



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:38 PM GMT

PDB ID : 4V55
Title : Crystal structure of the bacterial ribosome from Escherichia coli in complex with gentamicin and ribosome recycling factor (RRF).
Authors : Borovinskaya, M.A.; Pai, R.D.; Zhang, W.; Schuwirth, B.-S.; Holton, J.M.; Hirokawa, G.; Kaji, H.; Kaji, A.; Cate, J.H.D.
Deposited on : 2007-06-17
Resolution : 4.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

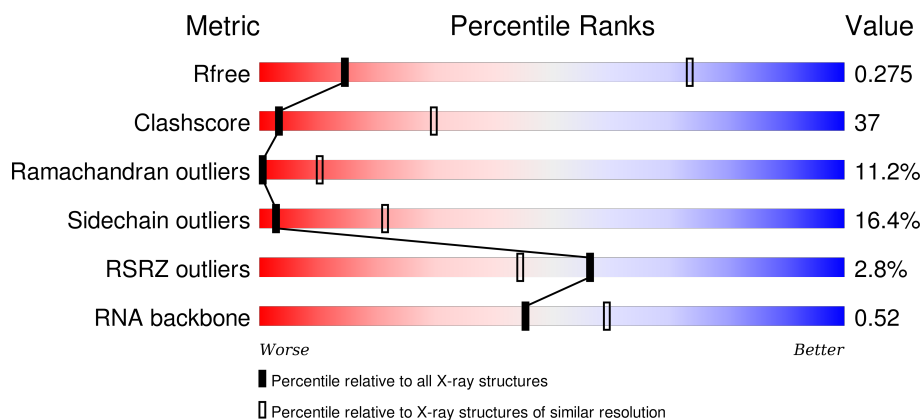
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1010 (4.42-3.56)
Clashscore	102246	1052 (4.40-3.60)
Ramachandran outliers	100387	1005 (4.40-3.60)
Sidechain outliers	100360	1013 (4.42-3.58)
RSRZ outliers	91569	1013 (4.42-3.56)
RNA backbone	2183	1079 (5.04-2.80)

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

Mol	Chain	Length	Quality of chain
1	AA	1542	<div> <div></div> <div>24% 62% 12% ..</div> </div>
1	CA	1542	<div> <div></div> <div>22% 65% 12% ..</div> </div>
2	AC	232	<div> <div></div> <div>29% 48% 11% 11%</div> </div>
2	CC	232	<div> <div></div> <div>28% 49% 12% 11%</div> </div>

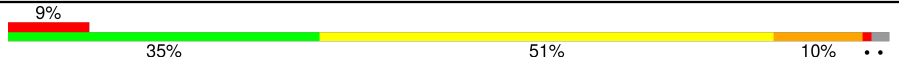
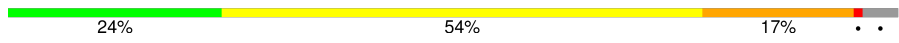

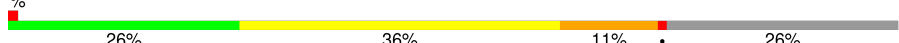
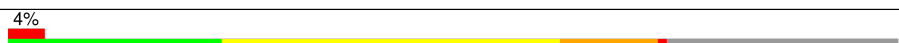
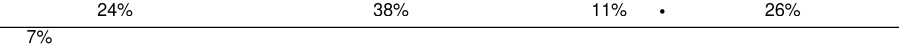
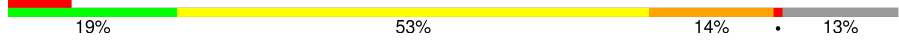
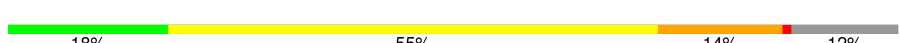
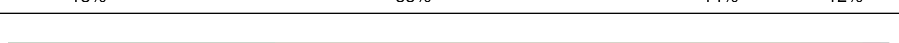

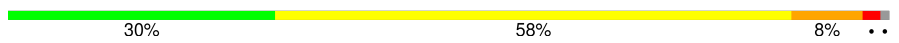
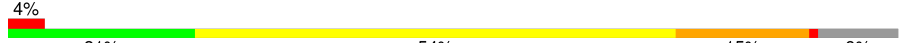
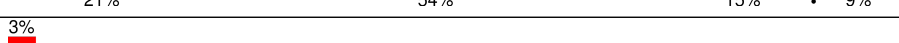
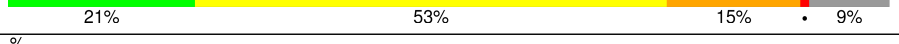

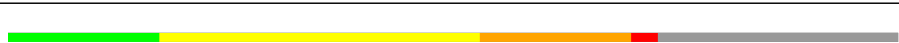
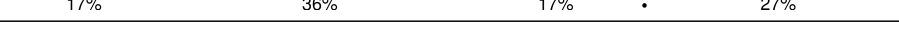
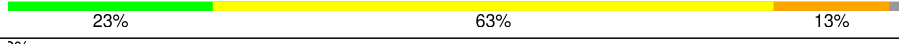
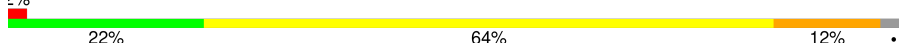
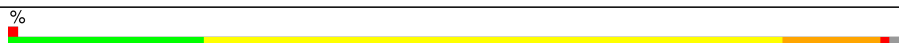
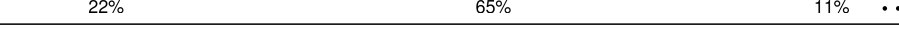


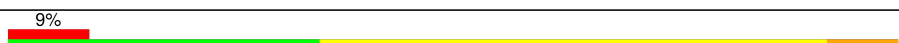

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Mol	Chain	Length	Quality of chain
3	AD	205	
3	CD	205	
4	AE	166	
4	CE	166	
5	AF	135	
5	CF	135	
6	AG	178	
6	CG	178	
7	AH	129	
7	CH	129	
8	AI	129	
8	CI	129	
9	AJ	103	
9	CJ	103	
10	AK	128	
10	CK	128	
11	AL	123	
11	CL	123	
12	AM	117	
12	CM	117	
13	AN	100	
13	CN	100	
14	AO	89	
14	CO	89	
15	AP	82	

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Mol	Chain	Length	Quality of chain
15	CP	82	
16	AQ	83	
16	CQ	83	
17	AR	74	
17	CR	74	
18	AS	91	
18	CS	91	
19	AT	86	
19	CT	86	
20	AB	240	
20	CB	240	
21	AU	70	
21	CU	70	
22	BA	120	
22	DA	120	
23	BB	2904	
23	DB	2904	
24	BI	141	
24	DI	141	
25	BC	272	
25	DC	272	
26	BD	209	
26	DD	209	
27	BK	123	
27	DK	123	

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Mol	Chain	Length	Quality of chain
28	BP	114	
28	DP	114	
29	BE	201	
29	DE	201	
30	BY	58	
30	DY	58	
31	B0	56	
31	D0	56	
32	B4	38	
32	D4	38	
33	B1	54	
33	D1	54	
34	B3	64	
34	D3	64	
35	BV	94	
35	DV	94	
36	B2	46	
36	D2	46	
37	BL	144	
37	DL	144	
38	BM	136	
38	DM	136	
39	BX	63	
39	DX	63	
40	BH	149	

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Mol	Chain	Length	Quality of chain
40	DH	149	
41	BJ	142	
41	DJ	142	
42	BN	127	
42	DN	127	
43	BO	117	
43	DO	117	
44	BQ	117	
44	DQ	117	
45	BS	110	
45	DS	110	
46	BU	103	
46	DU	103	
47	BF	178	
47	DF	178	
48	BG	176	
48	DG	176	
49	BR	103	
49	DR	103	
50	BT	100	
50	DT	100	
51	BZ	78	
51	DZ	78	
52	BW	84	
52	DW	84	

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Mol	Chain	Length	Quality of chain
53	B6	185	
53	D6	185	

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
54	MG	DB	3059	-	-	-	X
55	LLL	BB	3111	-	-	-	X
55	LLL	DB	3112	-	-	-	X

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 287083 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S rRNA.

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AG	150	Total	C	N	O	S	0	0	0
			1174	730	226	214	4			
6	CG	152	Total	C	N	O	S	0	0	0
			1196	745	230	217	4			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			
8	CI	127	Total	C	N	O	S	0	0	0
			1021	634	206	178	3			

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AO	88	Total	C	N	O	S	0	0	0
			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	81	Total	C	N	O	S	0	0	0
			657	417	122	115	3			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AS	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			
18	CS	80	Total	C	N	O	S	0	0	0
			644	413	121	108	2			

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

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

- Molecule 20 is a protein called 30S ribosomal protein S2.

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

- Molecule 21 is a protein called 30S ribosomal protein S21.

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

- Molecule 22 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	BA	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			
22	DA	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	BB	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			
23	DB	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			

- Molecule 24 is a protein called 50S ribosomal protein L11.

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

- Molecule 25 is a protein called 50S ribosomal protein L2.

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

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

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

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

- Molecule 27 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BK	121	Total	C	N	O	S	0	0	0
			930	582	179	164	5			
27	DK	121	Total	C	N	O	S	0	0	0
			930	582	179	164	5			

- Molecule 28 is a protein called 50S ribosomal protein L19.

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

- Molecule 29 is a protein called 50S ribosomal protein L4.

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

- Molecule 30 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BY	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			
30	DY	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			

- Molecule 31 is a protein called 50S ribosomal protein L32.

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

- Molecule 32 is a protein called 50S ribosomal protein L36.

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

- Molecule 33 is a protein called 50S ribosomal protein L33.

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

- Molecule 34 is a protein called 50S ribosomal protein L35.

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

- Molecule 35 is a protein called 50S ribosomal protein L25.

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

- Molecule 36 is a protein called 50S ribosomal protein L34.

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

- Molecule 37 is a protein called 50S ribosomal protein L15.

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

- Molecule 38 is a protein called 50S ribosomal protein L16.

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

- Molecule 39 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BX	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			
39	DX	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			

- Molecule 40 is a protein called 50S ribosomal protein L9.

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

- Molecule 41 is a protein called 50S ribosomal protein L13.

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

- Molecule 42 is a protein called 50S ribosomal protein L17.

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

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

- Molecule 43 is a protein called 50S ribosomal protein L18.

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

- Molecule 44 is a protein called 50S ribosomal protein L20.

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

- Molecule 45 is a protein called 50S ribosomal protein L22.

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

- Molecule 46 is a protein called 50S ribosomal protein L24.

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

- Molecule 47 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BF	178	Total	C	N	O	S	0	0	0
			1420	905	251	258	6			
47	DF	178	Total	C	N	O	S	0	0	0
			1420	905	251	258	6			

- Molecule 48 is a protein called 50S ribosomal protein L6.

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

- Molecule 49 is a protein called 50S ribosomal protein L21.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BZ	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			
51	DZ	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			

- Molecule 52 is a protein called 50S ribosomal protein L27.

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

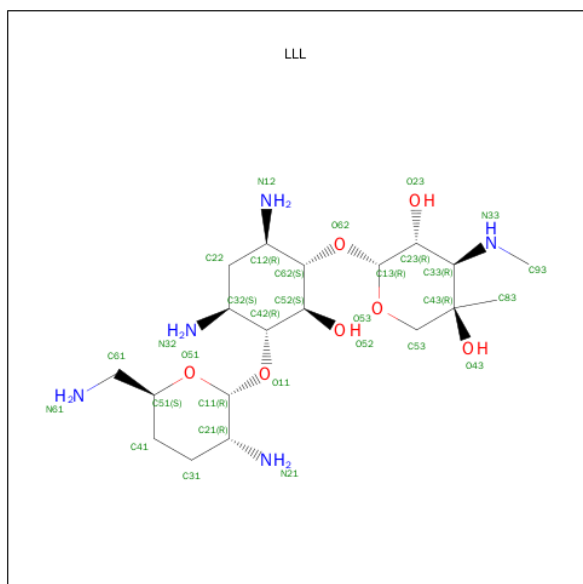
- Molecule 53 is a protein called 50S ribosomal protein RRF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B6	185	Total	C	N	O	S	0	0	0
			1478	924	270	282	2			
53	D6	185	Total	C	N	O	S	0	0	0
			1478	924	270	282	2			

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	DB	111	Total	Mg	0	0
			111	111		
54	BB	110	Total	Mg	0	0
			110	110		
54	AA	60	Total	Mg	0	0
			60	60		
54	CA	61	Total	Mg	0	0
			61	61		
54	CE	1	Total	Mg	0	0
			1	1		

- Molecule 55 is (2R,3R,4R,5R)-2-((1S,2S,3R,4S,6R)-4,6-DIAMINO-3-((2R,3R,6S)-3-AMINO-6-(AMINOMETHYL)-TETRAHYDRO-2H-PYRAN-2-YLOXY)-2-HYDROXYCYCLOHEXYLOXY)-5-METHYL-4-(METHYLAMINO)-TETRAHYDRO-2H-PYRAN-3,5-DIOL (three-letter code: LLL) (formula: C₁₉H₃₉N₅O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
55	AA	1	Total	C	N	O	0	0
			31	19	5	7		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
55	BB	1	Total	C	N	O	0	0
			31	19	5	7		
55	CA	1	Total	C	N	O	0	0
			31	19	5	7		
55	DB	1	Total	C	N	O	0	0
			31	19	5	7		

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

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

- Molecule 57 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	AA	287	Total	O	0	0
			287	287		
57	AE	3	Total	O	0	0
			3	3		
57	AK	1	Total	O	0	0
			1	1		
57	AL	3	Total	O	0	0
			3	3		
57	AN	4	Total	O	0	0
			4	4		
57	AT	2	Total	O	0	0
			2	2		
57	BB	492	Total	O	0	0
			492	492		
57	BC	6	Total	O	0	0
			6	6		
57	BD	1	Total	O	0	0
			1	1		
57	BE	3	Total	O	0	0
			3	3		
57	BL	3	Total	O	0	0
			3	3		
57	BT	1	Total	O	0	0
			1	1		

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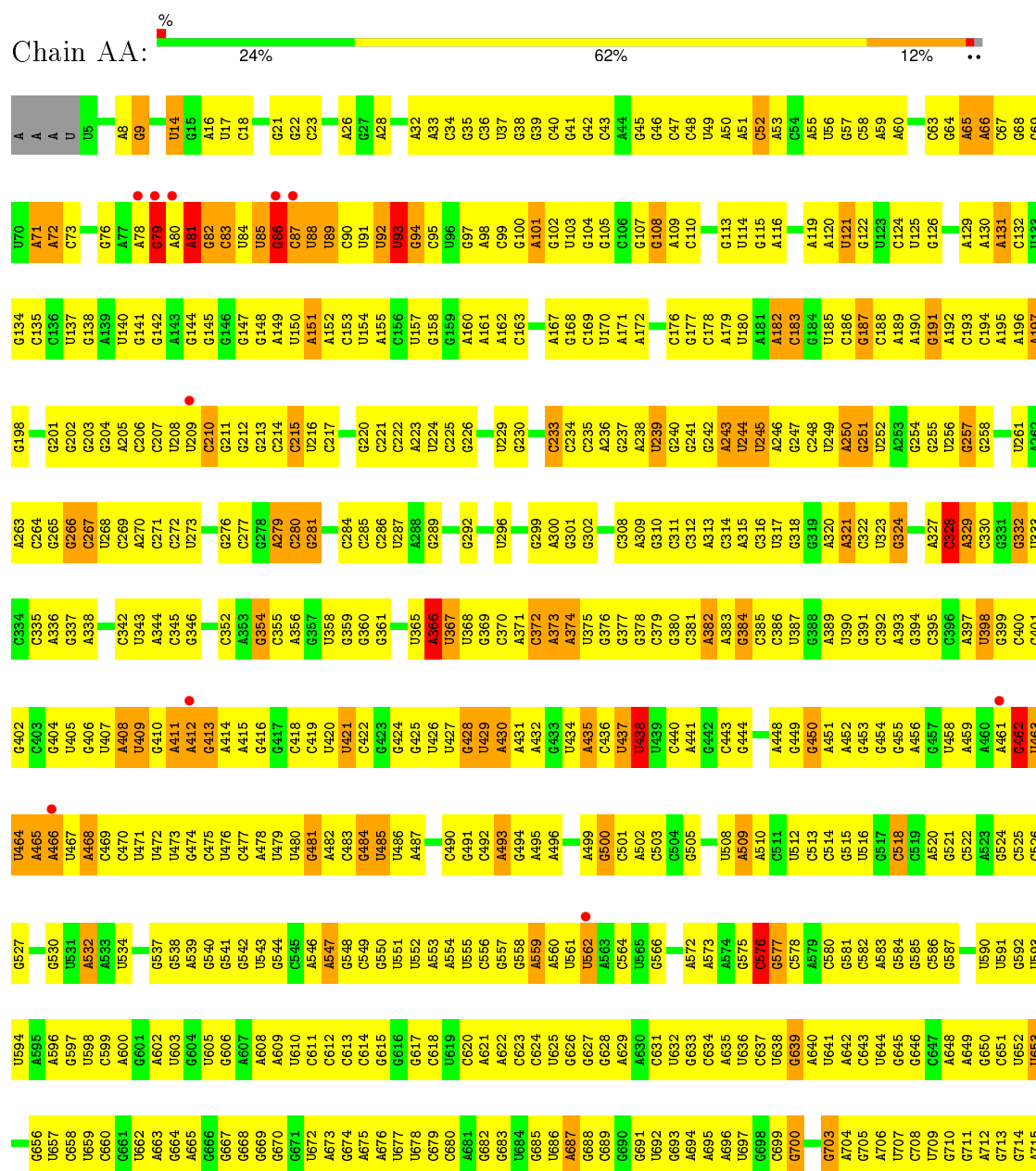
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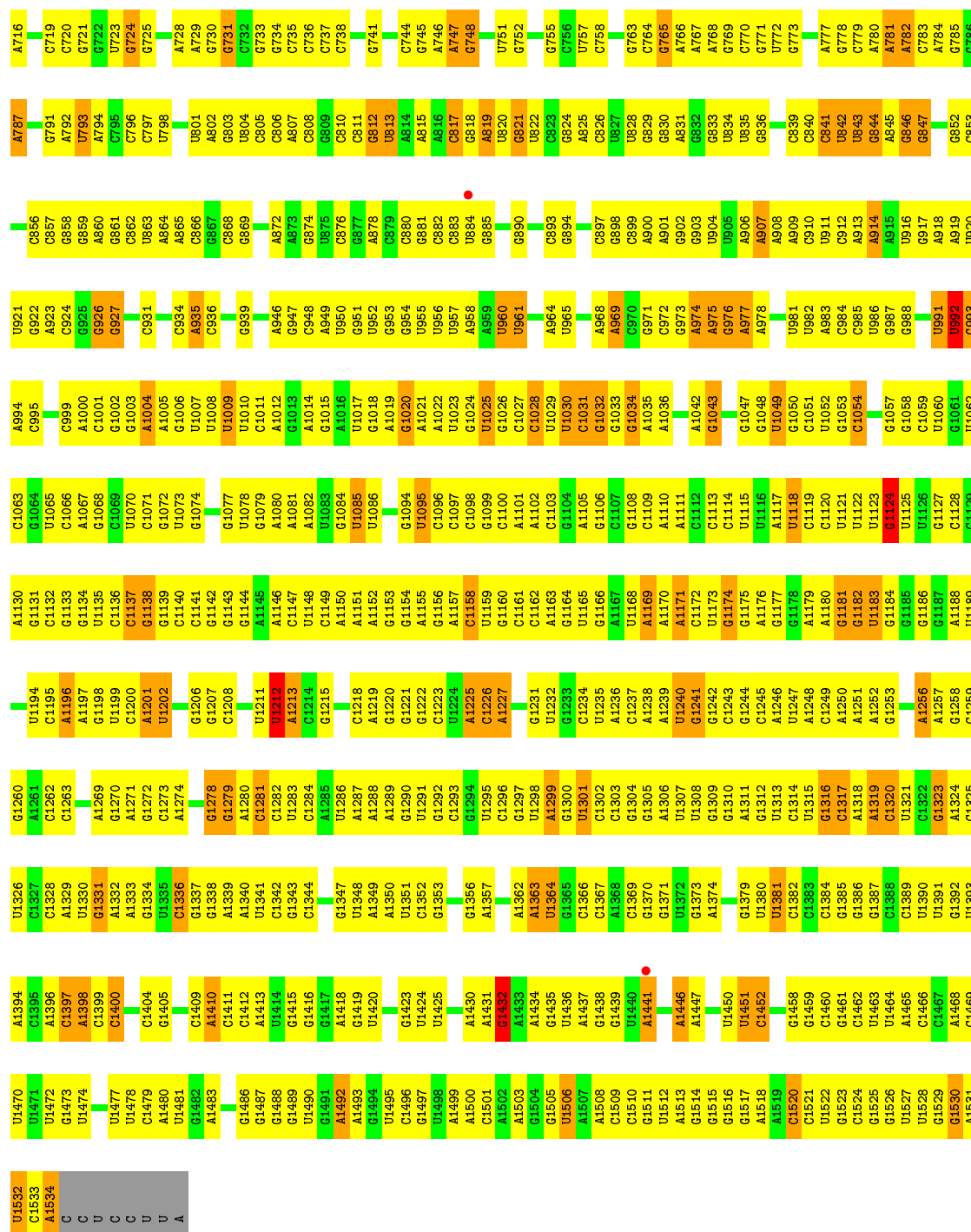
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	CA	296	Total 296	O 296	0	0
57	CE	3	Total 3	O 3	0	0
57	CK	1	Total 1	O 1	0	0
57	CL	3	Total 3	O 3	0	0
57	CN	4	Total 4	O 4	0	0
57	CT	2	Total 2	O 2	0	0
57	DB	500	Total 500	O 500	0	0
57	DC	6	Total 6	O 6	0	0
57	DE	2	Total 2	O 2	0	0
57	DL	2	Total 2	O 2	0	0
57	DR	1	Total 1	O 1	0	0
57	DT	1	Total 1	O 1	0	0

3 Residue-property plots

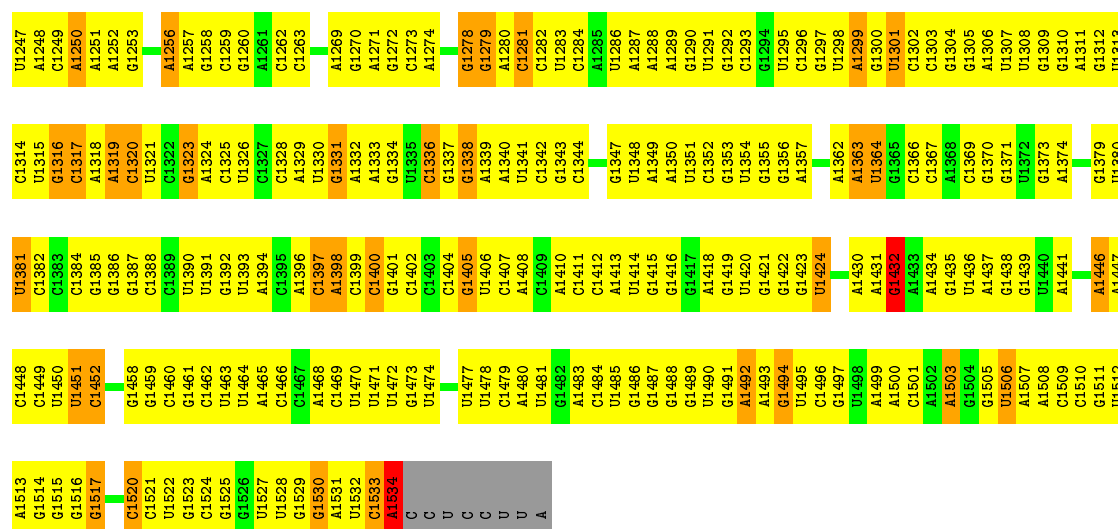
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: 16S rRNA

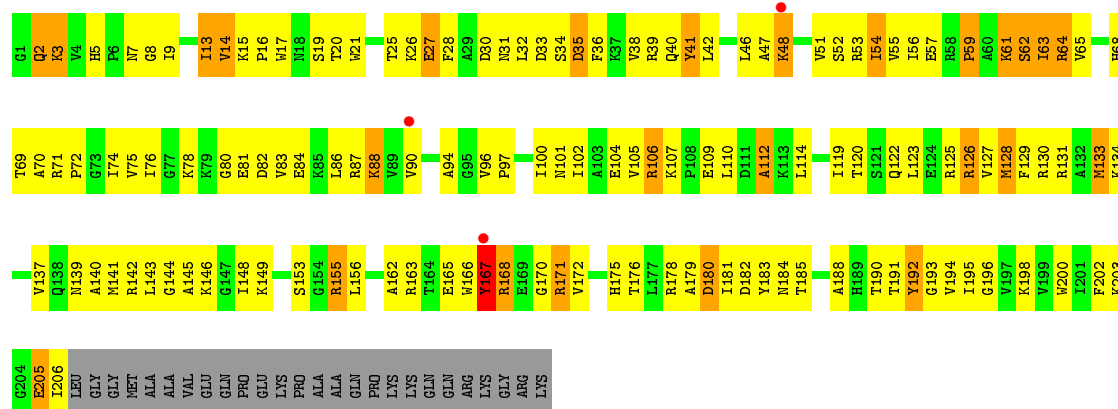




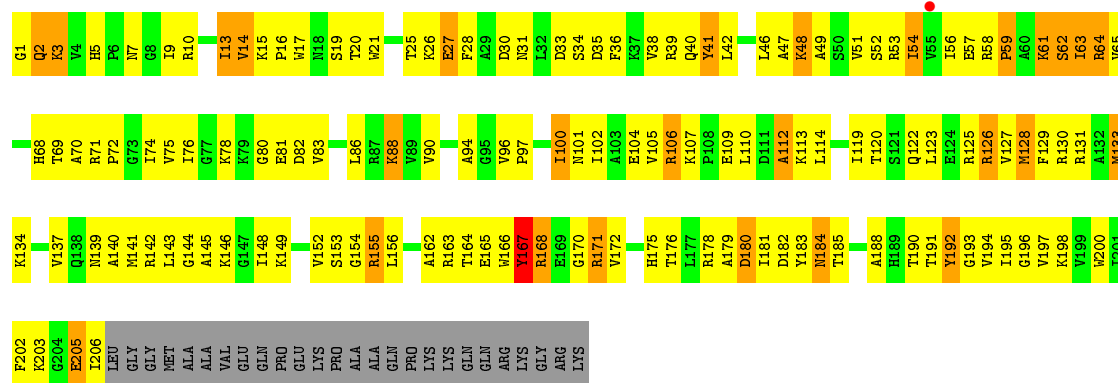
A1179	C1119	G1048	U981	A914	G852	A782	G711	A649	A523	A459	A397	A329	U261	A196	C136
A1180	C1120	U1049	U982	A915	C853	C783	G712	G650	G524	A460	U398	C330	A262	A197	C136
G1181	U1121	G1050	A983	U916	G784	A784	A713	C651	C525	A461	G399	G331	C264	G198	C137
U1122	C1051	G917	C984	G917	G785	G785	G713	U652	C526	G462	C400	G332	C264	G138	C138
U1123	C985	G918	C985	A918	G786	G786	G714	U653	C527	U463	C401	U333	G265	G201	A139
G1184	U1052	G1053	C986	A919	G787	G787	A715	U654	C528	U464	C402	U334	G266	G202	U140
U1125	C1054	G987	C987	U920	G858	U793	A716	G656	G529	A465	C403	C335	C267	G203	G141
G1186	U1126	G1057	G988	U921	G859	U794	G719	U657	G530	A466	C404	C336	U268	G142	G142
G1187	G1127	U991	U922	G922	G860	A794	C719	U658	U531	U467	U405	G337	U269	A143	A143
A1188	C1128	G1058	U992	A923	G861	C795	C720	U659	U532	A468	U406	G338	C270	C206	G144
U1189	C129	C924	C862	C924	C862	C796	G721	U660	A533	C469	U407	A338	C271	C207	G145
U1130	U1060	G993	U863	G925	U863	C797	G722	G661	U534	C470	A408	C342	C272	U208	G146
G1131	G1061	A924	A864	G926	A864	U798	U723	U662	G601	U471	U409	U343	U273	U209	G147
C1132	U1062	C995	A865	G927	A865	U799	G724	U663	A602	U472	G410	U344	C210	G210	G148
G1133	C1063	A996	C866	C930	C866	U801	G725	A663	U603	U473	A411	C345	G211	G211	A149
G1134	U1064	U997	G867	A802	A665	A802	A728	A666	G604	U474	A412	G346	G212	G212	U150
U1135	U1065	C998	C868	C931	G868	G803	A729	G667	U605	C475	G413	G352	G278	G278	A151
C1136	C1066	C999	C869	C932	G869	U804	A730	U668	G540	A476	A414	A353	C214	C214	A152
G1137	A1067	A1000	G870	G933	G870	C805	G731	G669	G542	C477	A415	G354	C215	C215	C153
U1138	C1068	C1001	A872	C934	A872	C806	G732	U670	U543	U478	G417	C355	U216	U216	U154
G1139	G1069	G1002	G873	A935	G873	C807	G733	G671	G544	U479	C418	C357	C217	C217	A155
C1140	U1070	G1003	U874	C936	U874	C808	G734	U672	C545	U480	C419	U358	G220	G220	U157
G1141	C1071	A1004	G875	C937	G875	C810	G735	A673	C546	U481	U420	U359	C221	C221	G158
G1142	G1072	A1005	C876	G939	C876	C811	G736	G674	G547	A482	U421	G359	C222	C222	G159
G1143	U1073	C911	G877	C940	G877	G812	C737	A675	G548	U483	C422	C360	A223	A223	A160
G1144	G1074	U1007	A878	G941	A878	U813	C738	G676	C549	U484	G423	G361	U224	U224	A161
U1145	U1075	U1008	C879	A946	C879	U814	C739	A677	G550	U485	G424	U365	G289	G289	A162
A1146	U1076	U1009	C880	A947	C880	A814	G740	U677	U551	U486	G425	U366	G292	G292	C163
C1147	G1077	U1010	G881	G947	G881	A815	G741	U678	U552	A487	U426	U367	U296	U296	U166
U1148	U1078	C1011	C882	C948	C882	A816	G742	U679	A553	C488	U427	U368	U231	U231	A167
C1149	G1079	A1012	C883	A949	C883	G817	G743	U680	U554	C489	G428	U369	G232	G232	G168
A1150	A1080	G1013	U884	U950	U884	G818	C744	A681	U555	C490	U429	U370	C233	C233	C169
U1151	A1081	A1014	G885	G951	G885	A819	G745	U682	C556	U491	U430	A371	C234	C234	U170
A1152	G1015	G1015	C886	G952	C886	U820	A746	U683	G557	C492	A431	C370	C235	C235	A171
G1084	G1084	A1016	G887	G953	G887	G821	A747	U684	C558	A493	A432	C372	G236	G236	A172
U1085	U1017	G954	G887	G954	G887	U822	G748	U685	A559	U494	G433	A373	G237	G237	U173
U1086	G1018	U955	G890	U955	G890	C823	A749	U686	A560	U495	G434	A374	U238	U238	A174
A1019	A1019	U956	U891	U956	U891	G824	C750	A687	U561	A496	U435	U375	U239	U239	C175
U1020	G1020	U957	A892	U957	A892	A825	U751	U688	U562	U499	A436	C307	G240	G240	C176
U1095	U1095	A958	C893	A958	C893	C826	G752	C688	A563	C500	U437	C308	G241	G241	G177
C1096	C1096	A959	G894	A959	G894	U827	G753	U689	C564	C501	U438	C309	G242	G242	C178
C1097	C1097	U960	G895	U960	G895	U828	G755	U690	C565	A502	G439	C310	G243	G243	A179
C1098	G1024	G895	G895	U961	G895	G829	G756	U691	G566	C503	C440	C311	U244	U244	U180
G1099	U1025	U961	C896	U961	C896	G830	G757	U692	G567	C504	A441	C312	U245	U245	A181
C1100	G1026	U962	C897	U962	C897	A831	C764	U693	G568	G505	G442	A392	U246	U246	A182
A1101	C1027	U963	C898	U963	C898	G832	G765	A695	A573	U508	C443	A393	G247	G247	C183
U1165	U1165	G966	C899	G966	C899	G833	A766	A696	A574	U509	G444	A394	C248	C248	G184
G1233	C1233	U166	A900	G967	A900	G834	A767	U697	C575	A510	G445	C395	U249	U249	U185
U1235	U1235	C967	A901	C967	A901	U834	A768	U698	C576	U508	G446	C396	G250	G250	C186
A1236	A1236	A968	G902	A968	G902	U835	A769	U699	C577	A511	G447	C397	G251	G251	A187
U1168	C1107	A969	G903	A969	G903	G836	C770	U700	C578	U512	G448	U387	U252	U252	C188
A1169	G1032	C970	U904	C970	U904	C839	G771	G701	C579	U513	G449	G388	G253	G253	A189
U1170	G1033	G971	U905	G971	U905	C840	A772	U702	C580	C513	A451	G389	G254	G254	A190
A1171	G1034	C972	A906	C972	A906	U841	U772	G703	C581	C514	A452	U390	G255	G255	A191
U1239	A1110	G973	A907	G973	A907	G842	G773	A704	C582	G514	G453	G391	U256	U256	A192
C1172	A1111	G973	A908	G973	A908	U843	A774	G705	C583	G515	G454	C392	G257	G257	C193
G1112	C1112	A1036	A909	A975	A909	U844	A775	A706	C584	C516	G455	A393	G258	G258	C194
C1113	C1113	A1036	A910	A976	A910	U845	G776	A707	C585	A520	G456	G394	G259	G259	A195
G1174	G1174	A1036	A911	A977	A911	A845	G777	A708	C586	G521	G457	G395	G260	G260	
G1175	G1175	A1042	C910	G976	C910	G844	G778	A709	C587	G522	G458	C396	G261	G261	
C1243	C1243	G1043	U911	G976	U911	A845	G779	A710	C588	G523	G459	G397	G262	G262	
G1244	G1244	G1043	C912	A977	C912	G845	G780	A711	C589	G524	G460	G398	G263	G263	
A1117	G1177	G846	A913	A978	A913	G847	A781	U709	C590	G525	U458	C399	G264	G264	
U1118	G1178	U1118	A913	A978	A913	G847	A781	U709	C591	G526	U459	C400	G265	G265	



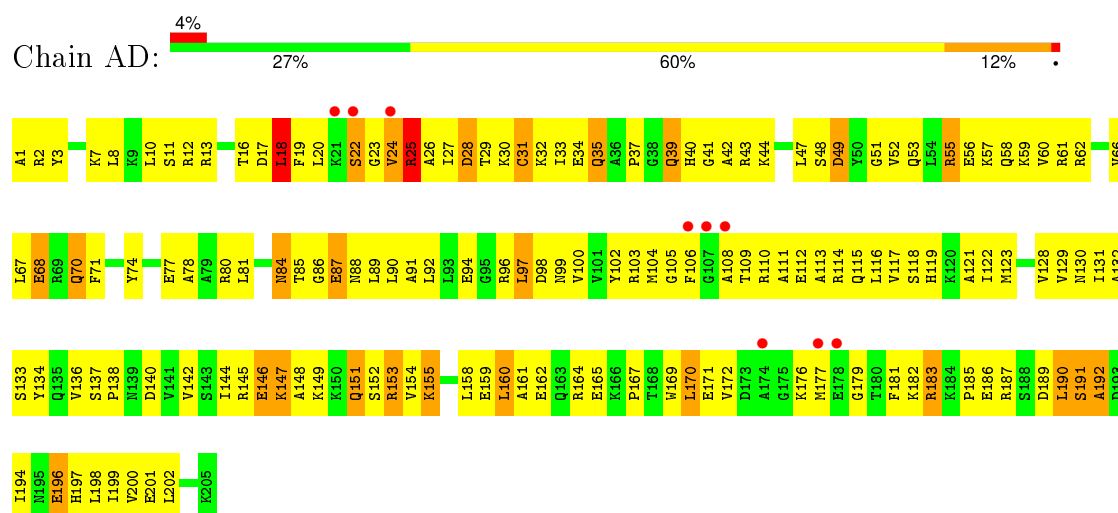
• Molecule 2: 30S ribosomal protein S3



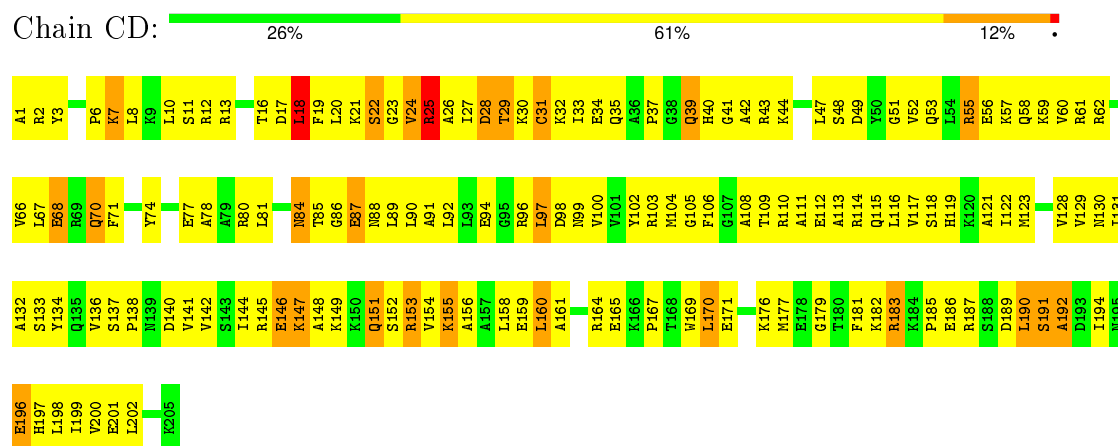
• Molecule 2: 30S ribosomal protein S3



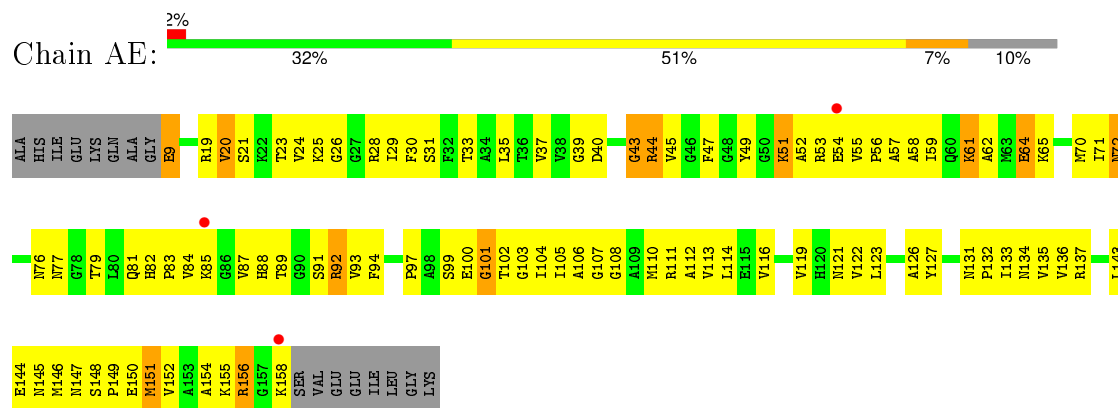
• Molecule 3: 30S ribosomal protein S4



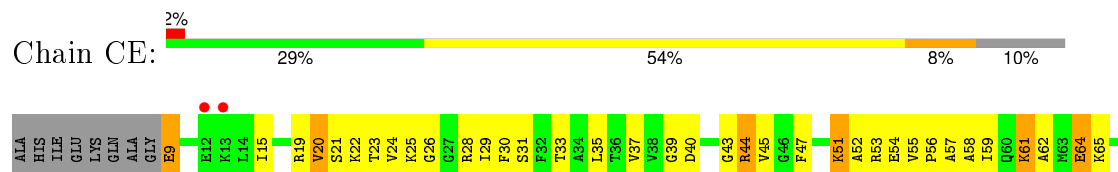
• Molecule 3: 30S ribosomal protein S4

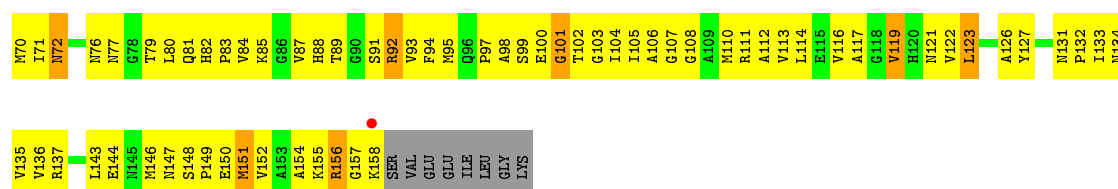


• Molecule 4: 30S ribosomal protein S5

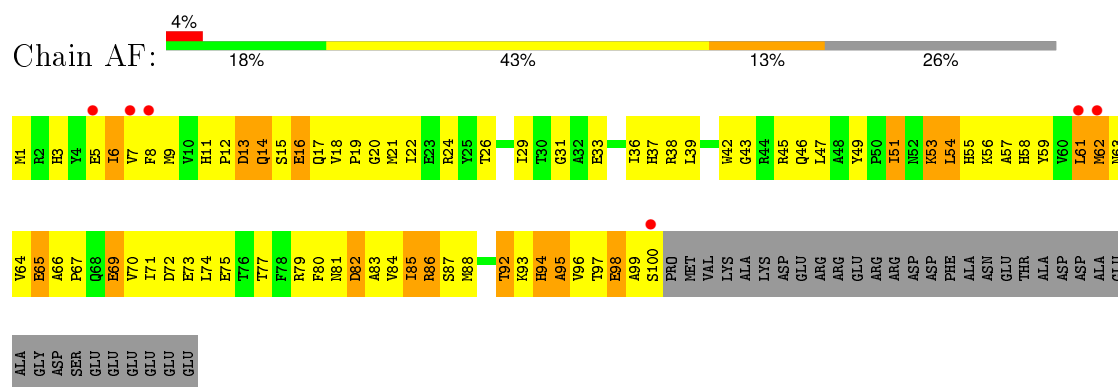


• Molecule 4: 30S ribosomal protein S5

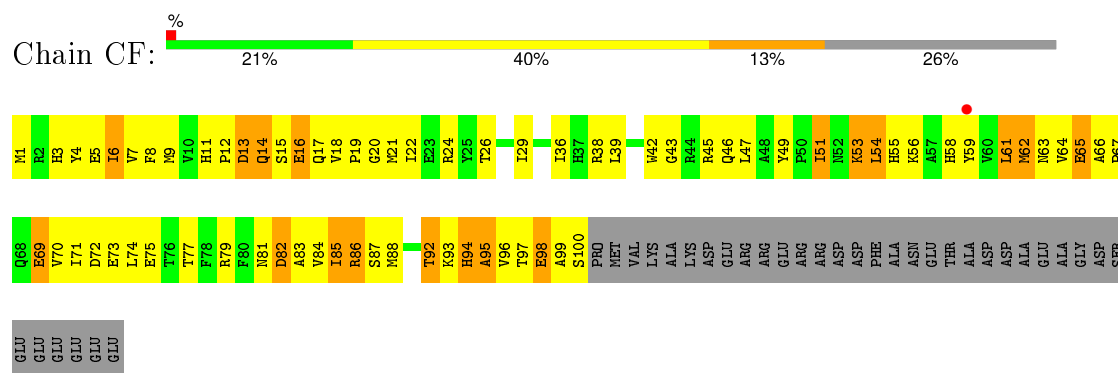




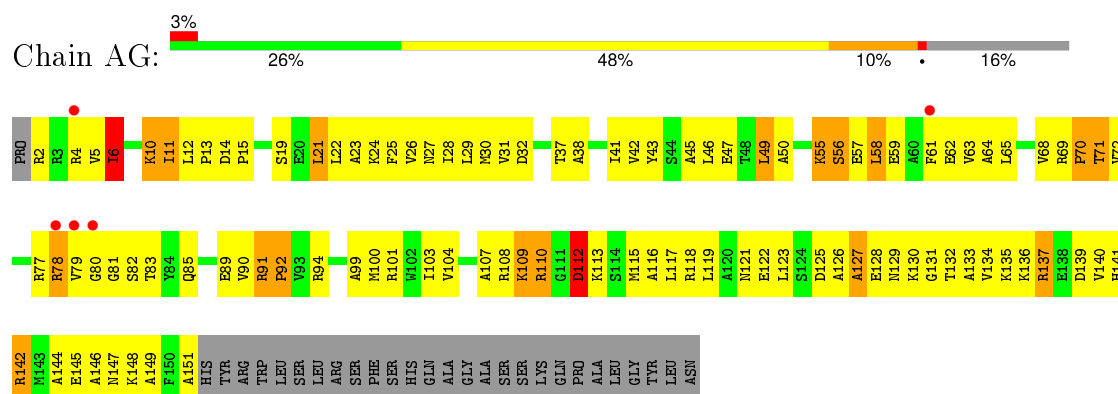
• Molecule 5: 30S ribosomal protein S6



• Molecule 5: 30S ribosomal protein S6

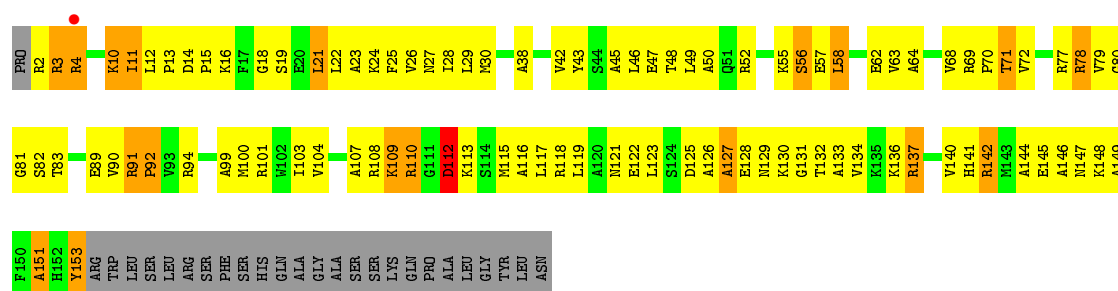


• Molecule 6: 30S ribosomal protein S7

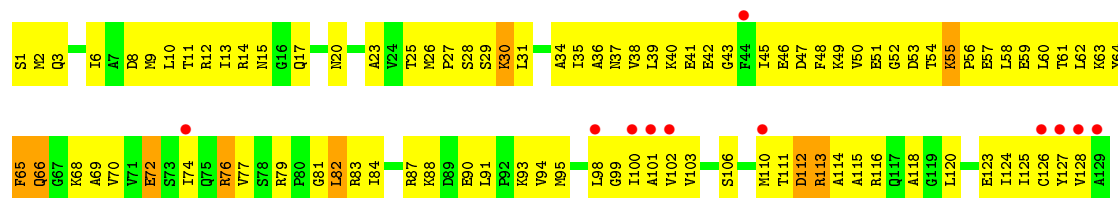


• Molecule 6: 30S ribosomal protein S7

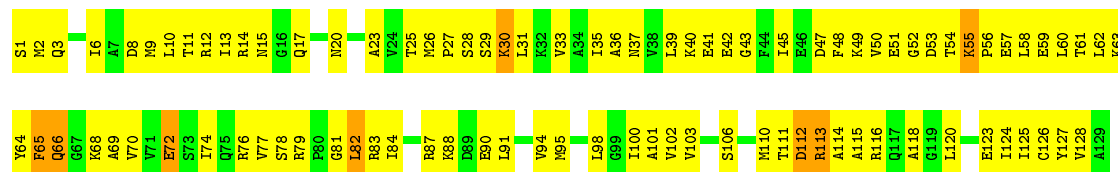




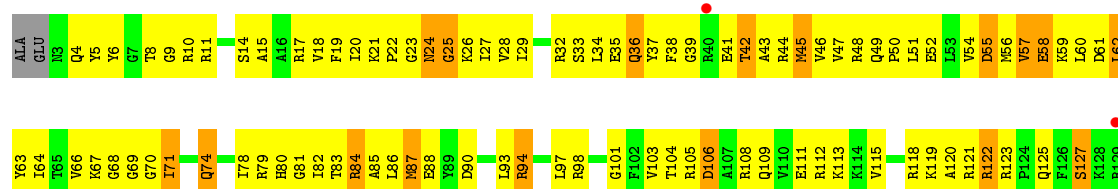
• Molecule 7: 30S ribosomal protein S8



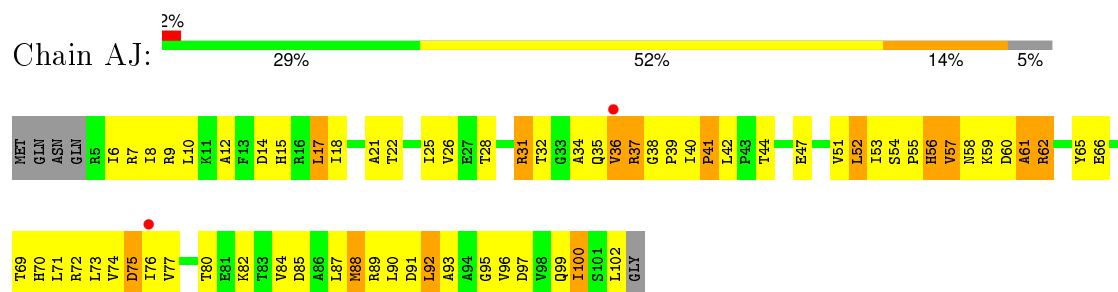
• Molecule 7: 30S ribosomal protein S8



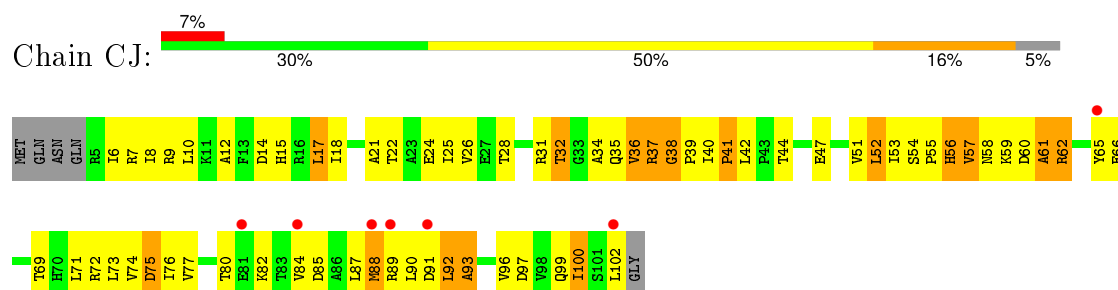
• Molecule 8: 30S ribosomal protein S9



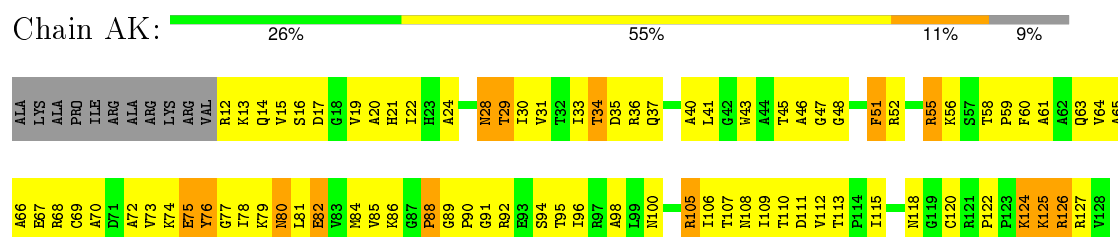
- Molecule 9: 30S ribosomal protein S10



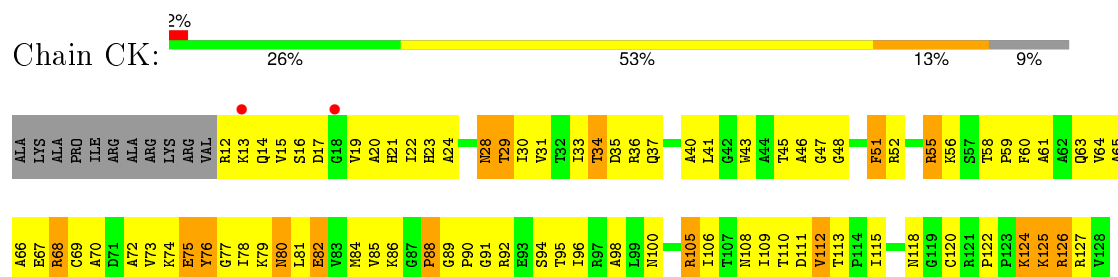
- Molecule 9: 30S ribosomal protein S10



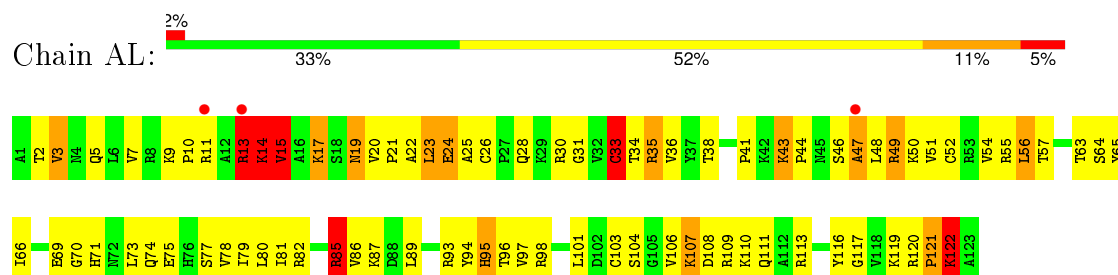
- Molecule 10: 30S ribosomal protein S11



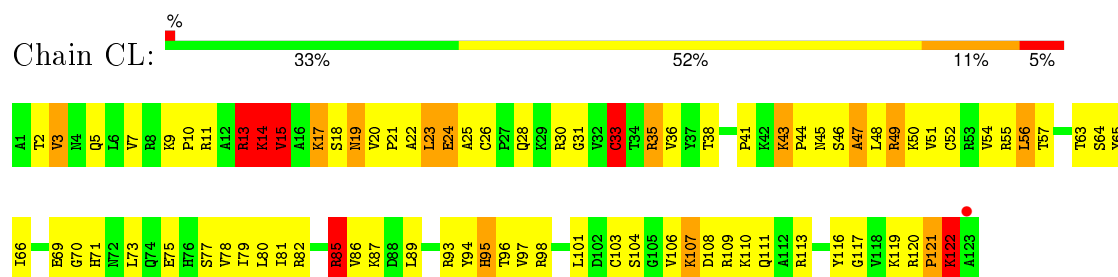
- Molecule 10: 30S ribosomal protein S11



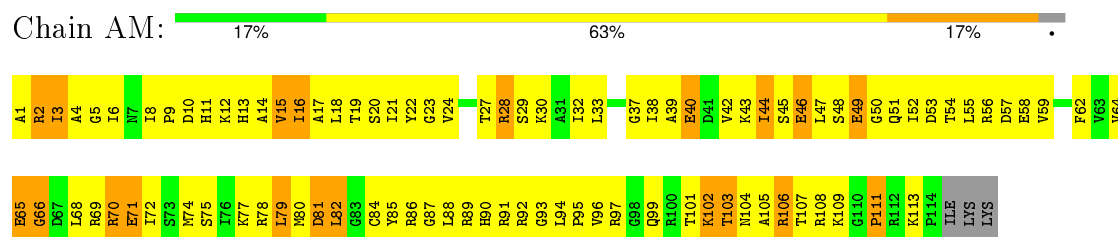
- Molecule 11: 30S ribosomal protein S12



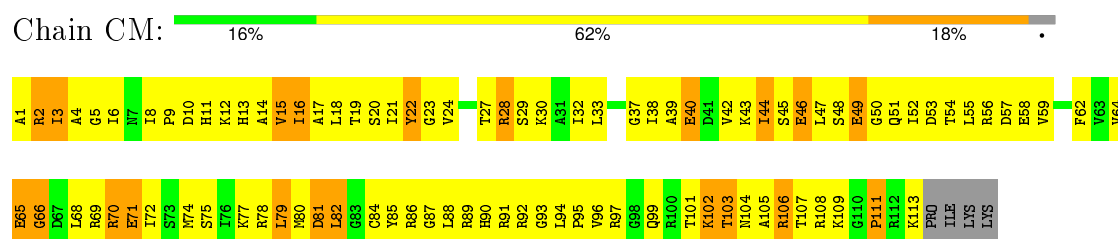
- Molecule 11: 30S ribosomal protein S12



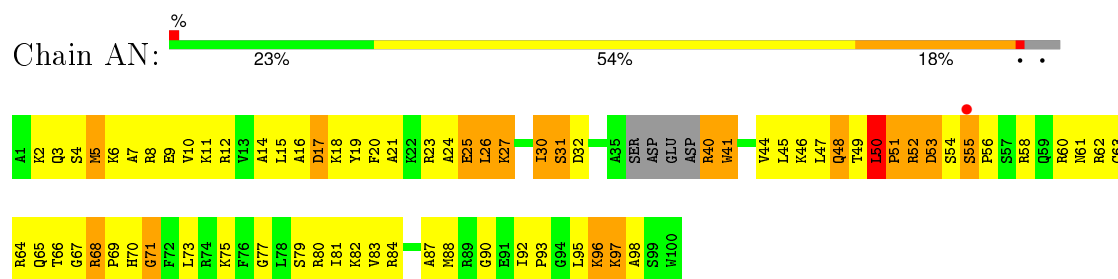
- Molecule 12: 30S ribosomal protein S13



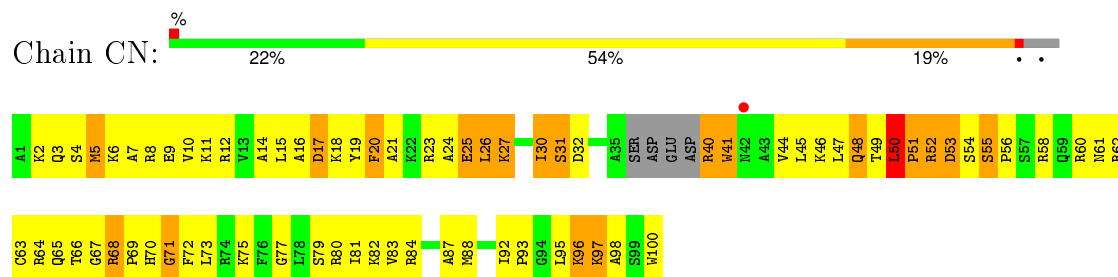
- Molecule 12: 30S ribosomal protein S13



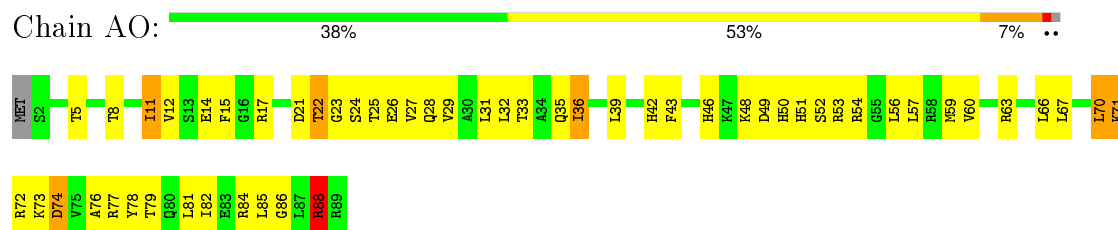
- Molecule 13: 30S ribosomal protein S14



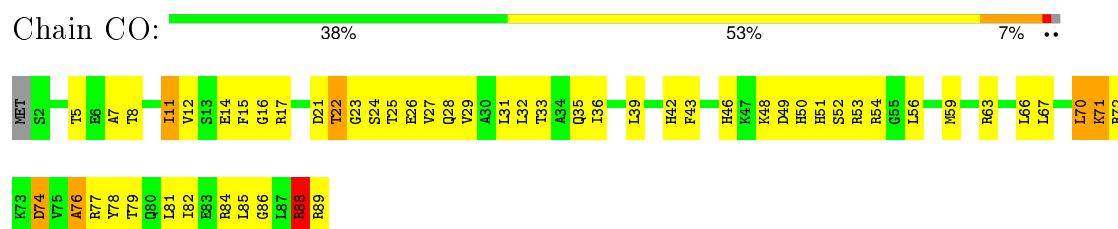
- Molecule 13: 30S ribosomal protein S14



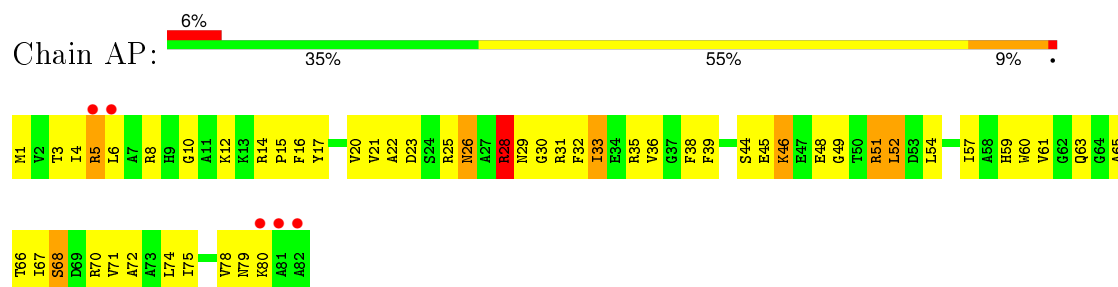
- Molecule 14: 30S ribosomal protein S15



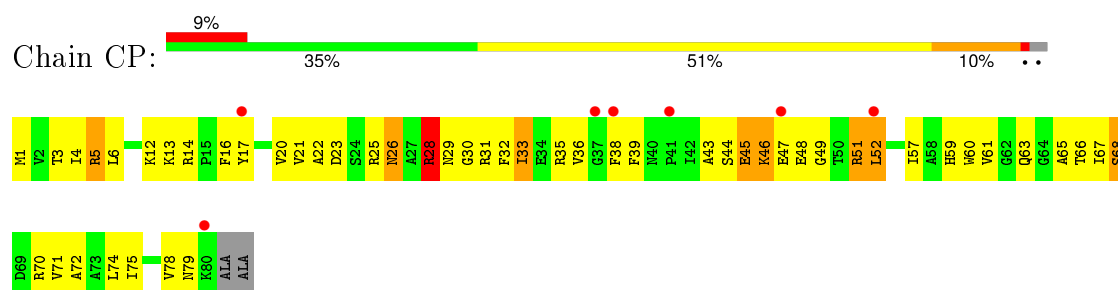
- Molecule 14: 30S ribosomal protein S15



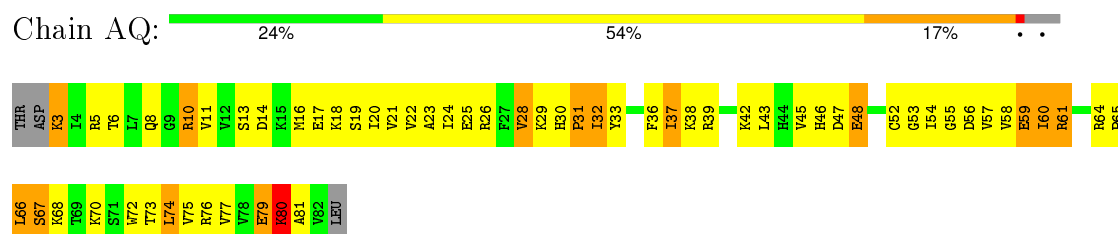
- Molecule 15: 30S ribosomal protein S16



- Molecule 15: 30S ribosomal protein S16



- Molecule 16: 30S ribosomal protein S17



- Molecule 16: 30S ribosomal protein S17

- Molecule 17: 30S ribosomal protein S18

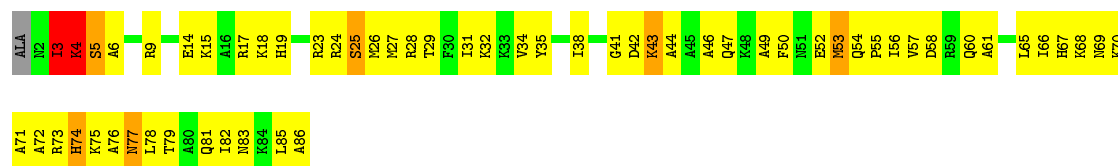
- Molecule 17: 30S ribosomal protein S18

- Molecule 18: 30S ribosomal protein S19

- Molecule 18: 30S ribosomal protein S19

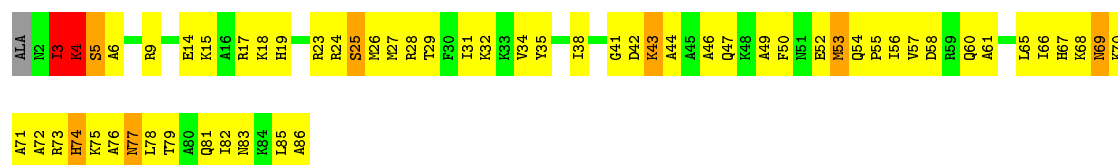
- Molecule 19: 30S ribosomal protein S20

Chain AT: 



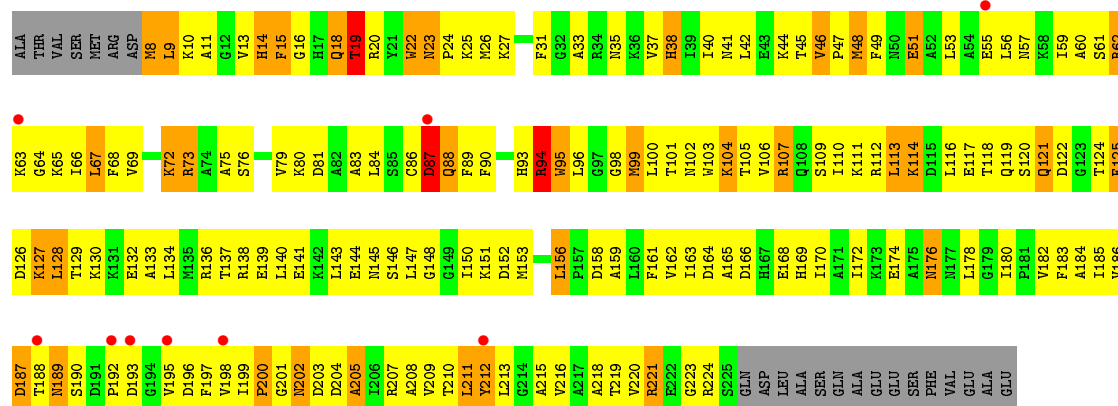
• Molecule 19: 30S ribosomal protein S20

Chain CT: 



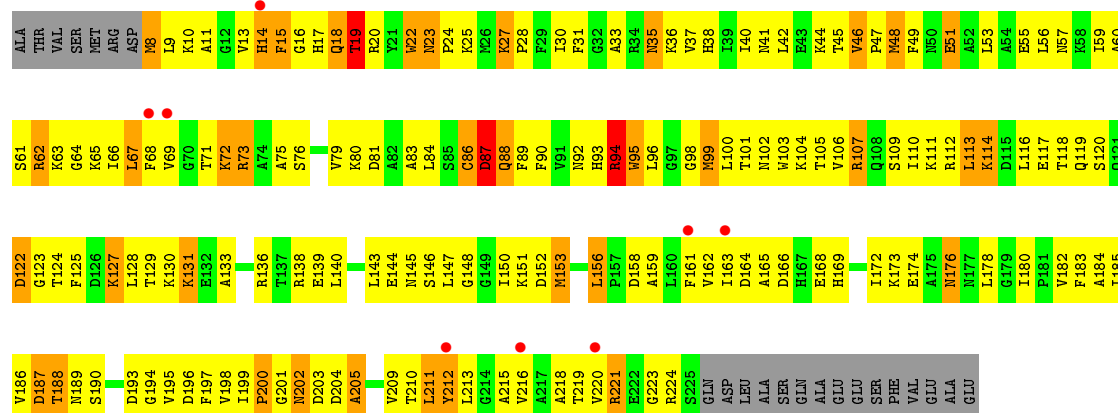
• Molecule 20: 30S ribosomal protein S2

Chain AB: 



• Molecule 20: 30S ribosomal protein S2

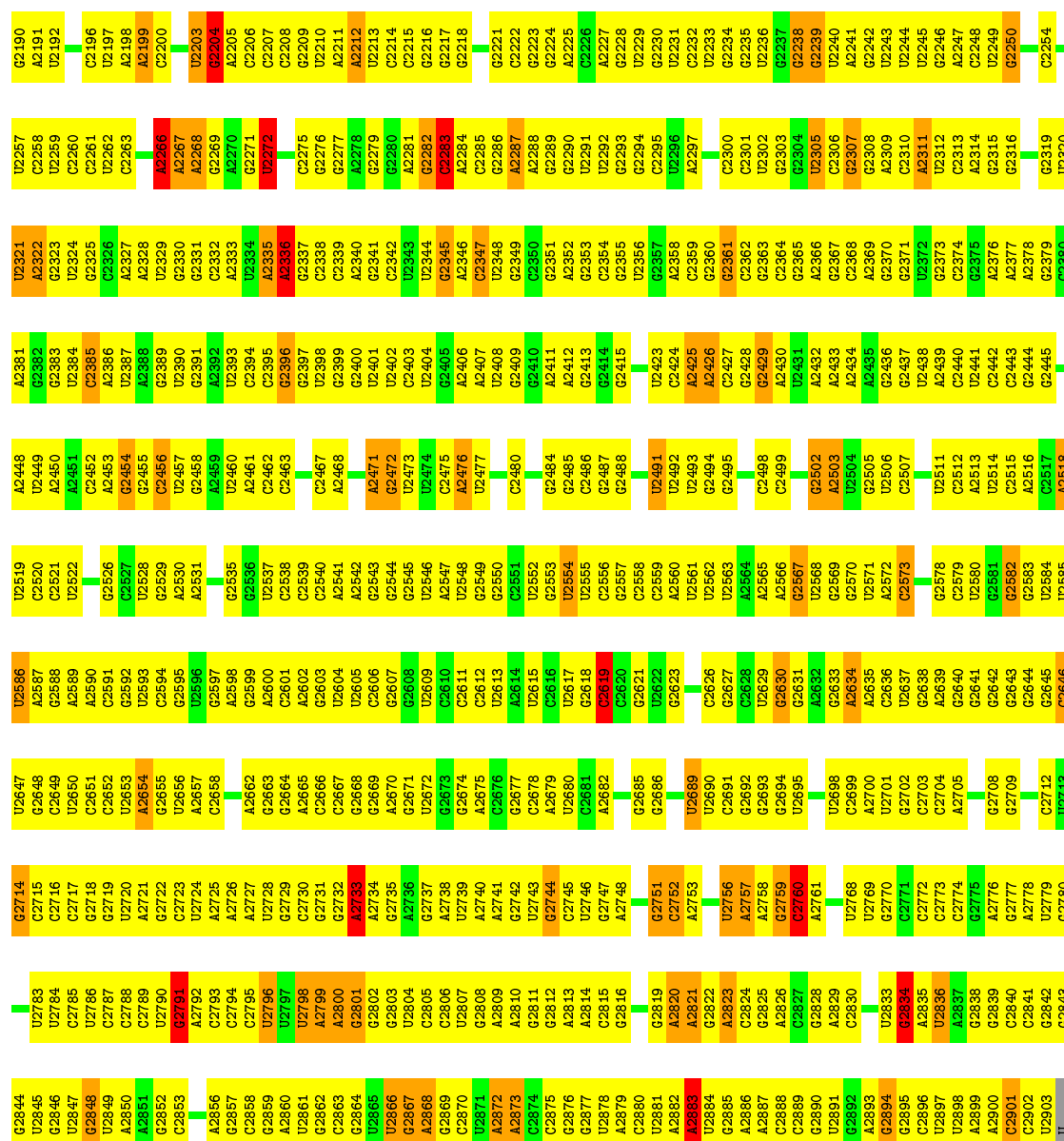
Chain CB: 



- 
- WORLD WIDE
PDB
PROTEIN DATA BANK

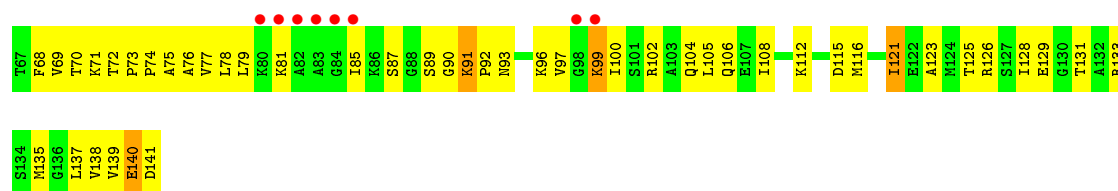
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G1136	A1070	A996	C935	G864	A734	G689	U546	G476	G408	C335	C268	U202	G136
G1137	G1071	A1000	U936	A865	A735	A609	A547	A477	G409	C336	C269	A203	U137
G1138	C1072	A1001	A937	A866	A736	C611	G548	A478	G410	C337	G271	G204	U138
G1139		G1002	G938	G869	A737	G612	G549	A479	G411	G338	G272	U206	U139
C1140			G939	U870	C737	G673	C550	A480	G412	U339	A273	A207	C140
U1141	G1076	C1007	G940	U871	C738	A674		A481	C413	A340	C274	C208	G141
A1142	U1077		U872	U877	A675	A675	G553	G482	C414	C341	C275	C209	A142
A1143	U1078		U873	C679	U615	U615	U554	A483	A415	A345	U276		C143
C1144	A1080	A1010	A941	U810	A616	U616	G555	A484	U416	A346	G277	G215	C144
C1145	U1081	G1011	A943	C812	A742	G617	A556	C485	U417	A347	A278	A216	C145
C1146	U1082	C1013	A945	C814	A743	G681	C557	C486	C418	A348	A279	A217	C146
A1147	U1083	A1014	G946	C815	U744	G682	C558		U419	A349	A280	A218	U148
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C1152	A1088	U1019	C951	A820	A753	U688	A563	G495	G426	A354	G285	A223	U153
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U1097	U1098	G1026	U958	U827	A632	G632	G570	A505	A433	C364		G230	A160
A1098	A1099	A1027	A959	C957	A633	U632	U571	A506	C433	U365	A294	G231	A161
C1162	A1099	A1028	G960	C958	A634	C698	A572	A507	U434	C366	A295	G232	U162
G1162	U1101	A1029	C961	A635	A764	A699	U573	A508	C435	U296	G296	G233	C163
G1163	C1102	U1032	G962	C962	C765	G700	A574	C509	A436	G370	G297	U234	C164
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		U1034	C964	U833	U767	U702	A576	U511	G438	G372	C299	C236	
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		U1046	A973	U842	G711	G647	A586	G520	U451	A383	A310	G247	G178
		G1047	A974	U843	G712	G648	C587	U521	U452	A384	A311	G248	C179
			A975	U844	G713	G649	U588	A522	A454	C385		G249	G180
			C975	U845	G714	C650	U589	C523	C455	G386	G315	A181	
			U913	C846	A715	G651	A590	A526	C456	U387	C316	G250	A182
			A917	C848	A716	U652	U591	A527	A457	G388	C317	A251	C183
			A918	U850	C717	U653	A592	A528	G458	U389	G318	G252	C184
			U919	C851	A718	A654	U593	A529	U459	U390	G319	C253	G185
			A920	U852	C719	G655	U594	C531	A460	U391	A320	G254	
			C921	C853	U720	G656	C595	A532	C461	U392	U321	A255	G189
			C922	C854	A721	U657	U596	A533	A461	U393	A322	A256	A190
			G923	C855	A722	U658	G597	U534	U464	C394	C323	C257	A191
				C856	G725	G659	U598	U535	A465	U395	A324	C258	C192
				C857	G726	C660	A599	G535	A466	U396	G325	G259	U193
				C858	A727	A661	C601	A538	G467	U397	G329	G260	G194
				C859	G728	G664	A602	G539	G468	A401	A330	G263	A195
				U860	G729	U665	A603	C540	G469	A402	C331	C264	A196
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WORLDWIDE
PDB
PROTEIN DATA BANK

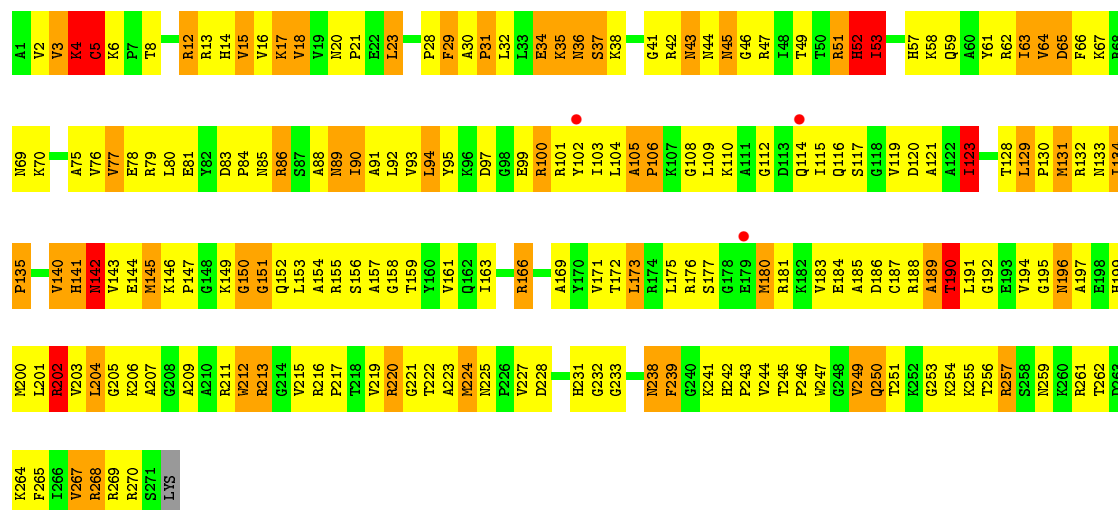




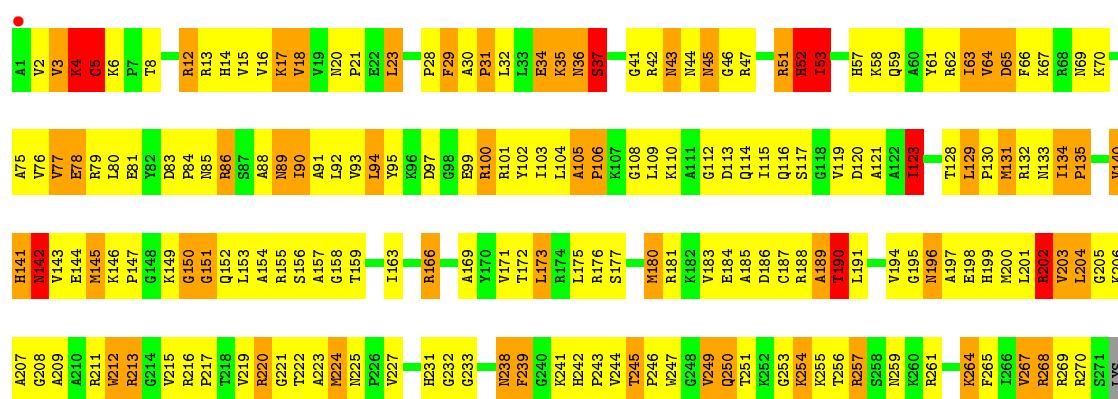




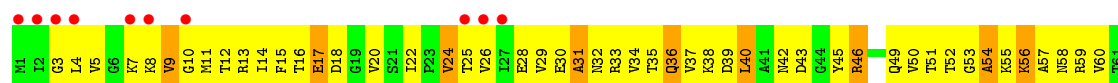
• Molecule 25: 50S ribosomal protein L2

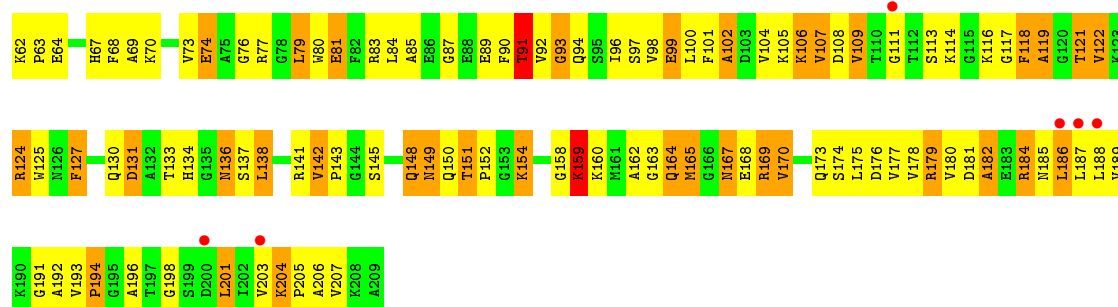


• Molecule 25: 50S ribosomal protein L2



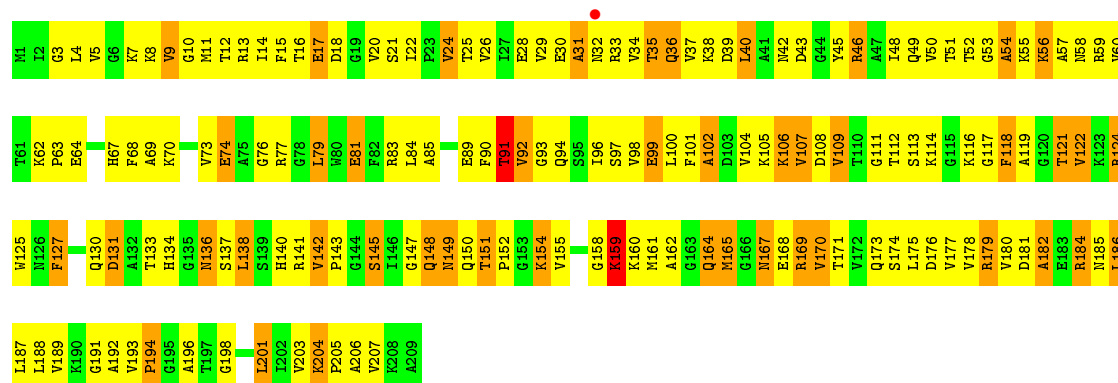
• Molecule 26: 50S ribosomal protein L3





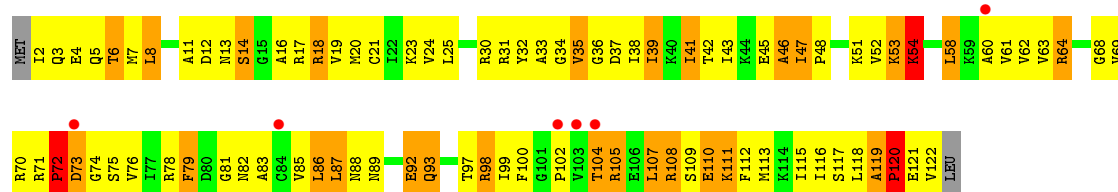
- Molecule 26: 50S ribosomal protein L3

Chain DD: 24% 54% 22%



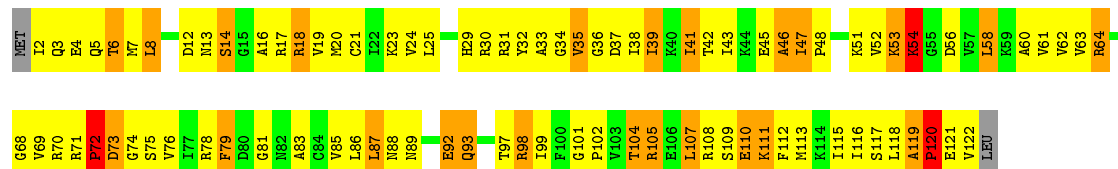
- Molecule 27: 50S ribosomal protein L14

Chain BK: 5% 25% 50% 21%



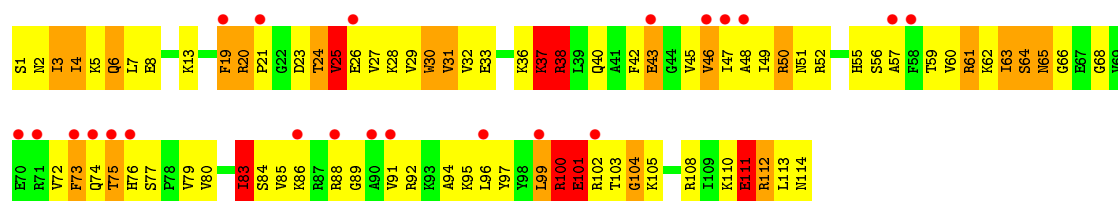
- Molecule 27: 50S ribosomal protein L14

Chain DK: 25% 51% 20%



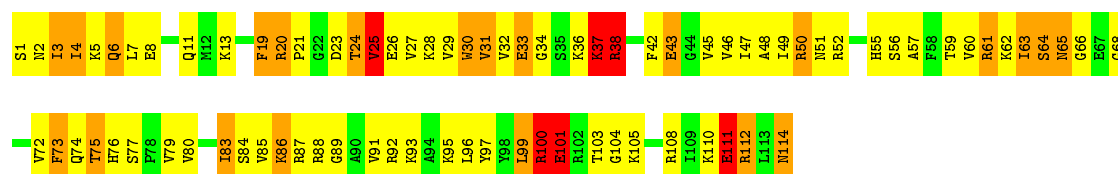
- Molecule 28: 50S ribosomal protein L19

Chain BP: 19% 28% 48% 18% 6%



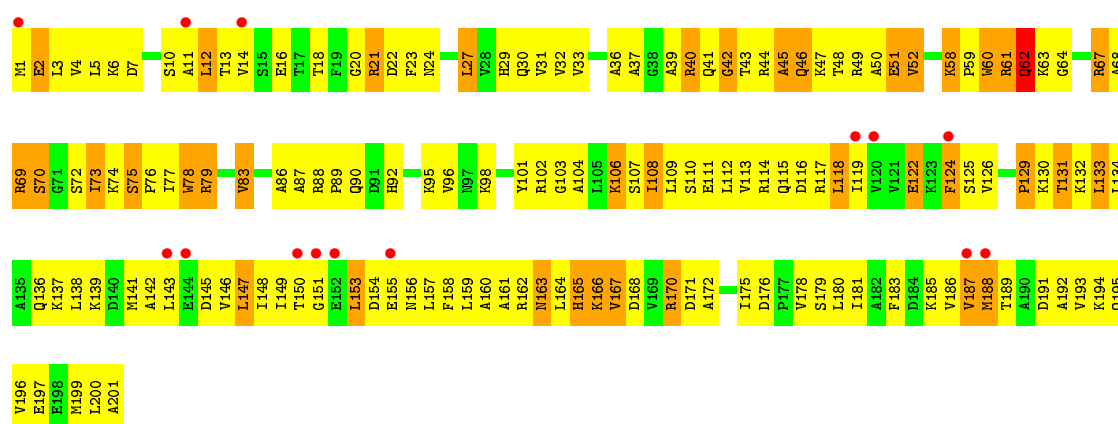
• Molecule 28: 50S ribosomal protein L19

Chain DP: 28% 47% 19% 5%



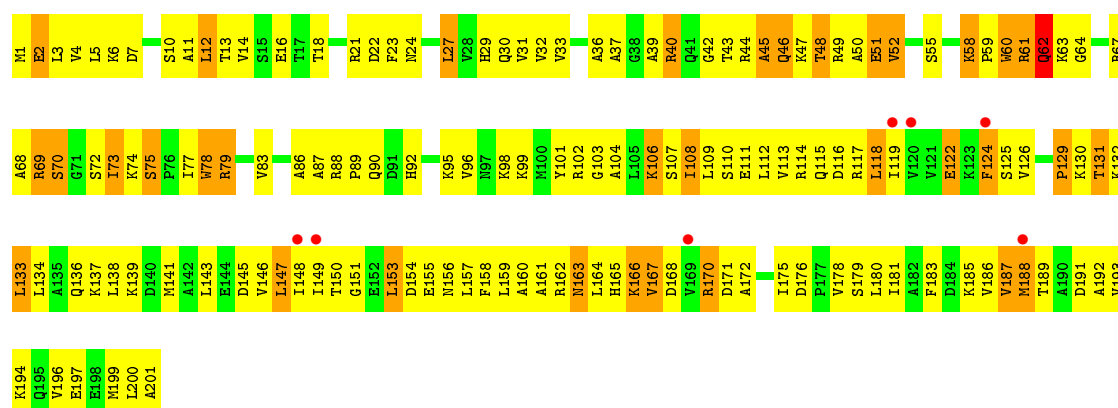
• Molecule 29: 50S ribosomal protein L4

Chain BE: 7% 24% 57% 19%

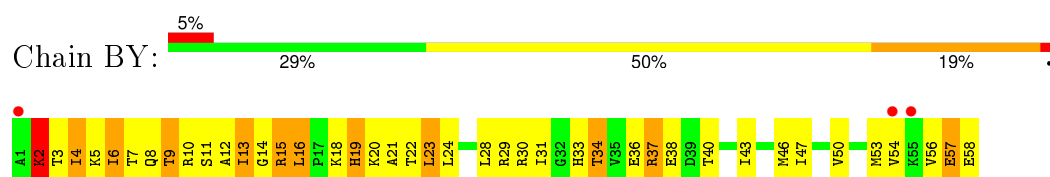


• Molecule 29: 50S ribosomal protein L4

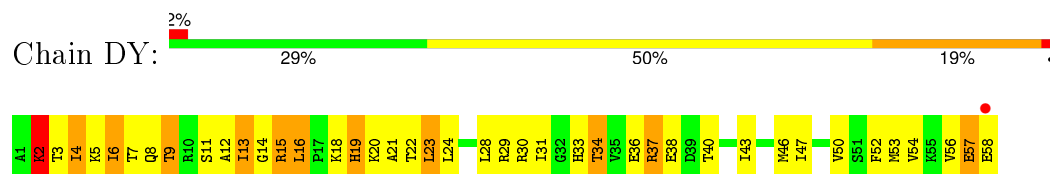
Chain DE: 3% 25% 57% 17%



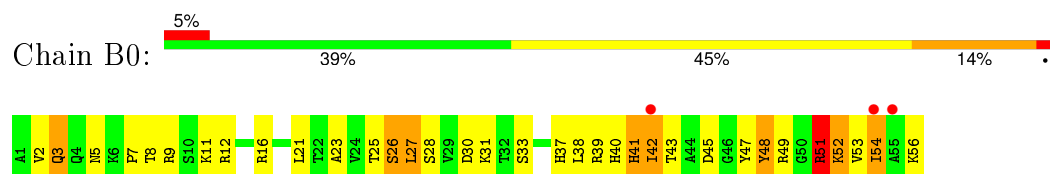
• Molecule 30: 50S ribosomal protein L30



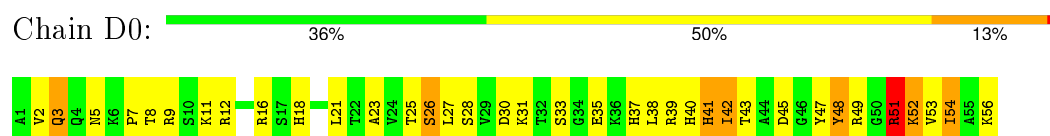
- Molecule 30: 50S ribosomal protein L30



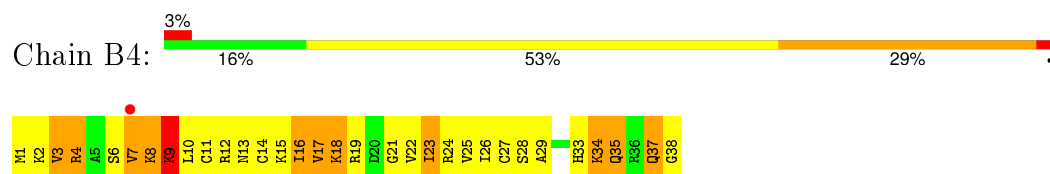
- Molecule 31: 50S ribosomal protein L32



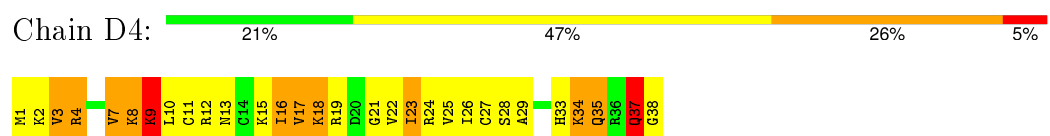
- Molecule 31: 50S ribosomal protein L32



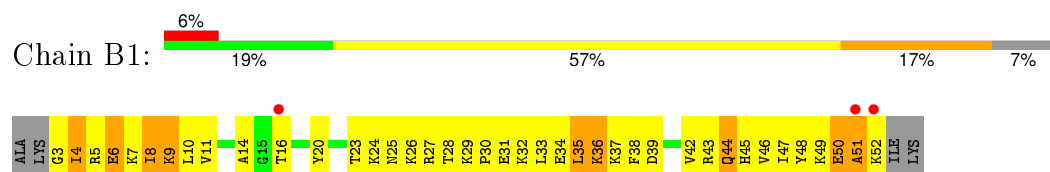
- Molecule 32: 50S ribosomal protein L36



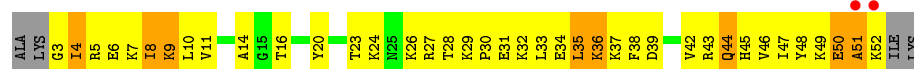
- Molecule 32: 50S ribosomal protein L36



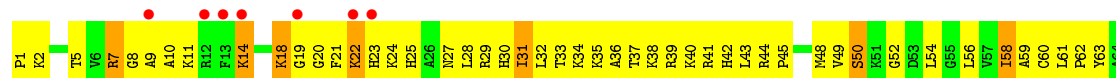
- Molecule 33: 50S ribosomal protein L33



- Molecule 33: 50S ribosomal protein L33



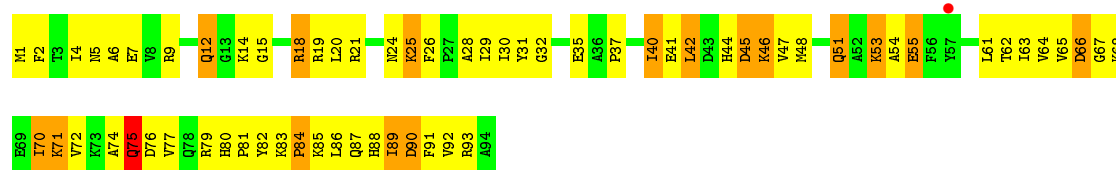
- Molecule 34: 50S ribosomal protein L35



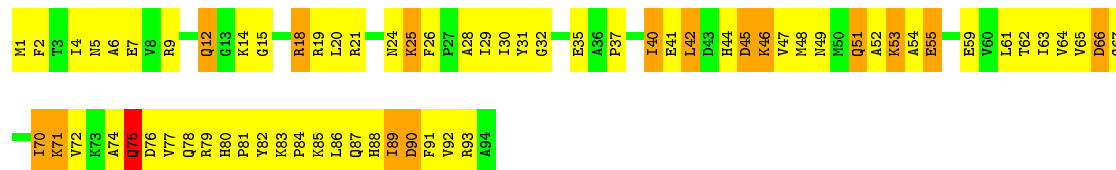
- Molecule 34: 50S ribosomal protein L35



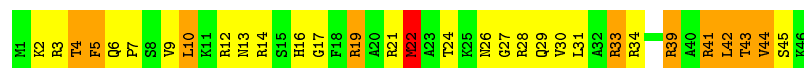
- Molecule 35: 50S ribosomal protein L25



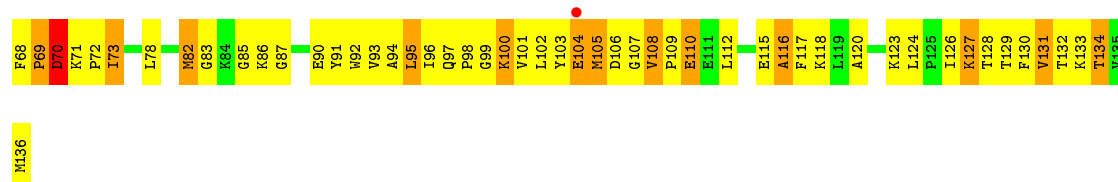
- Molecule 35: 50S ribosomal protein L25



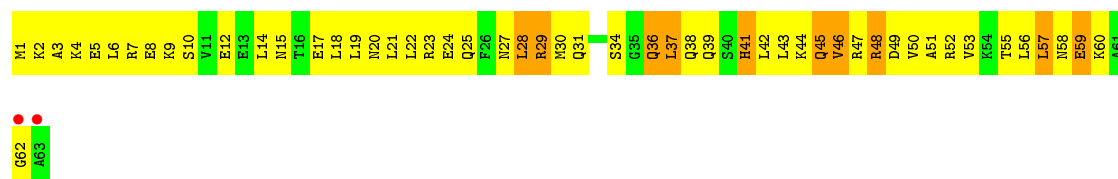
- Molecule 36: 50S ribosomal protein L34



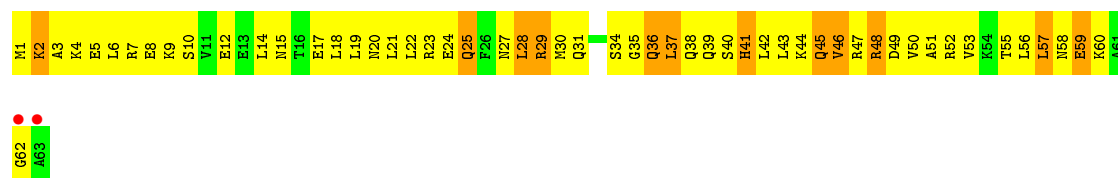
- Molecule 36: 50S ribosomal protein L34



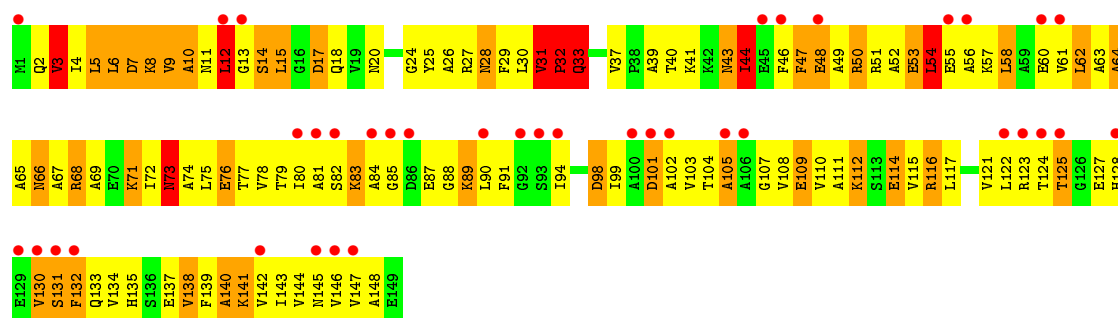
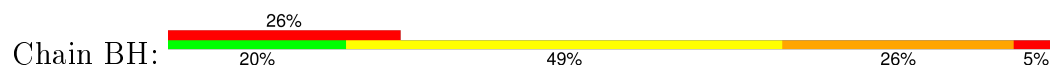
• Molecule 39: 50S ribosomal protein L29



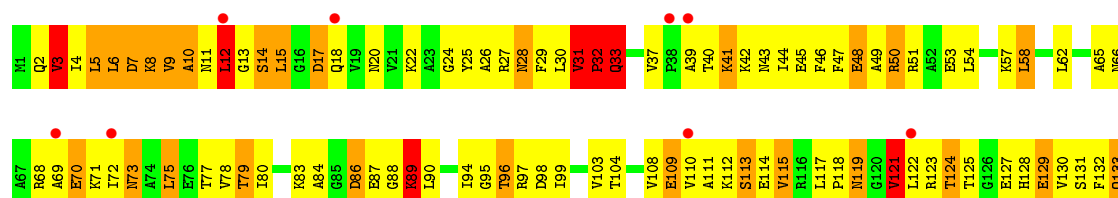
• Molecule 39: 50S ribosomal protein L29



• Molecule 40: 50S ribosomal protein L9

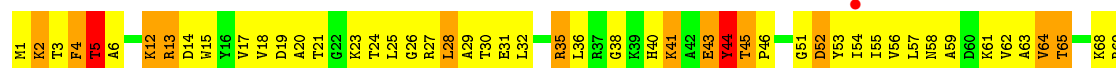


• Molecule 40: 50S ribosomal protein L9

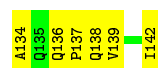
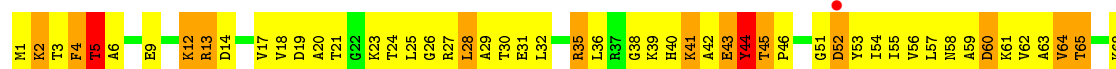




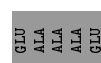
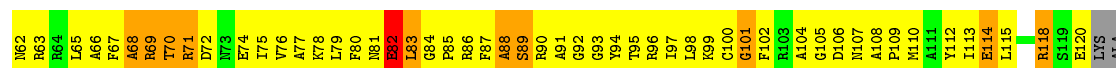
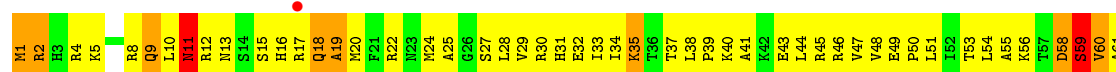
• Molecule 41: 50S ribosomal protein L13



• Molecule 41: 50S ribosomal protein L13



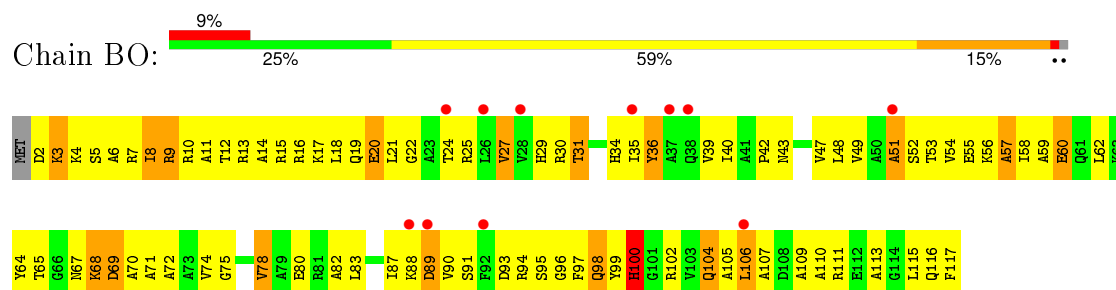
• Molecule 42: 50S ribosomal protein L17



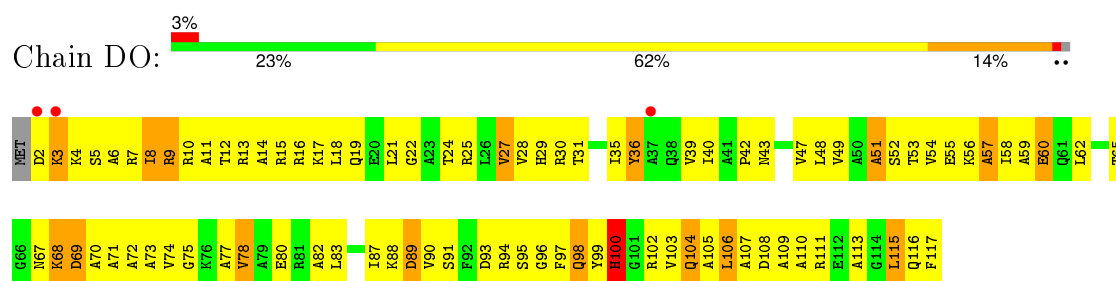
• Molecule 42: 50S ribosomal protein L17



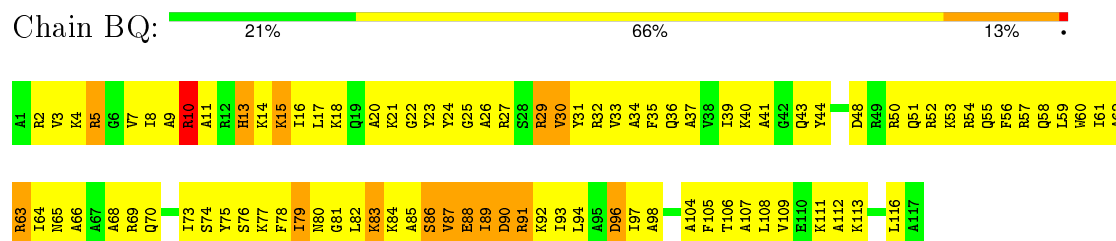
- Molecule 43: 50S ribosomal protein L18



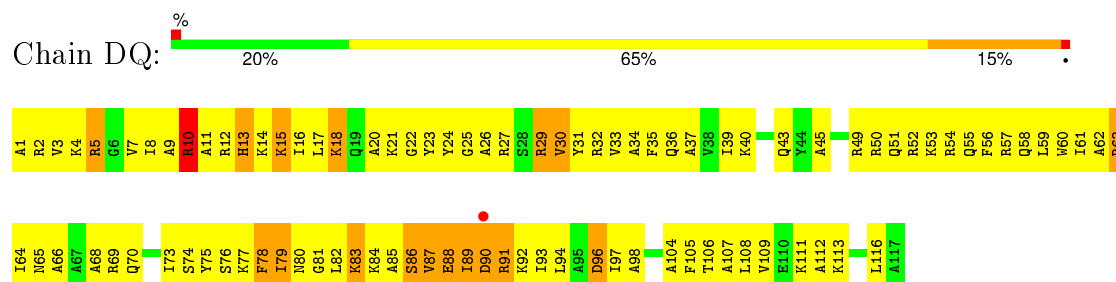
- Molecule 43: 50S ribosomal protein L18



- Molecule 44: 50S ribosomal protein L20

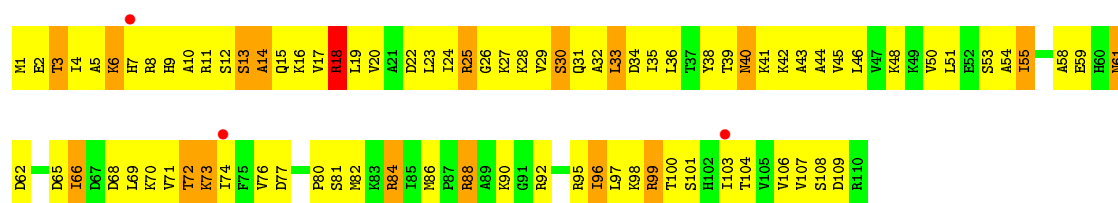


- Molecule 44: 50S ribosomal protein L20

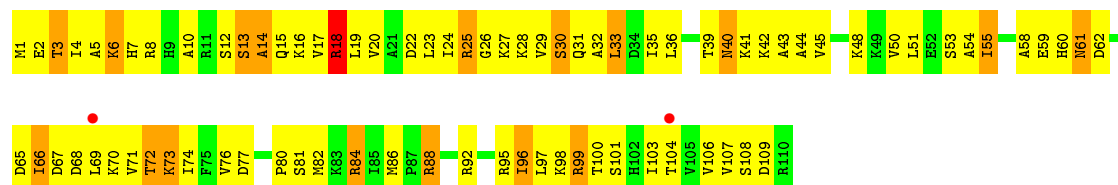


- Molecule 45: 50S ribosomal protein L22

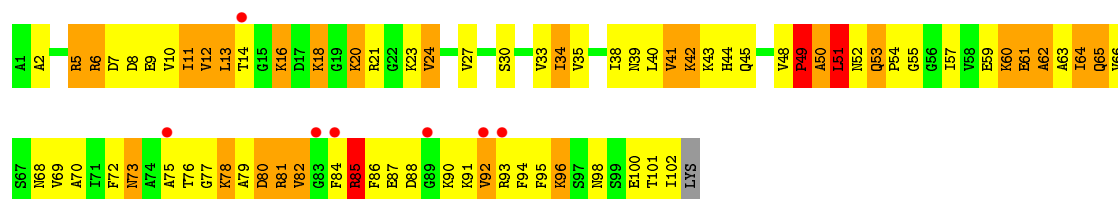




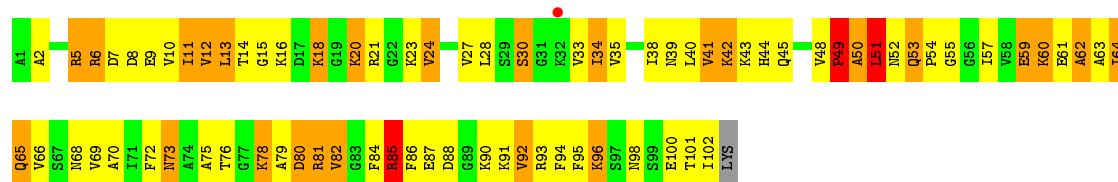
• Molecule 45: 50S ribosomal protein L22



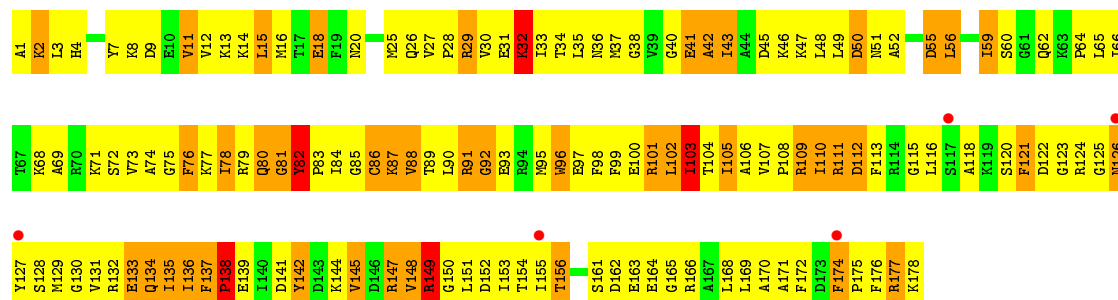
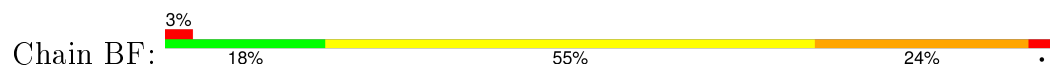
• Molecule 46: 50S ribosomal protein L24



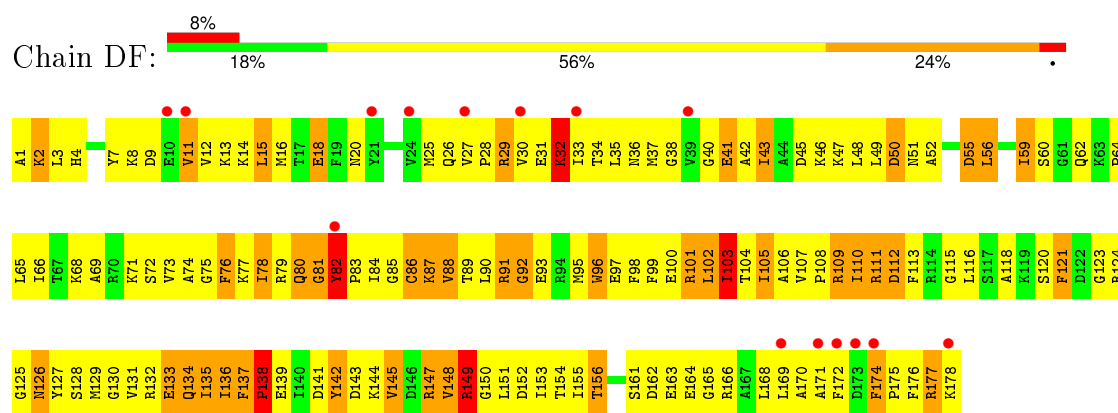
• Molecule 46: 50S ribosomal protein L24



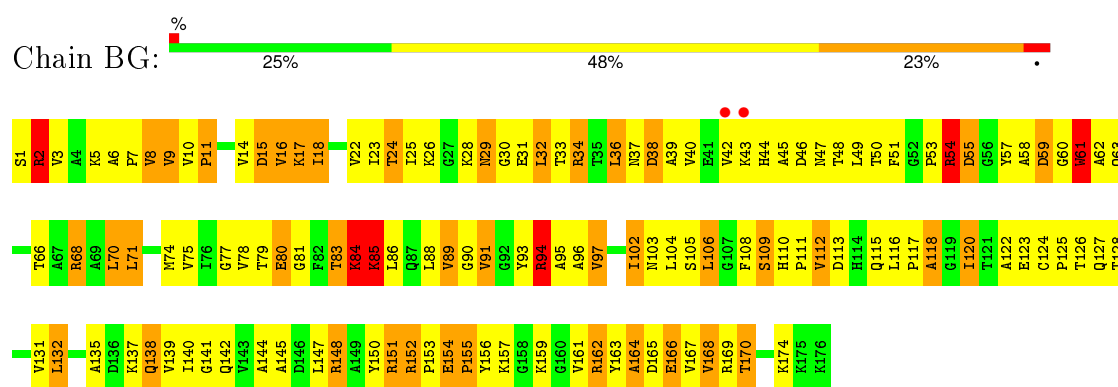
• Molecule 47: 50S ribosomal protein L5



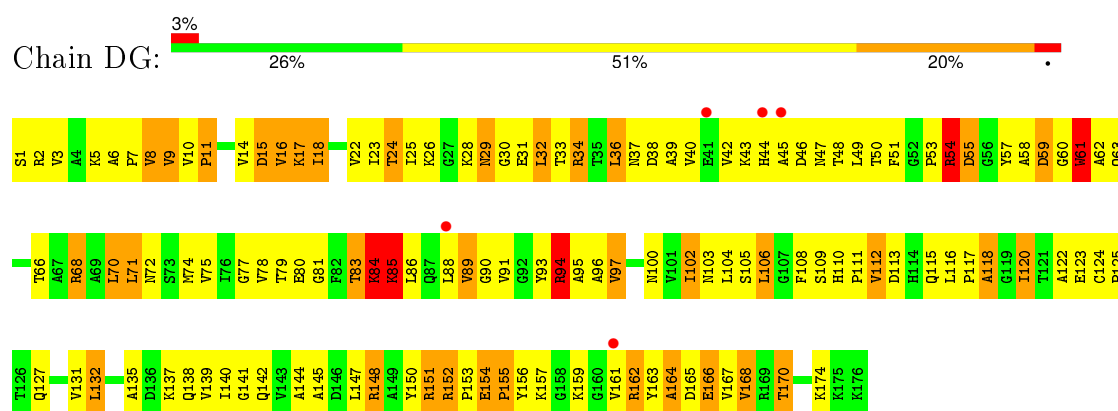
- Molecule 47: 50S ribosomal protein L5



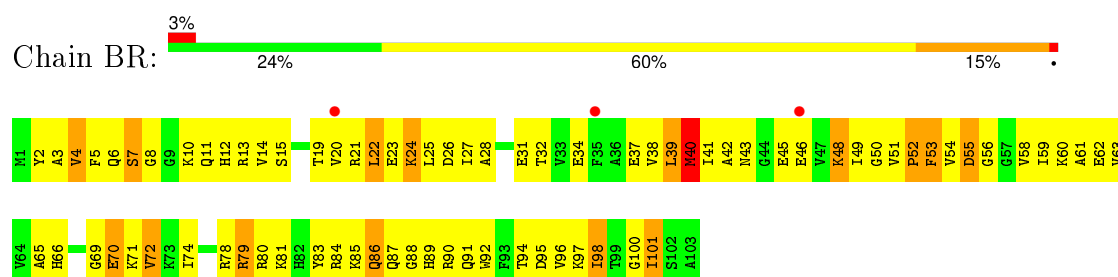
- Molecule 48: 50S ribosomal protein L6



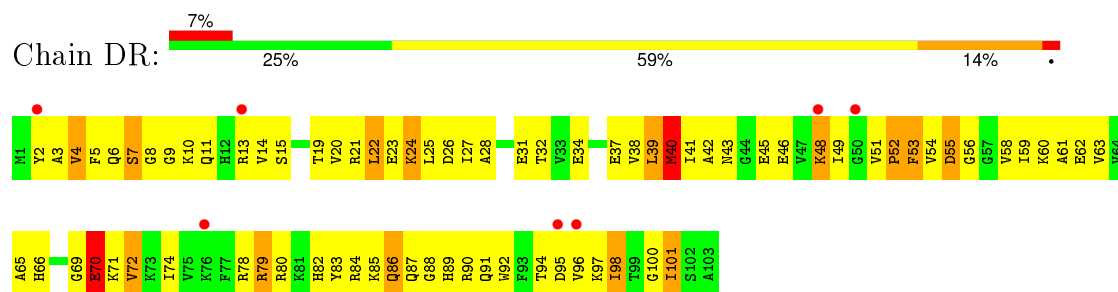
- Molecule 48: 50S ribosomal protein L6



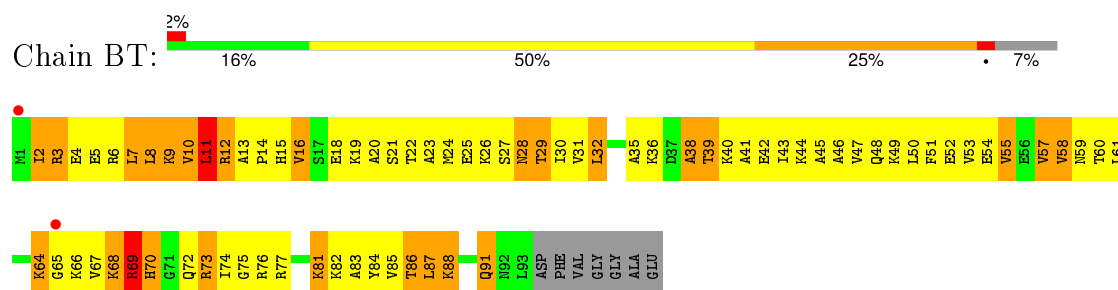
- Molecule 49: 50S ribosomal protein L21



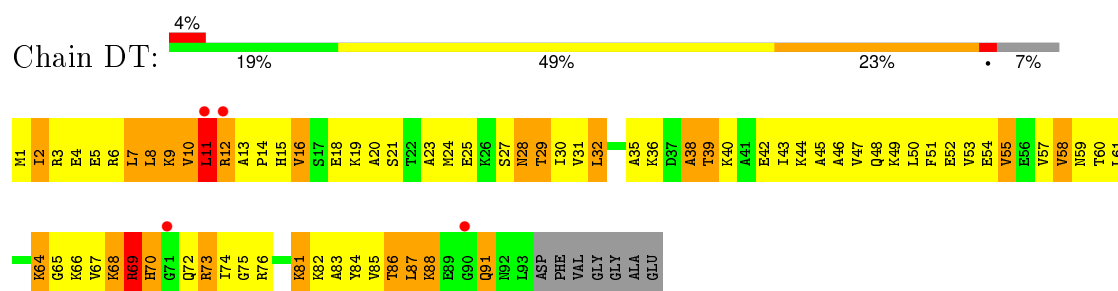
- Molecule 49: 50S ribosomal protein L21



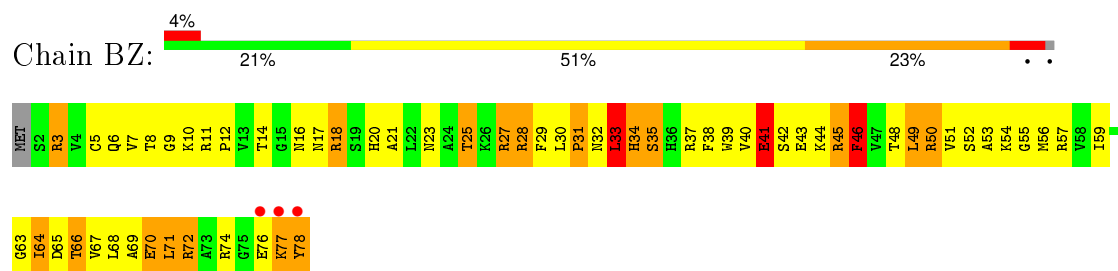
- Molecule 50: 50S ribosomal protein L23



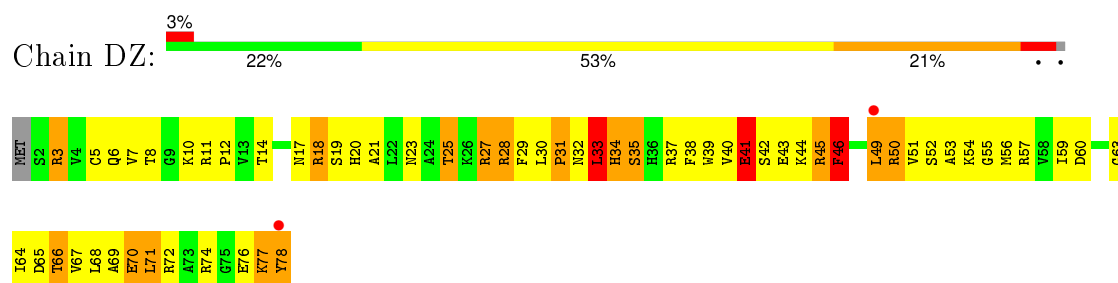
- Molecule 50: 50S ribosomal protein L23



- Molecule 51: 50S ribosomal protein L28

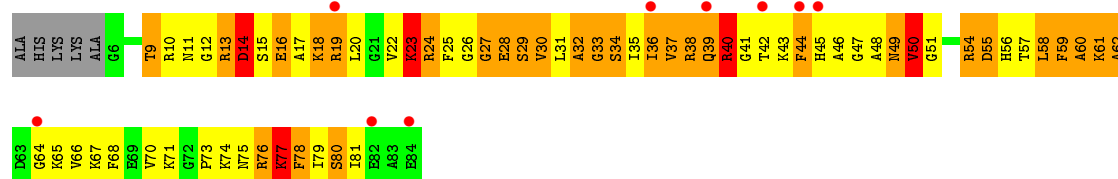


- Molecule 51: 50S ribosomal protein L28




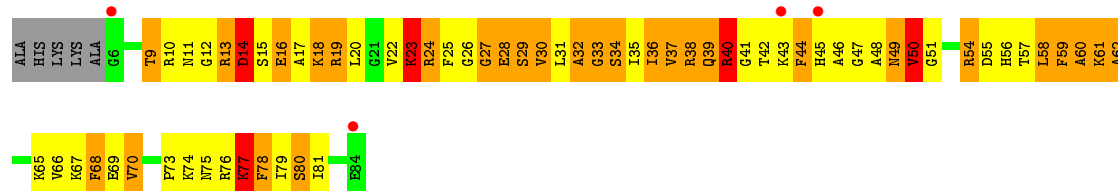
- Molecule 52: 50S ribosomal protein L27

Chain BW: 



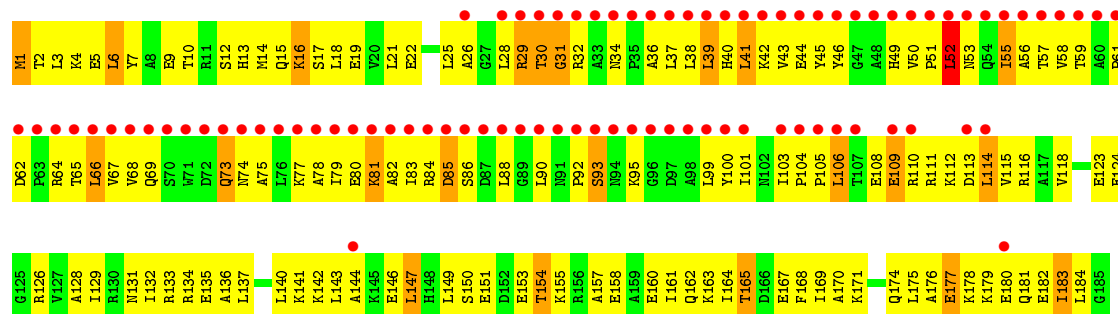
- Molecule 52: 50S ribosomal protein L27

Chain DW: 



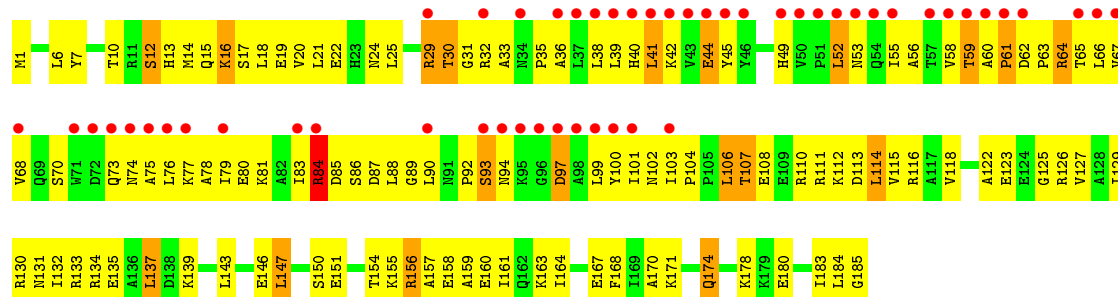
- Molecule 53: 50S ribosomal protein RRF

Chain B6: 



- Molecule 53: 50S ribosomal protein RRF

Chain D6: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.54Å 378.89Å 736.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 4.00 138.07 – 4.15	Depositor EDS
% Data completeness (in resolution range)	87.4 (40.00-4.00) 87.4 (138.07-4.15)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 4.15Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.261 , 0.305 0.237 , 0.275	Depositor DCC
R_{free} test set	18859 reflections (5.19%)	DCC
Wilson B-factor (Å ²)	133.1	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 74.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 382905 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	287083	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AA	0.29	3/36762 (0.0%)	0.78	21/57350 (0.0%)
1	CA	0.29	4/36762 (0.0%)	0.78	22/57350 (0.0%)
2	AC	0.23	0/1651	0.44	0/2225
2	CC	0.23	0/1651	0.44	0/2225
3	AD	0.23	0/1665	0.44	0/2227
3	CD	0.23	0/1665	0.44	0/2227
4	AE	0.23	0/1118	0.46	0/1504
4	CE	0.23	0/1118	0.46	0/1504
5	AF	0.24	0/835	0.45	0/1128
5	CF	0.24	0/835	0.45	0/1128
6	AG	0.23	0/1187	0.46	0/1591
6	CG	0.23	0/1211	0.46	0/1624
7	AH	0.23	0/989	0.44	0/1326
7	CH	0.23	0/989	0.44	0/1326
8	AI	0.24	0/1034	0.46	0/1375
8	CI	0.24	0/1033	0.46	0/1375
9	AJ	0.22	0/796	0.48	0/1077
9	CJ	0.22	0/796	0.48	0/1077
10	AK	0.24	0/893	0.46	0/1205
10	CK	0.24	0/893	0.46	0/1205
11	AL	0.22	0/969	0.50	0/1300
11	CL	0.22	0/969	0.50	0/1300
12	AM	0.21	0/892	0.46	0/1193
12	CM	0.21	0/884	0.46	0/1181
13	AN	0.24	0/785	0.45	0/1043
13	CN	0.24	0/785	0.45	0/1043
14	AO	0.23	0/722	0.47	0/964
14	CO	0.23	0/722	0.47	0/964
15	AP	0.25	0/659	0.46	0/884
15	CP	0.25	0/648	0.47	0/870
16	AQ	0.24	0/657	0.47	0/881
16	CQ	0.24	0/666	0.47	0/892

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AR	0.23	0/462	0.46	0/621
17	CR	0.23	0/462	0.46	0/621
18	AS	0.25	0/652	0.47	0/877
18	CS	0.25	0/660	0.48	0/888
19	AT	0.23	0/671	0.39	0/888
19	CT	0.23	0/671	0.39	0/888
20	AB	0.25	0/1735	0.45	0/2338
20	CB	0.25	0/1735	0.45	0/2338
21	AU	0.26	0/430	0.48	0/570
21	CU	0.26	0/430	0.48	0/570
22	BA	0.28	0/2803	0.76	1/4371 (0.0%)
22	DA	0.28	0/2803	0.76	0/4371
23	BB	0.28	6/68314 (0.0%)	0.78	48/106569 (0.0%)
23	DB	0.30	6/68314 (0.0%)	0.79	48/106569 (0.0%)
24	BI	0.24	0/1046	0.47	0/1410
24	DI	0.25	0/1046	0.48	0/1410
25	BC	0.22	0/2121	0.48	0/2852
25	DC	0.22	0/2121	0.48	0/2852
26	BD	0.24	0/1586	0.49	0/2134
26	DD	0.24	0/1586	0.49	0/2134
27	BK	0.24	0/939	0.55	0/1258
27	DK	0.24	0/939	0.55	0/1258
28	BP	0.24	0/929	0.51	0/1242
28	DP	0.24	0/929	0.51	0/1242
29	BE	0.24	0/1571	0.51	0/2113
29	DE	0.24	0/1571	0.51	0/2113
30	BY	0.23	0/453	0.49	0/605
30	DY	0.23	0/453	0.49	0/605
31	B0	0.22	0/450	0.55	0/599
31	D0	0.23	0/450	0.55	0/599
32	B4	0.23	0/303	0.47	0/397
32	D4	0.23	0/303	0.47	0/397
33	B1	0.27	0/416	0.49	0/554
33	D1	0.27	0/416	0.49	0/554
34	B3	0.24	0/513	0.48	0/676
34	D3	0.24	0/513	0.48	0/676
35	BV	0.25	0/766	0.43	0/1025
35	DV	0.25	0/766	0.43	0/1025
36	B2	0.25	0/380	0.48	0/498
36	D2	0.25	0/380	0.48	0/498
37	BL	0.23	0/1054	0.48	0/1403
37	DL	0.23	0/1054	0.48	0/1403
38	BM	0.25	0/1093	0.48	0/1460

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DM	0.25	0/1093	0.48	0/1460
39	BX	0.24	0/510	0.53	0/677
39	DX	0.24	0/510	0.53	0/677
40	BH	0.25	0/1122	0.48	0/1515
40	DH	0.25	0/1122	0.48	0/1515
41	BJ	0.24	0/1152	0.48	0/1551
41	DJ	0.23	0/1152	0.48	0/1551
42	BN	0.24	0/973	0.51	0/1301
42	DN	0.24	0/973	0.51	0/1301
43	BO	0.23	0/902	0.49	0/1209
43	DO	0.23	0/902	0.49	0/1209
44	BQ	0.25	0/960	0.49	0/1278
44	DQ	0.26	0/960	0.49	0/1278
45	BS	0.22	0/864	0.52	0/1156
45	DS	0.22	0/864	0.52	0/1156
46	BU	0.25	0/787	0.47	0/1051
46	DU	0.25	0/787	0.47	0/1051
47	BF	0.26	0/1444	0.52	0/1937
47	DF	0.26	0/1444	0.52	0/1937
48	BG	0.23	0/1343	0.47	0/1816
48	DG	0.23	0/1343	0.47	0/1816
49	BR	0.25	0/829	0.50	0/1107
49	DR	0.25	0/829	0.50	0/1107
50	BT	0.23	0/744	0.55	0/994
50	DT	0.22	0/744	0.55	0/994
51	BZ	0.25	0/635	0.51	0/848
51	DZ	0.25	0/635	0.52	0/848
52	BW	0.28	0/603	0.51	0/797
52	DW	0.28	0/603	0.51	0/797
53	B6	0.23	0/1497	0.52	1/2017 (0.0%)
53	D6	0.30	0/1497	0.58	1/2017 (0.0%)
All	All	0.28	19/309353 (0.0%)	0.71	142/462003 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	16
1	CA	0	17
23	BB	0	35

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Mol	Chain	#Chirality outliers	#Planarity outliers
23	DB	0	47
All	All	0	115

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	BB	1086	A	C5-C6	-16.56	1.26	1.41
23	DB	1086	A	C5-C6	-16.53	1.26	1.41
23	DB	1088	A	C6-N1	-10.57	1.28	1.35
23	BB	1088	A	C6-N1	-10.52	1.28	1.35
1	CA	1213	A	P-OP1	-9.61	1.32	1.49

The worst 5 of 142 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CA	1213	A	O5'-P-OP1	-31.90	72.42	110.70
1	AA	1213	A	O5'-P-OP2	-30.12	74.56	110.70
23	DB	2204	G	O5'-P-OP1	-29.74	75.02	110.70
23	BB	2204	G	O5'-P-OP2	-28.90	76.02	110.70
23	BB	2791	G	O5'-P-OP1	-28.07	77.02	110.70

There are no chirality outliers.

5 of 115 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	187	G	Sidechain
1	AA	281	G	Sidechain
1	AA	324	G	Sidechain
1	AA	437	U	Sidechain
1	AA	86	G	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32831	0	16521	1290	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CA	32831	0	16521	1350	0
2	AC	1624	0	1699	140	0
2	CC	1624	0	1699	146	0
3	AD	1643	0	1710	174	0
3	CD	1643	0	1710	170	0
4	AE	1105	0	1148	95	0
4	CE	1105	0	1148	96	0
5	AF	817	0	808	96	0
5	CF	817	0	808	94	0
6	AG	1174	0	1230	112	0
6	CG	1196	0	1246	106	0
7	AH	979	0	1034	95	0
7	CH	979	0	1034	96	0
8	AI	1022	0	1070	149	0
8	CI	1021	0	1070	149	0
9	AJ	786	0	828	77	0
9	CJ	786	0	828	80	0
10	AK	877	0	887	111	0
10	CK	877	0	887	114	0
11	AL	955	0	1019	92	0
11	CL	955	0	1019	91	0
12	AM	883	0	944	119	0
12	CM	876	0	937	120	0
13	AN	774	0	827	121	0
13	CN	774	0	827	131	0
14	AO	714	0	734	60	0
14	CO	714	0	734	54	0
15	AP	649	0	666	56	0
15	CP	638	0	656	57	0
16	AQ	648	0	691	71	0
16	CQ	657	0	702	67	0
17	AR	455	0	478	51	0
17	CR	455	0	478	56	0
18	AS	637	0	665	85	0
18	CS	644	0	675	87	0
19	AT	665	0	714	68	0
19	CT	665	0	714	70	0
20	AB	1704	0	1732	220	0
20	CB	1704	0	1732	211	0
21	AU	425	0	449	79	0
21	CU	425	0	449	89	0
22	BA	2507	0	1270	106	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	DA	2507	0	1270	108	0
23	BB	60995	0	30678	2536	0
23	DB	60995	0	30678	2543	0
24	BI	1032	0	1088	119	0
24	DI	1032	0	1088	181	0
25	BC	2082	0	2157	239	0
25	DC	2082	0	2157	241	0
26	BD	1565	0	1616	206	0
26	DD	1565	0	1616	216	0
27	BK	930	0	1000	122	0
27	DK	930	0	1000	122	0
28	BP	917	0	965	102	0
28	DP	917	0	965	108	0
29	BE	1552	0	1619	194	0
29	DE	1552	0	1619	181	0
30	BY	449	0	491	49	0
30	DY	449	0	491	55	0
31	B0	444	0	461	49	0
31	D0	444	0	461	47	0
32	B4	302	0	340	38	0
32	D4	302	0	340	44	0
33	B1	409	0	440	58	0
33	D1	409	0	440	54	0
34	B3	504	0	574	51	0
34	D3	504	0	574	48	0
35	BV	753	0	780	97	0
35	DV	753	0	780	102	0
36	B2	377	0	418	38	0
36	D2	377	0	418	38	0
37	BL	1045	0	1117	148	0
37	DL	1045	0	1117	153	0
38	BM	1074	0	1157	129	0
38	DM	1074	0	1157	121	0
39	BX	509	0	543	55	0
39	DX	509	0	543	60	0
40	BH	1111	0	1148	186	0
40	DH	1111	0	1148	158	0
41	BJ	1129	0	1162	136	0
41	DJ	1129	0	1162	137	0
42	BN	960	0	1000	130	0
42	DN	960	0	1000	129	0
43	BO	892	0	923	94	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	DO	892	0	923	96	0
44	BQ	947	0	1022	171	0
44	DQ	947	0	1022	178	0
45	BS	857	0	922	101	0
45	DS	857	0	922	101	0
46	BU	779	0	834	114	0
46	DU	779	0	834	109	0
47	BF	1420	0	1460	223	0
47	DF	1420	0	1460	216	0
48	BG	1323	0	1374	218	0
48	DG	1323	0	1374	195	0
49	BR	816	0	839	113	0
49	DR	816	0	839	128	0
50	BT	738	0	807	125	0
50	DT	738	0	807	121	0
51	BZ	625	0	652	82	0
51	DZ	625	0	652	82	0
52	BW	596	0	610	120	0
52	DW	596	0	610	126	0
53	B6	1478	0	1526	192	0
53	D6	1478	0	1526	150	0
54	AA	60	0	0	0	0
54	BB	110	0	0	0	0
54	CA	61	0	0	0	0
54	CE	1	0	0	0	0
54	DB	111	0	0	0	0
55	AA	31	0	39	0	0
55	BB	31	0	39	2	0
55	CA	31	0	39	3	0
55	DB	31	0	39	0	0
56	B4	1	0	0	0	0
56	D4	1	0	0	0	0
57	AA	287	0	0	1	0
57	AE	3	0	0	0	0
57	AK	1	0	0	0	0
57	AL	3	0	0	0	0
57	AN	4	0	0	0	0
57	AT	2	0	0	0	0
57	BB	492	0	0	8	0
57	BC	6	0	0	0	0
57	BD	1	0	0	0	0
57	BE	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	BL	3	0	0	0	0
57	BT	1	0	0	0	0
57	CA	296	0	0	2	0
57	CE	3	0	0	0	0
57	CK	1	0	0	0	0
57	CL	3	0	0	0	0
57	CN	4	0	0	0	0
57	CT	2	0	0	0	0
57	DB	500	0	0	7	0
57	DC	6	0	0	0	0
57	DE	2	0	0	0	0
57	DL	2	0	0	0	0
57	DR	1	0	0	0	0
57	DT	1	0	0	0	0
All	All	287083	0	193870	17818	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 37.

The worst 5 of 17818 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:DB:1099:G:H8	24:DI:3:LYS:N	1.36	1.20
40:BH:31:VAL:HB	40:BH:32:PRO:HD2	1.23	1.17
21:CU:36:PHE:HB3	21:CU:40:PRO:HD3	1.28	1.14
21:AU:36:PHE:HB3	21:AU:40:PRO:HD3	1.29	1.11
25:DC:144:GLU:HA	25:DC:151:GLY:HA2	1.33	1.11

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AC	204/232 (88%)	151 (74%)	38 (19%)	15 (7%)	1	21
2	CC	204/232 (88%)	152 (74%)	37 (18%)	15 (7%)	1	21
3	AD	203/205 (99%)	151 (74%)	39 (19%)	13 (6%)	2	26
3	CD	203/205 (99%)	148 (73%)	42 (21%)	13 (6%)	2	26
4	AE	148/166 (89%)	117 (79%)	25 (17%)	6 (4%)	3	37
4	CE	148/166 (89%)	117 (79%)	25 (17%)	6 (4%)	3	37
5	AF	98/135 (73%)	64 (65%)	25 (26%)	9 (9%)	1	16
5	CF	98/135 (73%)	65 (66%)	24 (24%)	9 (9%)	1	16
6	AG	148/178 (83%)	106 (72%)	33 (22%)	9 (6%)	2	27
6	CG	150/178 (84%)	112 (75%)	29 (19%)	9 (6%)	2	27
7	AH	127/129 (98%)	98 (77%)	23 (18%)	6 (5%)	3	33
7	CH	127/129 (98%)	96 (76%)	25 (20%)	6 (5%)	3	33
8	AI	125/129 (97%)	99 (79%)	17 (14%)	9 (7%)	1	23
8	CI	125/129 (97%)	98 (78%)	18 (14%)	9 (7%)	1	23
9	AJ	96/103 (93%)	70 (73%)	13 (14%)	13 (14%)	0	6
9	CJ	96/103 (93%)	71 (74%)	12 (12%)	13 (14%)	0	6
10	AK	115/128 (90%)	87 (76%)	22 (19%)	6 (5%)	2	31
10	CK	115/128 (90%)	87 (76%)	22 (19%)	6 (5%)	2	31
11	AL	121/123 (98%)	73 (60%)	33 (27%)	15 (12%)	0	8
11	CL	121/123 (98%)	75 (62%)	31 (26%)	15 (12%)	0	8
12	AM	112/117 (96%)	79 (70%)	24 (21%)	9 (8%)	1	19
12	CM	111/117 (95%)	76 (68%)	25 (22%)	10 (9%)	1	17
13	AN	92/100 (92%)	59 (64%)	26 (28%)	7 (8%)	1	20
13	CN	92/100 (92%)	60 (65%)	24 (26%)	8 (9%)	1	17
14	AO	86/89 (97%)	59 (69%)	22 (26%)	5 (6%)	2	28
14	CO	86/89 (97%)	60 (70%)	22 (26%)	4 (5%)	3	33
15	AP	80/82 (98%)	59 (74%)	16 (20%)	5 (6%)	2	27
15	CP	78/82 (95%)	56 (72%)	16 (20%)	6 (8%)	1	20
16	AQ	78/83 (94%)	58 (74%)	15 (19%)	5 (6%)	2	26
16	CQ	79/83 (95%)	59 (75%)	15 (19%)	5 (6%)	2	27
17	AR	53/74 (72%)	41 (77%)	9 (17%)	3 (6%)	2	29
17	CR	53/74 (72%)	41 (77%)	9 (17%)	3 (6%)	2	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	AS	77/91 (85%)	60 (78%)	12 (16%)	5 (6%)	1	26
18	CS	78/91 (86%)	61 (78%)	11 (14%)	6 (8%)	1	20
19	AT	83/86 (96%)	63 (76%)	15 (18%)	5 (6%)	2	27
19	CT	83/86 (96%)	62 (75%)	16 (19%)	5 (6%)	2	27
20	AB	216/240 (90%)	142 (66%)	57 (26%)	17 (8%)	1	19
20	CB	216/240 (90%)	134 (62%)	65 (30%)	17 (8%)	1	19
21	AU	49/70 (70%)	28 (57%)	11 (22%)	10 (20%)	0	2
21	CU	49/70 (70%)	28 (57%)	12 (24%)	9 (18%)	0	3
24	BI	139/141 (99%)	120 (86%)	14 (10%)	5 (4%)	4	41
24	DI	139/141 (99%)	114 (82%)	20 (14%)	5 (4%)	4	41
25	BC	269/272 (99%)	155 (58%)	66 (24%)	48 (18%)	0	3
25	DC	269/272 (99%)	155 (58%)	65 (24%)	49 (18%)	0	3
26	BD	207/209 (99%)	122 (59%)	54 (26%)	31 (15%)	0	5
26	DD	207/209 (99%)	124 (60%)	51 (25%)	32 (16%)	0	5
27	BK	119/123 (97%)	78 (66%)	24 (20%)	17 (14%)	0	6
27	DK	119/123 (97%)	78 (66%)	24 (20%)	17 (14%)	0	6
28	BP	112/114 (98%)	61 (54%)	32 (29%)	19 (17%)	0	4
28	DP	112/114 (98%)	61 (54%)	34 (30%)	17 (15%)	0	5
29	BE	199/201 (99%)	125 (63%)	50 (25%)	24 (12%)	0	8
29	DE	199/201 (99%)	125 (63%)	51 (26%)	23 (12%)	0	9
30	BY	56/58 (97%)	39 (70%)	12 (21%)	5 (9%)	1	17
30	DY	56/58 (97%)	39 (70%)	12 (21%)	5 (9%)	1	17
31	B0	54/56 (96%)	39 (72%)	8 (15%)	7 (13%)	0	7
31	D0	54/56 (96%)	39 (72%)	8 (15%)	7 (13%)	0	7
32	B4	36/38 (95%)	16 (44%)	10 (28%)	10 (28%)	0	0
32	D4	36/38 (95%)	16 (44%)	10 (28%)	10 (28%)	0	0
33	B1	48/54 (89%)	37 (77%)	7 (15%)	4 (8%)	1	18
33	D1	48/54 (89%)	36 (75%)	8 (17%)	4 (8%)	1	18
34	B3	62/64 (97%)	35 (56%)	21 (34%)	6 (10%)	1	14
34	D3	62/64 (97%)	34 (55%)	22 (36%)	6 (10%)	1	14
35	BV	92/94 (98%)	64 (70%)	22 (24%)	6 (6%)	1	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	DV	92/94 (98%)	62 (67%)	24 (26%)	6 (6%)	1	26
36	B2	44/46 (96%)	30 (68%)	10 (23%)	4 (9%)	1	16
36	D2	44/46 (96%)	30 (68%)	10 (23%)	4 (9%)	1	16
37	BL	141/144 (98%)	89 (63%)	31 (22%)	21 (15%)	0	5
37	DL	141/144 (98%)	89 (63%)	32 (23%)	20 (14%)	0	6
38	BM	134/136 (98%)	84 (63%)	29 (22%)	21 (16%)	0	5
38	DM	134/136 (98%)	83 (62%)	31 (23%)	20 (15%)	0	5
39	BX	61/63 (97%)	36 (59%)	17 (28%)	8 (13%)	0	7
39	DX	61/63 (97%)	36 (59%)	17 (28%)	8 (13%)	0	7
40	BH	147/149 (99%)	76 (52%)	46 (31%)	25 (17%)	0	4
40	DH	147/149 (99%)	91 (62%)	33 (22%)	23 (16%)	0	5
41	BJ	140/142 (99%)	85 (61%)	37 (26%)	18 (13%)	0	7
41	DJ	140/142 (99%)	85 (61%)	36 (26%)	19 (14%)	0	6
42	BN	118/127 (93%)	76 (64%)	29 (25%)	13 (11%)	0	10
42	DN	118/127 (93%)	77 (65%)	28 (24%)	13 (11%)	0	10
43	BO	114/117 (97%)	74 (65%)	29 (25%)	11 (10%)	1	14
43	DO	114/117 (97%)	75 (66%)	27 (24%)	12 (10%)	1	11
44	BQ	115/117 (98%)	75 (65%)	31 (27%)	9 (8%)	1	20
44	DQ	115/117 (98%)	75 (65%)	29 (25%)	11 (10%)	1	14
45	BS	108/110 (98%)	68 (63%)	29 (27%)	11 (10%)	1	13
45	DS	108/110 (98%)	66 (61%)	31 (29%)	11 (10%)	1	13
46	BU	100/103 (97%)	58 (58%)	23 (23%)	19 (19%)	0	3
46	DU	100/103 (97%)	59 (59%)	22 (22%)	19 (19%)	0	3
47	BF	176/178 (99%)	103 (58%)	44 (25%)	29 (16%)	0	4
47	DF	176/178 (99%)	105 (60%)	42 (24%)	29 (16%)	0	4
48	BG	174/176 (99%)	99 (57%)	42 (24%)	33 (19%)	0	3
48	DG	174/176 (99%)	101 (58%)	41 (24%)	32 (18%)	0	3
49	BR	101/103 (98%)	72 (71%)	20 (20%)	9 (9%)	1	17
49	DR	101/103 (98%)	74 (73%)	18 (18%)	9 (9%)	1	17
50	BT	91/100 (91%)	48 (53%)	23 (25%)	20 (22%)	0	1
50	DT	91/100 (91%)	46 (50%)	27 (30%)	18 (20%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	BZ	75/78 (96%)	50 (67%)	13 (17%)	12 (16%)	0	5
51	DZ	75/78 (96%)	50 (67%)	13 (17%)	12 (16%)	0	5
52	BW	77/84 (92%)	28 (36%)	23 (30%)	26 (34%)	0	0
52	DW	77/84 (92%)	28 (36%)	24 (31%)	25 (32%)	0	0
53	B6	183/185 (99%)	162 (88%)	16 (9%)	5 (3%)	6	47
53	D6	183/185 (99%)	152 (83%)	24 (13%)	7 (4%)	4	39
All	All	11607/12284 (94%)	7731 (67%)	2581 (22%)	1295 (11%)	0	10

5 of 1295 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AC	14	VAL
2	AC	54	ILE
2	AC	205	GLU
3	AD	24	VAL
3	AD	25	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AC	170/189 (90%)	144 (85%)	26 (15%)	3	24
2	CC	170/189 (90%)	143 (84%)	27 (16%)	3	23
3	AD	172/172 (100%)	146 (85%)	26 (15%)	3	25
3	CD	172/172 (100%)	147 (86%)	25 (14%)	4	27
4	AE	113/125 (90%)	95 (84%)	18 (16%)	3	23
4	CE	113/125 (90%)	96 (85%)	17 (15%)	3	25
5	AF	87/116 (75%)	76 (87%)	11 (13%)	5	31
5	CF	87/116 (75%)	76 (87%)	11 (13%)	5	31
6	AG	123/146 (84%)	105 (85%)	18 (15%)	4	26
6	CG	125/146 (86%)	106 (85%)	19 (15%)	3	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	AH	104/104 (100%)	96 (92%)	8 (8%)	16	55
7	CH	104/104 (100%)	97 (93%)	7 (7%)	20	60
8	AI	105/106 (99%)	91 (87%)	14 (13%)	5	30
8	CI	105/106 (99%)	89 (85%)	16 (15%)	3	25
9	AJ	86/90 (96%)	76 (88%)	10 (12%)	7	36
9	CJ	86/90 (96%)	76 (88%)	10 (12%)	7	36
10	AK	90/98 (92%)	77 (86%)	13 (14%)	4	27
10	CK	90/98 (92%)	75 (83%)	15 (17%)	3	21
11	AL	103/103 (100%)	86 (84%)	17 (16%)	3	21
11	CL	103/103 (100%)	85 (82%)	18 (18%)	2	18
12	AM	92/95 (97%)	77 (84%)	15 (16%)	3	22
12	CM	91/95 (96%)	76 (84%)	15 (16%)	3	21
13	AN	79/83 (95%)	62 (78%)	17 (22%)	1	10
13	CN	79/83 (95%)	62 (78%)	17 (22%)	1	10
14	AO	76/77 (99%)	69 (91%)	7 (9%)	11	46
14	CO	76/77 (99%)	69 (91%)	7 (9%)	11	46
15	AP	65/65 (100%)	59 (91%)	6 (9%)	11	46
15	CP	65/65 (100%)	59 (91%)	6 (9%)	11	46
16	AQ	74/77 (96%)	61 (82%)	13 (18%)	2	18
16	CQ	75/77 (97%)	63 (84%)	12 (16%)	3	23
17	AR	48/64 (75%)	40 (83%)	8 (17%)	3	21
17	CR	48/64 (75%)	39 (81%)	9 (19%)	2	15
18	AS	70/78 (90%)	56 (80%)	14 (20%)	1	13
18	CS	71/78 (91%)	57 (80%)	14 (20%)	1	13
19	AT	65/65 (100%)	55 (85%)	10 (15%)	3	24
19	CT	65/65 (100%)	55 (85%)	10 (15%)	3	24
20	AB	180/198 (91%)	148 (82%)	32 (18%)	2	17
20	CB	180/198 (91%)	150 (83%)	30 (17%)	3	21
21	AU	44/60 (73%)	32 (73%)	12 (27%)	0	5
21	CU	44/60 (73%)	32 (73%)	12 (27%)	0	5
24	BI	109/109 (100%)	107 (98%)	2 (2%)	66	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	DI	109/109 (100%)	103 (94%)	6 (6%)	27	66
25	BC	216/217 (100%)	179 (83%)	37 (17%)	2	19
25	DC	216/217 (100%)	176 (82%)	40 (18%)	2	15
26	BD	164/164 (100%)	135 (82%)	29 (18%)	2	18
26	DD	164/164 (100%)	134 (82%)	30 (18%)	2	16
27	BK	102/104 (98%)	80 (78%)	22 (22%)	1	10
27	DK	102/104 (98%)	81 (79%)	21 (21%)	1	12
28	BP	99/99 (100%)	80 (81%)	19 (19%)	2	14
28	DP	99/99 (100%)	80 (81%)	19 (19%)	2	14
29	BE	165/165 (100%)	143 (87%)	22 (13%)	5	30
29	DE	165/165 (100%)	142 (86%)	23 (14%)	4	29
30	BY	48/48 (100%)	38 (79%)	10 (21%)	1	11
30	DY	48/48 (100%)	38 (79%)	10 (21%)	1	11
31	B0	47/47 (100%)	38 (81%)	9 (19%)	2	14
31	D0	47/47 (100%)	38 (81%)	9 (19%)	2	14
32	B4	34/34 (100%)	28 (82%)	6 (18%)	2	18
32	D4	34/34 (100%)	29 (85%)	5 (15%)	4	26
33	B1	45/48 (94%)	40 (89%)	5 (11%)	8	38
33	D1	45/48 (94%)	41 (91%)	4 (9%)	12	48
34	B3	51/51 (100%)	45 (88%)	6 (12%)	6	35
34	D3	51/51 (100%)	46 (90%)	5 (10%)	10	43
35	BV	78/78 (100%)	64 (82%)	14 (18%)	2	17
35	DV	78/78 (100%)	64 (82%)	14 (18%)	2	17
36	B2	38/38 (100%)	28 (74%)	10 (26%)	0	6
36	D2	38/38 (100%)	28 (74%)	10 (26%)	0	6
37	BL	102/103 (99%)	91 (89%)	11 (11%)	8	39
37	DL	102/103 (99%)	91 (89%)	11 (11%)	8	39
38	BM	109/109 (100%)	87 (80%)	22 (20%)	1	12
38	DM	109/109 (100%)	87 (80%)	22 (20%)	1	12
39	BX	55/55 (100%)	46 (84%)	9 (16%)	3	21
39	DX	55/55 (100%)	46 (84%)	9 (16%)	3	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	BH	114/114 (100%)	79 (69%)	35 (31%)	0	3
40	DH	114/114 (100%)	89 (78%)	25 (22%)	1	10
41	BJ	116/116 (100%)	100 (86%)	16 (14%)	4	29
41	DJ	116/116 (100%)	100 (86%)	16 (14%)	4	29
42	BN	100/103 (97%)	84 (84%)	16 (16%)	3	23
42	DN	100/103 (97%)	84 (84%)	16 (16%)	3	23
43	BO	86/87 (99%)	71 (83%)	15 (17%)	2	18
43	DO	86/87 (99%)	72 (84%)	14 (16%)	3	22
44	BQ	89/89 (100%)	79 (89%)	10 (11%)	7	37
44	DQ	89/89 (100%)	79 (89%)	10 (11%)	7	37
45	BS	93/93 (100%)	77 (83%)	16 (17%)	2	19
45	DS	93/93 (100%)	77 (83%)	16 (17%)	2	19
46	BU	83/84 (99%)	65 (78%)	18 (22%)	1	10
46	DU	83/84 (99%)	65 (78%)	18 (22%)	1	10
47	BF	149/149 (100%)	117 (78%)	32 (22%)	1	10
47	DF	149/149 (100%)	117 (78%)	32 (22%)	1	10
48	BG	137/137 (100%)	110 (80%)	27 (20%)	1	13
48	DG	137/137 (100%)	112 (82%)	25 (18%)	2	16
49	BR	84/84 (100%)	71 (84%)	13 (16%)	3	24
49	DR	84/84 (100%)	70 (83%)	14 (17%)	3	21
50	BT	80/84 (95%)	64 (80%)	16 (20%)	1	13
50	DT	80/84 (95%)	64 (80%)	16 (20%)	1	13
51	BZ	67/68 (98%)	53 (79%)	14 (21%)	1	11
51	DZ	67/68 (98%)	56 (84%)	11 (16%)	3	21
52	BW	59/62 (95%)	42 (71%)	17 (29%)	0	4
52	DW	59/62 (95%)	42 (71%)	17 (29%)	0	4
53	B6	157/157 (100%)	137 (87%)	20 (13%)	5	31
53	D6	157/157 (100%)	134 (85%)	23 (15%)	4	26
All	All	9647/10014 (96%)	8066 (84%)	1581 (16%)	3	21

5 of 1581 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
49	BR	39	LEU
6	CG	110	ARG
47	DF	103	ILE
50	BT	68	LYS
2	CC	61	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 320 such sidechains are listed below:

Mol	Chain	Res	Type
48	BG	37	ASN
7	CH	3	GLN
46	DU	65	GLN
49	BR	86	GLN
2	CC	2	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1529/1542 (99%)	244 (15%)	21 (1%)
1	CA	1529/1542 (99%)	235 (15%)	19 (1%)
22	BA	116/120 (96%)	17 (14%)	0
22	DA	116/120 (96%)	16 (13%)	0
23	BB	2837/2904 (97%)	457 (16%)	17 (0%)
23	DB	2837/2904 (97%)	435 (15%)	22 (0%)
All	All	8964/9132 (98%)	1404 (15%)	79 (0%)

5 of 1404 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	14	U
1	AA	32	A
1	AA	39	G
1	AA	47	C

5 of 79 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	BB	2425	A
1	CA	372	C
23	DB	2336	A

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Mol	Chain	Res	Type
23	BB	2756	U
1	CA	243	A

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 349 ligands modelled in this entry, 345 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	LLL	AA	1661	-	30,33,33	2.25	11 (36%)	37,49,49	1.42	5 (13%)
55	LLL	BB	3111	-	30,33,33	2.21	11 (36%)	37,49,49	1.36	4 (10%)
55	LLL	CA	1662	-	30,33,33	2.25	11 (36%)	37,49,49	1.41	5 (13%)
55	LLL	DB	3112	-	30,33,33	2.25	11 (36%)	37,49,49	1.38	4 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	LLL	AA	1661	-	-	0/11/65/65	0/3/3/3
55	LLL	BB	3111	-	-	0/11/65/65	0/3/3/3
55	LLL	CA	1662	-	-	0/11/65/65	0/3/3/3
55	LLL	DB	3112	-	-	0/11/65/65	0/3/3/3

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	BB	3111	LLL	O51-C51	2.17	1.48	1.44
55	CA	1662	LLL	C52-C62	2.19	1.58	1.52
55	BB	3111	LLL	C22-C32	2.20	1.58	1.53
55	CA	1662	LLL	O51-C51	2.20	1.48	1.44
55	DB	3112	LLL	O51-C51	2.21	1.48	1.44

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	AA	1661	LLL	O43-C43-C83	-2.57	102.47	108.11
55	DB	3112	LLL	O43-C43-C83	-2.53	102.54	108.11
55	BB	3111	LLL	O43-C43-C83	-2.48	102.66	108.11
55	CA	1662	LLL	O43-C43-C83	-2.45	102.73	108.11
55	CA	1662	LLL	C13-O62-C62	2.33	124.09	118.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	BB	3111	LLL	2	0
55	CA	1662	LLL	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1530/1542 (99%)	-0.30	12 (0%) 87 82	13, 75, 157, 180	0
1	CA	1530/1542 (99%)	-0.36	2 (0%) 95 95	8, 52, 139, 180	0
2	AC	206/232 (88%)	-0.15	3 (1%) 76 66	5, 72, 147, 180	0
2	CC	206/232 (88%)	-0.06	1 (0%) 91 88	6, 72, 131, 180	0
3	AD	205/205 (100%)	0.25	9 (4%) 38 28	20, 95, 159, 180	0
3	CD	205/205 (100%)	-0.13	0 100 100	5, 56, 145, 180	0
4	AE	150/166 (90%)	0.21	3 (2%) 68 57	7, 69, 146, 180	0
4	CE	150/166 (90%)	0.22	3 (2%) 68 57	5, 49, 112, 180	0
5	AF	100/135 (74%)	0.30	6 (6%) 25 17	5, 69, 150, 177	0
5	CF	100/135 (74%)	0.04	1 (1%) 84 77	5, 72, 143, 166	0
6	AG	150/178 (84%)	0.06	5 (3%) 50 38	20, 97, 159, 175	0
6	CG	152/178 (85%)	-0.10	1 (0%) 89 84	29, 85, 147, 180	0
7	AH	129/129 (100%)	0.32	11 (8%) 13 10	26, 80, 143, 177	0
7	CH	129/129 (100%)	0.05	0 100 100	6, 49, 117, 174	0
8	AI	127/129 (98%)	0.06	2 (1%) 74 64	18, 89, 171, 180	0
8	CI	127/129 (98%)	-0.01	2 (1%) 74 64	22, 92, 160, 180	0
9	AJ	98/103 (95%)	0.27	2 (2%) 68 57	16, 92, 169, 180	0
9	CJ	98/103 (95%)	0.37	7 (7%) 19 13	26, 87, 153, 180	0
10	AK	117/128 (91%)	-0.12	0 100 100	7, 59, 119, 180	0
10	CK	117/128 (91%)	-0.15	2 (1%) 73 62	5, 52, 120, 180	0
11	AL	123/123 (100%)	0.15	3 (2%) 62 51	14, 78, 152, 180	0
11	CL	123/123 (100%)	-0.01	1 (0%) 87 82	5, 46, 127, 170	0
12	AM	114/117 (97%)	-0.14	0 100 100	40, 114, 180, 180	0
12	CM	113/117 (96%)	-0.19	0 100 100	27, 100, 173, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AN	96/100 (96%)	0.03	1 (1%) 84 77	8, 86, 158, 180	0
13	CN	96/100 (96%)	0.13	1 (1%) 84 77	14, 87, 147, 178	0
14	AO	88/89 (98%)	-0.32	0 100 100	5, 76, 128, 180	0
14	CO	88/89 (98%)	-0.17	0 100 100	10, 63, 132, 159	0
15	AP	82/82 (100%)	0.75	5 (6%) 25 16	24, 94, 154, 180	0
15	CP	80/82 (97%)	0.50	7 (8%) 12 9	5, 46, 128, 180	0
16	AQ	80/83 (96%)	0.07	0 100 100	36, 96, 168, 180	0
16	CQ	81/83 (97%)	0.06	0 100 100	5, 52, 135, 180	0
17	AR	55/74 (74%)	-0.00	1 (1%) 71 61	14, 70, 148, 180	0
17	CR	55/74 (74%)	0.46	3 (5%) 29 21	12, 64, 136, 180	0
18	AS	79/91 (86%)	0.46	6 (7%) 17 12	44, 120, 176, 180	0
18	CS	80/91 (87%)	-0.14	0 100 100	34, 107, 180, 180	0
19	AT	85/86 (98%)	-0.16	0 100 100	34, 101, 168, 180	0
19	CT	85/86 (98%)	-0.37	0 100 100	5, 62, 140, 180	0
20	AB	218/240 (90%)	0.19	9 (4%) 41 31	18, 97, 160, 180	0
20	CB	218/240 (90%)	0.16	8 (3%) 45 34	16, 93, 160, 180	0
21	AU	51/70 (72%)	0.04	1 (1%) 68 57	27, 89, 171, 180	0
21	CU	51/70 (72%)	-0.08	0 100 100	23, 81, 137, 180	0
22	BA	117/120 (97%)	-0.39	0 100 100	49, 85, 136, 180	0
22	DA	117/120 (97%)	-0.30	2 (1%) 73 62	36, 88, 148, 180	0
23	BB	2841/2904 (97%)	-0.09	21 (0%) 89 84	6, 60, 150, 180	0
23	DB	2841/2904 (97%)	-0.14	12 (0%) 93 90	5, 46, 154, 180	0
24	BI	141/141 (100%)	1.06	30 (21%) 1 2	72, 166, 180, 180	0
24	DI	141/141 (100%)	0.65	12 (8%) 13 10	63, 162, 180, 180	0
25	BC	271/272 (99%)	0.14	3 (1%) 82 75	5, 47, 107, 156	0
25	DC	271/272 (99%)	0.08	1 (0%) 93 90	5, 38, 99, 145	0
26	BD	209/209 (100%)	0.45	16 (7%) 16 11	8, 72, 145, 180	0
26	DD	209/209 (100%)	0.15	1 (0%) 91 88	5, 51, 131, 180	0
27	BK	121/123 (98%)	0.69	6 (4%) 32 24	16, 62, 142, 180	0
27	DK	121/123 (98%)	0.29	0 100 100	5, 42, 103, 180	0
28	BP	114/114 (100%)	1.19	22 (19%) 2 2	28, 86, 155, 173	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DP	114/114 (100%)	-0.18	0 100 100	5, 52, 119, 161	0
29	BE	201/201 (100%)	0.40	14 (6%) 19 13	5, 76, 143, 180	0
29	DE	201/201 (100%)	0.14	7 (3%) 48 37	5, 66, 138, 180	0
30	BY	58/58 (100%)	0.34	3 (5%) 31 23	22, 84, 137, 180	0
30	DY	58/58 (100%)	-0.00	1 (1%) 73 62	10, 66, 149, 158	0
31	B0	56/56 (100%)	0.21	3 (5%) 29 21	5, 81, 149, 180	0
31	D0	56/56 (100%)	-0.21	0 100 100	9, 54, 119, 180	0
32	B4	38/38 (100%)	0.12	1 (2%) 59 47	5, 71, 153, 168	0
32	D4	38/38 (100%)	0.03	0 100 100	17, 62, 132, 171	0
33	B1	50/54 (92%)	0.46	3 (6%) 25 17	32, 87, 132, 174	0
33	D1	50/54 (92%)	0.21	2 (4%) 42 31	24, 73, 125, 155	0
34	B3	64/64 (100%)	0.66	7 (10%) 7 6	19, 64, 105, 133	0
34	D3	64/64 (100%)	0.19	2 (3%) 52 40	6, 49, 107, 180	0
35	BV	94/94 (100%)	-0.06	1 (1%) 82 75	37, 92, 143, 180	0
35	DV	94/94 (100%)	-0.04	0 100 100	27, 94, 160, 180	0
36	B2	46/46 (100%)	0.05	0 100 100	5, 50, 123, 143	0
36	D2	46/46 (100%)	-0.08	0 100 100	7, 43, 103, 180	0
37	BL	143/144 (99%)	0.30	1 (0%) 89 84	7, 72, 131, 180	0
37	DL	143/144 (99%)	0.18	3 (2%) 67 56	5, 61, 128, 162	0
38	BM	136/136 (100%)	0.13	4 (2%) 55 42	16, 68, 144, 165	0
38	DM	136/136 (100%)	0.28	5 (3%) 45 34	5, 63, 134, 171	0
39	BX	63/63 (100%)	0.32	2 (3%) 51 38	24, 92, 169, 180	0
39	DX	63/63 (100%)	-0.05	2 (3%) 51 38	38, 94, 166, 180	0
40	BH	149/149 (100%)	1.33	38 (25%) 1 1	13, 125, 180, 180	0
40	DH	149/149 (100%)	0.45	10 (6%) 21 14	5, 109, 171, 180	0
41	BJ	142/142 (100%)	0.08	2 (1%) 78 68	13, 77, 132, 166	0
41	DJ	142/142 (100%)	-0.08	1 (0%) 89 84	5, 65, 128, 180	0
42	BN	120/127 (94%)	0.12	1 (0%) 87 82	5, 68, 136, 180	0
42	DN	120/127 (94%)	-0.35	0 100 100	5, 44, 116, 141	0
43	BO	116/117 (99%)	0.46	11 (9%) 10 8	29, 94, 144, 180	0
43	DO	116/117 (99%)	-0.06	3 (2%) 59 47	5, 93, 156, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BQ	117/117 (100%)	-0.34	0 100 100	5, 72, 134, 171	0
44	DQ	117/117 (100%)	0.10	1 (0%) 85 80	5, 50, 131, 156	0
45	BS	110/110 (100%)	0.51	3 (2%) 58 46	5, 67, 129, 180	0
45	DS	110/110 (100%)	0.35	2 (1%) 71 61	5, 50, 120, 157	0
46	BU	102/103 (99%)	0.79	7 (6%) 20 13	13, 88, 148, 177	0
46	DU	102/103 (99%)	0.04	1 (0%) 84 77	26, 93, 154, 180	0
47	BF	178/178 (100%)	0.35	5 (2%) 56 44	39, 115, 174, 180	0
47	DF	178/178 (100%)	0.68	15 (8%) 14 10	22, 106, 175, 180	0
48	BG	176/176 (100%)	0.28	2 (1%) 82 75	8, 102, 172, 180	0
48	DG	176/176 (100%)	0.08	5 (2%) 56 44	32, 104, 164, 180	0
49	BR	103/103 (100%)	0.20	3 (2%) 55 42	18, 99, 151, 173	0
49	DR	103/103 (100%)	0.35	7 (6%) 20 14	5, 85, 144, 180	0
50	BT	93/100 (93%)	0.28	2 (2%) 65 54	13, 83, 160, 180	0
50	DT	93/100 (93%)	0.37	4 (4%) 39 29	15, 79, 167, 180	0
51	BZ	77/78 (98%)	0.35	3 (3%) 43 32	12, 57, 112, 152	0
51	DZ	77/78 (98%)	-0.08	2 (2%) 59 47	5, 56, 101, 131	0
52	BW	79/84 (94%)	0.67	9 (11%) 7 6	19, 88, 139, 180	0
52	DW	79/84 (94%)	0.08	4 (5%) 32 23	5, 79, 143, 180	0
53	B6	185/185 (100%)	2.90	86 (46%) 0 1	23, 123, 180, 180	0
53	D6	185/185 (100%)	1.15	52 (28%) 1 1	5, 104, 180, 180	0
All	All	20787/21416 (97%)	0.06	584 (2%) 56 44	5, 69, 159, 180	0

The worst 5 of 584 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
53	B6	96	GLY	16.1
53	B6	97	ASP	15.6
53	B6	98	ALA	14.3
53	B6	88	LEU	11.4
53	B6	94	ASN	10.3

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
55	LLL	DB	3112	31/31	0.84	0.34	7.10	121,121,121,121	0
55	LLL	BB	3111	31/31	0.87	0.27	3.47	107,107,107,107	0
54	MG	DB	3059	1/1	0.69	0.23	2.64	166,166,166,166	0
55	LLL	CA	1662	31/31	0.94	0.22	1.73	14,14,14,14	0
54	MG	CA	1604	1/1	0.97	0.28	1.61	16,16,16,16	0
54	MG	BB	3013	1/1	0.81	0.18	1.51	92,92,92,92	0
54	MG	BB	3087	1/1	0.98	0.22	1.49	114,114,114,114	0
54	MG	BB	3108	1/1	0.92	0.22	1.17	44,44,44,44	0
54	MG	DB	3089	1/1	0.95	0.19	1.15	61,61,61,61	0
54	MG	AA	1653	1/1	0.97	0.18	0.70	87,87,87,87	0
54	MG	DB	3099	1/1	0.98	0.20	0.55	5,5,5,5	0
54	MG	DB	3092	1/1	0.96	0.15	0.46	56,56,56,56	0
54	MG	DB	3090	1/1	0.96	0.31	0.46	64,64,64,64	0
54	MG	DB	3051	1/1	0.98	0.20	0.22	32,32,32,32	0
55	LLL	AA	1661	31/31	0.95	0.21	0.20	21,21,21,21	0
54	MG	CA	1638	1/1	0.86	0.11	0.08	98,98,98,98	0
54	MG	DB	3035	1/1	0.93	0.19	0.00	75,75,75,75	0
54	MG	AA	1615	1/1	0.92	0.23	-0.11	106,106,106,106	0
54	MG	CA	1614	1/1	0.71	0.16	-0.19	90,90,90,90	0
54	MG	BB	3011	1/1	0.99	0.21	-0.30	29,29,29,29	0
54	MG	BB	3079	1/1	0.79	0.20	-0.31	63,63,63,63	0
54	MG	DB	3110	1/1	0.94	0.17	-0.35	38,38,38,38	0
54	MG	AA	1635	1/1	0.52	0.09	-0.37	103,103,103,103	0
54	MG	BB	3098	1/1	0.98	0.16	-0.45	16,16,16,16	0
54	MG	BB	3032	1/1	0.97	0.20	-0.46	49,49,49,49	0
54	MG	BB	3083	1/1	0.98	0.21	-0.49	28,28,28,28	0
54	MG	DB	3003	1/1	0.93	0.16	-0.57	33,33,33,33	0
54	MG	CA	1616	1/1	0.83	0.14	-0.58	88,88,88,88	0
54	MG	DB	3100	1/1	0.84	0.21	-0.61	46,46,46,46	0
54	MG	CA	1601	1/1	0.98	0.17	-0.62	5,5,5,5	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DB	3014	1/1	0.99	0.12	-0.62	43,43,43,43	0
54	MG	BB	3023	1/1	0.97	0.20	-0.70	11,11,11,11	0
54	MG	DB	3088	1/1	0.98	0.16	-0.78	46,46,46,46	0
54	MG	DB	3069	1/1	0.98	0.20	-0.79	14,14,14,14	0
54	MG	CA	1633	1/1	0.96	0.14	-0.80	50,50,50,50	0
54	MG	AA	1613	1/1	0.81	0.08	-0.82	71,71,71,71	0
54	MG	CA	1618	1/1	0.99	0.12	-0.88	30,30,30,30	0
54	MG	BB	3082	1/1	0.98	0.19	-0.90	5,5,5,5	0
54	MG	DB	3098	1/1	0.99	0.18	-0.92	28,28,28,28	0
54	MG	DB	3009	1/1	0.98	0.17	-0.94	18,18,18,18	0
54	MG	BB	3005	1/1	0.97	0.19	-1.03	20,20,20,20	0
54	MG	BB	3021	1/1	0.97	0.10	-1.04	51,51,51,51	0
54	MG	AA	1636	1/1	0.95	0.06	-1.05	93,93,93,93	0
54	MG	DB	3026	1/1	0.88	0.18	-1.06	54,54,54,54	0
54	MG	CA	1636	1/1	0.93	0.05	-1.10	92,92,92,92	0
54	MG	BB	3040	1/1	0.99	0.12	-1.15	27,27,27,27	0
54	MG	DB	3096	1/1	0.99	0.16	-1.16	20,20,20,20	0
54	MG	CA	1645	1/1	0.98	0.10	-1.16	66,66,66,66	0
54	MG	BB	3092	1/1	0.89	0.08	-1.18	45,45,45,45	0
54	MG	DB	3087	1/1	0.99	0.15	-1.19	75,75,75,75	0
54	MG	DB	3006	1/1	0.92	0.15	-1.27	15,15,15,15	0
54	MG	DB	3030	1/1	0.86	0.17	-1.28	10,10,10,10	0
54	MG	CA	1605	1/1	0.97	0.12	-1.35	18,18,18,18	0
54	MG	BB	3096	1/1	0.98	0.15	-1.39	67,67,67,67	0
56	ZN	D4	101	1/1	0.94	0.07	-1.51	45,45,45,45	0
54	MG	AA	1607	1/1	0.96	0.07	-1.51	42,42,42,42	0
56	ZN	B4	101	1/1	0.95	0.09	-1.64	64,64,64,64	0
54	MG	AA	1630	1/1	0.92	0.11	-1.65	88,88,88,88	0
54	MG	BB	3086	1/1	0.96	0.17	-1.82	18,18,18,18	0
54	MG	BB	3019	1/1	0.86	0.09	-1.86	40,40,40,40	0
54	MG	AA	1609	1/1	0.99	0.11	-1.87	5,5,5,5	0
54	MG	BB	3037	1/1	0.90	0.11	-1.90	44,44,44,44	0
54	MG	CA	1617	1/1	0.98	0.08	-1.91	5,5,5,5	0
54	MG	AA	1601	1/1	0.91	0.12	-1.93	41,41,41,41	0
54	MG	DB	3068	1/1	0.96	0.17	-1.95	22,22,22,22	0
54	MG	BB	3029	1/1	0.96	0.11	-1.97	17,17,17,17	0
54	MG	DB	3055	1/1	0.88	0.13	-1.98	41,41,41,41	0
54	MG	BB	3048	1/1	0.95	0.10	-2.05	7,7,7,7	0
54	MG	BB	3090	1/1	0.98	0.10	-2.14	91,91,91,91	0
54	MG	DB	3085	1/1	0.96	0.13	-2.26	49,49,49,49	0
54	MG	AA	1610	1/1	0.98	0.06	-2.27	62,62,62,62	0
54	MG	BB	3074	1/1	0.97	0.14	-2.41	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BB	3077	1/1	0.96	0.07	-2.48	83,83,83,83	0
54	MG	CA	1612	1/1	0.98	0.07	-2.50	72,72,72,72	0
54	MG	DB	3078	1/1	0.99	0.08	-2.56	32,32,32,32	0
54	MG	BB	3110	1/1	0.95	0.09	-2.59	40,40,40,40	0
54	MG	AA	1638	1/1	0.98	0.07	-2.60	20,20,20,20	0
54	MG	DB	3070	1/1	0.98	0.10	-2.72	38,38,38,38	0
54	MG	BB	3085	1/1	0.99	0.11	-2.88	43,43,43,43	0
54	MG	DB	3007	1/1	0.97	0.11	-2.88	13,13,13,13	0
54	MG	AA	1629	1/1	0.99	0.05	-2.89	26,26,26,26	0
54	MG	BB	3016	1/1	0.99	0.13	-2.91	91,91,91,91	0
54	MG	DB	3103	1/1	0.98	0.11	-3.01	42,42,42,42	0
54	MG	DB	3072	1/1	0.90	0.09	-3.02	54,54,54,54	0
54	MG	BB	3012	1/1	0.98	0.09	-3.06	53,53,53,53	0
54	MG	BB	3081	1/1	0.88	0.17	-3.12	16,16,16,16	0
54	MG	DB	3074	1/1	0.92	0.09	-3.12	17,17,17,17	0
54	MG	DB	3047	1/1	0.98	0.11	-3.12	19,19,19,19	0
54	MG	BB	3062	1/1	0.98	0.05	-3.15	27,27,27,27	0
54	MG	BB	3001	1/1	0.95	0.07	-3.33	29,29,29,29	0
54	MG	BB	3002	1/1	0.96	0.08	-3.34	30,30,30,30	0
54	MG	BB	3069	1/1	0.98	0.14	-3.64	10,10,10,10	0
54	MG	AA	1603	1/1	0.96	0.10	-3.64	14,14,14,14	0
54	MG	DB	3108	1/1	0.97	0.10	-3.66	5,5,5,5	0
54	MG	AA	1654	1/1	0.95	0.07	-3.72	82,82,82,82	0
54	MG	BB	3035	1/1	0.93	0.13	-3.80	82,82,82,82	0
54	MG	DB	3012	1/1	0.98	0.09	-3.85	12,12,12,12	0
54	MG	BB	3088	1/1	0.92	0.08	-4.18	36,36,36,36	0
54	MG	DB	3001	1/1	0.97	0.09	-4.27	6,6,6,6	0
54	MG	DB	3056	1/1	0.99	0.12	-4.41	12,12,12,12	0
54	MG	BB	3094	1/1	0.98	0.13	-4.43	47,47,47,47	0
54	MG	CA	1632	1/1	0.98	0.08	-4.60	18,18,18,18	0
54	MG	CA	1643	1/1	0.84	0.07	-4.69	32,32,32,32	0
54	MG	DB	3010	1/1	0.98	0.09	-4.75	16,16,16,16	0
54	MG	BB	3103	1/1	0.96	0.09	-4.89	20,20,20,20	0
54	MG	CA	1656	1/1	0.97	0.06	-4.96	11,11,11,11	0
54	MG	DB	3080	1/1	0.93	0.08	-5.03	5,5,5,5	0
54	MG	BB	3065	1/1	0.94	0.06	-5.04	5,5,5,5	0
54	MG	AA	1641	1/1	0.92	0.04	-5.08	69,69,69,69	0
54	MG	BB	3052	1/1	0.97	0.08	-5.16	36,36,36,36	0
54	MG	CA	1640	1/1	0.97	0.08	-5.20	5,5,5,5	0
54	MG	BB	3056	1/1	0.97	0.06	-5.46	31,31,31,31	0
54	MG	CA	1653	1/1	0.98	0.04	-5.52	51,51,51,51	0
54	MG	DB	3002	1/1	0.98	0.08	-6.11	6,6,6,6	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	CA	1655	1/1	0.99	0.07	-8.88	25,25,25,25	0
54	MG	AA	1643	1/1	0.97	0.03	-9.25	29,29,29,29	0
54	MG	CA	1651	1/1	0.95	0.11	-	38,38,38,38	0
54	MG	DB	3041	1/1	0.98	0.08	-	34,34,34,34	0
54	MG	AA	1649	1/1	0.91	0.06	-	82,82,82,82	0
54	MG	CA	1630	1/1	0.97	0.29	-	52,52,52,52	0
54	MG	BB	3101	1/1	0.98	0.05	-	5,5,5,5	0
54	MG	BB	3102	1/1	0.98	0.04	-	31,31,31,31	0
54	MG	CA	1658	1/1	0.83	0.34	-	53,53,53,53	0
54	MG	BB	3063	1/1	0.98	0.14	-	28,28,28,28	0
54	MG	DB	3066	1/1	0.68	0.30	-	158,158,158,158	0
54	MG	CA	1647	1/1	0.97	0.07	-	65,65,65,65	0
54	MG	DB	3022	1/1	0.94	0.08	-	71,71,71,71	0
54	MG	DB	3033	1/1	0.90	0.12	-	43,43,43,43	0
54	MG	DB	3019	1/1	0.98	0.06	-	5,5,5,5	0
54	MG	BB	3105	1/1	0.99	0.05	-	60,60,60,60	0
54	MG	DB	3048	1/1	0.99	0.08	-	34,34,34,34	0
54	MG	BB	3055	1/1	0.98	0.19	-	53,53,53,53	0
54	MG	BB	3042	1/1	0.56	0.12	-	135,135,135,135	0
54	MG	AA	1640	1/1	0.98	0.09	-	56,56,56,56	0
54	MG	DB	3097	1/1	0.94	0.18	-	64,64,64,64	0
54	MG	BB	3066	1/1	0.98	0.14	-	25,25,25,25	0
54	MG	CA	1607	1/1	0.96	0.07	-	83,83,83,83	0
54	MG	CA	1652	1/1	0.94	0.17	-	65,65,65,65	0
54	MG	AA	1650	1/1	0.69	0.14	-	122,122,122,122	0
54	MG	CA	1606	1/1	0.93	0.13	-	138,138,138,138	0
54	MG	BB	3106	1/1	0.98	0.11	-	39,39,39,39	0
54	MG	BB	3009	1/1	0.96	0.14	-	96,96,96,96	0
54	MG	AA	1616	1/1	0.97	0.06	-	42,42,42,42	0
54	MG	DB	3024	1/1	0.95	0.14	-	45,45,45,45	0
54	MG	CA	1609	1/1	0.91	0.04	-	84,84,84,84	0
54	MG	BB	3104	1/1	0.99	0.16	-	28,28,28,28	0
54	MG	AA	1617	1/1	0.97	0.12	-	100,100,100,100	0
54	MG	BB	3044	1/1	0.97	0.08	-	52,52,52,52	0
54	MG	DB	3046	1/1	0.97	0.07	-	11,11,11,11	0
54	MG	CE	201	1/1	0.80	0.22	-	113,113,113,113	0
54	MG	CA	1642	1/1	0.93	0.13	-	108,108,108,108	0
54	MG	CA	1657	1/1	0.92	0.24	-	89,89,89,89	0
54	MG	BB	3022	1/1	0.95	0.29	-	37,37,37,37	0
54	MG	AA	1622	1/1	0.54	0.39	-	163,163,163,163	0
54	MG	DB	3079	1/1	0.98	0.12	-	34,34,34,34	0
54	MG	AA	1606	1/1	0.87	0.08	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DB	3038	1/1	0.95	0.15	-	37,37,37,37	0
54	MG	DB	3028	1/1	0.98	0.18	-	58,58,58,58	0
54	MG	DB	3101	1/1	0.99	0.25	-	25,25,25,25	0
54	MG	DB	3005	1/1	0.98	0.17	-	45,45,45,45	0
54	MG	DB	3029	1/1	0.88	0.13	-	59,59,59,59	0
54	MG	BB	3050	1/1	0.95	0.10	-	33,33,33,33	0
54	MG	DB	3008	1/1	0.96	0.14	-	17,17,17,17	0
54	MG	BB	3030	1/1	0.98	0.04	-	70,70,70,70	0
54	MG	DB	3077	1/1	0.98	0.08	-	15,15,15,15	0
54	MG	DB	3043	1/1	0.99	0.08	-	32,32,32,32	0
54	MG	CA	1660	1/1	0.92	0.10	-	63,63,63,63	0
54	MG	DB	3004	1/1	0.99	0.13	-	69,69,69,69	0
54	MG	DB	3044	1/1	0.98	0.07	-	21,21,21,21	0
54	MG	BB	3093	1/1	0.70	0.37	-	131,131,131,131	0
54	MG	AA	1645	1/1	0.89	0.09	-	95,95,95,95	0
54	MG	CA	1641	1/1	0.81	0.17	-	42,42,42,42	0
54	MG	BB	3046	1/1	0.98	0.08	-	64,64,64,64	0
54	MG	AA	1639	1/1	0.59	0.34	-	134,134,134,134	0
54	MG	AA	1659	1/1	0.68	0.45	-	180,180,180,180	0
54	MG	BB	3036	1/1	0.96	0.13	-	62,62,62,62	0
54	MG	AA	1602	1/1	0.73	0.18	-	147,147,147,147	0
54	MG	CA	1650	1/1	0.99	0.07	-	33,33,33,33	0
54	MG	CA	1661	1/1	0.96	0.10	-	48,48,48,48	0
54	MG	DB	3082	1/1	0.98	0.08	-	57,57,57,57	0
54	MG	DB	3013	1/1	0.88	0.14	-	41,41,41,41	0
54	MG	CA	1626	1/1	0.96	0.24	-	41,41,41,41	1
54	MG	BB	3076	1/1	0.99	0.06	-	20,20,20,20	0
54	MG	AA	1620	1/1	0.85	0.06	-	113,113,113,113	0
54	MG	AA	1637	1/1	0.66	2.40	-	151,151,151,151	0
54	MG	CA	1659	1/1	0.92	0.09	-	90,90,90,90	0
54	MG	CA	1654	1/1	0.94	0.10	-	59,59,59,59	0
54	MG	DB	3063	1/1	0.96	0.06	-	19,19,19,19	0
54	MG	AA	1644	1/1	0.94	0.13	-	98,98,98,98	0
54	MG	BB	3018	1/1	0.92	0.18	-	50,50,50,50	0
54	MG	BB	3057	1/1	0.90	0.36	-	65,65,65,65	0
54	MG	BB	3089	1/1	0.98	0.19	-	25,25,25,25	0
54	MG	AA	1625	1/1	0.27	0.87	-	84,84,84,84	1
54	MG	DB	3023	1/1	0.97	0.10	-	17,17,17,17	0
54	MG	BB	3031	1/1	0.95	0.13	-	63,63,63,63	0
54	MG	CA	1625	1/1	0.95	0.17	-	6,6,6,6	0
54	MG	BB	3078	1/1	0.91	0.21	-	101,101,101,101	0
54	MG	BB	3033	1/1	0.47	0.65	-	141,141,141,141	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DB	3021	1/1	0.99	0.08	-	51,51,51,51	0
54	MG	BB	3049	1/1	0.88	0.15	-	35,35,35,35	0
54	MG	AA	1628	1/1	0.97	0.12	-	59,59,59,59	0
54	MG	BB	3043	1/1	0.82	0.08	-	122,122,122,122	0
54	MG	BB	3071	1/1	0.96	0.09	-	89,89,89,89	0
54	MG	DB	3039	1/1	0.97	0.08	-	69,69,69,69	0
54	MG	AA	1658	1/1	0.86	0.09	-	85,85,85,85	0
54	MG	DB	3083	1/1	0.95	0.17	-	83,83,83,83	0
54	MG	BB	3020	1/1	0.95	0.09	-	36,36,36,36	0
54	MG	AA	1656	1/1	0.71	0.80	-	161,161,161,161	0
54	MG	CA	1634	1/1	0.96	0.11	-	23,23,23,23	0
54	MG	CA	1613	1/1	0.97	0.11	-	40,40,40,40	0
54	MG	DB	3075	1/1	0.98	0.12	-	35,35,35,35	0
54	MG	AA	1632	1/1	0.64	0.26	-	62,62,62,62	0
54	MG	CA	1623	1/1	0.76	0.08	-	173,173,173,173	0
54	MG	BB	3067	1/1	0.95	0.13	-	24,24,24,24	0
54	MG	BB	3061	1/1	0.91	0.10	-	56,56,56,56	0
54	MG	BB	3060	1/1	0.99	0.08	-	22,22,22,22	0
54	MG	DB	3076	1/1	0.98	0.14	-	104,104,104,104	0
54	MG	CA	1603	1/1	0.97	0.09	-	29,29,29,29	0
54	MG	AA	1611	1/1	0.98	0.09	-	77,77,77,77	0
54	MG	BB	3107	1/1	0.96	0.09	-	30,30,30,30	0
54	MG	DB	3036	1/1	0.95	0.08	-	20,20,20,20	0
54	MG	CA	1624	1/1	0.93	0.12	-	56,56,56,56	0
54	MG	AA	1624	1/1	0.93	0.10	-	77,77,77,77	0
54	MG	BB	3025	1/1	0.99	0.06	-	42,42,42,42	0
54	MG	CA	1648	1/1	0.97	0.19	-	14,14,14,14	0
54	MG	CA	1611	1/1	0.97	0.06	-	57,57,57,57	0
54	MG	AA	1626	1/1	0.54	0.18	-	49,49,49,49	1
54	MG	BB	3100	1/1	0.94	0.21	-	151,151,151,151	0
54	MG	DB	3084	1/1	0.98	0.14	-	16,16,16,16	0
54	MG	DB	3016	1/1	0.95	0.07	-	25,25,25,25	0
54	MG	DB	3093	1/1	0.94	0.17	-	10,10,10,10	0
54	MG	DB	3015	1/1	0.89	0.10	-	24,24,24,24	0
54	MG	DB	3027	1/1	0.96	0.17	-	28,28,28,28	0
54	MG	BB	3038	1/1	0.95	0.23	-	152,152,152,152	0
54	MG	BB	3034	1/1	0.96	0.24	-	59,59,59,59	0
54	MG	BB	3095	1/1	0.95	0.11	-	81,81,81,81	0
54	MG	DB	3102	1/1	0.97	0.09	-	22,22,22,22	0
54	MG	BB	3070	1/1	0.98	0.19	-	59,59,59,59	0
54	MG	BB	3028	1/1	0.97	0.15	-	61,61,61,61	0
54	MG	DB	3058	1/1	0.83	0.85	-	162,162,162,162	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	CA	1635	1/1	0.83	0.14	-	98,98,98,98	0
54	MG	CA	1627	1/1	0.52	0.32	-	69,69,69,69	1
54	MG	DB	3109	1/1	0.95	0.09	-	83,83,83,83	0
54	MG	BB	3010	1/1	0.84	0.13	-	40,40,40,40	0
54	MG	BB	3045	1/1	0.99	0.04	-	38,38,38,38	0
54	MG	AA	1618	1/1	0.95	0.13	-	93,93,93,93	0
54	MG	CA	1602	1/1	0.99	0.12	-	11,11,11,11	0
54	MG	BB	3058	1/1	0.97	0.09	-	11,11,11,11	0
54	MG	DB	3060	1/1	0.55	0.10	-	104,104,104,104	0
54	MG	BB	3073	1/1	0.99	0.23	-	38,38,38,38	0
54	MG	AA	1621	1/1	0.97	0.17	-	26,26,26,26	0
54	MG	DB	3111	1/1	0.97	0.18	-	32,32,32,32	0
54	MG	AA	1646	1/1	0.73	0.18	-	104,104,104,104	0
54	MG	BB	3051	1/1	0.96	0.18	-	65,65,65,65	0
54	MG	BB	3026	1/1	0.95	0.21	-	43,43,43,43	0
54	MG	DB	3107	1/1	0.98	0.07	-	11,11,11,11	0
54	MG	DB	3061	1/1	0.94	0.09	-	69,69,69,69	0
54	MG	CA	1639	1/1	0.98	0.07	-	7,7,7,7	0
54	MG	DB	3105	1/1	0.97	0.08	-	30,30,30,30	0
54	MG	CA	1629	1/1	0.89	0.12	-	65,65,65,65	1
54	MG	DB	3037	1/1	0.93	0.17	-	54,54,54,54	0
54	MG	AA	1612	1/1	0.96	0.13	-	88,88,88,88	0
54	MG	DB	3095	1/1	0.96	0.12	-	88,88,88,88	0
54	MG	BB	3109	1/1	0.98	0.07	-	59,59,59,59	0
54	MG	BB	3059	1/1	0.99	0.11	-	60,60,60,60	0
54	MG	DB	3034	1/1	0.81	0.20	-	69,69,69,69	0
54	MG	DB	3094	1/1	0.98	0.10	-	55,55,55,55	0
54	MG	BB	3003	1/1	0.92	0.09	-	51,51,51,51	0
54	MG	BB	3027	1/1	0.95	0.13	-	42,42,42,42	0
54	MG	CA	1644	1/1	0.98	0.07	-	68,68,68,68	0
54	MG	BB	3041	1/1	0.96	0.15	-	8,8,8,8	0
54	MG	AA	1633	1/1	0.97	0.03	-	48,48,48,48	0
54	MG	BB	3008	1/1	0.89	0.20	-	75,75,75,75	0
54	MG	DB	3062	1/1	0.97	0.04	-	67,67,67,67	0
54	MG	DB	3073	1/1	0.98	0.21	-	67,67,67,67	0
54	MG	AA	1651	1/1	0.86	0.09	-	112,112,112,112	0
54	MG	DB	3042	1/1	0.94	0.07	-	23,23,23,23	0
54	MG	CA	1649	1/1	0.91	0.14	-	127,127,127,127	0
54	MG	DB	3054	1/1	0.96	0.06	-	29,29,29,29	0
54	MG	DB	3017	1/1	0.96	0.10	-	5,5,5,5	0
54	MG	BB	3097	1/1	0.80	0.07	-	88,88,88,88	0
54	MG	DB	3025	1/1	0.97	0.18	-	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DB	3053	1/1	0.92	0.09	-	80,80,80,80	0
54	MG	AA	1619	1/1	0.64	0.25	-	180,180,180,180	0
54	MG	AA	1655	1/1	0.94	0.07	-	54,54,54,54	0
54	MG	BB	3039	1/1	0.97	0.07	-	5,5,5,5	0
54	MG	BB	3064	1/1	0.98	0.08	-	37,37,37,37	0
54	MG	DB	3049	1/1	0.98	0.07	-	9,9,9,9	0
54	MG	CA	1619	1/1	0.70	0.19	-	70,70,70,70	0
54	MG	BB	3075	1/1	0.97	0.16	-	29,29,29,29	0
54	MG	DB	3057	1/1	0.80	0.10	-	77,77,77,77	0
54	MG	BB	3017	1/1	0.93	0.17	-	73,73,73,73	0
54	MG	DB	3040	1/1	0.98	0.09	-	18,18,18,18	0
54	MG	BB	3007	1/1	0.98	0.07	-	53,53,53,53	0
54	MG	BB	3072	1/1	0.90	0.14	-	79,79,79,79	0
54	MG	AA	1604	1/1	0.98	0.10	-	19,19,19,19	0
54	MG	BB	3015	1/1	0.99	0.08	-	42,42,42,42	0
54	MG	AA	1652	1/1	0.97	0.08	-	90,90,90,90	0
54	MG	AA	1642	1/1	0.97	0.12	-	41,41,41,41	0
54	MG	BB	3053	1/1	0.89	0.07	-	79,79,79,79	0
54	MG	DB	3071	1/1	0.98	0.05	-	37,37,37,37	0
54	MG	DB	3065	1/1	0.97	0.06	-	45,45,45,45	0
54	MG	DB	3020	1/1	0.94	0.20	-	13,13,13,13	0
54	MG	DB	3011	1/1	0.97	0.27	-	33,33,33,33	0
54	MG	AA	1648	1/1	0.95	0.07	-	40,40,40,40	0
54	MG	DB	3086	1/1	0.98	0.20	-	52,52,52,52	0
54	MG	AA	1605	1/1	0.97	0.09	-	47,47,47,47	0
54	MG	CA	1621	1/1	0.91	0.53	-	110,110,110,110	0
54	MG	CA	1608	1/1	0.96	0.09	-	139,139,139,139	0
54	MG	AA	1634	1/1	0.97	0.07	-	67,67,67,67	0
54	MG	BB	3080	1/1	0.79	0.20	-	77,77,77,77	0
54	MG	CA	1646	1/1	0.91	0.08	-	99,99,99,99	0
54	MG	DB	3045	1/1	0.92	0.07	-	68,68,68,68	0
54	MG	CA	1637	1/1	0.98	0.07	-	92,92,92,92	0
54	MG	BB	3054	1/1	0.96	0.14	-	46,46,46,46	0
54	MG	BB	3004	1/1	0.93	0.19	-	73,73,73,73	0
54	MG	AA	1608	1/1	0.49	0.29	-	147,147,147,147	0
54	MG	DB	3104	1/1	0.96	0.19	-	71,71,71,71	0
54	MG	AA	1657	1/1	0.75	0.42	-	124,124,124,124	0
54	MG	AA	1627	1/1	0.79	0.19	-	68,68,68,68	0
54	MG	AA	1660	1/1	0.94	0.08	-	37,37,37,37	0
54	MG	DB	3031	1/1	0.98	0.07	-	24,24,24,24	0
54	MG	BB	3006	1/1	0.99	0.08	-	20,20,20,20	0
54	MG	DB	3064	1/1	0.92	0.10	-	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DB	3091	1/1	0.99	0.14	-	5,5,5,5	0
54	MG	DB	3067	1/1	0.97	0.14	-	16,16,16,16	0
54	MG	AA	1631	1/1	0.94	0.12	-	88,88,88,88	0
54	MG	DB	3018	1/1	0.97	0.10	-	22,22,22,22	0
54	MG	DB	3081	1/1	0.95	0.11	-	19,19,19,19	0
54	MG	DB	3106	1/1	0.94	0.18	-	64,64,64,64	0
54	MG	CA	1622	1/1	0.98	0.10	-	18,18,18,18	0
54	MG	CA	1610	1/1	0.96	0.07	-	75,75,75,75	0
54	MG	CA	1620	1/1	0.93	0.14	-	37,37,37,37	0
54	MG	BB	3024	1/1	0.95	0.06	-	44,44,44,44	0
54	MG	CA	1615	1/1	0.93	0.09	-	180,180,180,180	0
54	MG	BB	3047	1/1	0.96	0.13	-	116,116,116,116	0
54	MG	DB	3050	1/1	0.97	0.14	-	123,123,123,123	0
54	MG	BB	3014	1/1	0.96	0.13	-	58,58,58,58	0
54	MG	BB	3084	1/1	0.98	0.20	-	77,77,77,77	0
54	MG	AA	1623	1/1	0.83	0.65	-	73,73,73,73	1
54	MG	CA	1631	1/1	0.98	0.10	-	40,40,40,40	0
54	MG	AA	1614	1/1	0.71	0.11	-	113,113,113,113	0
54	MG	BB	3091	1/1	0.97	0.10	-	37,37,37,37	0
54	MG	DB	3052	1/1	0.91	0.23	-	113,113,113,113	0
54	MG	AA	1647	1/1	0.55	0.99	-	180,180,180,180	0
54	MG	CA	1628	1/1	0.94	0.07	-	44,44,44,44	0
54	MG	BB	3068	1/1	1.00	0.05	-	61,61,61,61	0
54	MG	DB	3032	1/1	0.96	0.09	-	51,51,51,51	0
54	MG	BB	3099	1/1	0.95	0.16	-	56,56,56,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.