS	637	0	665	79	0
19	AT	665	0	714	56	0
19	CT	665	0	714	58	0
20	AU	425	0	449	65	0
20	CU	425	0	449	70	0
21	AA	32895	0	16553	1800	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	3133	0
24	DA	60995	0	30679	3843	0
25	BB	2529	0	1281	109	0
26	BC	2082	0	2157	226	0
26	DC	2082	0	2157	230	0
27	BD	1565	0	1616	200	0
27	DD	1565	0	1616	162	0
28	BE	1552	0	1619	158	0
28	DE	1552	0	1619	170	0
29	BF	1410	0	1447	144	0
29	DF	1420	0	1460	183	0
30	BG	1323	0	1374	149	0
30	DG	1323	0	1374	116	0
31	BH	1111	0	1148	108	0
31	DH	1111	0	1148	100	0
32	BI	1032	0	1088	116	0
32	DI	1032	0	1088	69	0
33	BJ	1129	0	1162	160	0
33	DJ	1129	0	1162	122	0
34	BK	938	0	1012	102	0
34	DK	938	0	1012	114	0
35	BL	1045	0	1117	133	0
35	DL	1045	0	1117	130	0
36	BM	1074	0	1157	129	0
36	DM	1074	0	1157	96	0
37	BN	960	0	1000	102	0
37	DN	960	0	1000	107	0
38	BO	892	0	923	82	0
38	DO	892	0	923	90	0
39	BP	917	0	965	120	0
39	DP	917	0	965	87	0
40	BQ	947	0	1022	147	0
40	DQ	947	0	1022	120	0
41	BR	816	0	839	102	0
41	DR	816	0	839	90	0
42	BS	857	0	922	89	0
42	DS	857	0	922	83	0
43	BT	738	0	807	103	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	DT	738	0	807	96	0
44	BU	779	0	834	65	0
44	DU	779	0	834	93	0
45	BV	753	0	780	54	0
45	DV	753	0	780	98	0
46	BW	596	0	610	179	0
46	DW	596	0	610	105	0
47	BX	625	0	655	68	0
47	DX	625	0	655	76	0
48	BY	509	0	543	45	0
48	DY	509	0	543	55	0
49	BZ	449	0	491	41	0
49	DZ	449	0	491	40	0
50	B0	444	0	461	36	0
50	D0	444	0	461	63	0
51	B1	409	0	440	43	0
51	D1	409	0	440	33	0
52	B2	377	0	418	28	0
52	D2	377	0	418	42	0
53	B3	504	0	574	41	0
53	D3	504	0	574	54	0
54	B4	302	0	340	40	0
54	D4	302	0	340	27	0
55	CA	32831	0	16521	2003	0
56	DB	2507	0	1270	160	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	19249	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 19249 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	4
1	CB	216/241 (90%)	144 (67%)	50 (23%)	22 (10%)	0	8
2	AC	204/233 (88%)	140 (69%)	48 (24%)	16 (8%)	1	13
2	CC	204/233 (88%)	136 (67%)	52 (26%)	16 (8%)	1	13
3	AD	203/206 (98%)	143 (70%)	43 (21%)	17 (8%)	1	11
3	CD	203/206 (98%)	136 (67%)	46 (23%)	21 (10%)	0	7
4	AE	148/167 (89%)	105 (71%)	27 (18%)	16 (11%)	0	6
4	CE	148/167 (89%)	100 (68%)	34 (23%)	14 (10%)	0	9
5	AF	98/135 (73%)	68 (69%)	22 (22%)	8 (8%)	1	11
5	CF	98/135 (73%)	65 (66%)	27 (28%)	6 (6%)	1	18
6	AG	149/179 (83%)	103 (69%)	36 (24%)	10 (7%)	1	17
6	CG	148/179 (83%)	84 (57%)	44 (30%)	20 (14%)	0	4
7	AH	127/130 (98%)	90 (71%)	27 (21%)	10 (8%)	1	13
7	CH	127/130 (98%)	88 (69%)	30 (24%)	9 (7%)	1	15
8	AI	125/130 (96%)	81 (65%)	32 (26%)	12 (10%)	0	9
8	CI	125/130 (96%)	88 (70%)	33 (26%)	4 (3%)	4	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	AJ	96/103 (93%)	69 (72%)	16 (17%)	11 (12%)	0	5
9	CJ	96/103 (93%)	62 (65%)	22 (23%)	12 (12%)	0	5
10	AK	115/129 (89%)	84 (73%)	22 (19%)	9 (8%)	1	13
10	CK	115/129 (89%)	86 (75%)	19 (16%)	10 (9%)	1	11
11	AL	121/124 (98%)	82 (68%)	27 (22%)	12 (10%)	0	8
11	CL	121/124 (98%)	86 (71%)	26 (22%)	9 (7%)	1	14
12	AM	112/118 (95%)	89 (80%)	16 (14%)	7 (6%)	1	18
12	CM	111/118 (94%)	71 (64%)	28 (25%)	12 (11%)	0	6
13	AN	92/101 (91%)	63 (68%)	18 (20%)	11 (12%)	0	5
13	CN	91/101 (90%)	62 (68%)	24 (26%)	5 (6%)	2	21
14	AO	86/89 (97%)	64 (74%)	20 (23%)	2 (2%)	6	37
14	CO	86/89 (97%)	67 (78%)	19 (22%)	0	100	100
15	AP	80/82 (98%)	52 (65%)	22 (28%)	6 (8%)	1	14
15	CP	78/82 (95%)	52 (67%)	20 (26%)	6 (8%)	1	13
16	AQ	78/84 (93%)	47 (60%)	20 (26%)	11 (14%)	0	4
16	CQ	78/84 (93%)	57 (73%)	16 (20%)	5 (6%)	1	18
17	AR	53/75 (71%)	39 (74%)	11 (21%)	3 (6%)	1	20
17	CR	53/75 (71%)	39 (74%)	11 (21%)	3 (6%)	1	20
18	AS	77/92 (84%)	61 (79%)	13 (17%)	3 (4%)	3	27
18	CS	77/92 (84%)	55 (71%)	20 (26%)	2 (3%)	5	34
19	AT	83/87 (95%)	63 (76%)	14 (17%)	6 (7%)	1	15
19	CT	83/87 (95%)	59 (71%)	21 (25%)	3 (4%)	3	29
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	2
26	BC	269/273 (98%)	192 (71%)	48 (18%)	29 (11%)	0	6
26	DC	269/273 (98%)	169 (63%)	73 (27%)	27 (10%)	0	8
27	BD	207/209 (99%)	141 (68%)	35 (17%)	31 (15%)	0	3
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	8
28	DE	199/201 (99%)	129 (65%)	49 (25%)	21 (11%)	0	7
29	BF	175/179 (98%)	133 (76%)	26 (15%)	16 (9%)	1	10

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	BV	92/94 (98%)	76 (83%)	15 (16%)	1 (1%)	14	50
45	DV	92/94 (98%)	59 (64%)	25 (27%)	8 (9%)	1	11
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	17
47	DX	75/78 (96%)	49 (65%)	19 (25%)	7 (9%)	0	10
48	BY	61/63 (97%)	39 (64%)	15 (25%)	7 (12%)	0	5
48	DY	61/63 (97%)	45 (74%)	11 (18%)	5 (8%)	1	11
49	BZ	56/59 (95%)	43 (77%)	10 (18%)	3 (5%)	2	21
49	DZ	56/59 (95%)	35 (62%)	14 (25%)	7 (12%)	0	5
50	B0	54/57 (95%)	39 (72%)	8 (15%)	7 (13%)	0	4
50	D0	54/57 (95%)	39 (72%)	8 (15%)	7 (13%)	0	4
51	B1	48/55 (87%)	32 (67%)	9 (19%)	7 (15%)	0	3
51	D1	48/55 (87%)	37 (77%)	7 (15%)	4 (8%)	1	11
52	B2	44/46 (96%)	36 (82%)	6 (14%)	2 (4%)	2	24
52	D2	44/46 (96%)	30 (68%)	9 (20%)	5 (11%)	0	5
53	B3	62/65 (95%)	50 (81%)	10 (16%)	2 (3%)	4	31
53	D3	62/65 (95%)	42 (68%)	15 (24%)	5 (8%)	1	12
54	B4	36/38 (95%)	27 (75%)	6 (17%)	3 (8%)	1	11
54	D4	36/38 (95%)	22 (61%)	8 (22%)	6 (17%)	0	3
All	All	11238/11970 (94%)	7515 (67%)	2516 (22%)	1207 (11%)	0	6

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%)	147 (82%)	33 (18%)	1	10
1	CB	180/199 (90%)	158 (88%)	22 (12%)	5	24
2	AC	170/190 (90%)	148 (87%)	22 (13%)	4	23
2	CC	170/190 (90%)	146 (86%)	24 (14%)	3	20
3	AD	172/173 (99%)	147 (86%)	25 (14%)	3	19
3	CD	172/173 (99%)	152 (88%)	20 (12%)	5	27
4	AE	113/126 (90%)	93 (82%)	20 (18%)	2	12
4	CE	113/126 (90%)	100 (88%)	13 (12%)	5	27
5	AF	87/116 (75%)	75 (86%)	12 (14%)	3	21
5	CF	87/116 (75%)	74 (85%)	13 (15%)	3	18
6	AG	124/147 (84%)	117 (94%)	7 (6%)	21	53
6	CG	123/147 (84%)	95 (77%)	28 (23%)	1	6
7	AH	104/105 (99%)	92 (88%)	12 (12%)	5	27
7	CH	104/105 (99%)	91 (88%)	13 (12%)	4	23
8	AI	105/107 (98%)	90 (86%)	15 (14%)	3	19
8	CI	105/107 (98%)	91 (87%)	14 (13%)	4	22
9	AJ	86/90 (96%)	74 (86%)	12 (14%)	3	20
9	CJ	86/90 (96%)	77 (90%)	9 (10%)	7	30
10	AK	90/99 (91%)	80 (89%)	10 (11%)	6	29
10	CK	90/99 (91%)	80 (89%)	10 (11%)	6	29
11	AL	103/104 (99%)	85 (82%)	18 (18%)	2	12
11	CL	103/104 (99%)	88 (85%)	15 (15%)	3	18
12	AM	92/96 (96%)	87 (95%)	5 (5%)	22	54
12	CM	91/96 (95%)	74 (81%)	17 (19%)	1	10
13	AN	79/84 (94%)	73 (92%)	6 (8%)	13	43
13	CN	79/84 (94%)	68 (86%)	11 (14%)	3	21
14	AO	76/77 (99%)	72 (95%)	4 (5%)	22	54
14	CO	76/77 (99%)	72 (95%)	4 (5%)	22	54
15	AP	65/65 (100%)	60 (92%)	5 (8%)	13	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	CP	65/65 (100%)	59 (91%)	6 (9%)	9	36
16	AQ	74/78 (95%)	60 (81%)	14 (19%)	1	9
16	CQ	74/78 (95%)	64 (86%)	10 (14%)	4	22
17	AR	48/65 (74%)	46 (96%)	2 (4%)	30	58
17	CR	48/65 (74%)	46 (96%)	2 (4%)	30	58
18	AS	70/79 (89%)	63 (90%)	7 (10%)	7	32
18	CS	70/79 (89%)	59 (84%)	11 (16%)	2	16
19	AT	65/66 (98%)	55 (85%)	10 (15%)	2	17
19	CT	65/66 (98%)	56 (86%)	9 (14%)	3	21
20	AU	44/61 (72%)	37 (84%)	7 (16%)	2	16
20	CU	44/61 (72%)	35 (80%)	9 (20%)	1	7
26	BC	216/218 (99%)	173 (80%)	43 (20%)	1	8
26	DC	216/218 (99%)	191 (88%)	25 (12%)	5	27
27	BD	164/164 (100%)	136 (83%)	28 (17%)	2	13
27	DD	164/164 (100%)	144 (88%)	20 (12%)	5	24
28	BE	165/165 (100%)	130 (79%)	35 (21%)	1	7
28	DE	165/165 (100%)	152 (92%)	13 (8%)	12	42
29	BF	148/150 (99%)	130 (88%)	18 (12%)	5	24
29	DF	149/150 (99%)	124 (83%)	25 (17%)	2	14
30	BG	137/138 (99%)	107 (78%)	30 (22%)	1	6
30	DG	137/138 (99%)	120 (88%)	17 (12%)	4	24
31	BH	114/114 (100%)	97 (85%)	17 (15%)	3	18
31	DH	114/114 (100%)	95 (83%)	19 (17%)	2	14
32	BI	109/110 (99%)	94 (86%)	15 (14%)	3	21
32	DI	109/110 (99%)	102 (94%)	7 (6%)	17	48
33	BJ	116/116 (100%)	90 (78%)	26 (22%)	1	6
33	DJ	116/116 (100%)	106 (91%)	10 (9%)	10	39
34	BK	103/104 (99%)	84 (82%)	19 (18%)	1	10
34	DK	103/104 (99%)	85 (82%)	18 (18%)	2	12
35	BL	102/103 (99%)	81 (79%)	21 (21%)	1	7
35	DL	102/103 (99%)	90 (88%)	12 (12%)	5	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	BM	109/109 (100%)	90 (83%)	19 (17%)	2	12
36	DM	109/109 (100%)	100 (92%)	9 (8%)	11	40
37	BN	100/103 (97%)	81 (81%)	19 (19%)	1	9
37	DN	100/103 (97%)	85 (85%)	15 (15%)	3	18
38	BO	86/87 (99%)	69 (80%)	17 (20%)	1	8
38	DO	86/87 (99%)	78 (91%)	8 (9%)	9	35
39	BP	99/100 (99%)	79 (80%)	20 (20%)	1	8
39	DP	99/100 (99%)	91 (92%)	8 (8%)	11	41
40	BQ	89/90 (99%)	73 (82%)	16 (18%)	1	11
40	DQ	89/90 (99%)	79 (89%)	10 (11%)	6	28
41	BR	84/84 (100%)	69 (82%)	15 (18%)	2	11
41	DR	84/84 (100%)	70 (83%)	14 (17%)	2	14
42	BS	93/93 (100%)	73 (78%)	20 (22%)	1	7
42	DS	93/93 (100%)	79 (85%)	14 (15%)	3	18
43	BT	80/84 (95%)	61 (76%)	19 (24%)	0	5
43	DT	80/84 (95%)	74 (92%)	6 (8%)	13	44
44	BU	83/85 (98%)	69 (83%)	14 (17%)	2	13
44	DU	83/85 (98%)	72 (87%)	11 (13%)	4	22
45	BV	78/78 (100%)	64 (82%)	14 (18%)	2	11
45	DV	78/78 (100%)	68 (87%)	10 (13%)	4	23
46	BW	59/63 (94%)	43 (73%)	16 (27%)	0	3
46	DW	59/63 (94%)	44 (75%)	15 (25%)	0	4
47	BX	67/68 (98%)	53 (79%)	14 (21%)	1	7
47	DX	67/68 (98%)	58 (87%)	9 (13%)	4	22
48	BY	55/55 (100%)	44 (80%)	11 (20%)	1	8
48	DY	55/55 (100%)	52 (94%)	3 (6%)	21	53
49	BZ	48/49 (98%)	34 (71%)	14 (29%)	0	2
49	DZ	48/49 (98%)	41 (85%)	7 (15%)	3	18
50	B0	47/48 (98%)	42 (89%)	5 (11%)	6	30
50	D0	47/48 (98%)	42 (89%)	5 (11%)	6	30
51	B1	45/49 (92%)	37 (82%)	8 (18%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	D1	45/49 (92%)	41 (91%)	4 (9%)	9	37
52	B2	38/38 (100%)	32 (84%)	6 (16%)	2	16
52	D2	38/38 (100%)	34 (90%)	4 (10%)	7	30
53	B3	51/52 (98%)	44 (86%)	7 (14%)	3	21
53	D3	51/52 (98%)	42 (82%)	9 (18%)	2	12
54	B4	34/34 (100%)	30 (88%)	4 (12%)	5	26
54	D4	34/34 (100%)	29 (85%)	5 (15%)	3	18
All	All	9331/9756 (96%)	7983 (86%)	1348 (14%)	3	19

5 of 1348 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
42	BS	41	LYS
54	B4	9	LYS
41	DR	95	ASP
43	BT	8	LEU
46	BW	71	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 323 such sidechains are listed below:

Mol	Chain	Res	Type
45	BV	51	GLN
4	CE	77	ASN
45	DV	51	GLN
47	BX	5	GLN
1	CB	167	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1532/1533 (99%)	465 (30%)	230 (15%)
22	AV	17/17 (100%)	2 (11%)	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%)	1 (20%)	1 (20%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
24	BA	2850/2903 (98%)	925 (32%)	497 (17%)
24	DA	2838/2903 (97%)	1020 (35%)	505 (17%)
25	BB	117/118 (99%)	32 (27%)	22 (18%)
55	CA	1529/1530 (99%)	516 (33%)	245 (16%)
56	DB	116/117 (99%)	29 (25%)	13 (11%)
All	All	9059/9184 (98%)	3000 (33%)	1517 (16%)

5 of 3000 RNA backbone outliers are listed below:

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

5 of 1517 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
24	BA	2638	G
55	CA	497	G
24	DA	2283	C
24	BA	2778	A
55	CA	82	G

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AB	218/241 (90%)	1.99	83 (38%) 0 0	170, 274, 284, 290	0
1	CB	218/241 (90%)	0.79	36 (16%) 1 1	159, 222, 233, 241	0
2	AC	206/233 (88%)	0.43	11 (5%) 26 23	133, 162, 187, 202	0
2	CC	206/233 (88%)	0.59	16 (7%) 13 10	140, 172, 212, 228	0
3	AD	205/206 (99%)	0.25	11 (5%) 25 22	122, 157, 195, 218	0
3	CD	205/206 (99%)	-0.27	0 100 100	112, 131, 152, 165	0
4	AE	150/167 (89%)	2.91	84 (56%) 0 0	108, 211, 223, 227	0
4	CE	150/167 (89%)	0.50	15 (10%) 7 6	100, 156, 171, 176	0
5	AF	100/135 (74%)	0.30	7 (7%) 16 12	197, 229, 250, 260	0
5	CF	100/135 (74%)	0.85	18 (18%) 1 1	164, 186, 203, 209	0
6	AG	151/179 (84%)	0.34	17 (11%) 5 5	158, 192, 220, 237	0
6	CG	150/179 (83%)	0.34	20 (13%) 3 3	142, 194, 228, 244	0
7	AH	129/130 (99%)	0.34	12 (9%) 8 7	127, 155, 181, 193	0
7	CH	129/130 (99%)	0.81	23 (17%) 1 1	152, 177, 195, 203	0
8	AI	127/130 (97%)	0.71	18 (14%) 2 3	142, 193, 220, 233	0
8	CI	127/130 (97%)	0.52	14 (11%) 5 5	155, 195, 223, 232	0
9	AJ	98/103 (95%)	0.31	6 (6%) 21 16	135, 181, 216, 239	0
9	CJ	98/103 (95%)	0.83	14 (14%) 2 3	155, 196, 230, 240	0
10	AK	117/129 (90%)	0.74	14 (11%) 4 4	132, 195, 243, 254	0
10	CK	117/129 (90%)	0.31	6 (5%) 28 24	125, 155, 181, 196	0
11	AL	123/124 (99%)	0.15	4 (3%) 46 38	89, 106, 131, 150	0
11	CL	123/124 (99%)	0.67	13 (10%) 6 5	117, 139, 155, 161	0
12	AM	114/118 (96%)	0.61	14 (12%) 4 4	157, 219, 252, 264	0
12	CM	113/118 (95%)	0.71	15 (13%) 3 3	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%)	0.28	5 (5%) 27 24	142, 165, 217, 227	0
13	CN	95/101 (94%)	1.05	15 (15%) 2 1	155, 207, 265, 284	0
14	AO	88/89 (98%)	-0.20	0 100 100	138, 168, 199, 219	0
14	CO	88/89 (98%)	-0.06	1 (1%) 80 76	142, 174, 193, 201	0
15	AP	82/82 (100%)	0.79	11 (13%) 3 3	117, 144, 178, 192	0
15	CP	80/82 (97%)	1.48	23 (28%) 0 0	151, 180, 203, 207	0
16	AQ	80/84 (95%)	0.64	5 (6%) 20 15	90, 113, 135, 144	0
16	CQ	80/84 (95%)	1.11	16 (20%) 1 1	99, 123, 145, 163	0
17	AR	55/75 (73%)	0.81	8 (14%) 2 2	175, 198, 219, 234	0
17	CR	55/75 (73%)	0.24	3 (5%) 25 21	148, 165, 180, 187	0
18	AS	79/92 (85%)	1.49	27 (34%) 0 0	171, 203, 244, 257	0
18	CS	79/92 (85%)	1.52	26 (32%) 0 0	223, 265, 319, 334	0
19	AT	85/87 (97%)	0.12	3 (3%) 44 36	114, 141, 164, 180	0
19	CT	85/87 (97%)	1.16	25 (29%) 0 0	194, 242, 275, 283	0
20	AU	51/71 (71%)	0.76	6 (11%) 4 4	133, 168, 248, 252	0
20	CU	51/71 (71%)	0.19	2 (3%) 39 32	126, 150, 183, 193	0
21	AA	1533/1533 (100%)	-0.47	13 (0%) 86 83	76, 150, 233, 282	0
22	AV	17/17 (100%)	0.19	1 (5%) 22 17	142, 154, 182, 203	0
22	AX	17/17 (100%)	-0.25	1 (5%) 22 17	139, 144, 186, 195	0
22	CV	17/17 (100%)	0.05	1 (5%) 22 17	158, 162, 193, 208	0
22	CX	17/17 (100%)	2.35	8 (47%) 0 0	187, 193, 221, 222	0
23	AW	6/6 (100%)	0.13	0 100 100	136, 138, 143, 152	0
23	CW	6/6 (100%)	0.47	0 100 100	160, 160, 168, 179	0
24	BA	2854/2903 (98%)	-0.38	39 (1%) 75 69	52, 81, 194, 355	0
24	DA	2841/2903 (97%)	0.27	139 (4%) 29 25	132, 200, 303, 402	0
25	BB	118/118 (100%)	-0.62	0 100 100	66, 101, 133, 171	0
26	BC	271/273 (99%)	-0.08	3 (1%) 80 76	60, 99, 129, 161	0
26	DC	271/273 (99%)	0.60	25 (9%) 9 7	133, 157, 179, 190	0
27	BD	209/209 (100%)	-0.18	2 (0%) 82 78	55, 75, 114, 129	0
27	DD	209/209 (100%)	1.42	68 (32%) 0 0	147, 200, 232, 242	0
28	BE	201/201 (100%)	-0.17	2 (0%) 82 78	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%)	1.26	46 (22%) 0 0	154, 282, 335, 351	0
29	BF	177/179 (98%)	1.04	32 (18%) 1 1	120, 166, 201, 215	0
29	DF	178/179 (99%)	2.08	76 (42%) 0 0	307, 314, 321, 323	0
30	BG	176/177 (99%)	0.09	3 (1%) 70 64	83, 108, 134, 152	0
30	DG	176/177 (99%)	1.59	55 (31%) 0 0	186, 221, 245, 259	0
31	BH	149/149 (100%)	2.05	57 (38%) 0 0	110, 239, 259, 264	0
31	DH	149/149 (100%)	1.54	42 (28%) 0 0	186, 240, 256, 260	0
32	BI	141/142 (99%)	2.13	60 (42%) 0 0	243, 307, 359, 366	0
32	DI	141/142 (99%)	3.16	87 (61%) 0 0	367, 394, 412, 419	0
33	BJ	142/142 (100%)	-0.30	0 100 100	59, 76, 102, 132	0
33	DJ	142/142 (100%)	1.24	35 (24%) 0 0	161, 201, 223, 233	0
34	BK	122/123 (99%)	-0.09	1 (0%) 86 83	55, 73, 113, 169	0
34	DK	122/123 (99%)	1.24	36 (29%) 0 0	151, 171, 189, 198	0
35	BL	143/144 (99%)	-0.27	1 (0%) 87 85	55, 93, 124, 136	0
35	DL	143/144 (99%)	1.19	38 (26%) 0 0	166, 240, 288, 297	0
36	BM	136/136 (100%)	-0.08	1 (0%) 87 85	58, 81, 111, 138	0
36	DM	136/136 (100%)	1.76	55 (40%) 0 0	144, 181, 210, 232	0
37	BN	120/127 (94%)	-0.07	0 100 100	61, 76, 96, 141	0
37	DN	120/127 (94%)	2.05	52 (43%) 0 0	183, 222, 252, 266	0
38	BO	116/117 (99%)	-0.05	1 (0%) 84 80	96, 105, 123, 147	0
38	DO	116/117 (99%)	2.44	56 (48%) 0 0	286, 293, 297, 303	0
39	BP	114/115 (99%)	-0.07	0 100 100	64, 81, 119, 134	0
39	DP	114/115 (99%)	1.41	33 (28%) 0 0	179, 203, 220, 230	0
40	BQ	117/118 (99%)	-0.47	0 100 100	56, 77, 99, 120	0
40	DQ	117/118 (99%)	1.13	25 (21%) 0 0	184, 211, 240, 247	0
41	BR	103/103 (100%)	-0.22	0 100 100	55, 87, 114, 131	0
41	DR	103/103 (100%)	2.21	45 (43%) 0 0	173, 249, 271, 277	0
42	BS	110/110 (100%)	-0.34	0 100 100	55, 70, 105, 159	0
42	DS	110/110 (100%)	1.74	39 (35%) 0 0	159, 223, 269, 278	0
43	BT	93/100 (93%)	0.11	2 (2%) 62 55	65, 105, 142, 151	0
43	DT	93/100 (93%)	2.27	47 (50%) 0 0	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%)	0.32	5 (4%) 29 25	89, 114, 136, 158	0
44	DU	102/104 (98%)	3.17	60 (58%) 0 0	272, 312, 355, 358	0
45	BV	94/94 (100%)	-0.15	0 100 100	71, 90, 116, 126	0
45	DV	94/94 (100%)	1.19	23 (24%) 0 0	228, 241, 252, 254	0
46	BW	79/85 (92%)	-0.02	2 (2%) 57 49	68, 86, 136, 156	0
46	DW	79/85 (92%)	3.13	54 (68%) 0 0	156, 216, 233, 252	0
47	BX	77/78 (98%)	-0.20	0 100 100	65, 101, 124, 137	0
47	DX	77/78 (98%)	0.78	10 (12%) 3 4	157, 185, 209, 224	0
48	BY	63/63 (100%)	-0.02	3 (4%) 30 26	101, 123, 149, 159	0
48	DY	63/63 (100%)	1.20	16 (25%) 0 0	264, 288, 316, 329	0
49	BZ	58/59 (98%)	0.14	1 (1%) 70 64	64, 74, 111, 141	0
49	DZ	58/59 (98%)	1.12	12 (20%) 1 1	188, 215, 238, 248	0
50	B0	56/57 (98%)	-0.52	0 100 100	54, 77, 113, 132	0
50	D0	56/57 (98%)	1.32	11 (19%) 1 1	157, 230, 260, 265	0
51	B1	50/55 (90%)	0.58	4 (8%) 12 10	76, 100, 118, 132	0
51	D1	50/55 (90%)	1.67	18 (36%) 0 0	174, 207, 228, 238	0
52	B2	46/46 (100%)	-0.27	0 100 100	62, 75, 103, 137	0
52	D2	46/46 (100%)	0.69	4 (8%) 10 8	155, 182, 198, 202	0
53	B3	64/65 (98%)	-0.30	0 100 100	58, 73, 96, 120	0
53	D3	64/65 (98%)	1.23	14 (21%) 0 0	180, 194, 211, 215	0
54	B4	38/38 (100%)	-0.03	0 100 100	69, 84, 110, 120	0
54	D4	38/38 (100%)	1.23	11 (28%) 0 0	171, 187, 198, 203	0
55	CA	1530/1530 (100%)	-0.14	34 (2%) 62 55	109, 171, 272, 362	0
56	DB	117/117 (100%)	0.07	2 (1%) 70 64	219, 294, 300, 302	0
All	All	20511/21154 (96%)	0.38	2158 (10%) 6 5	52, 166, 293, 419	0

The worst 5 of 2158 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AB	194	GLY	17.7
31	BH	87	GLU	14.6
4	AE	145	ASN	14.0
24	BA	2179	C	13.7
29	DF	129	MET	13.7

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	DA	3002	1/1	-0.26	1.16	212,212,212,212	0
57	MG	DA	3073	1/1	-0.05	0.20	312,312,312,312	0
57	MG	DA	3020	1/1	0.16	2.42	229,229,229,229	0
57	MG	DA	3045	1/1	0.23	0.24	188,188,188,188	0
57	MG	DA	3132	1/1	0.24	0.26	198,198,198,198	0
57	MG	DA	3063	1/1	0.35	1.56	157,157,157,157	0
57	MG	DA	3003	1/1	0.36	1.42	229,229,229,229	0
57	MG	DA	3109	1/1	0.38	0.91	145,145,145,145	0
57	MG	CA	1610	1/1	0.39	0.22	181,181,181,181	0
57	MG	DA	3083	1/1	0.40	0.08	303,303,303,303	0
57	MG	DJ	201	1/1	0.40	0.55	183,183,183,183	0
57	MG	CA	1602	1/1	0.42	0.16	177,177,177,177	0
57	MG	CA	1627	1/1	0.44	0.35	136,136,136,136	0
57	MG	D4	101	1/1	0.45	1.38	183,183,183,183	0
57	MG	DA	3015	1/1	0.46	1.27	164,164,164,164	0
57	MG	DA	3108	1/1	0.46	0.65	172,172,172,172	0
57	MG	DA	3071	1/1	0.51	0.30	184,184,184,184	0
57	MG	BA	3070	1/1	0.51	0.17	158,158,158,158	0
57	MG	DA	3125	1/1	0.53	0.31	187,187,187,187	0
57	MG	DA	3064	1/1	0.55	0.51	157,157,157,157	0
57	MG	AA	1624	1/1	0.56	0.17	131,131,131,131	0
57	MG	DA	3106	1/1	0.57	0.35	228,228,228,228	0
57	MG	AA	1619	1/1	0.57	0.48	162,162,162,162	0
57	MG	DA	3006	1/1	0.58	0.17	296,296,296,296	0
57	MG	DA	3049	1/1	0.58	0.11	249,249,249,249	0
57	MG	CA	1622	1/1	0.58	0.09	216,216,216,216	0
57	MG	DA	3016	1/1	0.59	1.32	175,175,175,175	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3092	1/1	0.60	0.27	198,198,198,198	0
57	MG	CA	1620	1/1	0.61	0.49	150,150,150,150	0
57	MG	DA	3128	1/1	0.61	0.65	132,132,132,132	0
57	MG	CA	1607	1/1	0.62	0.22	134,134,134,134	0
57	MG	CA	1619	1/1	0.62	0.92	135,135,135,135	0
57	MG	DA	3078	1/1	0.62	0.64	144,144,144,144	0
57	MG	DA	3018	1/1	0.64	0.40	248,248,248,248	0
57	MG	DA	3058	1/1	0.64	0.92	162,162,162,162	0
57	MG	DA	3087	1/1	0.65	0.16	208,208,208,208	0
57	MG	CA	1606	1/1	0.66	0.14	124,124,124,124	0
57	MG	DA	3094	1/1	0.67	0.68	173,173,173,173	0
57	MG	CA	1617	1/1	0.67	0.28	183,183,183,183	0
57	MG	DA	3044	1/1	0.67	0.24	210,210,210,210	0
57	MG	DA	3069	1/1	0.68	0.52	139,139,139,139	0
57	MG	DA	3068	1/1	0.68	0.33	143,143,143,143	0
57	MG	DA	3129	1/1	0.69	1.36	132,132,132,132	0
57	MG	CA	1603	1/1	0.69	0.17	141,141,141,141	0
57	MG	DA	3059	1/1	0.69	0.28	136,136,136,136	0
57	MG	AA	1617	1/1	0.69	0.29	150,150,150,150	0
57	MG	DA	3082	1/1	0.69	0.42	220,220,220,220	0
57	MG	AA	1630	1/1	0.70	0.28	99,99,99,99	0
57	MG	DA	3095	1/1	0.71	0.19	152,152,152,152	0
57	MG	DA	3029	1/1	0.71	0.62	179,179,179,179	0
57	MG	DA	3010	1/1	0.71	0.26	210,210,210,210	0
57	MG	AA	1636	1/1	0.72	0.36	154,154,154,154	0
57	MG	DA	3121	1/1	0.72	0.45	206,206,206,206	0
57	MG	DA	3037	1/1	0.72	0.20	204,204,204,204	0
57	MG	DA	3072	1/1	0.72	0.43	182,182,182,182	0
57	MG	DA	3039	1/1	0.73	0.27	186,186,186,186	0
57	MG	DA	3113	1/1	0.73	0.19	182,182,182,182	0
57	MG	DA	3060	1/1	0.73	0.78	132,132,132,132	0
57	MG	DA	3097	1/1	0.73	0.34	156,156,156,156	0
57	MG	DA	3022	1/1	0.73	0.77	152,152,152,152	0
57	MG	DA	3013	1/1	0.74	0.29	165,165,165,165	0
57	MG	DA	3051	1/1	0.75	0.23	160,160,160,160	0
57	MG	DA	3107	1/1	0.75	0.14	137,137,137,137	0
57	MG	CA	1616	1/1	0.75	0.33	199,199,199,199	0
57	MG	AA	1610	1/1	0.75	0.12	155,155,155,155	0
57	MG	DA	3093	1/1	0.75	0.14	208,208,208,208	0
57	MG	DA	3110	1/1	0.75	0.17	219,219,219,219	0
57	MG	DA	3033	1/1	0.76	0.14	162,162,162,162	0
57	MG	DA	3070	1/1	0.76	0.09	147,147,147,147	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	CA	1634	1/1	0.76	0.11	153,153,153,153	0
57	MG	DA	3041	1/1	0.77	0.40	176,176,176,176	0
57	MG	DA	3005	1/1	0.77	1.13	197,197,197,197	0
57	MG	DB	201	1/1	0.78	0.15	224,224,224,224	0
57	MG	DA	3119	1/1	0.78	0.13	147,147,147,147	0
57	MG	BA	3098	1/1	0.78	0.37	72,72,72,72	0
57	MG	DA	3075	1/1	0.78	0.96	155,155,155,155	0
57	MG	BA	3115	1/1	0.78	0.53	65,65,65,65	0
57	MG	AA	1614	1/1	0.78	0.18	150,150,150,150	0
57	MG	DA	3084	1/1	0.78	0.35	214,214,214,214	0
57	MG	DA	3054	1/1	0.78	0.34	155,155,155,155	0
57	MG	CA	1614	1/1	0.78	0.56	146,146,146,146	0
57	MG	DA	3081	1/1	0.78	0.23	182,182,182,182	0
57	MG	CA	1624	1/1	0.78	0.29	99,99,99,99	0
57	MG	AA	1637	1/1	0.79	0.57	118,118,118,118	0
57	MG	CA	1632	1/1	0.79	0.15	210,210,210,210	0
57	MG	DA	3124	1/1	0.79	0.35	168,168,168,168	0
57	MG	DA	3030	1/1	0.79	0.30	164,164,164,164	0
57	MG	DA	3048	1/1	0.79	0.14	203,203,203,203	0
57	MG	DA	3008	1/1	0.79	0.13	198,198,198,198	0
57	MG	DA	3038	1/1	0.79	0.43	197,197,197,197	0
57	MG	DA	3001	1/1	0.79	0.29	206,206,206,206	0
57	MG	DA	3096	1/1	0.80	0.31	190,190,190,190	0
57	MG	CA	1611	1/1	0.80	0.29	132,132,132,132	0
57	MG	DA	3111	1/1	0.80	0.30	160,160,160,160	0
57	MG	DA	3062	1/1	0.80	1.23	160,160,160,160	0
57	MG	DA	3036	1/1	0.80	0.47	212,212,212,212	0
57	MG	DA	3101	1/1	0.80	0.17	155,155,155,155	0
57	MG	DC	301	1/1	0.80	0.18	135,135,135,135	0
57	MG	DA	3079	1/1	0.80	0.22	148,148,148,148	0
57	MG	CA	1629	1/1	0.80	0.23	157,157,157,157	0
57	MG	AA	1633	1/1	0.81	0.16	128,128,128,128	0
57	MG	BA	3101	1/1	0.81	0.14	54,54,54,54	0
57	MG	DA	3025	1/1	0.81	0.09	135,135,135,135	0
57	MG	CA	1642	1/1	0.81	0.12	170,170,170,170	0
57	MG	BA	3095	1/1	0.81	0.21	92,92,92,92	0
57	MG	AA	1628	1/1	0.81	0.28	134,134,134,134	0
57	MG	DA	3019	1/1	0.81	0.19	245,245,245,245	0
57	MG	DA	3011	1/1	0.82	1.01	184,184,184,184	0
57	MG	BA	3046	1/1	0.82	0.19	77,77,77,77	0
57	MG	AA	1627	1/1	0.82	1.47	142,142,142,142	0
57	MG	AA	1641	1/1	0.82	0.43	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3131	1/1	0.82	0.44	181,181,181,181	0
57	MG	BA	3092	1/1	0.82	0.08	127,127,127,127	0
57	MG	DA	3047	1/1	0.82	0.25	208,208,208,208	0
57	MG	AA	1604	1/1	0.82	0.08	157,157,157,157	0
57	MG	DA	3088	1/1	0.82	0.30	180,180,180,180	0
57	MG	DA	3076	1/1	0.82	1.13	145,145,145,145	0
57	MG	BA	3028	1/1	0.82	0.33	57,57,57,57	0
57	MG	AA	1609	1/1	0.82	0.14	118,118,118,118	0
57	MG	BA	3075	1/1	0.82	0.32	58,58,58,58	0
57	MG	DA	3074	1/1	0.83	1.75	187,187,187,187	0
57	MG	AA	1625	1/1	0.83	0.32	114,114,114,114	0
57	MG	CA	1636	1/1	0.83	1.56	120,120,120,120	0
57	MG	DA	3043	1/1	0.83	0.16	208,208,208,208	0
57	MG	CA	1639	1/1	0.83	0.12	266,266,266,266	0
57	MG	DA	3032	1/1	0.83	0.15	161,161,161,161	0
57	MG	CA	1633	1/1	0.83	0.14	123,123,123,123	0
57	MG	BA	3133	1/1	0.84	0.58	73,73,73,73	0
57	MG	AA	1635	1/1	0.84	0.17	148,148,148,148	0
57	MG	DA	3017	1/1	0.84	0.19	187,187,187,187	0
57	MG	DA	3085	1/1	0.84	0.23	167,167,167,167	0
57	MG	DA	3091	1/1	0.84	0.93	174,174,174,174	0
57	MG	DA	3120	1/1	0.84	0.22	159,159,159,159	0
57	MG	BA	3015	1/1	0.85	0.60	55,55,55,55	0
57	MG	CA	1625	1/1	0.85	0.49	127,127,127,127	0
57	MG	DA	3028	1/1	0.85	0.47	165,165,165,165	0
57	MG	DC	302	1/1	0.85	0.20	140,140,140,140	0
57	MG	BA	3026	1/1	0.85	0.44	59,59,59,59	0
57	MG	BA	3124	1/1	0.85	0.96	59,59,59,59	0
57	MG	DA	3014	1/1	0.86	0.28	162,162,162,162	0
57	MG	BA	3131	1/1	0.86	0.59	68,68,68,68	0
57	MG	AA	1632	1/1	0.86	0.10	117,117,117,117	0
57	MG	DA	3050	1/1	0.86	0.22	180,180,180,180	0
57	MG	DA	3007	1/1	0.86	0.47	250,250,250,250	0
57	MG	AA	1607	1/1	0.86	0.45	113,113,113,113	0
57	MG	BA	3086	1/1	0.86	0.12	60,60,60,60	0
57	MG	DA	3026	1/1	0.86	1.01	160,160,160,160	0
57	MG	DA	3098	1/1	0.86	0.33	170,170,170,170	0
57	MG	BA	3032	1/1	0.86	0.13	57,57,57,57	0
57	MG	BA	3007	1/1	0.86	0.17	111,111,111,111	0
57	MG	CA	1640	1/1	0.86	0.59	118,118,118,118	0
57	MG	DA	3117	1/1	0.87	0.45	170,170,170,170	0
57	MG	DA	3123	1/1	0.87	0.20	225,225,225,225	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3040	1/1	0.87	0.26	171,171,171,171	0
57	MG	BA	3047	1/1	0.87	0.19	78,78,78,78	0
57	MG	DA	3023	1/1	0.87	0.23	148,148,148,148	0
57	MG	AA	1601	1/1	0.87	0.12	133,133,133,133	0
57	MG	CA	1612	1/1	0.87	0.17	124,124,124,124	0
57	MG	BA	3011	1/1	0.87	0.30	62,62,62,62	0
57	MG	CA	1641	1/1	0.87	0.17	151,151,151,151	0
57	MG	DA	3099	1/1	0.88	0.19	211,211,211,211	0
57	MG	AA	1634	1/1	0.88	0.12	121,121,121,121	0
57	MG	BA	3077	1/1	0.88	0.15	63,63,63,63	0
57	MG	BA	3090	1/1	0.88	0.11	63,63,63,63	0
57	MG	BA	3004	1/1	0.88	0.22	86,86,86,86	0
57	MG	BB	201	1/1	0.88	0.49	118,118,118,118	0
57	MG	DA	3066	1/1	0.88	0.12	150,150,150,150	0
57	MG	BA	3014	1/1	0.88	0.26	55,55,55,55	0
57	MG	DA	3080	1/1	0.88	0.12	134,134,134,134	0
57	MG	DA	3102	1/1	0.88	0.15	141,141,141,141	0
57	MG	BA	3056	1/1	0.88	0.30	64,64,64,64	0
57	MG	CA	1613	1/1	0.88	0.11	121,121,121,121	0
57	MG	DA	3130	1/1	0.88	0.17	170,170,170,170	0
57	MG	BA	3037	1/1	0.88	0.23	58,58,58,58	0
57	MG	BA	3019	1/1	0.88	0.12	86,86,86,86	0
57	MG	AA	1620	1/1	0.89	0.17	186,186,186,186	0
57	MG	DA	3027	1/1	0.89	0.14	171,171,171,171	0
57	MG	CA	1608	1/1	0.89	0.19	121,121,121,121	0
57	MG	CA	1615	1/1	0.89	0.21	156,156,156,156	0
57	MG	BA	3079	1/1	0.89	0.06	110,110,110,110	0
57	MG	CA	1635	1/1	0.89	0.10	142,142,142,142	0
57	MG	DA	3115	1/1	0.89	0.14	154,154,154,154	0
57	MG	DA	3103	1/1	0.90	0.15	150,150,150,150	0
57	MG	DA	3067	1/1	0.90	0.15	147,147,147,147	0
57	MG	BA	3118	1/1	0.90	0.09	60,60,60,60	0
57	MG	DA	3100	1/1	0.90	0.32	150,150,150,150	0
57	MG	BA	3062	1/1	0.90	0.68	55,55,55,55	0
57	MG	DA	3042	1/1	0.90	0.26	179,179,179,179	0
57	MG	BA	3081	1/1	0.90	0.10	56,56,56,56	0
57	MG	DA	3118	1/1	0.90	0.25	181,181,181,181	0
57	MG	BA	3112	1/1	0.90	0.22	64,64,64,64	0
57	MG	BA	3030	1/1	0.90	0.40	58,58,58,58	0
57	MG	DA	3090	1/1	0.90	0.09	200,200,200,200	0
57	MG	AA	1605	1/1	0.90	0.20	124,124,124,124	0
57	MG	BB	202	1/1	0.91	0.14	127,127,127,127	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	AA	1621	1/1	0.91	0.27	80,80,80,80	0
57	MG	BA	3121	1/1	0.91	0.11	64,64,64,64	0
57	MG	DA	3055	1/1	0.91	0.13	136,136,136,136	0
57	MG	BA	3052	1/1	0.91	0.11	54,54,54,54	0
57	MG	BA	3051	1/1	0.91	0.14	57,57,57,57	0
57	MG	CA	1628	1/1	0.91	1.01	99,99,99,99	0
57	MG	BA	3093	1/1	0.91	0.29	104,104,104,104	0
57	MG	DA	3056	1/1	0.91	0.19	141,141,141,141	0
57	MG	AA	1611	1/1	0.91	0.23	126,126,126,126	0
57	MG	BA	3105	1/1	0.91	0.18	55,55,55,55	0
57	MG	BA	3060	1/1	0.92	0.36	56,56,56,56	0
57	MG	DA	3034	1/1	0.92	0.14	158,158,158,158	0
57	MG	DA	3086	1/1	0.92	0.27	196,196,196,196	0
57	MG	CA	1609	1/1	0.92	0.15	131,131,131,131	0
57	MG	DA	3031	1/1	0.92	0.16	159,159,159,159	0
57	MG	BA	3103	1/1	0.92	0.07	81,81,81,81	0
57	MG	AA	1629	1/1	0.92	0.21	161,161,161,161	0
57	MG	BA	3107	1/1	0.92	0.18	67,67,67,67	0
57	MG	CA	1637	1/1	0.92	0.28	112,112,112,112	0
57	MG	AA	1603	1/1	0.92	0.09	93,93,93,93	0
57	MG	BA	3085	1/1	0.92	0.42	59,59,59,59	0
57	MG	BA	3044	1/1	0.92	0.08	88,88,88,88	0
57	MG	DA	3004	1/1	0.92	0.21	206,206,206,206	0
57	MG	DA	3057	1/1	0.92	0.28	133,133,133,133	0
57	MG	AA	1638	1/1	0.92	0.19	107,107,107,107	0
57	MG	CA	1630	1/1	0.92	0.19	99,99,99,99	0
57	MG	BA	3127	1/1	0.92	0.10	57,57,57,57	0
57	MG	DA	3035	1/1	0.93	0.11	155,155,155,155	0
57	MG	BA	3058	1/1	0.93	0.48	63,63,63,63	0
57	MG	BA	3035	1/1	0.93	0.28	72,72,72,72	0
57	MG	DA	3089	1/1	0.93	0.44	179,179,179,179	0
57	MG	DA	3024	1/1	0.93	0.17	162,162,162,162	0
57	MG	DA	3065	1/1	0.93	0.37	152,152,152,152	0
57	MG	DA	3127	1/1	0.93	0.80	138,138,138,138	0
57	MG	BA	3123	1/1	0.93	0.12	79,79,79,79	0
57	MG	AA	1623	1/1	0.93	0.11	129,129,129,129	0
57	MG	AA	1602	1/1	0.93	0.37	97,97,97,97	0
57	MG	AA	1631	1/1	0.93	0.20	114,114,114,114	0
57	MG	CA	1618	1/1	0.93	0.28	148,148,148,148	0
57	MG	DA	3009	1/1	0.93	0.22	199,199,199,199	0
57	MG	BA	3088	1/1	0.93	0.12	77,77,77,77	0
57	MG	BB	204	1/1	0.93	0.09	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3052	1/1	0.93	0.12	144,144,144,144	0
57	MG	DA	3021	1/1	0.93	0.36	151,151,151,151	0
57	MG	CA	1631	1/1	0.94	0.22	130,130,130,130	0
57	MG	DA	3104	1/1	0.94	0.27	142,142,142,142	0
57	MG	BA	3122	1/1	0.94	0.22	57,57,57,57	0
57	MG	BA	3048	1/1	0.94	0.22	91,91,91,91	0
57	MG	BA	3043	1/1	0.94	0.19	68,68,68,68	0
57	MG	CA	1601	1/1	0.94	0.13	224,224,224,224	0
57	MG	AA	1643	1/1	0.94	0.11	101,101,101,101	0
57	MG	BA	3002	1/1	0.94	0.36	61,61,61,61	0
57	MG	AA	1608	1/1	0.94	0.23	105,105,105,105	0
57	MG	BA	3024	1/1	0.94	0.15	60,60,60,60	0
57	MG	DA	3116	1/1	0.94	0.14	133,133,133,133	0
57	MG	BA	3102	1/1	0.94	0.20	57,57,57,57	0
57	MG	DA	3077	1/1	0.94	0.12	162,162,162,162	0
57	MG	BA	3005	1/1	0.94	0.15	91,91,91,91	0
57	MG	BD	301	1/1	0.94	0.20	55,55,55,55	0
57	MG	BA	3083	1/1	0.94	0.06	59,59,59,59	0
57	MG	BA	3104	1/1	0.94	0.18	55,55,55,55	0
57	MG	DA	3046	1/1	0.94	0.25	172,172,172,172	0
57	MG	CA	1604	1/1	0.94	0.04	117,117,117,117	0
57	MG	AA	1642	1/1	0.94	0.26	90,90,90,90	0
57	MG	DA	3122	1/1	0.94	0.28	146,146,146,146	0
57	MG	BA	3071	1/1	0.94	0.33	55,55,55,55	0
57	MG	DA	3053	1/1	0.94	0.17	144,144,144,144	0
57	MG	DA	3114	1/1	0.94	0.26	135,135,135,135	0
57	MG	BA	3069	1/1	0.94	0.11	65,65,65,65	0
57	MG	AA	1613	1/1	0.94	0.11	95,95,95,95	0
57	MG	AA	1640	1/1	0.94	0.07	160,160,160,160	0
57	MG	BA	3036	1/1	0.94	0.09	65,65,65,65	0
57	MG	BA	3018	1/1	0.94	0.08	80,80,80,80	0
57	MG	BA	3099	1/1	0.94	0.09	58,58,58,58	0
57	MG	CA	1623	1/1	0.95	0.30	123,123,123,123	0
57	MG	BA	3135	1/1	0.95	0.34	60,60,60,60	0
57	MG	AA	1616	1/1	0.95	0.27	161,161,161,161	0
57	MG	BA	3125	1/1	0.95	0.24	58,58,58,58	0
57	MG	BA	3010	1/1	0.95	0.13	64,64,64,64	0
57	MG	BA	3057	1/1	0.95	0.35	61,61,61,61	0
57	MG	BA	3009	1/1	0.95	0.09	61,61,61,61	0
57	MG	BA	3020	1/1	0.95	0.36	63,63,63,63	0
57	MG	BA	3061	1/1	0.95	0.38	56,56,56,56	0
57	MG	BA	3094	1/1	0.95	0.12	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3111	1/1	0.95	0.09	55,55,55,55	0
57	MG	BA	3063	1/1	0.95	0.12	54,54,54,54	0
57	MG	BA	3076	1/1	0.95	0.18	62,62,62,62	0
57	MG	BA	3114	1/1	0.95	0.11	88,88,88,88	0
57	MG	BA	3053	1/1	0.95	0.08	57,57,57,57	0
57	MG	AA	1612	1/1	0.95	0.09	106,106,106,106	0
57	MG	BA	3059	1/1	0.95	0.09	69,69,69,69	0
57	MG	DA	3012	1/1	0.95	0.32	168,168,168,168	0
57	MG	BA	3080	1/1	0.96	0.15	93,93,93,93	0
57	MG	BA	3084	1/1	0.96	0.22	61,61,61,61	0
57	MG	BA	3008	1/1	0.96	0.13	59,59,59,59	0
57	MG	BA	3016	1/1	0.96	0.26	56,56,56,56	0
57	MG	AA	1639	1/1	0.96	0.08	143,143,143,143	0
57	MG	DA	3061	1/1	0.96	0.11	134,134,134,134	0
57	MG	BA	3120	1/1	0.96	0.17	59,59,59,59	0
57	MG	BA	3029	1/1	0.96	0.07	54,54,54,54	0
57	MG	BA	3132	1/1	0.96	0.27	61,61,61,61	0
57	MG	BA	3113	1/1	0.96	0.12	54,54,54,54	0
57	MG	BA	3064	1/1	0.96	0.07	55,55,55,55	0
57	MG	BA	3003	1/1	0.96	0.07	90,90,90,90	0
57	MG	CA	1638	1/1	0.96	0.10	226,226,226,226	0
57	MG	AA	1626	1/1	0.96	0.30	136,136,136,136	0
57	MG	BA	3078	1/1	0.96	0.07	100,100,100,100	0
57	MG	BA	3119	1/1	0.96	0.41	68,68,68,68	0
57	MG	BA	3055	1/1	0.96	0.11	62,62,62,62	0
57	MG	BA	3022	1/1	0.96	0.23	55,55,55,55	0
57	MG	BA	3126	1/1	0.96	0.24	70,70,70,70	0
57	MG	BA	3068	1/1	0.96	0.17	65,65,65,65	0
57	MG	AA	1606	1/1	0.96	0.12	119,119,119,119	0
57	MG	BA	3049	1/1	0.96	0.07	61,61,61,61	0
58	ZN	D4	102	1/1	0.96	0.07	99,99,99,99	0
57	MG	BA	3027	1/1	0.96	0.08	59,59,59,59	0
57	MG	BA	3134	1/1	0.97	0.15	55,55,55,55	0
57	MG	BA	3042	1/1	0.97	0.11	68,68,68,68	0
57	MG	BA	3067	1/1	0.97	0.17	57,57,57,57	0
57	MG	BA	3073	1/1	0.97	0.09	61,61,61,61	0
57	MG	BA	3025	1/1	0.97	0.10	59,59,59,59	0
57	MG	DA	3112	1/1	0.97	0.14	143,143,143,143	0
57	MG	BA	3072	1/1	0.97	0.31	55,55,55,55	0
57	MG	BA	3091	1/1	0.97	0.13	88,88,88,88	0
57	MG	DA	3105	1/1	0.97	0.12	159,159,159,159	0
57	MG	CA	1605	1/1	0.97	0.12	115,115,115,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3100	1/1	0.97	0.15	74,74,74,74	0
57	MG	BA	3065	1/1	0.97	0.06	55,55,55,55	0
57	MG	BA	3097	1/1	0.97	0.08	65,65,65,65	0
57	MG	BA	3089	1/1	0.97	0.18	66,66,66,66	0
57	MG	BA	3128	1/1	0.97	0.14	64,64,64,64	0
57	MG	BA	3040	1/1	0.97	0.17	58,58,58,58	0
57	MG	BA	3116	1/1	0.97	0.17	55,55,55,55	0
57	MG	DA	3126	1/1	0.97	0.17	199,199,199,199	0
57	MG	BA	3066	1/1	0.97	0.13	61,61,61,61	0
57	MG	BA	3110	1/1	0.97	0.09	61,61,61,61	0
57	MG	BA	3013	1/1	0.97	0.17	55,55,55,55	0
57	MG	BA	3045	1/1	0.97	0.32	80,80,80,80	0
57	MG	BA	3041	1/1	0.98	0.23	60,60,60,60	0
57	MG	CA	1626	1/1	0.98	0.31	139,139,139,139	0
57	MG	BA	3106	1/1	0.98	0.15	58,58,58,58	0
57	MG	BA	3109	1/1	0.98	0.21	60,60,60,60	0
57	MG	BA	3017	1/1	0.98	0.12	56,56,56,56	0
57	MG	BA	3096	1/1	0.98	0.22	61,61,61,61	0
57	MG	BA	3012	1/1	0.98	0.13	54,54,54,54	0
57	MG	AA	1615	1/1	0.98	0.12	153,153,153,153	0
57	MG	BA	3001	1/1	0.98	0.06	61,61,61,61	0
57	MG	BA	3074	1/1	0.98	0.16	54,54,54,54	0
57	MG	BA	3039	1/1	0.98	0.13	57,57,57,57	0
57	MG	BA	3136	1/1	0.98	0.37	64,64,64,64	0
57	MG	BA	3130	1/1	0.98	0.16	68,68,68,68	0
57	MG	BA	3108	1/1	0.98	0.18	58,58,58,58	0
57	MG	BA	3050	1/1	0.98	0.14	56,56,56,56	0
57	MG	CA	1621	1/1	0.98	0.14	115,115,115,115	0
57	MG	BA	3006	1/1	0.98	0.06	101,101,101,101	0
57	MG	BA	3082	1/1	0.98	0.12	55,55,55,55	0
57	MG	BA	3054	1/1	0.98	0.07	62,62,62,62	0
57	MG	BA	3087	1/1	0.98	0.14	61,61,61,61	0
57	MG	BA	3038	1/1	0.98	0.14	59,59,59,59	0
57	MG	AA	1622	1/1	0.98	0.10	113,113,113,113	0
57	MG	AA	1618	1/1	0.98	0.16	131,131,131,131	0
57	MG	BA	3034	1/1	0.99	0.17	57,57,57,57	0
57	MG	BA	3033	1/1	0.99	0.17	56,56,56,56	0
57	MG	BA	3129	1/1	0.99	0.10	55,55,55,55	0
57	MG	BA	3031	1/1	0.99	0.23	59,59,59,59	0
57	MG	BA	3021	1/1	0.99	0.31	59,59,59,59	0
57	MG	BB	203	1/1	0.99	0.10	69,69,69,69	0
57	MG	BA	3117	1/1	0.99	0.15	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	ZN	B4	101	1/1	0.99	0.09	99,99,99,99	0
57	MG	BA	3023	1/1	0.99	0.14	59,59,59,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.