



# wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 06:38 PM BST

PDB ID : 4V50  
Title : Crystal Structure of Ribosome with messenger RNA and the Anticodon stem-loop of P-site tRNA.  
Authors : Berk, V.; Zhang, W.; Pai, R.D.; Cate, J.H.D.  
Deposited on : 2006-08-16  
Resolution : 3.22 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

---

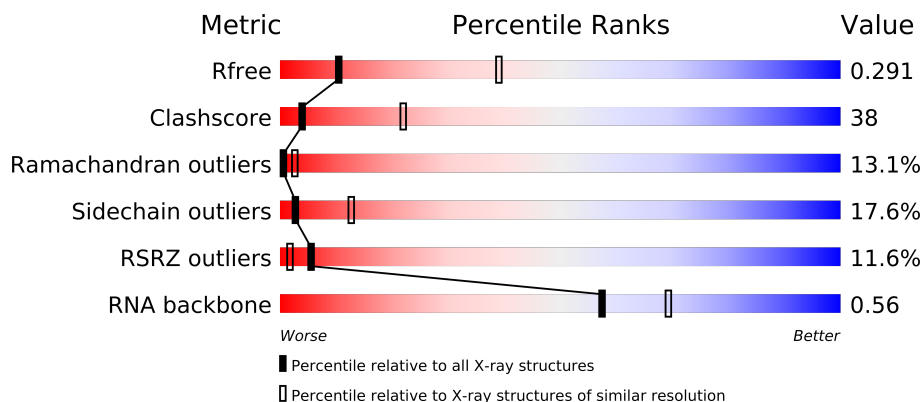
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable23397  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23397

# 1 Overall quality at a glance

The reported resolution of this entry is 3.22 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))
$R_{free}$	66092	1205 (3.30-3.14)
Clashscore	79885	1072 (3.28-3.16)
Ramachandran outliers	78287	1052 (3.28-3.16)
Sidechain outliers	78261	1051 (3.28-3.16)
RSRZ outliers	66119	1206 (3.30-3.14)
RNA backbone	1838	1004 (3.74-2.70)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	AA	1542	
1	CA	1542	
2	AW	17	
2	CW	17	
3	AX	6	
3	CX	6	
4	AB	240	
4	CB	240	
5	AC	232	
5	CC	232	
6	AD	205	
6	CD	205	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
7	AE	166	
7	CE	166	
8	AF	135	
8	CF	135	
9	AG	178	
9	CG	178	
10	AH	129	
10	CH	129	
11	AI	129	
11	CI	129	
12	AJ	103	
12	CJ	103	
13	AK	128	
13	CK	128	
14	AL	123	
14	CL	123	
15	AM	117	
15	CM	117	
16	AN	100	
16	CN	100	
17	AO	88	
17	CO	88	
18	AP	82	
18	CP	82	
19	AQ	83	
19	CQ	83	
20	AR	74	
20	CR	74	
21	AS	91	
21	CS	91	
22	AT	86	
22	CT	86	
23	AU	70	
23	CU	70	
24	BA	120	
24	DA	120	
25	BB	2904	
25	DB	2904	
26	BC	272	
26	DC	272	
27	BD	209	
27	DD	209	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
28	BE	201	
28	DE	201	
29	BF	178	
29	DF	178	
30	BG	176	
30	DG	176	
31	BH	149	
31	DH	149	
32	BI	141	
32	DI	141	
33	BJ	142	
33	DJ	142	
34	BK	123	
34	DK	123	
35	BL	144	
35	DL	144	
36	BM	136	
36	DM	136	
37	BN	127	
37	DN	127	
38	BO	117	
38	DO	117	
39	BP	114	
39	DP	114	
40	BQ	117	
40	DQ	117	
41	BR	103	
41	DR	103	
42	BS	110	
42	DS	110	
43	BT	100	
43	DT	100	
44	BU	103	
44	DU	103	
45	BV	94	
45	DV	94	
46	BW	84	
46	DW	84	
47	BX	77	
47	DX	77	
48	BY	63	
48	DY	63	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
49	BZ	58	
49	DZ	58	
50	B0	56	
50	D0	56	
51	B1	54	
51	D1	54	
52	B2	46	
52	D2	46	
53	B3	64	
53	D3	64	
54	B4	38	
54	D4	38	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
55	MG	AA	1614	-	X
55	MG	AA	1617	-	X
55	MG	AA	1625	-	X
55	MG	AA	1626	-	X
55	MG	AA	1627	-	X
55	MG	AA	1628	-	X
55	MG	AA	1632	-	X
55	MG	AA	1637	-	X
55	MG	AA	1639	-	X
55	MG	AA	1643	-	X
55	MG	AA	1650	-	X
55	MG	AA	1652	-	X
55	MG	AA	1653	-	X
55	MG	AA	1655	-	X
55	MG	AA	1656	-	X
55	MG	AA	1658	-	X
55	MG	BB	3014	-	X
55	MG	BB	3016	-	X
55	MG	BB	3031	-	X
55	MG	BB	3033	-	X
55	MG	BB	3057	-	X
55	MG	BB	3063	-	X
55	MG	BB	3093	-	X
55	MG	CA	1606	-	X
55	MG	CA	1613	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Geometry	Electron density
55	MG	CA	1627	-	X
55	MG	CA	1638	-	X
55	MG	CA	1639	-	X
55	MG	CA	1640	-	X
55	MG	CA	1646	-	X
55	MG	CA	1655	-	X
55	MG	DB	3029	-	X
55	MG	DB	3032	-	X
55	MG	DB	3034	-	X
55	MG	DB	3043	-	X
55	MG	DB	3052	-	X
55	MG	DB	3058	-	X
55	MG	DB	3065	-	X
55	MG	DB	3070	-	X
55	MG	DB	3082	-	X
55	MG	DB	3088	-	X

## 2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 285033 atoms, of which 0 are hydrogen and 0 are deuterium.

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 ribosomal RNA.

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 RNA chain called PHE TRNA (UNMODIFIED BASES).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AW	17	Total	C	N	O	P	0	0	0
			360	161	64	118	17			
2	CW	17	Total	C	N	O	P	0	0	0
			360	161	64	118	17			

- Molecule 3 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AX	6	Total	C	N	O	P	0	0	0
			125	56	18	45	6			
3	CX	6	Total	C	N	O	P	0	0	0
			125	56	18	45	6			

- Molecule 4 is a protein called 30S ribosomal protein S2.

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

- Molecule 5 is a protein called 30S ribosomal protein S3.

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

- Molecule 6 is a protein called 30S ribosomal protein S4.

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

- Molecule 7 is a protein called 30S ribosomal protein S5.

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

- Molecule 8 is a protein called 30S ribosomal protein S6.

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

- Molecule 9 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AG	150	Total	C	N	O	S	0	0	0
			1174	730	226	214	4			
9	CG	150	Total	C	N	O	S	0	0	0
			1174	730	226	214	4			

- Molecule 10 is a protein called 30S ribosomal protein S8.

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

*Continued on next page...*



*Continued from previous page...*

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

- Molecule 11 is a protein called 30S ribosomal protein S9.

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

- Molecule 12 is a protein called 30S ribosomal protein S10.

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

- Molecule 13 is a protein called 30S ribosomal protein S11.

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

- Molecule 14 is a protein called 30S ribosomal protein S12.

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

- Molecule 15 is a protein called 30S ribosomal protein S13.

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

- Molecule 16 is a protein called 30S ribosomal protein S14.

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

- Molecule 17 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AO	88	Total	C	N	O	S	0	0	0
			716	440	146	129	1			
17	CO	88	Total	C	N	O	S	0	0	0
			716	440	146	129	1			

- Molecule 18 is a protein called 30S ribosomal protein S16.

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

- Molecule 19 is a protein called 30S ribosomal protein S17.

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

- Molecule 20 is a protein called 30S ribosomal protein S18.

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

- Molecule 21 is a protein called 30S ribosomal protein S19.

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

- Molecule 22 is a protein called 30S ribosomal protein S20.

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

- Molecule 23 is a protein called 30S ribosomal protein S21.

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

- Molecule 24 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 25 is a RNA chain called 23S ribosomal RNA.

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

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

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

*Continued on next page...*

*Continued from previous page...*

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

*Continued on next page...*

*Continued from previous page...*

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	BB	118	Total	Mg	0	0
			118	118		
55	CN	1	Total	Mg	0	0
			1	1		
55	CA	56	Total	Mg	0	0
			56	56		
55	AA	60	Total	Mg	0	0
			60	60		
55	AX	2	Total	Mg	0	0
			2	2		
55	BJ	1	Total	Mg	0	0
			1	1		
55	CX	1	Total	Mg	0	0
			1	1		
55	DB	119	Total	Mg	0	0
			119	119		

- 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 287 287	0	0
57	AX	9	Total O 9 9	0	0
57	AE	3	Total O 3 3	0	0
57	AI	1	Total O 1 1	0	0
57	AK	2	Total O 2 2	0	0
57	AL	2	Total O 2 2	0	0
57	AN	1	Total O 1 1	0	0
57	AP	1	Total O 1 1	0	0
57	AT	2	Total O 2 2	0	0
57	BB	532	Total O 532 532	0	0
57	BC	7	Total O 7 7	0	0
57	BE	3	Total O 3 3	0	0
57	BH	3	Total O 3 3	0	0
57	BJ	3	Total O 3 3	0	0
57	BL	2	Total O 2 2	0	0
57	BN	3	Total O 3 3	0	0
57	B2	1	Total O 1 1	0	0
57	B4	5	Total O 5 5	0	0
57	CA	264	Total O 264 264	0	0
57	CX	6	Total O 6 6	0	0
57	CE	2	Total O 2 2	0	0
57	CI	3	Total O 3 3	0	0

Continued on next page...

*Continued from previous page...*

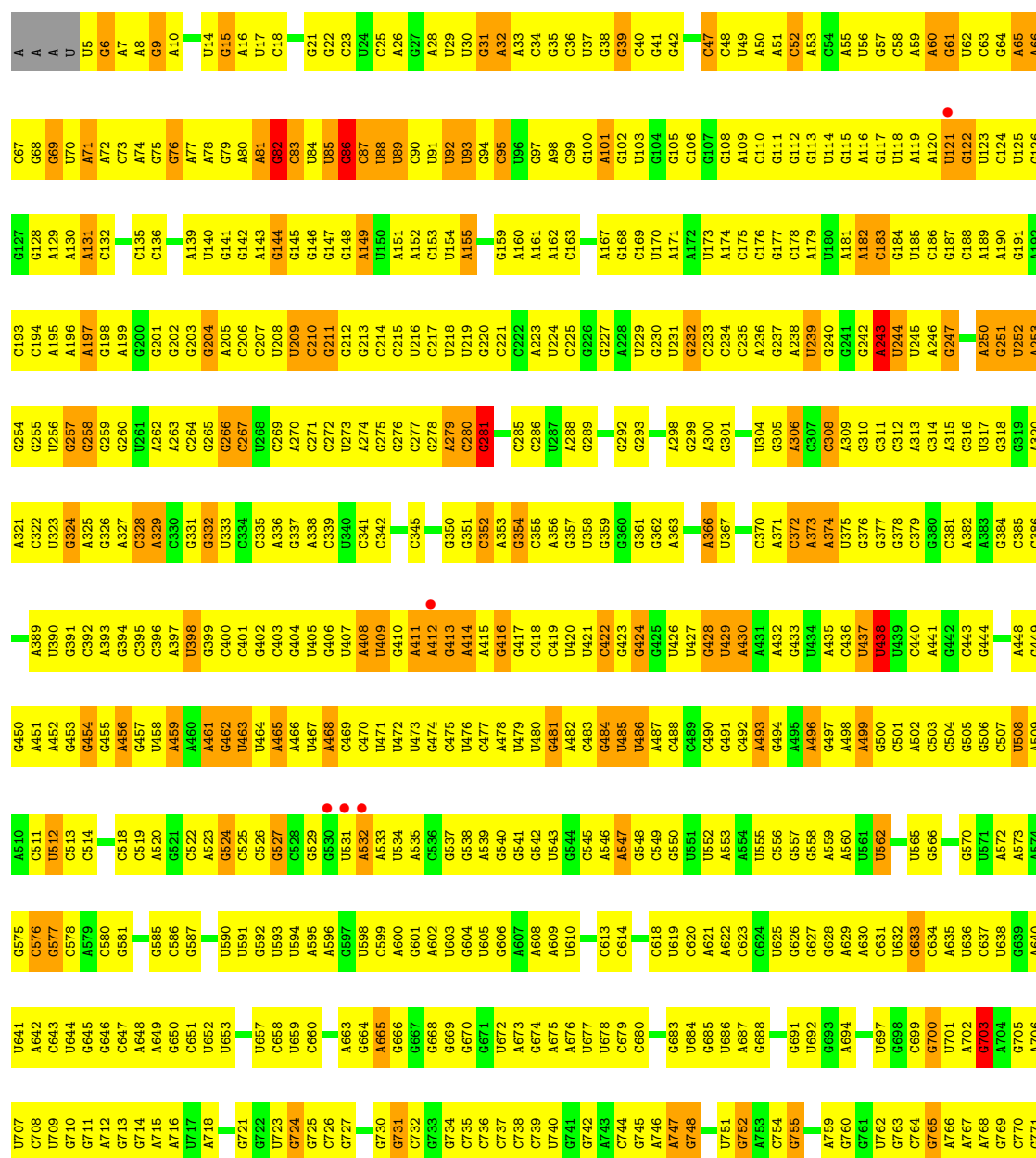
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	CL	1	Total 1	O 1	0	0
57	CN	1	Total 1	O 1	0	0
57	CP	1	Total 1	O 1	0	0
57	CT	3	Total 3	O 3	0	0
57	CU	1	Total 1	O 1	0	0
57	DB	531	Total 531	O 531	0	0
57	DC	7	Total 7	O 7	0	0
57	DD	1	Total 1	O 1	0	0
57	DE	3	Total 3	O 3	0	0
57	DJ	2	Total 2	O 2	0	0
57	DL	3	Total 3	O 3	0	0
57	DN	3	Total 3	O 3	0	0
57	DT	1	Total 1	O 1	0	0
57	D2	1	Total 1	O 1	0	0
57	D4	4	Total 4	O 4	0	0

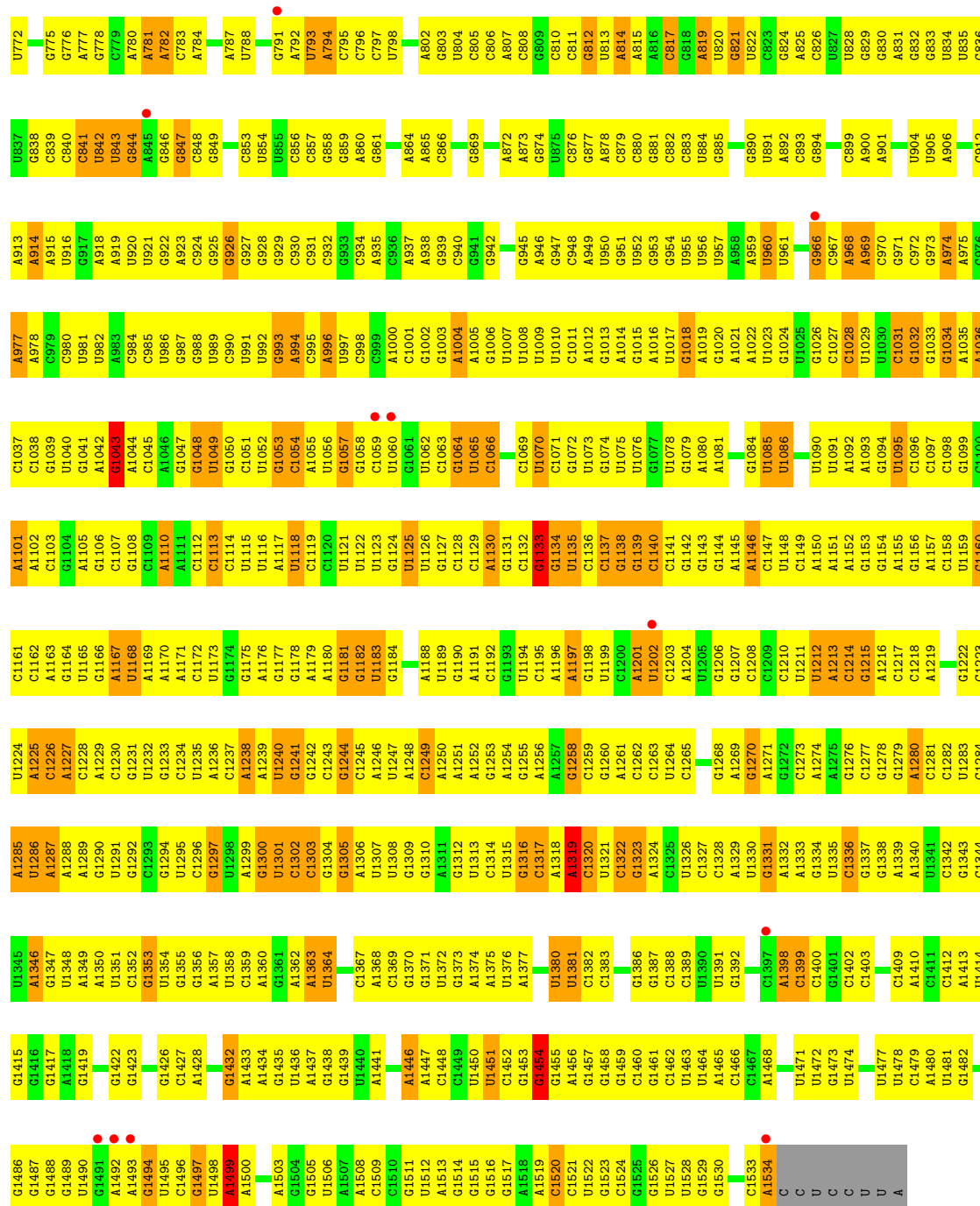
### 3 Residue-property plots

These plots are drawn for all protein, RNA 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 ( $\text{RSRZ} > 2$ ). 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 ribosomal RNA

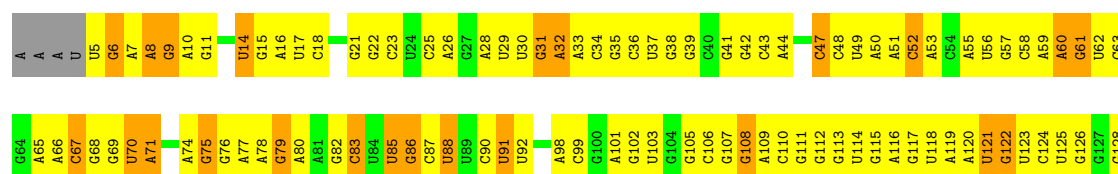
Chain AA: 



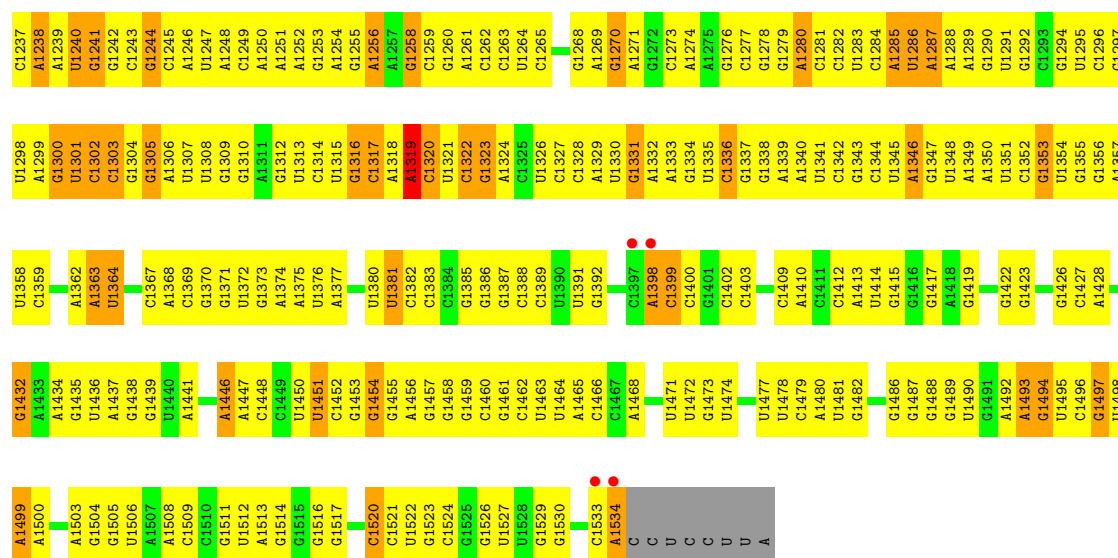


● Molecule 1: 16S ribosomal RNA

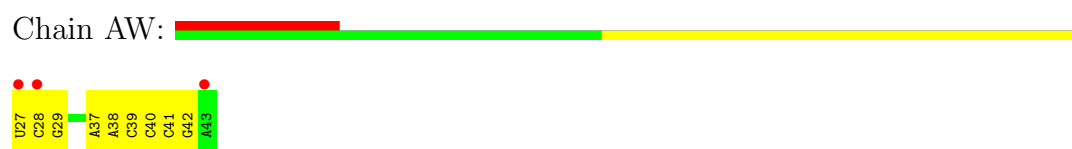
Chain CA:



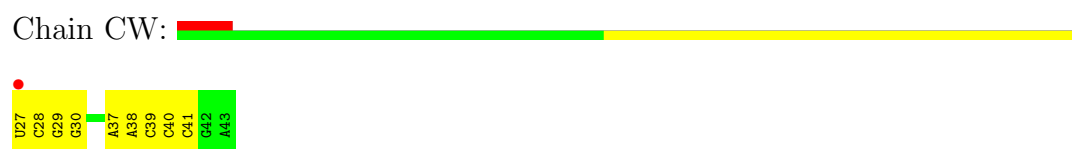
G1177	A1117	U1052	U992	G926	C856	U793	U723	U657	U594	G524	A460	C395	G326	G257	C194	A129
G1178	U1118	G1053	G993	G927	C857	A794	G724	C658	A595	C525	A461	C396	A327	G258	A195	A130
A1180	C1120	A1054	A994	G928	G858	C795	G726	C660	A596	C526	G462	U998	C328	A197	A196	A131
G1181	U1121	U1055	C995	G929	G859	C796	G727	C661	G597	G527	U463	U999	C329	G198	A199	U133
G1182	U1122	G1056	A996	C930	A860	C797	G728	A663	C598	U531	A465	C400	G330	C264	G199	G134
U1183	U1123	G1058	C998	C932	C862	G799	A729	G664	A600	A832	A466	C401	G332	G265	G200	U135
G1184	G1125	C1059	G999	G933	U863	G800	G730	A665	A601	U534	A467	C402	U333	G267	G201	C136
G1185	U1126	U1060	A1000	C934	A864	A801	G731	G666	A602	U534	A468	G403	C334	C267	G202	
G1186	G1127	A1061	C1001	A935	A865	A802	C732	G667	U603	G537	C469	G404	A336	C269	G203	A139
G1187	U1128	G1062	G1002	C936	C866	G803	C732	G668	G604	U538	C470	U405	A337	U268	G204	U140
A1188	C1129	G1063	G1003	A937	U869	U804	G735	G669	U605	G539	U471	G406	G337	G270	A205	G141
U1189	U1129	G1064	A1004	A938	U869	C805	G736	G670	G606	G540	U472	U407	A338	C271	C206	G142
G1190	A1130	U1065	A1005	G939	U869	C806	C737	G671	A607	G541	U473	A408		C272	C207	A143
A1191	G1131	C1066	G1006	C940	A872	A807	C738	A672	A608	G542	U474	U409	C341	U273	U208	A144
C1192	C1132	U1067	U1007		A873	C808	C739	A673	A609	U543	C475	G410	C342	G274	U209	G145
G1193	U1133	C1069	U1008	G944	G874	G809	U740	G674	G610	G544	U476	A411	G345	G275	C210	G146
U1194	G1134	U1070	U1009	G945	U875	C810	G741	A675	G611	G545	U477	A412		G276	G211	G147
C1195	U1135	C1071	U1010	A946	C876	C811	G742	A676	C613	C546	U478	G413	G380	C277	G212	G148
A1196	C1136	G1072	C1011	G947	G877	G812	A743	A677	C614	A546	U479	A414	G381	G278	G213	A149
A1197	C1137	U1073	A1012	C948	A878	U813	C744	U678	G615	A547	U480	A415	G351	A279	C214	U150
G1198	G1138	G1074	G1013	A949	C879	A814	G745	G548	G616	G548	G481	G416	C352	C280	G215	A151
U1199	U1139	U1075	A1014	U950	C880	A815	A746	C549	U617	C549	A482	G417	A353	U216	U216	A152
C1200	C1140	U1076	G1015	G951	C881	A816	A747	G550	C483	G550	C483	C418	G354	C217	C153	U154
A1201	C1141	G1077	A1016	U952	C882	C817	G748	G551	U618	U551	G484	C419	C355	U218	U154	
U1202	G1142	U1078	G1017	G953	C883	C818		U552	C620	U552	U485	U420	A356	U219	U155	
C1203	G1143	G1079	U1018	G954	C884	G819	U751	U553	A621	A553	U486	U421	G357	G220	G220	
A1204	A1144	A1080	A1019	U955	G885	A820	G752	A554	A622	A554	A487	C422	U358	C221	G221	G159
U1205	A1145	U1081	G1020	U956	G886	G821	A753	U555	C488	U555	C488	G423	G359	C222	C222	A160
G1206	A1146	G1084	A1021	U957	G887	U822	C754	C556	C489	C556	C489	G424	G360	U223	U223	A161
U1207	C1147	U1085	A1022	A958	G888	C823	G755	G557	C490	G557	C490	U425	G361	U224	U224	C163
C1208	U1148	U1086	G1023	A959	G889	G824		G558	C491	G558	C491	U426	G362	C225	C225	
U1209	C1149	U1087	U1024	U960	C893	A825		U559	C492	A559	C492	U427				
C1210	A1150	U1090	U1025	U961	G894	A826	U759	U560	G493	U560	G494	U428	A366	U229	U229	A167
U1211	A1151	U1091	G1026			U828	G761	A694	G494	U561	G494	U429	U367	G230	G230	G168
A1212	G1152	A1092	C1027	G966	C899	G829	U762	G700	A630	U562	A496	U430	U368	U231	U231	C169
A1213	G1153	A1093	G1028	C967	A900	G830	G763	A701	A635	U565	A497		A371	G232	G232	U170
C1214	G1154	G1094	U1029	A968	A901	A831	C764	G698	U632	G666	A498		C370	C233	C233	A171
G1215	A1155	U1095	U1030	A969	U904	G832	G765	C699	U633	U566	A499		C372	C234	C234	A172
A1216	G1156	C1096	G1031	C970	U905	G833	A766	G700	C634	G666	A499		C373	C235	C235	U173
C1217	U1157	C1097	G1032	G971	U906	U834	A767	A702	A636	G570	G500	U438	A374	A236	A236	A174
C1218	C1158	C1098	G1033	C972	A906	U835	A768	G703	U636	U571	C501	U439	C307	G237	G237	C175
A1219	U1159	G1099	G1034	G973	U907	G836	G769	G703	C637	A572	A502	C440	C308	A238	A238	G176
G1220	G1160	C1100	A1035	A974	A909	U837	C770	A573	U638	A573	C503	A441	A309	U239	U239	G177
C1221	C1161	A1101	A1036	A975	C910	G838	G771	A574	G639	A574	C504	G442	G377	G240	G240	C178
G1222	A1162	A1102	C1037	G976	U911	C839	U772	G575	A640	G575	G505	C443	G378	G241	G241	A179
C1223	A1163	C1103	G1038	A977	C912	C840		C576	U641	C576	G506	G444	C379	G242	G242	U180
U1224	G1164	G1104	G1039	A978	A913	U841	G775	G577	A642	G577	C507		G380	A243	A243	A181
A1225	U1165	A1105	U1040		A914	U842	G776	G578	C643	C578	U508		C381	U244	U244	A182
C1226	G1166	C1106	G1041	U981	A915	U843	A777	A579	U644	A579	A509	G449	A382	U245	U245	C183
A1227	A1167	C1107	A1042	U982	U916	G844		C580	G645	C580	A510	G450	A383	A246	A246	G184
C1228	U1168	G1108	G1043	A983	G917	A845	A780	G581	G646	G581	A511	C451	A384	G247	G247	U185
A1229	A1169	C1109	A1044	C984	A918	G846	A781	G585	U647	G585	U512	A452	C385	A250	A250	C186
C1230	A1170	A1110	C1045	C985	A919	G847	A782	G586	C647	G586	U513	G453	C386	G187	G187	A188
G1231	C1171	A1111	A1046	U986	U920	C848	C783	G586	A649	C586	C514	G454	A389	U252	U252	A190
U1232	U1172	G1112	G1047	G987	U921	G849		U590	C650	U590	C518	G455	U390	G251	G251	A189
G1233	U1173	C1113	G1048	G988	G922	U921	A784	C586	C651	U591	C522	A456	G391	A253	A253	G191
C1234	G1174	C1114	U1049	U989	A923	C853	A787	G586	C652	G592	C522	U457	U391	G254	G254	A192
U1235	U1175	U1115	G1050	U990	C924	U854	U788	G592	U653	U593	A523	U458	G394	U256	U256	C193
A1236	A1176	U1116	C1051	U991	G925	U955	G722	G722								



- Molecule 2: PHE TRNA (UNMODIFIED BASES)



- Molecule 2: PHE TRNA (UNMODIFIED BASES)



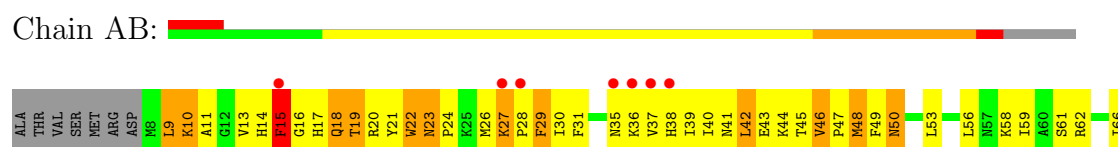
- Molecule 3: MRNA

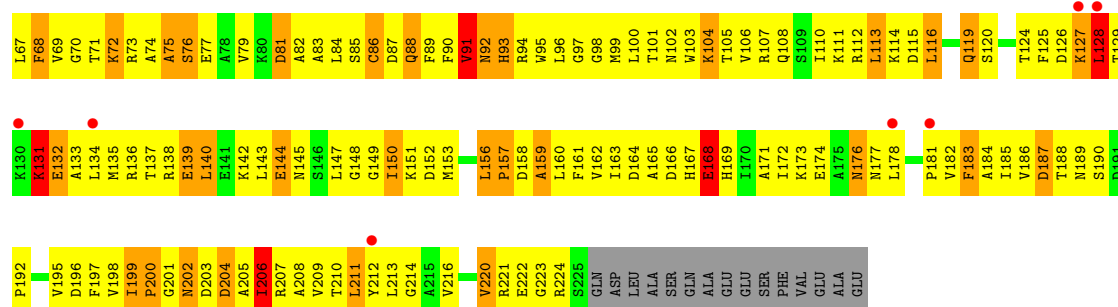


- Molecule 3: MRNA



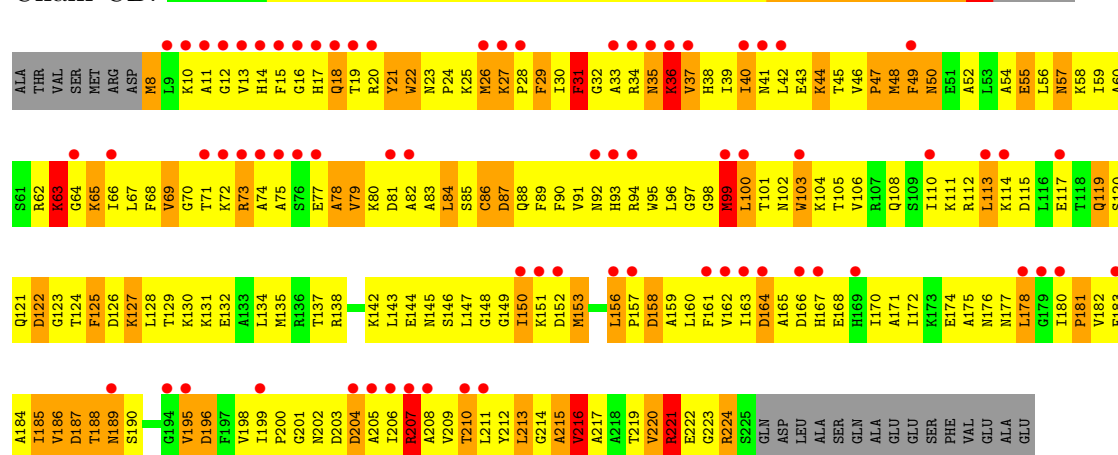
- Molecule 4: 30S ribosomal protein S2





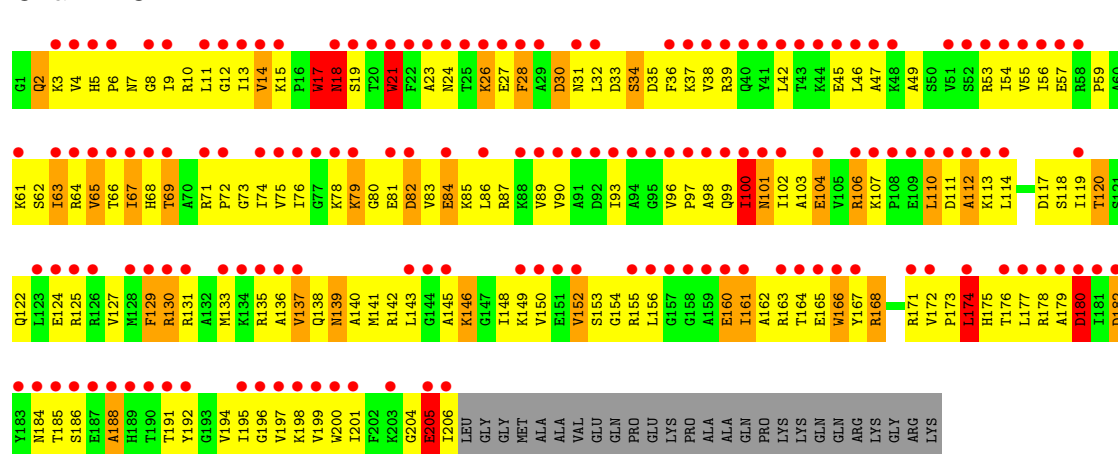
• Molecule 4: 30S ribosomal protein S2

Chain CB:



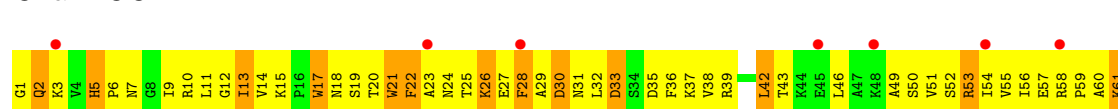
• Molecule 5: 30S ribosomal protein S3

Chain AC:

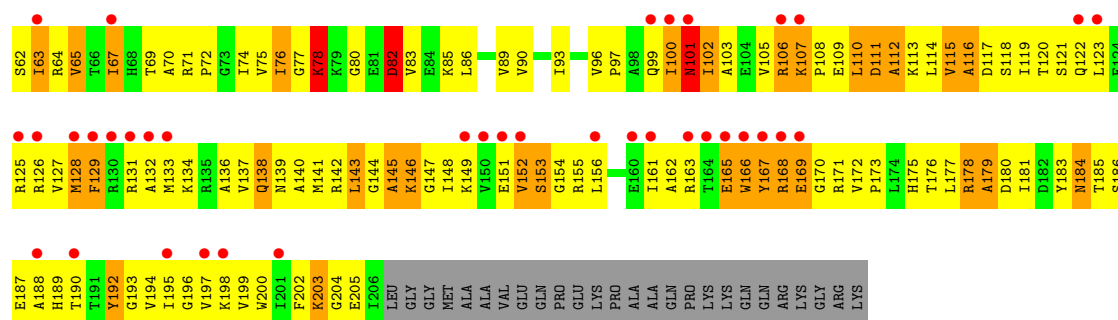


• Molecule 5: 30S ribosomal protein S3

Chain CC:

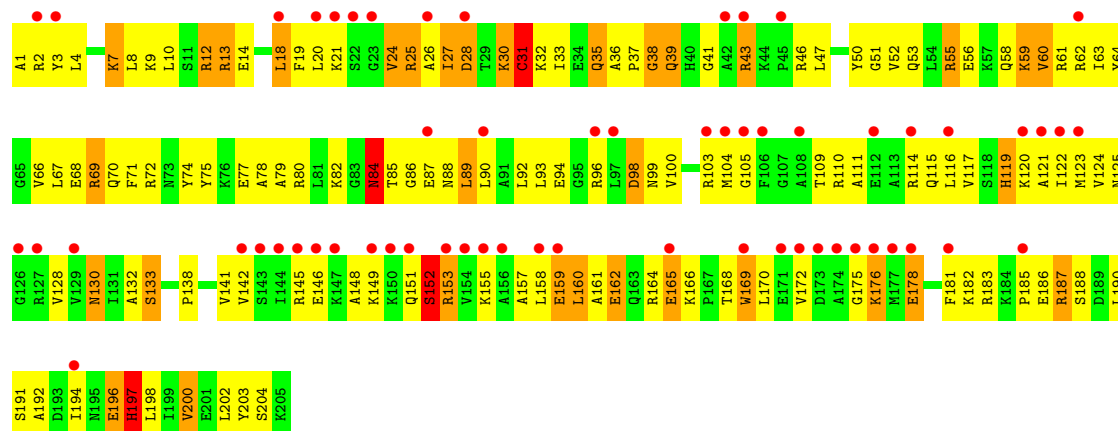






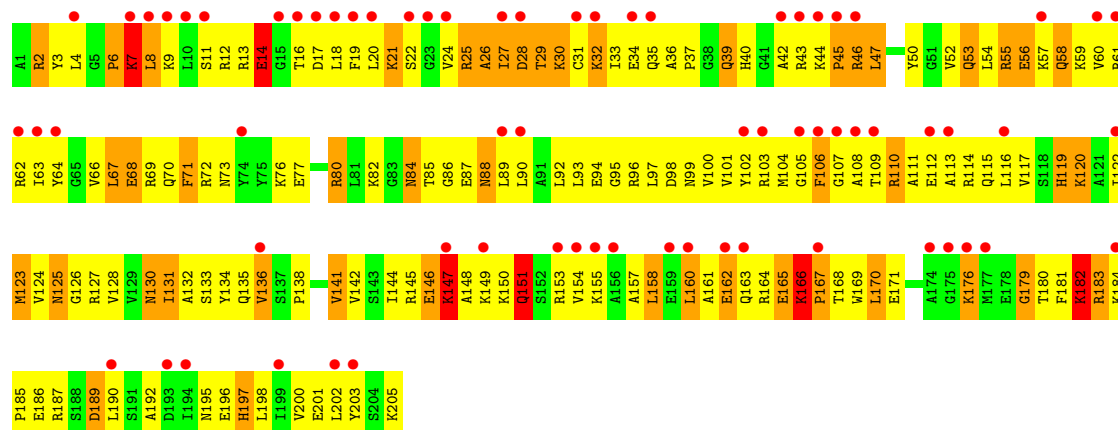
• Molecule 6: 30S ribosomal protein S4

Chain AD:



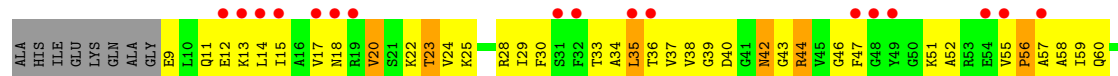
• Molecule 6: 30S ribosomal protein S4

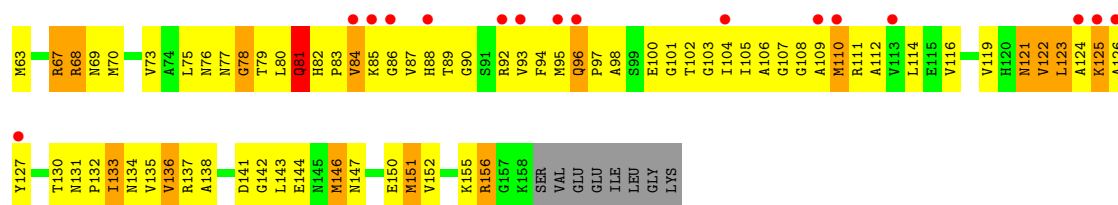
Chain CD:



• Molecule 7: 30S ribosomal protein S5

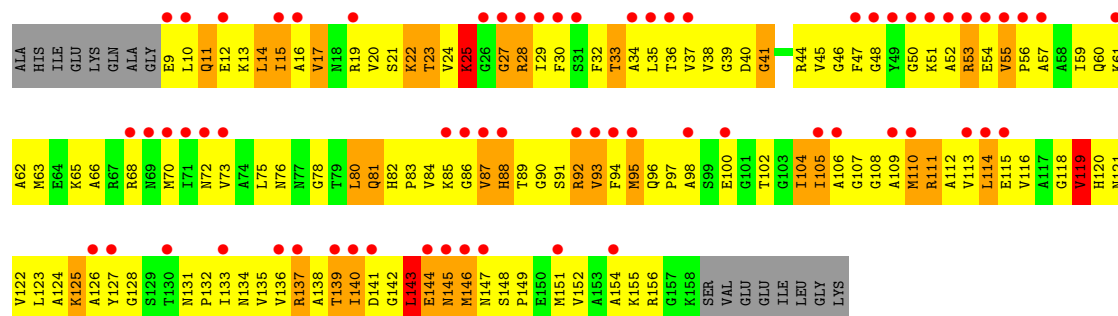
Chain AE:





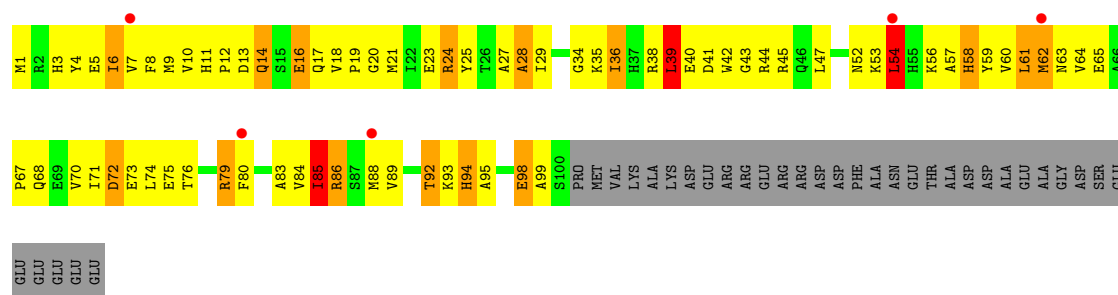
• Molecule 7: 30S ribosomal protein S5

Chain CE:



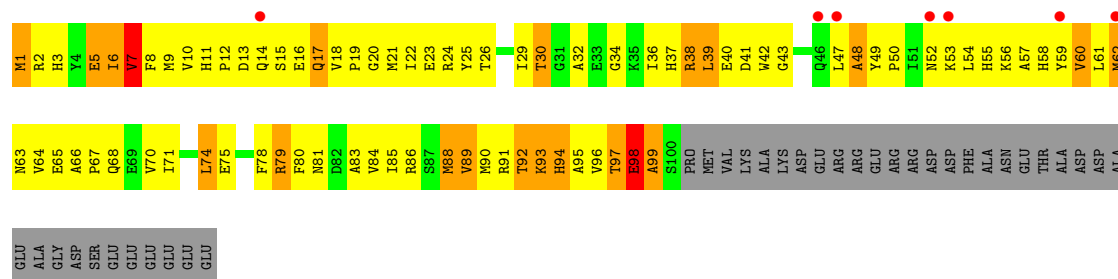
• Molecule 8: 30S ribosomal protein S6

Chain AF:



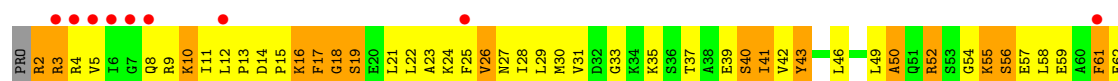
• Molecule 8: 30S ribosomal protein S6

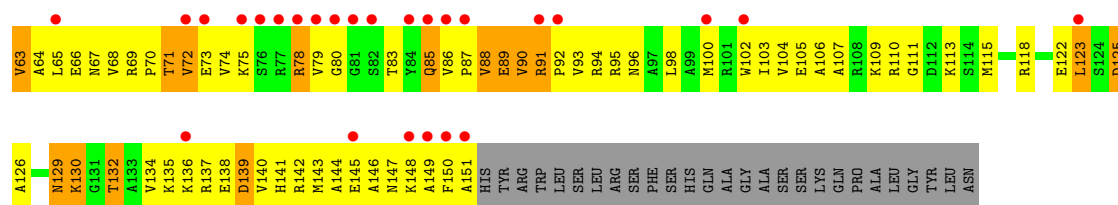
Chain CF:



• Molecule 9: 30S ribosomal protein S7

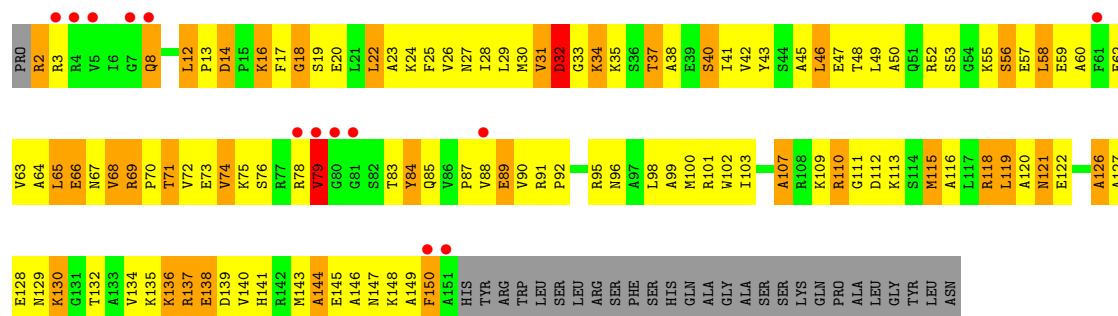
Chain AG:





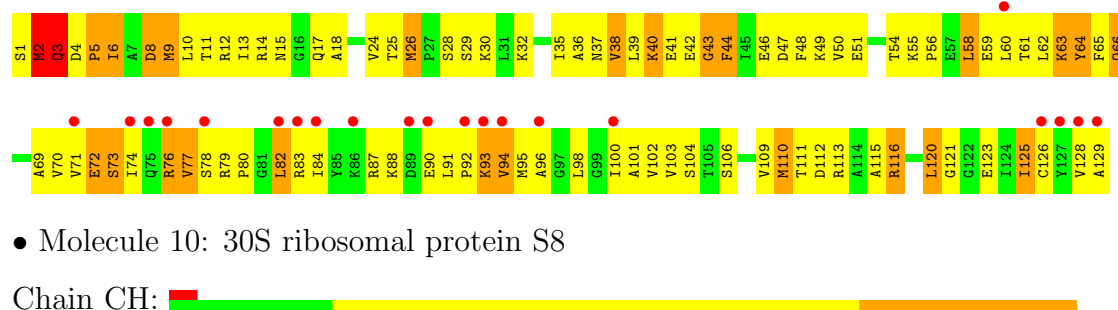
• Molecule 9: 30S ribosomal protein S7

Chain CG:



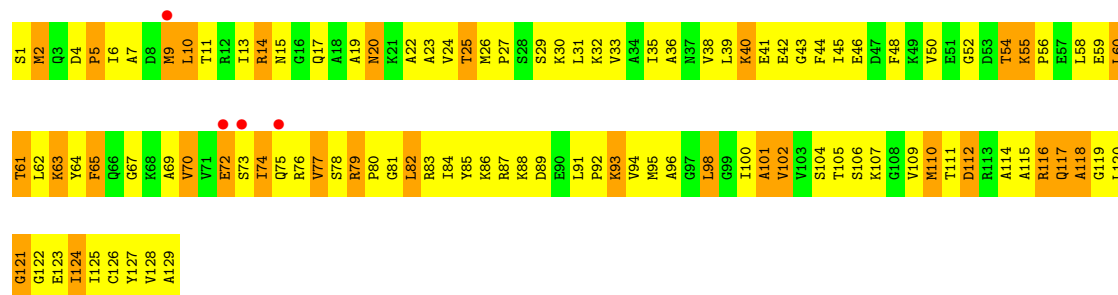
• Molecule 10: 30S ribosomal protein S8

Chain AH:



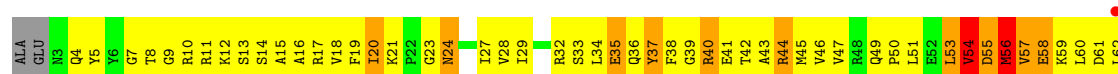
• Molecule 10: 30S ribosomal protein S8

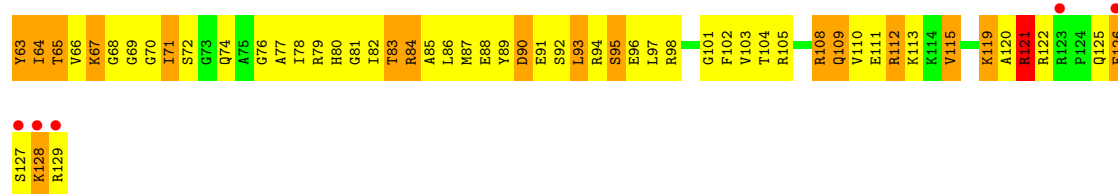
Chain CH:



• Molecule 11: 30S ribosomal protein S9

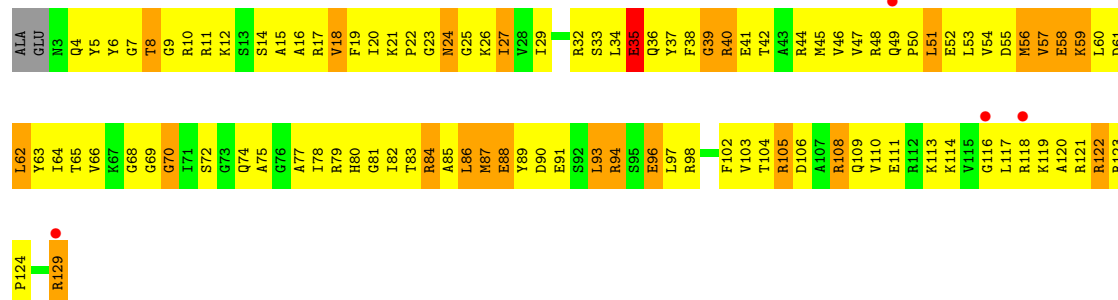
Chain AI:





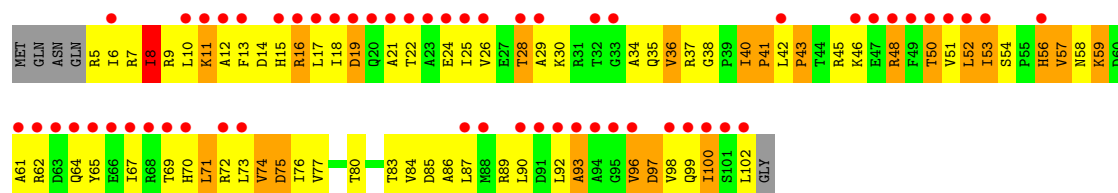
• Molecule 11: 30S ribosomal protein S9

Chain CI:



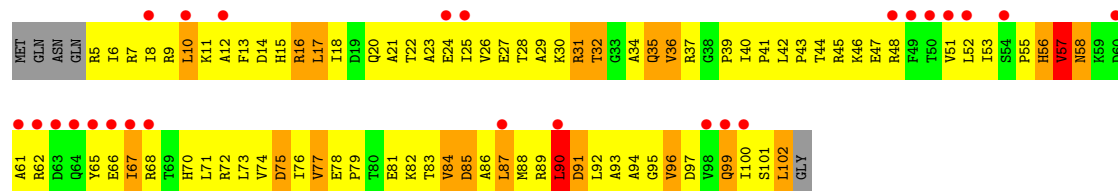
• Molecule 12: 30S ribosomal protein S10

Chain AJ:



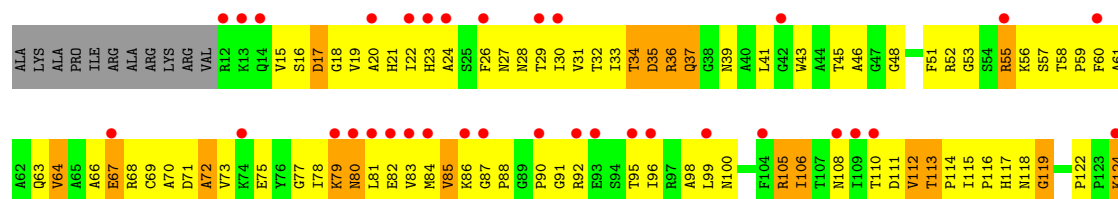
• Molecule 12: 30S ribosomal protein S10

Chain CJ:



• Molecule 13: 30S ribosomal protein S11

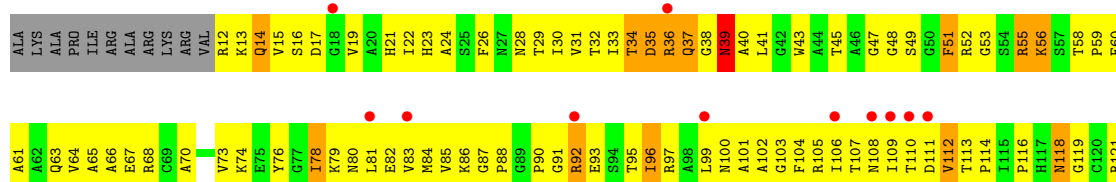
Chain AK:





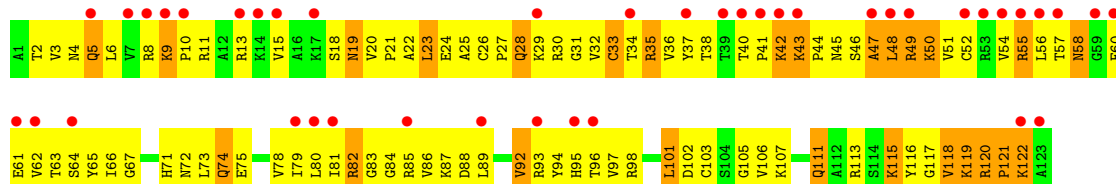
- Molecule 13: 30S ribosomal protein S11

Chain CK:



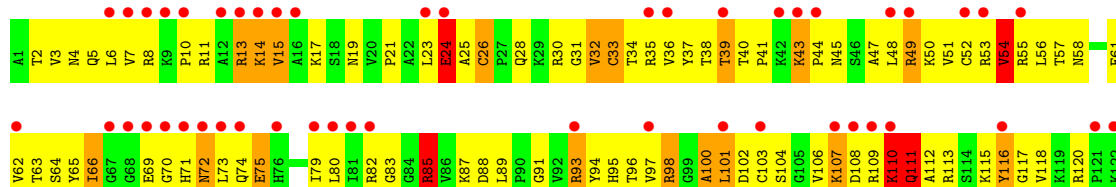
- Molecule 14: 30S ribosomal protein S12

Chain AL:



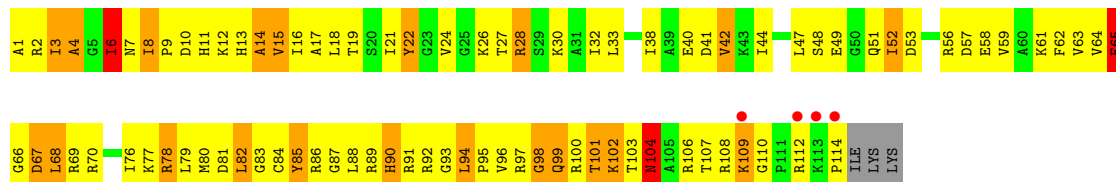
- Molecule 14: 30S ribosomal protein S12

Chain CL:



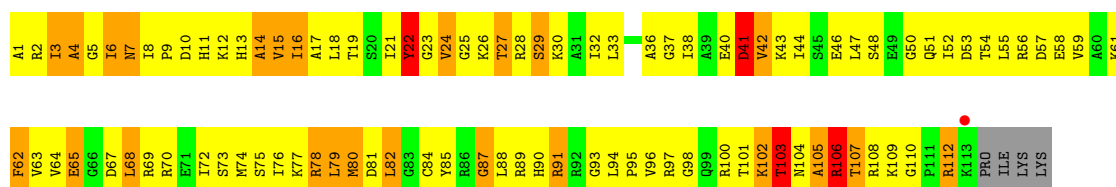
- Molecule 15: 30S ribosomal protein S13

Chain AM:



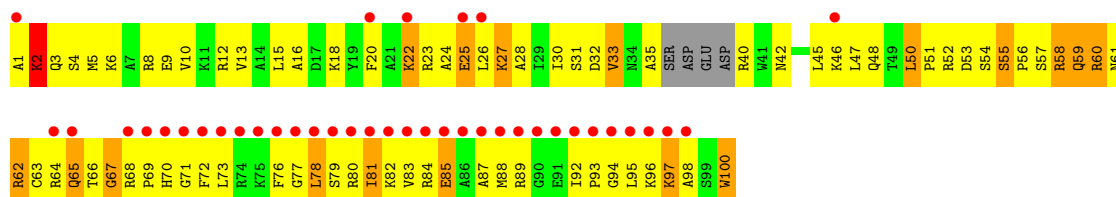
- Molecule 15: 30S ribosomal protein S13

Chain CM:



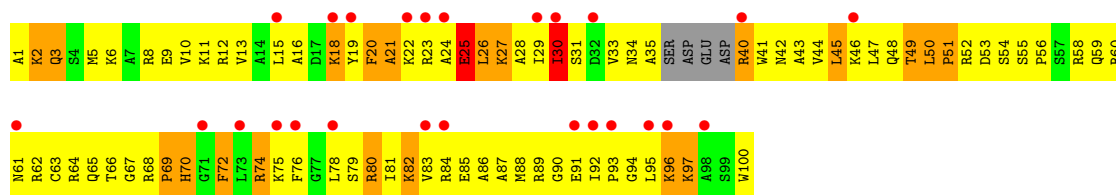
• Molecule 16: 30S ribosomal protein S14

Chain AN:



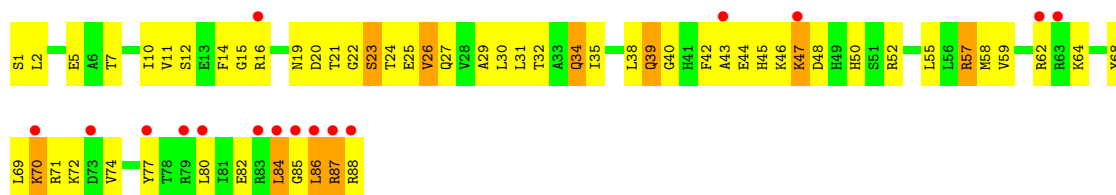
• Molecule 16: 30S ribosomal protein S14

Chain CN:



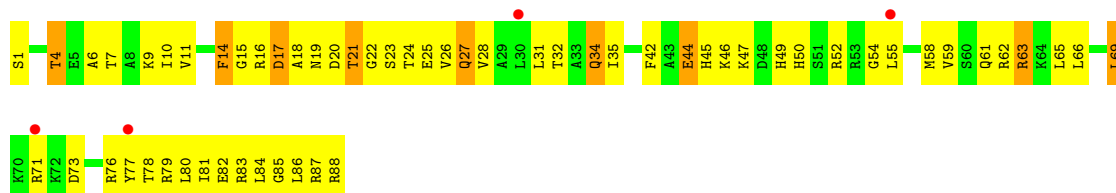
• Molecule 17: 30S ribosomal protein S15

Chain AO:



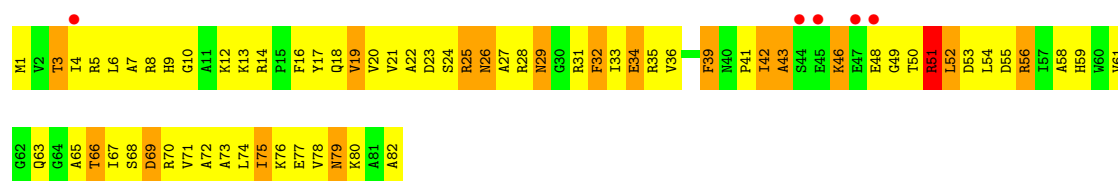
• Molecule 17: 30S ribosomal protein S15

Chain CO:



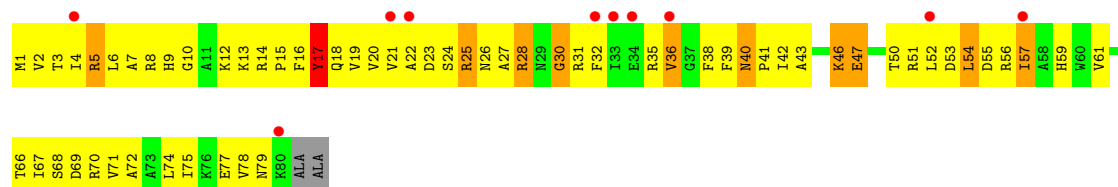
• Molecule 18: 30S ribosomal protein S16

Chain AP:



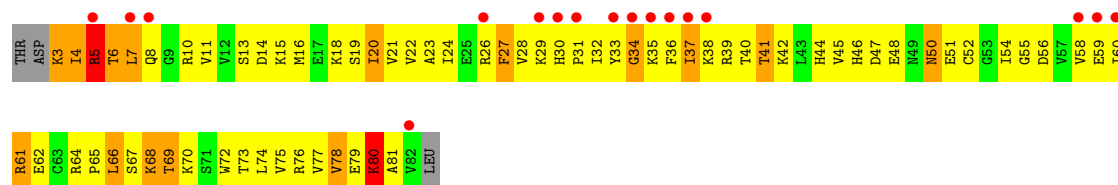
• Molecule 18: 30S ribosomal protein S16

Chain CP:



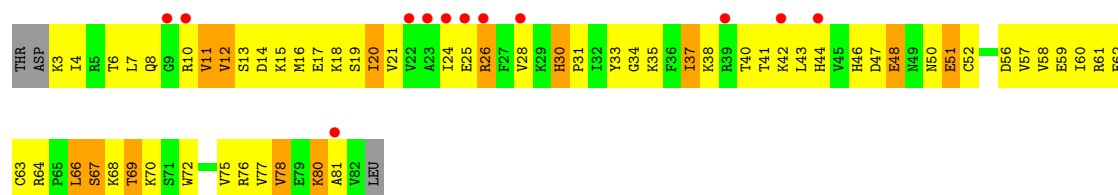
• Molecule 19: 30S ribosomal protein S17

Chain AQ:



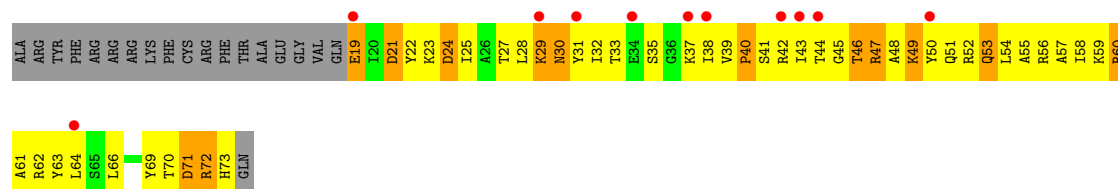
• Molecule 19: 30S ribosomal protein S17

Chain CQ:



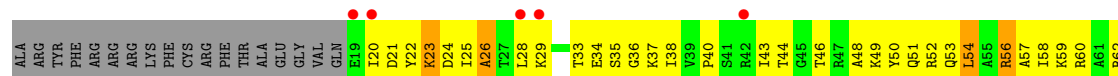
• Molecule 20: 30S ribosomal protein S18

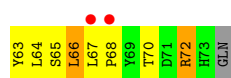
Chain AR:



• Molecule 20: 30S ribosomal protein S18

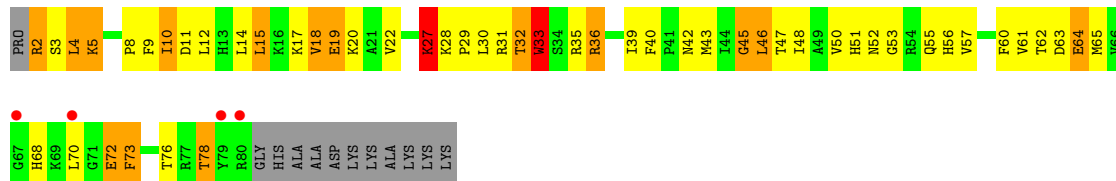
Chain CR:





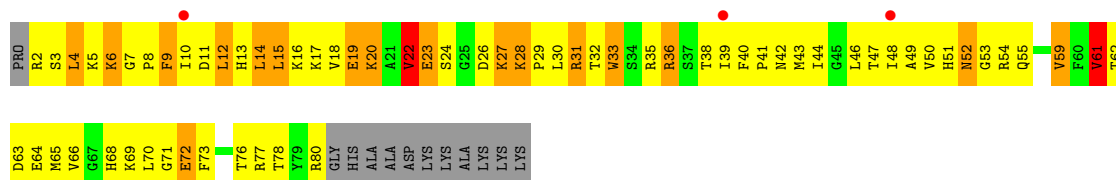
- Molecule 21: 30S ribosomal protein S19

Chain AS:



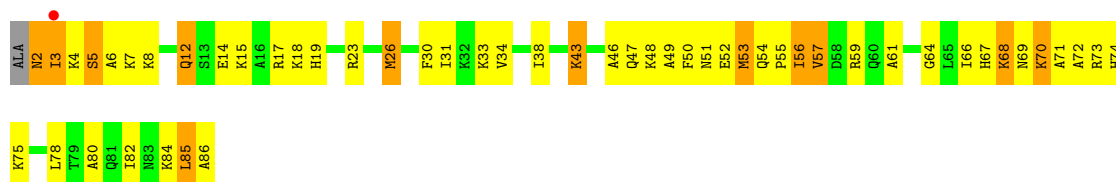
- Molecule 21: 30S ribosomal protein S19

Chain CS:



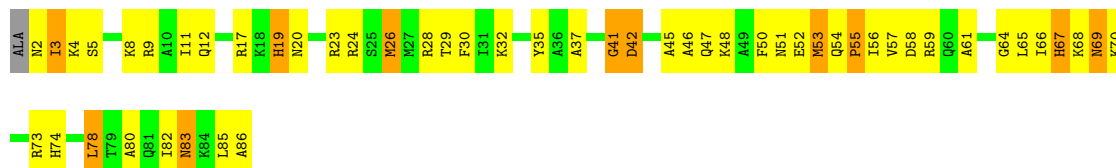
- Molecule 22: 30S ribosomal protein S20

Chain AT:



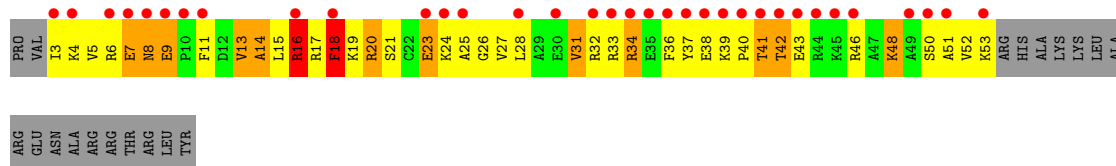
- Molecule 22: 30S ribosomal protein S20

Chain CT:



- Molecule 23: 30S ribosomal protein S21

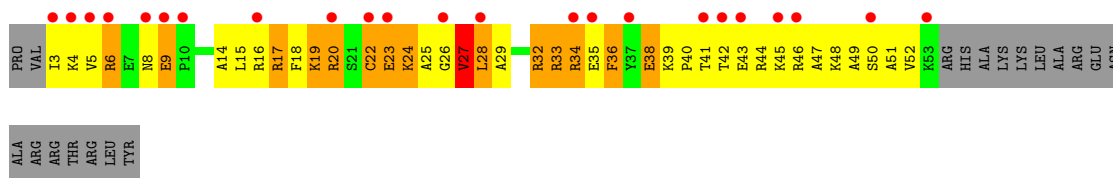
Chain AU:



- Molecule 23: 30S ribosomal protein S21

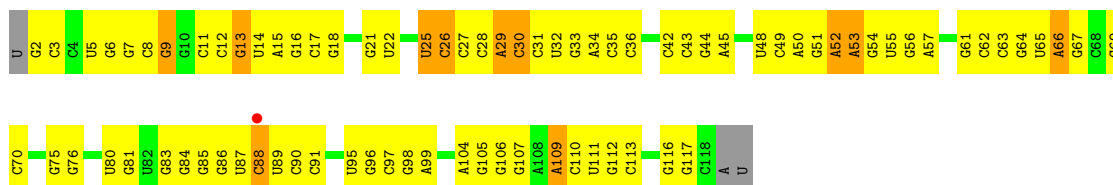


Chain CU:



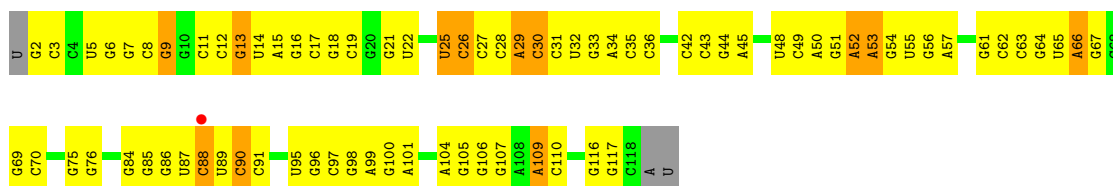
- Molecule 24: 5S ribosomal RNA

Chain BA:



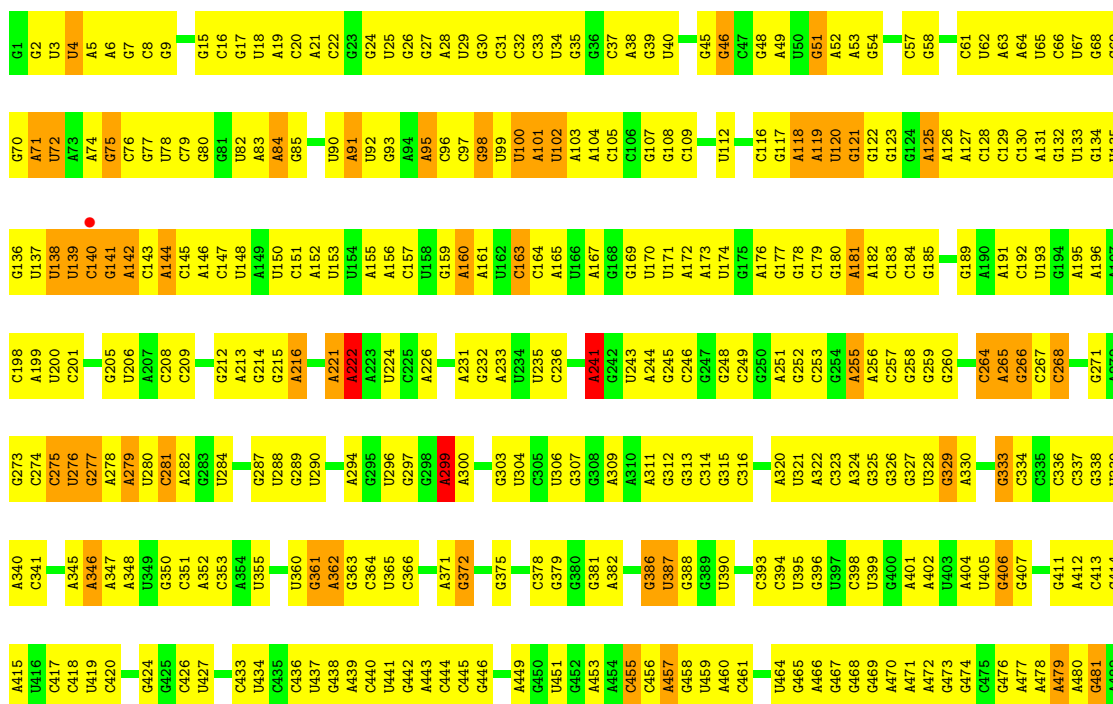
- Molecule 24: 5S ribosomal RNA

Chain DA:



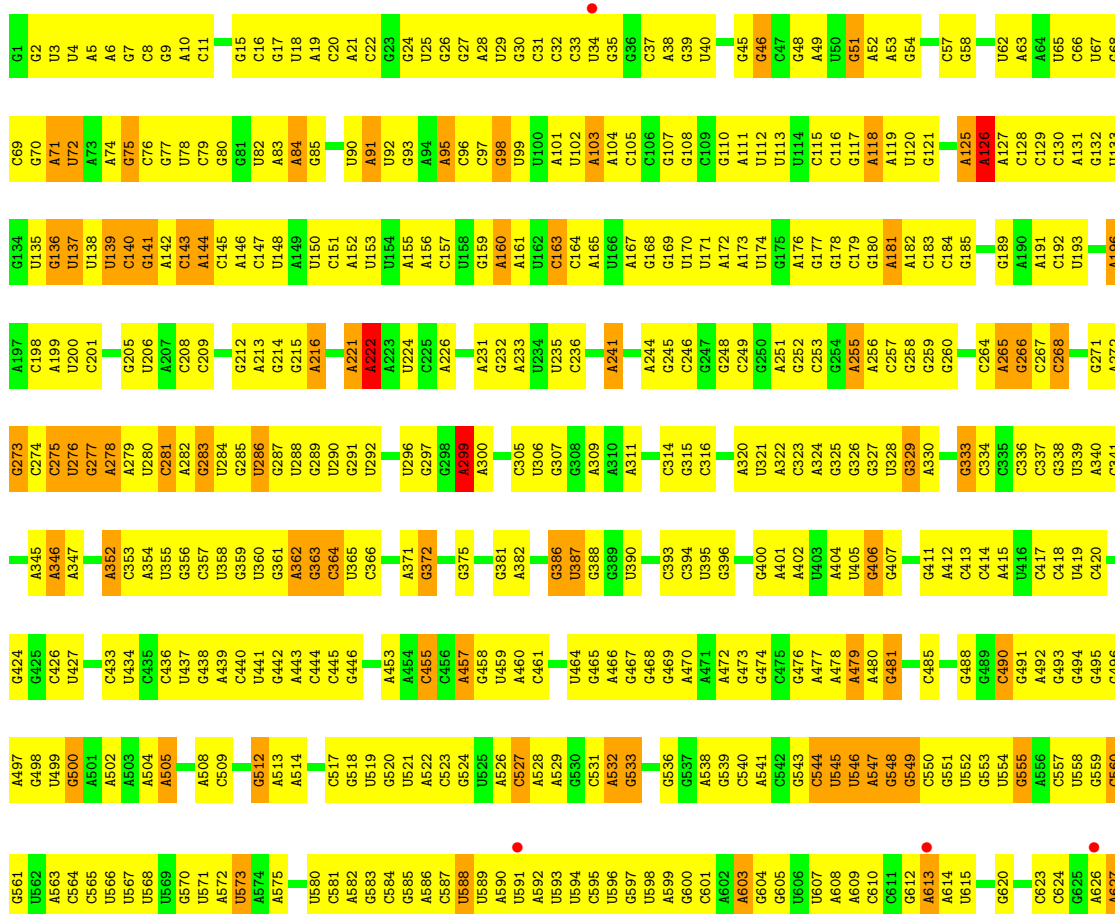
- Molecule 25: 23S ribosomal RNA

Chain BB:



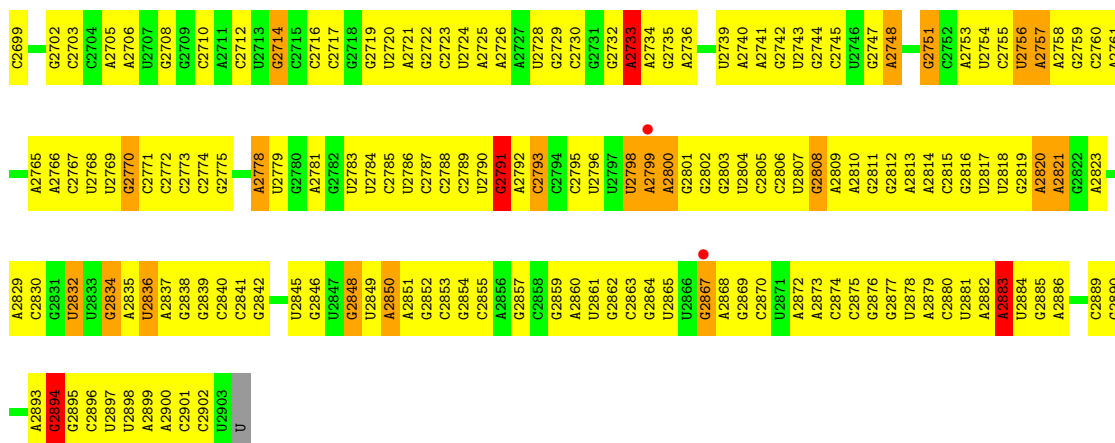
C1446	C1447	G1448	G1449	G1450	G1451	G1452	A1453	C1454	C1455	U1458	G1459	U1460	C1461	C1462	C1463	G1464	G1465	U1466	A1469	A1470	G1471	C1472	G1473	U1474	G1475	U1476	U1477	G1478	G1482	U1483	U1484	U1485	U1486	U1487	C1488	C1489	A1490	G1491	G1492	C1493	U1494	A1495	A1496	U1497	C1498	A1504	A1505	U1506	C1507	A1508	A1509	G1510	G1511	U1512			
G1374	U1379	G1380	G1381	G1382	A1383	A1384	A1385	C1386	A1387	U1394	A1395	U1396	U1397	C1398	C1399	U1400	G1401	U1402	A1403	A1404	U1405	U1406	G1407	U1408	U1409	G1410	U1411	U1412	A1413	U1414	G1415	G1416	C1417	G1418	A1419	U1420	G1421	U1426	A1427	C1428	G1429	A1430	G1432	A1433	A1434	U1437	U1438	U1439	U1440	U1442	U1443	U1444	U1445				
G1309	G1310	G1311	U1312	U1313	U1314	C1315	U1316	U1317	U1318	C1319	A1320	A1321	A1322	C1323	G1324	U1325	U1326	A1327	A1328	U1329	G1333	G1334	C1335	A1336	G1337	U1340	G1341	U1344	G1345	G1346	A1347	C1348	C1349	C1350	C1351	U1352	A1353	A1354	G1355	G1356	C1357	G1360	G1361	C1362	C1363	G1364	A1365	A1366	A1367	G1368	C1369	C1370	G1371	U1372			
G1238	G1239	U1240	A1241	U1242	C1243	A1244	G1245	U1248	U1249	G1250	A1253	A1254	U1255	G1256	C1257	U1258	G1259	A1260	U1266	U1267	U1268	A1269	C1270	G1271	U1272	U1273	A1274	U1275	C1276	G1279	G1280	G1281	U1282	G1283	A1284	A1285	A1286	A1287	C1289	C1290	C1291	G1292	C1293	G1296	C1297	G1300	A1301	A1302	C1306	A1307	U1308						
A1165	G1166	A1169	U1170	G1171	C1172	U1173	U1174	U1175	U1176	G1177	C1178	G1179	U1180	U1181	G1182	U1183	U1184	G1187	U1188	A1189	G1190	G1191	C1192	G1193	C1196	U1197	U1198	U1199	C1200	U1203	A1204	A1205	G1206	G1210	C1211	G1212	A1213	U1219	G1220	C1221	U1224	G1225	A1226	G1227	G1228	C1229	A1230	U1231	G1232	G1236	A1237						
A1098	G1099	C1100	U1101	C1104	U1105	G1106	G1107	U1108	C1109	U1110	A1111	G1112	G1115	G1116	C1117	C1118	U1119	G1120	C1121	G1125	A1126	A1127	U1130	G1131	U1132	A1133	A1134	C1135	G1136	G1137	G1138	A1139	C1140	U1141	A1142	A1143	A1144	C1145	C1146	A1147	U1148	G1149	C1150	A1151	C1152	C1153	A1156	G1157	C1158	U1159	G1160	G1163	C1164				
A1029	C1030	U1031	A1032	U1033	G1036	G1037	U1038	A1039	A1040	G1041	G1042	C1045	A1046	U1047	A1048	C1049	A1050	G1051	C1052	A1053	A1054	G1055	G1056	U1057	U1058	G1059	U1060	U1061	G1062	G1063	C1064	U1065	G1068	A1069	U1070	C1071	C1072	C1076	A1077	A1080	U1081	U1082	U1083	A1084	A1085	A1086	U1087	A1088	A1089	A1090	G1091	C1092	U1097				
G950	C956	U957	U958	A959	A960	C961	G962	C963	C964	U967	C968	G969	U970	A973	G974	A981	C982	A983	C986	C987	A988	G989	A990	C991	C992	C995	A996	G997	C998	U999	A1000	A1001	C1005	A1010	G1011	U1012	C1013	A1014	U1015	G1016	C1017	U1018	U1019	A1020	A1021	G1022	U1023	G1024	G1025	A1028							
C817	G818	A819	A820	A821	G822	C823	U824	A825	U826	U827	U828	U832	A833	G834	C835	G836	C837	C838	U839	G840	G841	U842	A845	U846	U847	C848	U849	U850	C851	U852	A853	G854	G855	G856	G857	G858	U859	U860	A863	G864	C865	G869	U870	U871	U872	C873	G874	C875	A877	A878	G	G	G	C816			
U746	U747	G748	A749	A752	U753	U754	U755	U756	G757	U762	G763	G765	U766	U767	G768	U769	G770	G771	C772	U773	G774	G775	G776	G777	U778	U779	G780	A781	U782	A783	G784	G785	A788	U789	U790	C791	A794	C795	G796	G797	U803	A804	G805	G806	G807	U810	U811	C812	U813	C814	C815	C816					
C610	C611	G612	A613	A614	U615	A616	G620	C623	C624	G625	A626	A627	G628	G629	C630	C631	A632	A633	C634	C635	G636	A637	G638	C640	A643	A644	C645	U646	G647	G648	G649	C650	G651	U652	U653	A654	A655	G656	U657	U658	G659	C660	A661	G664	U665	A666	U667	A668	A603	G669	G670	G605	U686	U607	C672	C673	G674
A483	C484	C485	G488	G489	C490	G491	A492	C493	G494	G495	G496	A497	U498	U499	C500	A501	A502	A503	A504	A505	A508	C509	G512	A513	A514	C517	G518	U519	G520	U521	A522	G523	G524	U525	U526	C527	A528	U529	G530	C531	A532	G533	U534	G535	A538	G539	C540	A541	C542	G543	C544	U545	U546	A547			

G2472	A2406	A2336	A2273	C2207	C2146	C2084	C2021	U1946	G1875	A1809	G1743	A1669	A1583	G1514
C2475	A2407	G2337	A2274	C2208	A2147	U2085	U2022	C1947	G1878	A1810	A1744	G1874	U1584	A1515
A2476	U2408	C2338	A2278	G2209	U2148	U2086	G2023	G1948	C1879	U1811	A1745	A1585	C1586	G1516
U2477	G2410	C2339	G2279	U2210	U2149	G2087	G2024	G1949	U1880	U1812	A1746	A1586	A1587	G1517
A2478	G2411	A2341	G2280	A2212	C2150	A2088	C2025	U1955	U1881	G1813	U1747	A1590	U1523	U1523
U2479	A2412	C2342	A2281	U2213	U2151	U2096	U2026	U1956	U1882	A1814	C1748	A1591	G1524	G1524
C2480	G2413	G2345	G2282	C2215	G2152	C2091	G2027	C1957	U1883	A1815	A1749	U1880	A1592	A1525
G2481	G2414	C2346	G2283	C2216	C2153	U2092	U2028	C1958	G1884	C1816	G1750	G1881	C1592	A1526
G2485	G2415	A2347	C2284	G2217	U2155	G2093	G2029	G1959	A1885	U1818	G1682	G1882	A1593	G1527
G2486	C2416	U2348	G2285	G2218	G2156	A2094	A2030	A1960	U1886	U1819	G1684	G1883	U1594	U1594
C2487	G2417	G2349	G2286	U2219	G2157	C2095	G2031	C1961	C1887	U1820	C1754	G1884	C1595	A1532
G2488	A2418	A2352	G2287	U2220	A	C2096	A2032	C1962	U1888	G1821	G1756	C1885	C1533	C1533
U2489	U2419	C2353	A2288	G2221	G	U2097	U2034	U1963	A1889	C1822	A1757	G1887	U1534	U1534
U2490	U2420	G2354	G2289	C2222	C	U2098	G2035	G1964	A1890	G1823	U1758	U1888	A1535	A1535
U2491	U2421	C2355	U2291	G2223	C	U2099	G2036	C1965	C1891	U1824	U1759	U1889	C1536	C1536
U2492	A2425	U2356	U2292	G2224	G	A2101	A2037	A1966	C1892	U1825	C1760	A1890	G1537	G1537
U2493	A2426	U2357	G2293	A2225	C	C2102	G2038	C1967	C1893	G1826	C1761	C1691	G1538	G1538
C2498	C2427	G2359	G2294	G2228	C	C2103	U2039	G1968	C1894	U1827	A1762	A1608	U1539	U1539
C2499	G2428	U2360	G2295	U2229	U	C2104	G2040	A1969	G1895	G1828	G1763	A1609	G1540	G1540
U2500	A2429	G2361	U2296	G2230	A	U2105	U2041	A1970	U1896	U1829	C1764	A1610	U1542	U1542
C2501	G2430	C2362	A2297	U2231	G	U2106	A2042	U1971	G1897	C1830	U1765	A1616	G1543	G1543
G2502	U2431	G2363	U2298	C2232	A	G2107	C2043	G1972	U1898	C1833	G1766	A1700	A1544	A1544
A2503	U2432	C2364	U2299	U2233	A	U2108	C2044	G1973	A1899	U1834	G1767	C1704	A1545	A1545
U2504	A2434	G2365	C2300	G2234	A	G2110	G2046	C1974	G1902	C1837	A1773	A1705	G1546	G1546
U2505	U2435	A2366	G2301	G2235	U	U	G2047	A1981	G1903	C1838	C1774	A1623	C1547	C1547
U2506	G2436	G2367	C2302	U2236	A	G	G2048	C1985	G1904	G1839	U1775	U1709	U1624	U1624
C2507	U2437	C2368	U2305	G2238	C	U	G2049	C1986	C1905	U1842	G1776	C1625	A1548	A1548
G2508	U2438	A2369	C2306	U2240	C	A	C2051	C1987	G1906	U1843	U1777	A1711	A1549	A1549
U2511	C2440	G2370	G2307	A2241	C	G	A2052	A1988	C1907	G1842	U1778	U1712	C1550	C1550
U2512	U2441	C2373	U2308	G2242	C	A	C2055	U1991	C1908	C1843	U1779	A1713	A1551	A1551
C2513	C2442	C2374	C2309	U2243	U	U	G2056	G1992	C1909	G1844	U1780	U1714	A1552	A1552
U2514	G2443	A2377	C2310	U2244	U	A	G2057	U1993	A1913	G1845	U1781	G1715	A1553	A1553
C2515	G2444	U2378	U2312	U2245	U	G	G2058	C1994	C1914	U1847	A1783	A1717	C1556	C1556
A2516	G2445	C2379	C2313	G2246	U	G	U2059	U1995	U1915	A1848	A1784	A1640	C1557	C1557
C2517	G2446	C2380	A2314	G2247	A2183	U	A2060	C1996	G1921	G1849	U1785	U1720	C1558	C1558
A2518	U2447	A2381	G2315	U2248	A2184	G	G2061	C1997	U1922	U1850	A1786	G1721	U1559	U1559
U2519	U2448	G2382	G2316	U2249	U2185	G	A2062	A1998	U1923	A1853	A1787	A1722	G1561	G1561
C2520	G2449	C2383	A2317	G2250	U2186	A	C2063	C1999	C1924	U1854	G1788	G1723	U1562	U1562
C2521	U2450	U2384	G2318	G2253	U2187	G	C2064	C2000	U1925	U1855	A1789	G1724	U1563	U1563
U2522	G2455	C2385	G2319	G2254	U2188	G	C2065	C2001	U1926	U1856	A1790	U1725	C1564	C1564
G2523	C2456	A2386	U2320	U2257	G2190	C	C2066	G2002	A1927	G1857	C1726	U1643	G1567	G1567
U2524	U2457	U2387	U2321	C2258	U2191	U	G2069	A2003	A1928	A1858	C1727	C1728	G1568	G1568
G2529	G2458	G2391	A2322	U2259	U2192	U	C2070	C2008	G1929	C1795	U1729	A1654	A1569	A1569
A2530	U2460	C2392	U2323	C2260	G2193	U	A2071	A2009	G1930	U1796	C1730	A1655	A1570	A1570
U2531	A2461	U2393	G2325	C2261	U2194	G	C2072	G2010	U1931	G1863	C1731	C1656	A1571	A1571
G2532	C2462	C2394	G2326	U2262	U2195	A2134	U2073	U2011	G1935	U1864	U1798	U1657	A1572	A1572
U2533	G2463	C2395	C2327	C2263	U2196	G2135	C2074	G2012	U1865	U1866	G1799	C1658	G1573	G1573
A2534	C2464	A2396	U2328	G2264	C2197	U	U2075	A2013	A1937	C1867	C1800	G1659	C1574	C1574
G2535	C2465	C2396	C2329	A2266	U2198	U2139	U2076	A2014	C1868	C1867	A1801	G1660	C1575	C1575
U2536	G2466	G2400	A2330	C2267	C2200	G2140	A2077	A2015	A1938	C1869	A1802	U1736	U1576	U1576
G2537	C2467	U2401	G2331	A2268	C2201	G2141	C2078	U2016	U1939	C1870	A1803	G1737	C1577	C1577
C2538	U2468	U2402	C2332	G2269	U2203	A2142	U2079	U2017	U1940	C1871	A1805	A1738	U1578	U1578
C2539	G2469	U2403	U2333	A2270	G2204	G2143	U2079	G2018	U1943	A1872	C1806	A1739	A1579	A1579
C2540	U2470	U2404	U2334	G2271	A2205	C2144	A2082	A2019	U1944	C1873	G1807	G1740	A1580	A1580
	A2471	G2405	U2335	U2272	C2206	C2145	G2083	A2020	G1945	C1874	A1808	U1742	G1581	G1581
													G1582	G1582



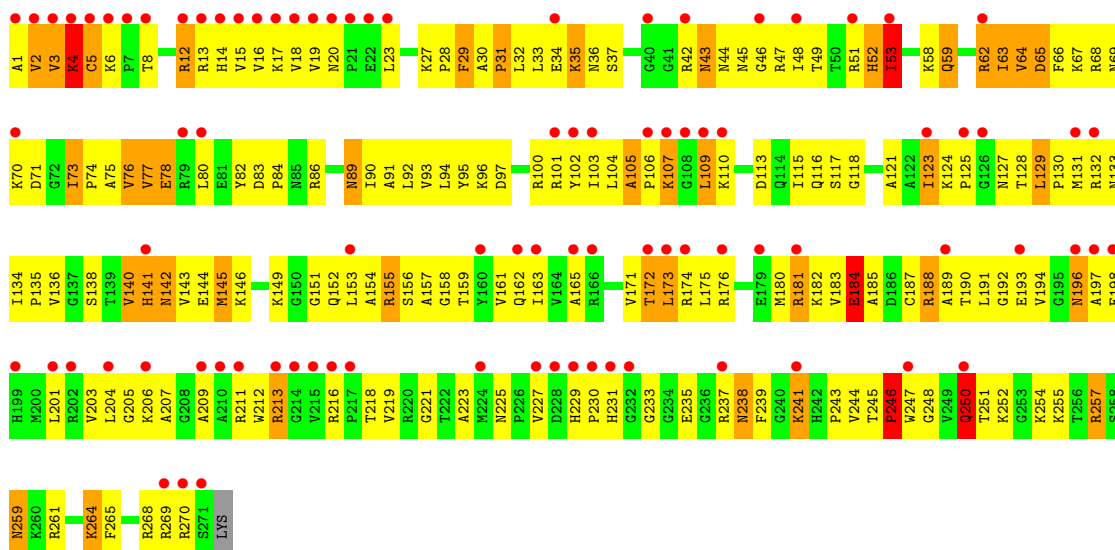
WORLDWIDE  
 **PDB**  
PROTEIN DATA BANK

WORLDWIDE  
PDB  
PROTEIN DATA BANK



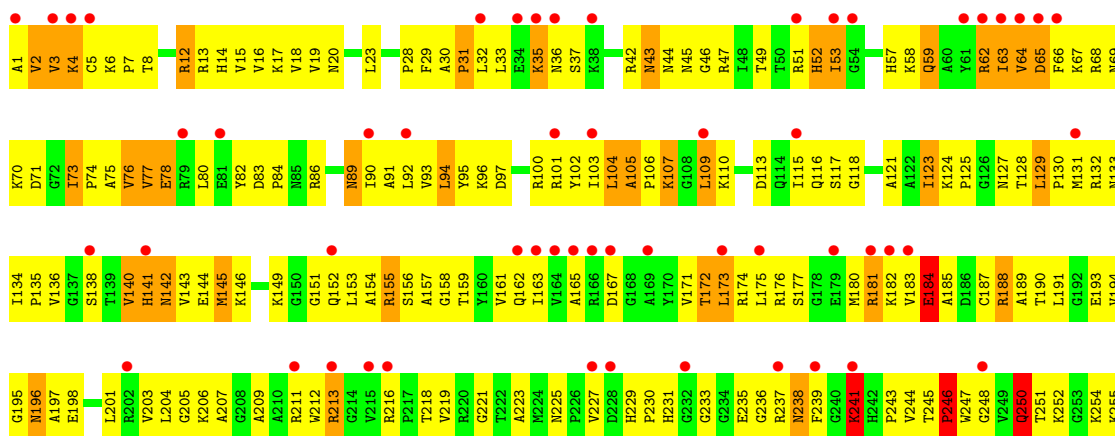
• Molecule 26: 50S ribosomal protein L2

Chain BC:



• Molecule 26: 50S ribosomal protein L2

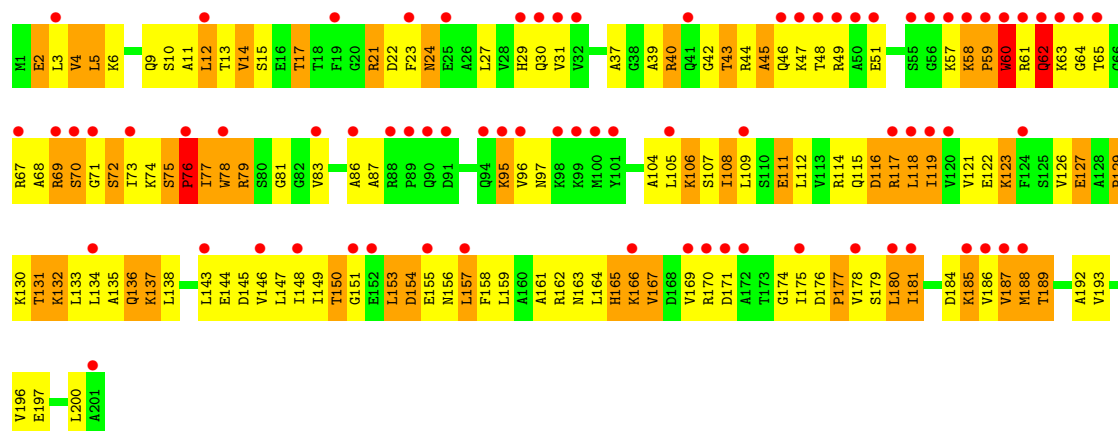
Chain DC:





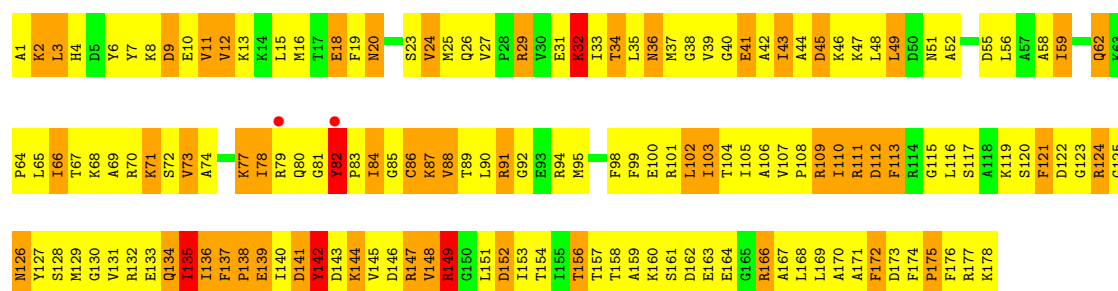


Chain DE:



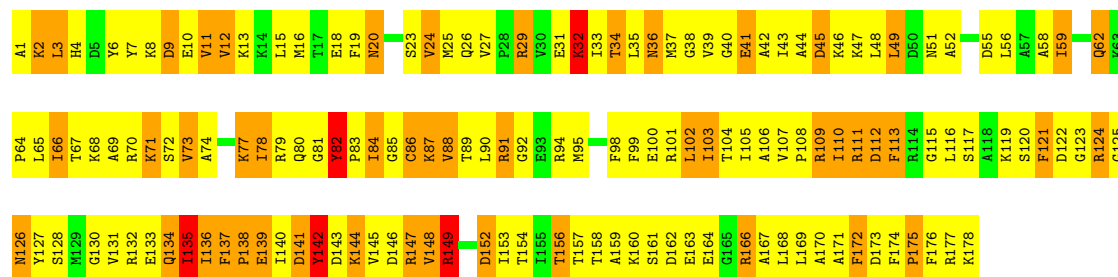
- Molecule 29: 50S ribosomal protein L5

Chain BF:



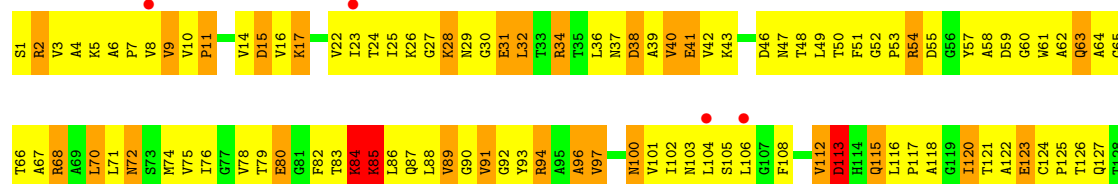
- Molecule 29: 50S ribosomal protein L5

Chain DF:



- Molecule 30: 50S ribosomal protein L6

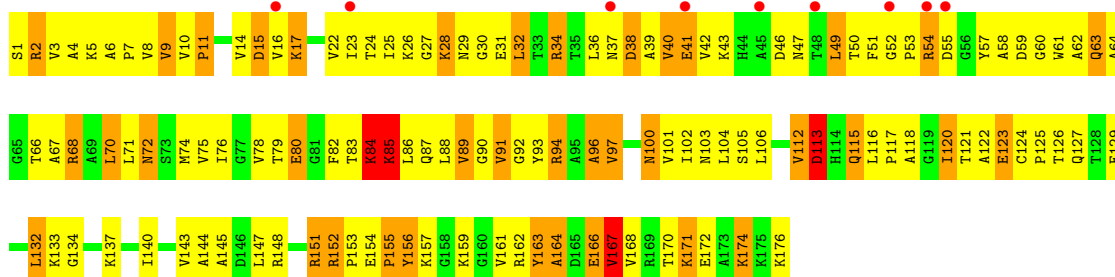
Chain BG:





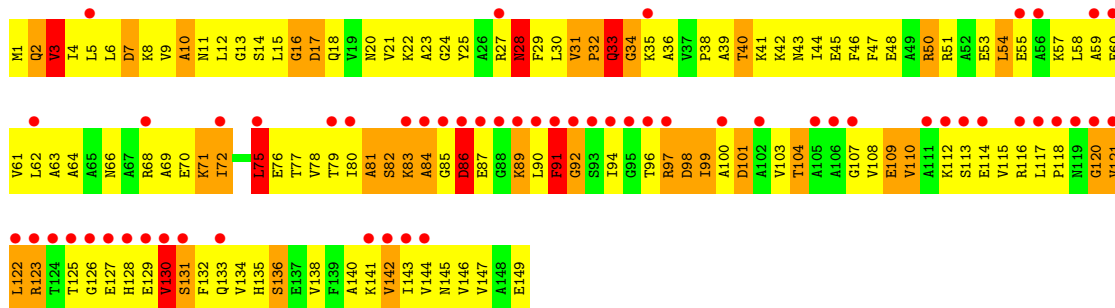
- Molecule 30: 50S ribosomal protein L6

Chain DG:



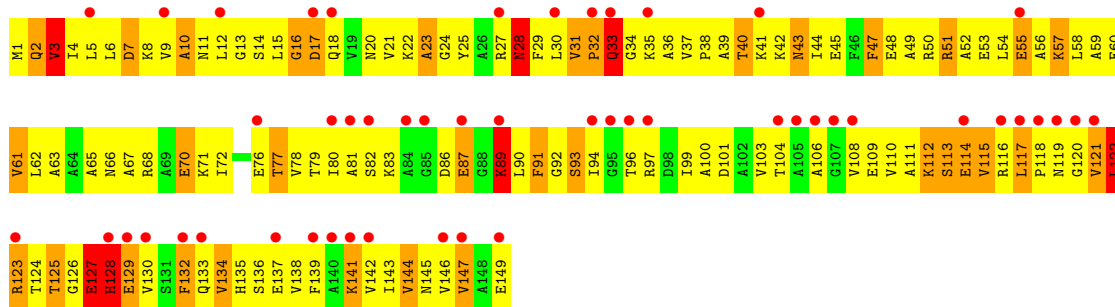
- Molecule 31: 50S ribosomal protein L9

Chain BH:



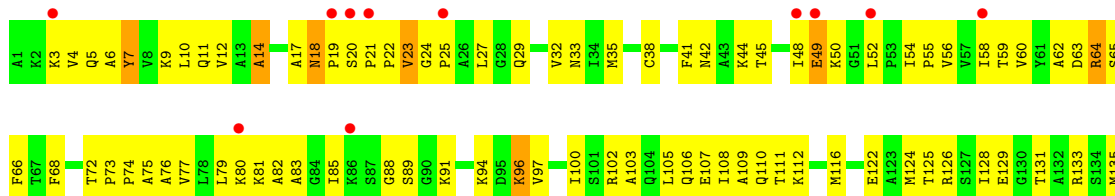
- Molecule 31: 50S ribosomal protein L9

Chain DH:



- Molecule 32: 50S ribosomal protein L11

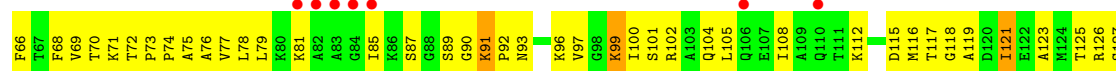
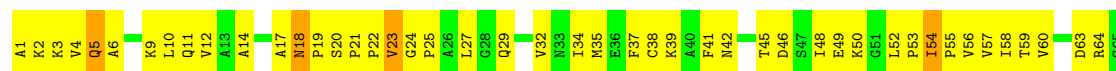
Chain BI:





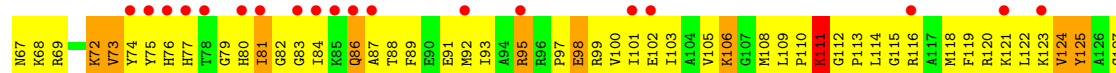
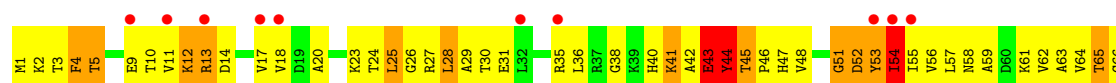
- Molecule 32: 50S ribosomal protein L11

Chain DI:



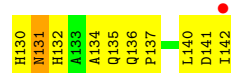
- Molecule 33: 50S ribosomal protein L13

Chain BJ:



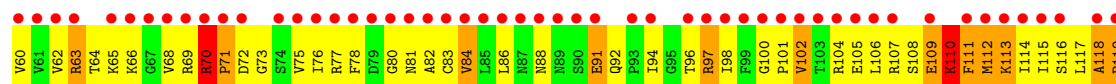
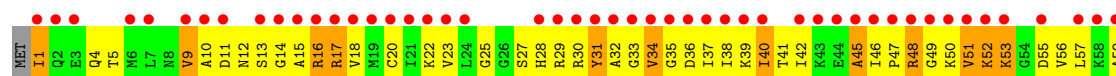
- Molecule 33: 50S ribosomal protein L13

Chain DJ:



- Molecule 34: 50S ribosomal protein L14

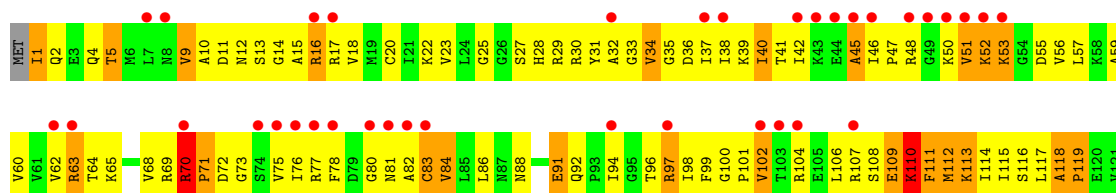
Chain BK:





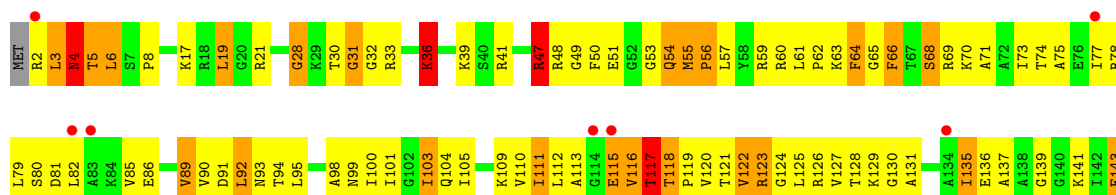
- Molecule 34: 50S ribosomal protein L14

Chain DK:



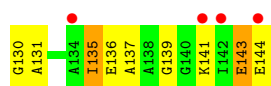
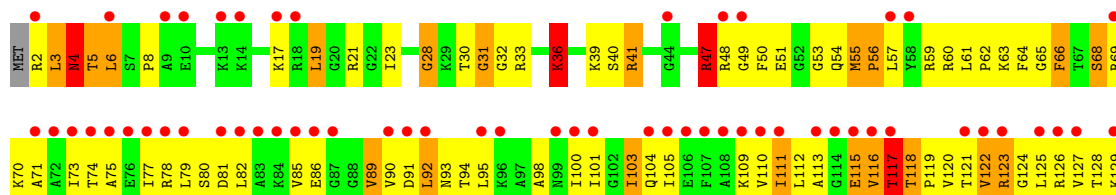
- Molecule 35: 50S ribosomal protein L15

Chain BL:



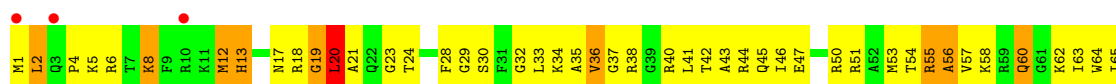
- Molecule 35: 50S ribosomal protein L15

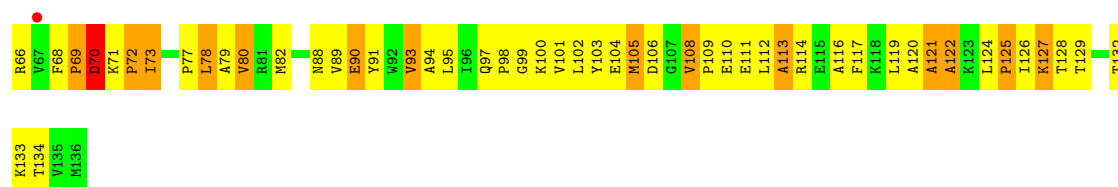
Chain DL:



- Molecule 36: 50S ribosomal protein L16

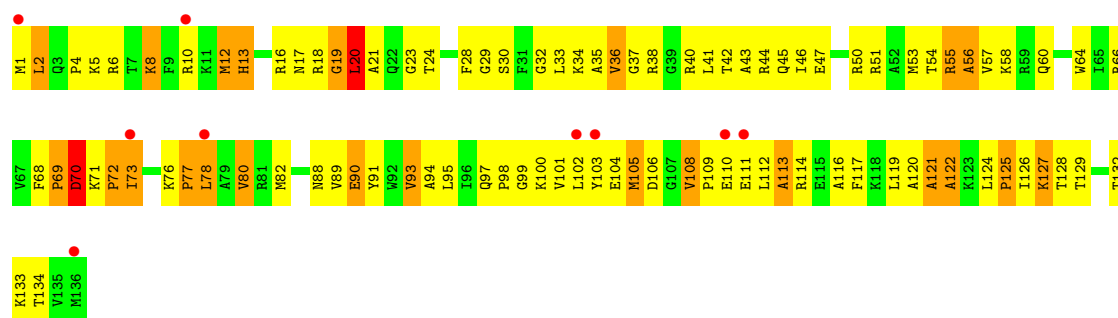
Chain BM:





• Molecule 36: 50S ribosomal protein L16

Chain DM:



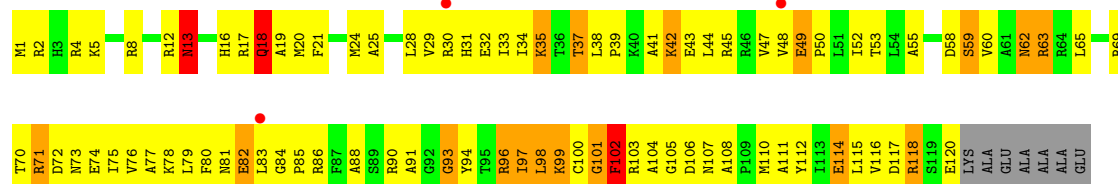
• Molecule 37: 50S ribosomal protein L17

Chain BN:



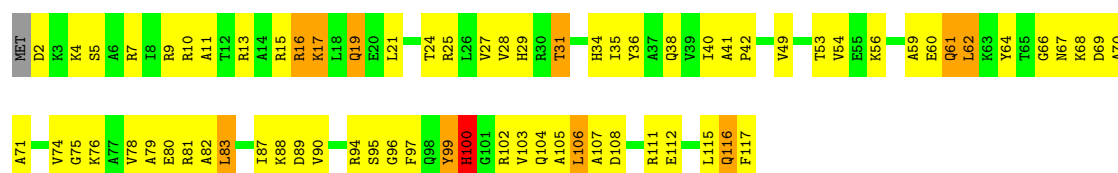
• Molecule 37: 50S ribosomal protein L17

Chain DN:



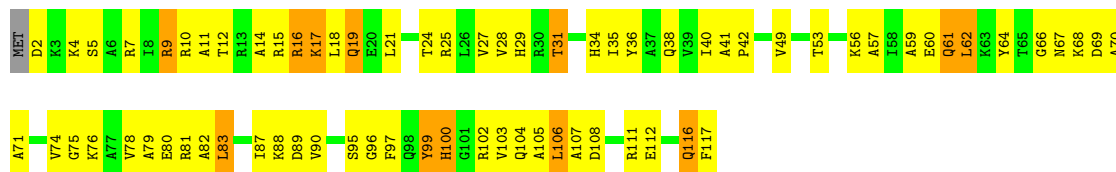
• Molecule 38: 50S ribosomal protein L18

Chain BO:



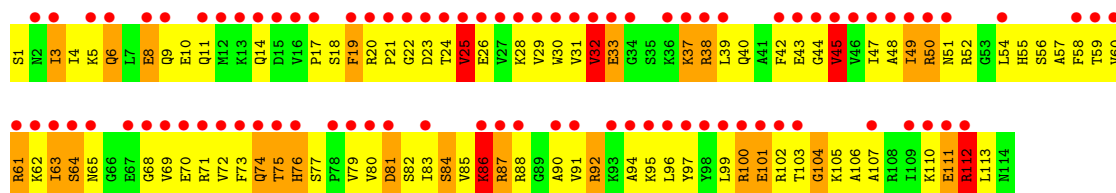
- Molecule 38: 50S ribosomal protein L18

Chain DO:



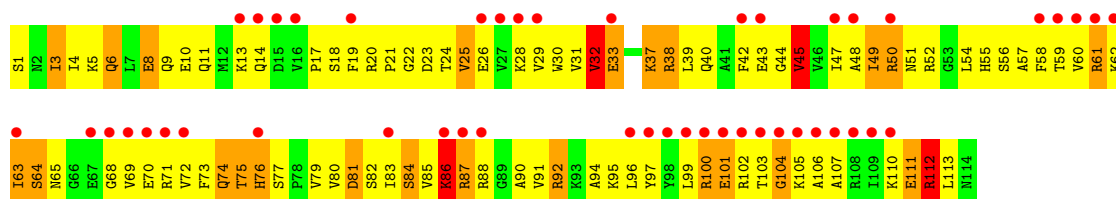
- Molecule 39: 50S ribosomal protein L19

Chain BP:



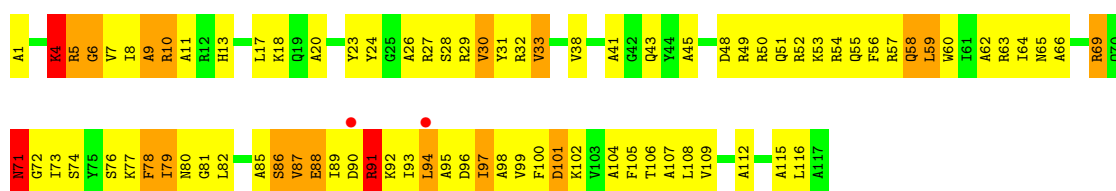
- Molecule 39: 50S ribosomal protein L19

Chain DP:



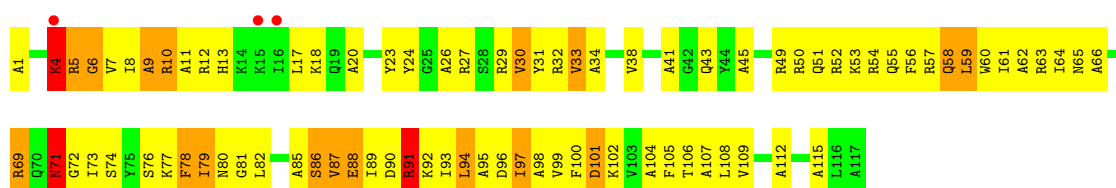
- Molecule 40: 50S ribosomal protein L20

Chain BQ:



- Molecule 40: 50S ribosomal protein L20

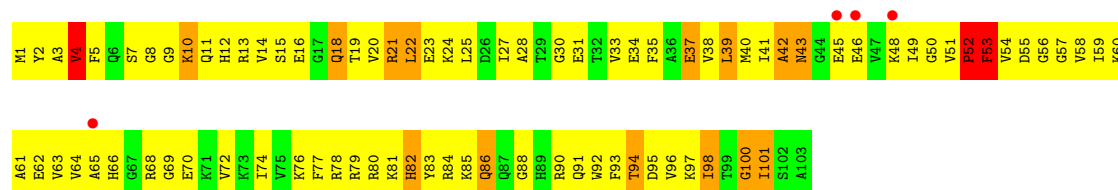
Chain DQ:



- Molecule 41: 50S ribosomal protein L21

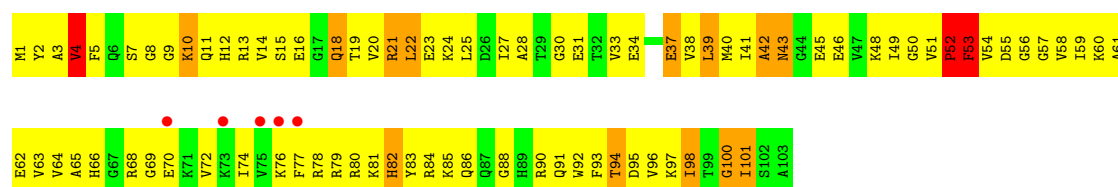
Chain BR:





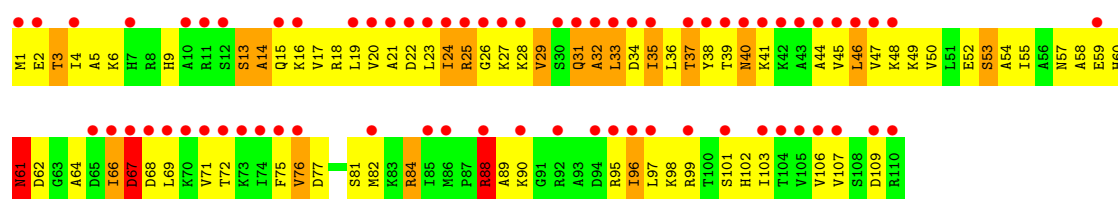
• Molecule 41: 50S ribosomal protein L21

Chain DR:



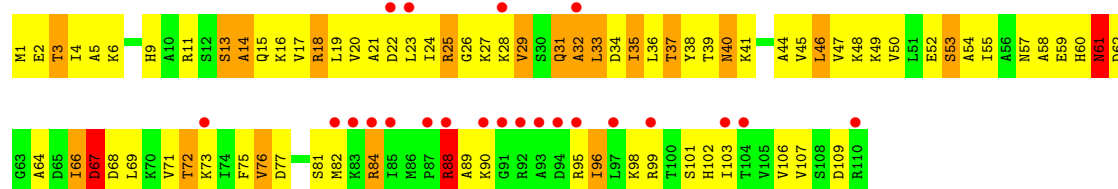
• Molecule 42: 50S ribosomal protein L22

Chain BS:



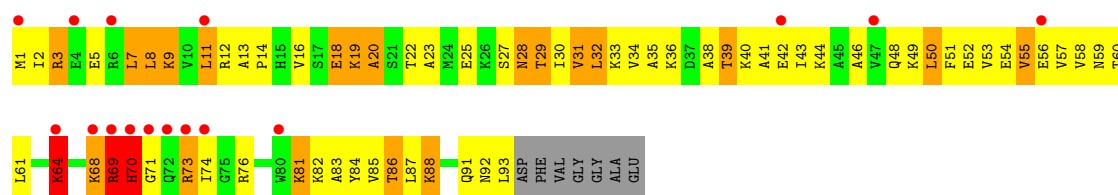
• Molecule 42: 50S ribosomal protein L22

Chain DS:



• Molecule 43: 50S ribosomal protein L23

Chain BT:



• Molecule 43: 50S ribosomal protein L23

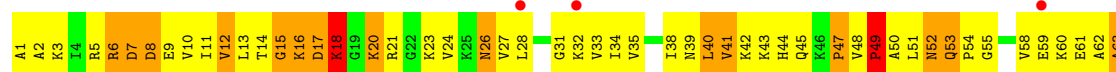
Chain DT:





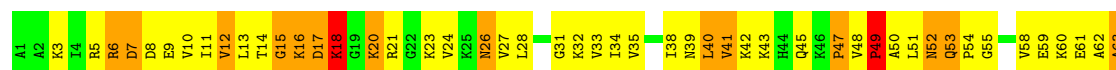
• Molecule 44: 50S ribosomal protein L24

Chain BU:



• Molecule 44: 50S ribosomal protein L24

Chain DU:



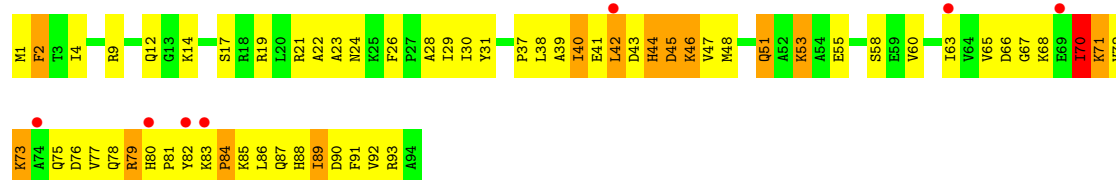
• Molecule 45: 50S ribosomal protein L25

Chain BV:



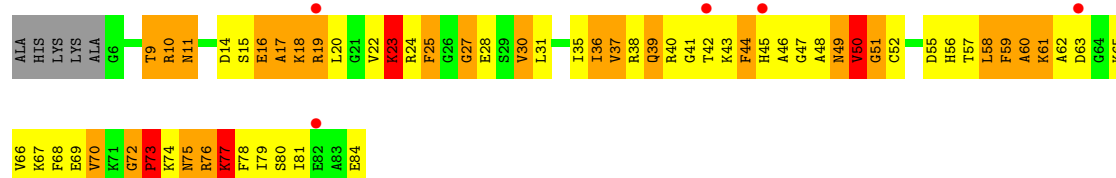
• Molecule 45: 50S ribosomal protein L25

Chain DV:



• Molecule 46: 50S ribosomal protein L27

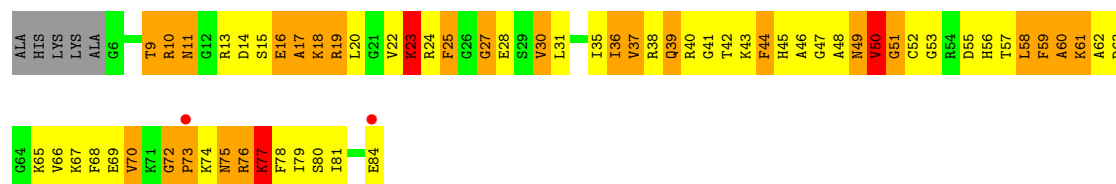
Chain BW:





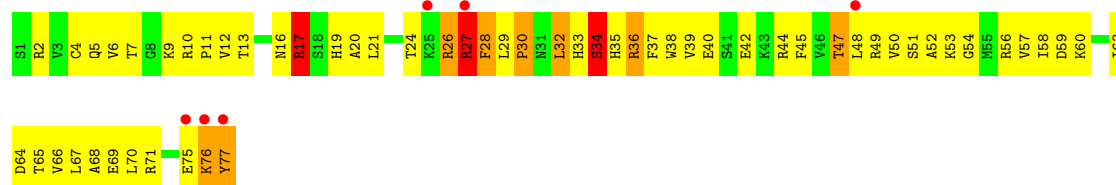
- Molecule 46: 50S ribosomal protein L27

Chain DW:



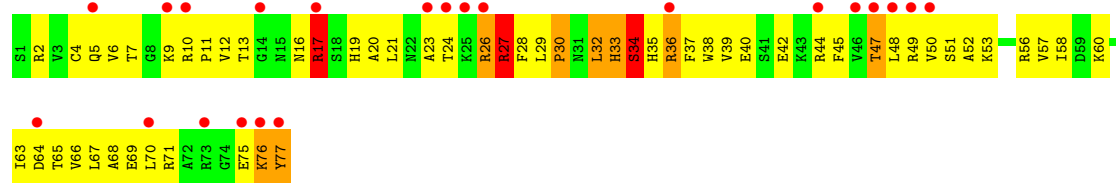
- Molecule 47: 50S ribosomal protein L28

Chain BX:



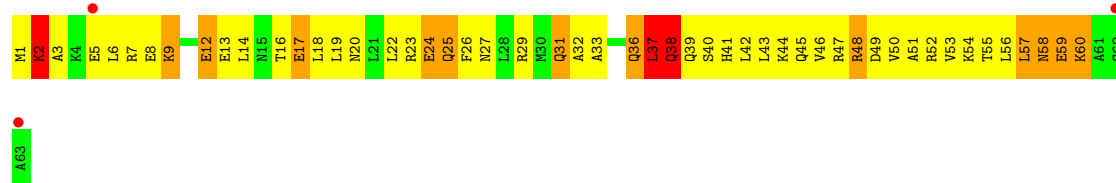
- Molecule 47: 50S ribosomal protein L28

Chain DX:



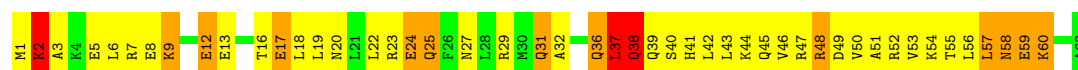
- Molecule 48: 50S ribosomal protein L29

Chain BY:



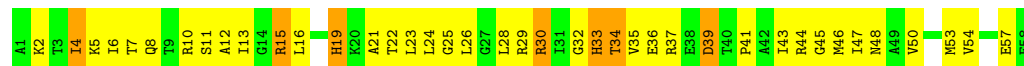
- Molecule 48: 50S ribosomal protein L29

Chain DY:

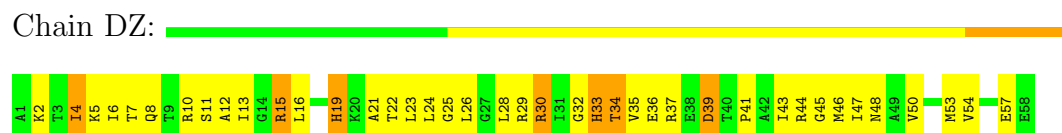


- Molecule 49: 50S ribosomal protein L30

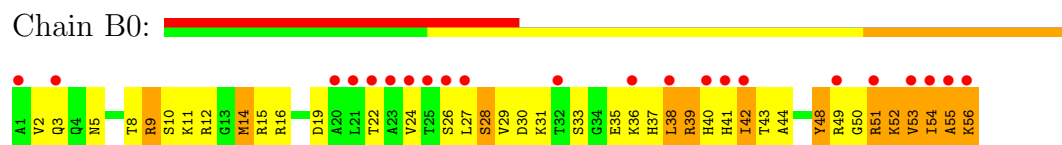
Chain BZ:



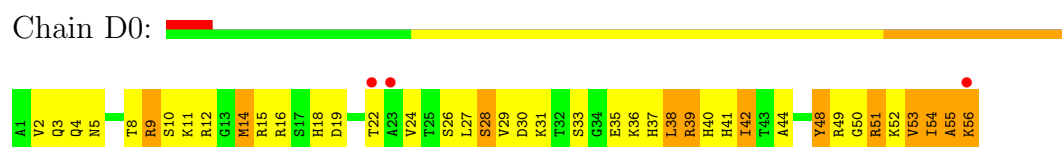
- Molecule 49: 50S ribosomal protein L30



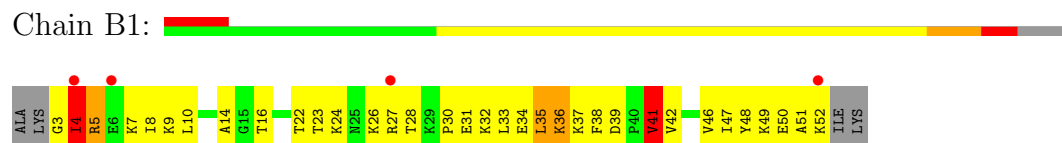
- Molecule 50: 50S ribosomal protein L32



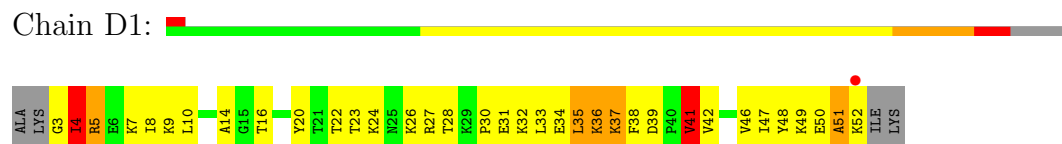
- Molecule 50: 50S ribosomal protein L32



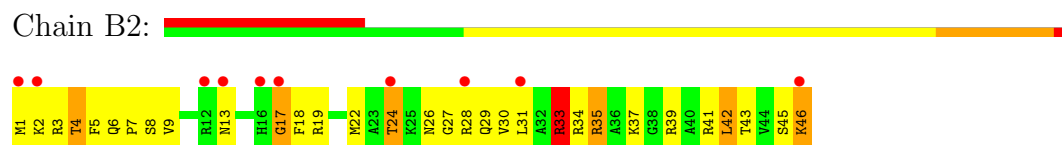
- Molecule 51: 50S ribosomal protein L33



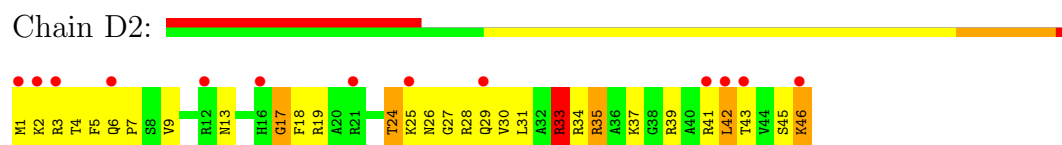
- Molecule 51: 50S ribosomal protein L33



- Molecule 52: 50S ribosomal protein L34

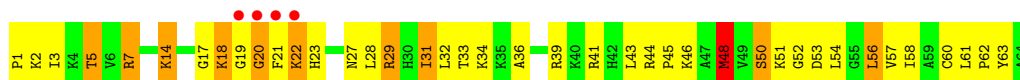


- Molecule 52: 50S ribosomal protein L34



- Molecule 53: 50S ribosomal protein L35





- Molecule 53: 50S ribosomal protein L35

Chain D3:



- Molecule 54: 50S ribosomal protein L36

Chain B4:



- Molecule 54: 50S ribosomal protein L36

Chain D4:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.78Å 395.22Å 744.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.00 – 3.22 184.07 – 3.22	Depositor EDS
% Data completeness (in resolution range)	(Not available) (70.00-3.22) 75.7 (184.07-3.22)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.11 (at 3.19Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.287 , 0.320 0.265 , 0.291	Depositor DCC
$R_{free}$ test set	37294 reflections (5.21%)	DCC
Wilson B-factor (Å <sup>2</sup> )	80.0	Xtriage
Anisotropy	0.720	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.21 , 25.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 753156 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	285033	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	AA	0.25	0/36762	0.74	11/57350 (0.0%)
1	CA	0.25	0/36762	0.73	7/57350 (0.0%)
2	AW	0.32	0/401	0.75	0/622
2	CW	0.31	0/401	0.74	0/622
3	AX	0.48	0/138	0.88	0/212
3	CX	0.49	0/138	0.88	0/212
4	AB	0.25	0/1735	0.44	0/2338
4	CB	0.25	0/1735	0.45	0/2338
5	AC	0.23	0/1651	0.44	0/2225
5	CC	0.23	0/1651	0.44	0/2225
6	AD	0.23	0/1665	0.44	0/2227
6	CD	0.23	0/1665	0.45	0/2227
7	AE	0.23	0/1118	0.45	0/1504
7	CE	0.23	0/1118	0.47	0/1504
8	AF	0.24	0/835	0.44	0/1128
8	CF	0.24	0/835	0.45	0/1128
9	AG	0.23	0/1187	0.43	0/1591
9	CG	0.23	0/1187	0.44	0/1591
10	AH	0.23	0/989	0.47	0/1326
10	CH	0.23	0/989	0.46	0/1326
11	AI	0.24	0/1034	0.45	0/1375
11	CI	0.24	0/1034	0.44	0/1375
12	AJ	0.22	0/796	0.47	0/1077
12	CJ	0.22	0/796	0.47	0/1077
13	AK	0.24	0/893	0.46	0/1205
13	CK	0.24	0/893	0.45	0/1205
14	AL	0.22	0/969	0.46	0/1300
14	CL	0.22	0/969	0.46	0/1300
15	AM	0.21	0/892	0.46	0/1193
15	CM	0.22	0/884	0.46	0/1181
16	AN	0.24	0/785	0.43	0/1043
16	CN	0.24	0/786	0.44	0/1046

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AO	0.23	0/724	0.44	0/966
17	CO	0.23	0/724	0.44	0/966
18	AP	0.25	0/659	0.45	0/884
18	CP	0.25	0/648	0.43	0/870
19	AQ	0.23	0/657	0.46	0/881
19	CQ	0.24	0/657	0.46	0/881
20	AR	0.23	0/462	0.45	0/621
20	CR	0.23	0/462	0.46	0/621
21	AS	0.25	0/652	0.43	0/877
21	CS	0.25	0/652	0.45	0/877
22	AT	0.23	0/671	0.42	0/888
22	CT	0.23	0/671	0.41	0/888
23	AU	0.26	0/430	0.45	0/570
23	CU	0.26	0/430	0.44	0/570
24	BA	0.24	0/2803	0.72	0/4371
24	DA	0.24	0/2803	0.73	0/4371
25	BB	0.27	7/68314 (0.0%)	0.77	53/106569 (0.0%)
25	DB	0.28	7/68314 (0.0%)	0.77	62/106569 (0.1%)
26	BC	0.22	0/2121	0.52	0/2852
26	DC	0.22	0/2121	0.52	0/2852
27	BD	0.25	0/1586	0.60	0/2134
27	DD	0.25	0/1586	0.60	0/2134
28	BE	0.24	0/1571	0.61	2/2113 (0.1%)
28	DE	0.24	0/1571	0.61	2/2113 (0.1%)
29	BF	0.26	0/1444	0.59	0/1937
29	DF	0.27	0/1444	0.59	0/1937
30	BG	0.23	0/1343	0.52	0/1816
30	DG	0.23	0/1343	0.52	0/1816
31	BH	0.28	0/1122	0.56	1/1515 (0.1%)
31	DH	0.26	0/1122	0.52	0/1515
32	BI	0.24	0/1046	0.46	0/1410
32	DI	0.24	0/1046	0.46	0/1410
33	BJ	0.24	0/1152	0.59	0/1551
33	DJ	0.24	0/1152	0.59	0/1551
34	BK	0.25	0/939	0.81	2/1258 (0.2%)
34	DK	0.25	0/939	0.81	2/1258 (0.2%)
35	BL	0.23	0/1054	0.58	0/1403
35	DL	0.23	0/1054	0.58	0/1403
36	BM	0.26	0/1093	0.56	0/1460
36	DM	0.26	0/1093	0.56	0/1460
37	BN	0.25	0/973	0.62	0/1301
37	DN	0.25	0/973	0.62	0/1301
38	BO	0.24	0/902	0.55	0/1209

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	DO	0.23	0/902	0.55	0/1209
39	BP	0.25	0/929	0.60	0/1242
39	DP	0.25	0/929	0.60	0/1242
40	BQ	0.26	0/960	0.65	0/1278
40	DQ	0.26	0/960	0.65	0/1278
41	BR	0.26	0/829	0.58	0/1107
41	DR	0.26	0/829	0.58	0/1107
42	BS	0.23	0/864	0.61	1/1156 (0.1%)
42	DS	0.23	0/864	0.61	1/1156 (0.1%)
43	BT	0.23	0/744	0.73	2/994 (0.2%)
43	DT	0.23	0/744	0.73	2/994 (0.2%)
44	BU	0.26	0/787	0.56	0/1051
44	DU	0.26	0/787	0.56	0/1051
45	BV	0.25	0/766	0.46	0/1025
45	DV	0.25	0/766	0.46	0/1025
46	BW	0.31	0/603	0.65	0/797
46	DW	0.31	0/603	0.65	0/797
47	BX	0.25	0/635	0.58	0/848
47	DX	0.25	0/635	0.58	0/848
48	BY	0.24	0/510	0.64	0/677
48	DY	0.25	0/510	0.64	0/677
49	BZ	0.24	0/453	0.55	0/605
49	DZ	0.23	0/453	0.55	0/605
50	B0	0.23	0/450	0.65	0/599
50	D0	0.22	0/450	0.65	0/599
51	B1	0.27	0/416	0.55	0/554
51	D1	0.27	0/416	0.55	0/554
52	B2	0.26	0/380	0.58	0/498
52	D2	0.26	0/380	0.58	0/498
53	B3	0.26	0/513	0.66	2/676 (0.3%)
53	D3	0.26	0/513	0.66	2/676 (0.3%)
54	B4	0.24	0/303	0.54	0/397
54	D4	0.23	0/303	0.54	0/397
All	All	0.26	14/307402 (0.0%)	0.70	152/459589 (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

*Continued on next page...*

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	CA	0	15
25	BB	0	37
25	DB	0	36
All	All	0	104

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BB	1086	A	C5-C6	-16.31	1.26	1.41
25	DB	1086	A	C5-C6	-16.20	1.26	1.41
25	DB	1088	A	C6-N1	-10.54	1.28	1.35
25	BB	1088	A	C6-N1	-10.43	1.28	1.35
25	DB	1060	U	C2-N3	7.83	1.43	1.37

The worst 5 of 152 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	DB	2204	G	O5'-P-OP1	-29.28	75.56	110.70
25	DB	2791	G	O5'-P-OP2	-29.23	75.63	110.70
25	BB	2791	G	O5'-P-OP1	-28.43	76.59	110.70
25	BB	2204	G	O5'-P-OP2	-27.54	77.65	110.70
25	DB	2204	G	O5'-P-OP2	18.17	132.50	110.70

There are no chirality outliers.

5 of 104 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	82	G	Sidechain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32831	0	16521	1479	0
1	CA	32831	0	16521	1483	0
2	AW	360	0	185	9	0
2	CW	360	0	185	9	0
3	AX	125	0	63	6	0
3	CX	125	0	63	5	0
4	AB	1704	0	1732	269	0
4	CB	1704	0	1732	320	0
5	AC	1624	0	1699	212	0
5	CC	1624	0	1699	251	0
6	AD	1643	0	1710	195	0
6	CD	1643	0	1710	260	0
7	AE	1105	0	1148	159	0
7	CE	1105	0	1148	217	0
8	AF	817	0	808	94	0
8	CF	817	0	808	123	0
9	AG	1174	0	1230	146	0
9	CG	1174	0	1230	167	0
10	AH	979	0	1034	120	0
10	CH	979	0	1034	166	0
11	AI	1022	0	1070	188	0
11	CI	1022	0	1070	193	0
12	AJ	786	0	828	125	0
12	CJ	786	0	828	121	0
13	AK	877	0	887	117	0
13	CK	877	0	887	141	0
14	AL	955	0	1019	139	0
14	CL	955	0	1019	119	0
15	AM	883	0	944	127	0
15	CM	876	0	937	165	0
16	AN	774	0	827	128	0
16	CN	774	0	828	133	0
17	AO	716	0	742	62	0
17	CO	716	0	742	70	0
18	AP	649	0	666	101	0
18	CP	638	0	656	103	0
19	AQ	648	0	691	97	0
19	CQ	648	0	691	75	0
20	AR	455	0	478	76	0
20	CR	455	0	478	54	0
21	AS	637	0	665	83	0
21	CS	637	0	665	109	0
22	AT	665	0	714	57	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	CT	665	0	714	60	0
23	AU	425	0	449	77	0
23	CU	425	0	449	88	0
24	BA	2507	0	1270	87	0
24	DA	2507	0	1270	76	0
25	BB	60995	0	30678	2083	0
25	DB	60995	0	30678	2153	0
26	BC	2082	0	2157	218	0
26	DC	2082	0	2157	215	0
27	BD	1565	0	1616	219	0
27	DD	1565	0	1616	215	0
28	BE	1552	0	1619	163	0
28	DE	1552	0	1619	165	0
29	BF	1420	0	1460	254	0
29	DF	1420	0	1460	241	0
30	BG	1323	0	1374	181	0
30	DG	1323	0	1374	175	0
31	BH	1111	0	1148	203	0
31	DH	1111	0	1148	174	0
32	BI	1032	0	1088	108	0
32	DI	1032	0	1088	184	0
33	BJ	1129	0	1162	155	0
33	DJ	1129	0	1162	167	0
34	BK	930	0	1003	99	0
34	DK	930	0	1003	96	0
35	BL	1045	0	1117	123	0
35	DL	1045	0	1117	123	0
36	BM	1074	0	1157	109	0
36	DM	1074	0	1157	105	0
37	BN	960	0	1000	103	0
37	DN	960	0	1000	102	0
38	BO	892	0	923	77	0
38	DO	892	0	923	73	0
39	BP	917	0	965	118	0
39	DP	917	0	965	111	0
40	BQ	947	0	1022	133	0
40	DQ	947	0	1022	140	0
41	BR	816	0	839	111	0
41	DR	816	0	839	114	0
42	BS	857	0	922	95	0
42	DS	857	0	922	96	0
43	BT	738	0	807	109	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	DT	738	0	807	118	0
44	BU	779	0	834	111	0
44	DU	779	0	834	105	0
45	BV	753	0	780	75	0
45	DV	753	0	780	71	0
46	BW	596	0	610	149	0
46	DW	596	0	610	146	0
47	BX	625	0	655	79	0
47	DX	625	0	655	78	0
48	BY	509	0	543	84	0
48	DY	509	0	543	75	0
49	BZ	449	0	491	47	0
49	DZ	449	0	491	40	0
50	B0	444	0	461	45	0
50	D0	444	0	461	48	0
51	B1	409	0	440	31	0
51	D1	409	0	440	32	0
52	B2	377	0	418	32	0
52	D2	377	0	418	29	0
53	B3	504	0	574	49	0
53	D3	504	0	574	48	0
54	B4	302	0	340	27	0
54	D4	302	0	340	28	0
55	AA	60	0	0	0	0
55	AX	2	0	0	0	0
55	BB	118	0	0	0	0
55	BJ	1	0	0	0	0
55	CA	56	0	0	0	0
55	CN	1	0	0	0	0
55	CX	1	0	0	0	0
55	DB	119	0	0	0	0
56	B4	1	0	0	0	0
56	D4	1	0	0	0	0
57	AA	287	0	0	5	0
57	AE	3	0	0	0	0
57	AI	1	0	0	0	0
57	AK	2	0	0	0	0
57	AL	2	0	0	0	0
57	AN	1	0	0	0	0
57	AP	1	0	0	0	0
57	AT	2	0	0	0	0
57	AX	9	0	0	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	B2	1	0	0	0	0
57	B4	5	0	0	0	0
57	BB	532	0	0	7	0
57	BC	7	0	0	0	0
57	BE	3	0	0	0	0
57	BH	3	0	0	0	0
57	BJ	3	0	0	0	0
57	BL	2	0	0	1	0
57	BN	3	0	0	0	0
57	CA	264	0	0	4	0
57	CE	2	0	0	0	0
57	CI	3	0	0	1	0
57	CL	1	0	0	0	0
57	CN	1	0	0	0	0
57	CP	1	0	0	0	0
57	CT	3	0	0	0	0
57	CU	1	0	0	0	0
57	CX	6	0	0	1	0
57	D2	1	0	0	0	0
57	D4	4	0	0	0	0
57	DB	531	0	0	5	0
57	DC	7	0	0	0	0
57	DD	1	0	0	0	0
57	DE	3	0	0	0	0
57	DJ	2	0	0	0	0
57	DL	3	0	0	0	0
57	DN	3	0	0	0	0
57	DT	1	0	0	0	0
All	All	285033	0	191150	17782	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 38.

The worst 5 of 17782 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
37:DN:101:GLY:HA2	37:DN:110:MET:H	1.04	1.18
27:BD:148:GLN:HG3	27:BD:152:PRO:HG2	1.29	1.15
34:BK:70:ARG:HB3	34:BK:71:PRO:CD	1.76	1.14
37:BN:101:GLY:HA2	37:BN:110:MET:H	1.06	1.13
28:DE:46:GLN:HG3	28:DE:87:ALA:HB3	1.31	1.12

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	AB	216/240 (90%)	133 (62%)	59 (27%)	24 (11%)	1	5
4	CB	216/240 (90%)	106 (49%)	71 (33%)	39 (18%)	0	1
5	AC	204/232 (88%)	134 (66%)	50 (24%)	20 (10%)	1	7
5	CC	204/232 (88%)	119 (58%)	57 (28%)	28 (14%)	0	2
6	AD	203/205 (99%)	123 (61%)	56 (28%)	24 (12%)	1	4
6	CD	203/205 (99%)	122 (60%)	54 (27%)	27 (13%)	0	2
7	AE	148/166 (89%)	101 (68%)	38 (26%)	9 (6%)	2	19
7	CE	148/166 (89%)	78 (53%)	50 (34%)	20 (14%)	0	2
8	AF	98/135 (73%)	63 (64%)	24 (24%)	11 (11%)	1	4
8	CF	98/135 (73%)	52 (53%)	30 (31%)	16 (16%)	0	1
9	AG	148/178 (83%)	107 (72%)	31 (21%)	10 (7%)	2	15
9	CG	148/178 (83%)	89 (60%)	40 (27%)	19 (13%)	0	3
10	AH	127/129 (98%)	83 (65%)	31 (24%)	13 (10%)	1	6
10	CH	127/129 (98%)	78 (61%)	35 (28%)	14 (11%)	1	5
11	AI	125/129 (97%)	78 (62%)	33 (26%)	14 (11%)	1	4
11	CI	125/129 (97%)	74 (59%)	44 (35%)	7 (6%)	3	23
12	AJ	96/103 (93%)	55 (57%)	27 (28%)	14 (15%)	0	2
12	CJ	96/103 (93%)	60 (62%)	22 (23%)	14 (15%)	0	2
13	AK	115/128 (90%)	75 (65%)	30 (26%)	10 (9%)	1	9
13	CK	115/128 (90%)	82 (71%)	25 (22%)	8 (7%)	2	14
14	AL	121/123 (98%)	80 (66%)	30 (25%)	11 (9%)	1	8
14	CL	121/123 (98%)	80 (66%)	24 (20%)	17 (14%)	0	2
15	AM	112/117 (96%)	75 (67%)	22 (20%)	15 (13%)	0	2
15	CM	111/117 (95%)	66 (60%)	29 (26%)	16 (14%)	0	2
16	AN	92/100 (92%)	61 (66%)	25 (27%)	6 (6%)	2	17

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	CN	94/100 (94%)	46 (49%)	29 (31%)	19 (20%)	0	0
17	AO	86/88 (98%)	69 (80%)	14 (16%)	3 (4%)	6	37
17	CO	86/88 (98%)	70 (81%)	14 (16%)	2 (2%)	10	52
18	AP	80/82 (98%)	46 (58%)	26 (32%)	8 (10%)	1	7
18	CP	78/82 (95%)	53 (68%)	17 (22%)	8 (10%)	1	6
19	AQ	78/83 (94%)	51 (65%)	16 (20%)	11 (14%)	0	2
19	CQ	78/83 (94%)	51 (65%)	20 (26%)	7 (9%)	1	8
20	AR	53/74 (72%)	39 (74%)	9 (17%)	5 (9%)	1	8
20	CR	53/74 (72%)	37 (70%)	12 (23%)	4 (8%)	2	12
21	AS	77/91 (85%)	53 (69%)	19 (25%)	5 (6%)	2	17
21	CS	77/91 (85%)	55 (71%)	18 (23%)	4 (5%)	3	25
22	AT	83/86 (96%)	63 (76%)	11 (13%)	9 (11%)	1	5
22	CT	83/86 (96%)	59 (71%)	20 (24%)	4 (5%)	4	27
23	AU	49/70 (70%)	21 (43%)	17 (35%)	11 (22%)	0	0
23	CU	49/70 (70%)	27 (55%)	16 (33%)	6 (12%)	1	3
26	BC	269/272 (99%)	166 (62%)	68 (25%)	35 (13%)	0	3
26	DC	269/272 (99%)	168 (62%)	63 (23%)	38 (14%)	0	2
27	BD	207/209 (99%)	113 (55%)	56 (27%)	38 (18%)	0	1
27	DD	207/209 (99%)	110 (53%)	56 (27%)	41 (20%)	0	0
28	BE	199/201 (99%)	126 (63%)	43 (22%)	30 (15%)	0	1
28	DE	199/201 (99%)	127 (64%)	42 (21%)	30 (15%)	0	1
29	BF	176/178 (99%)	97 (55%)	40 (23%)	39 (22%)	0	0
29	DF	176/178 (99%)	95 (54%)	43 (24%)	38 (22%)	0	0
30	BG	174/176 (99%)	94 (54%)	54 (31%)	26 (15%)	0	1
30	DG	174/176 (99%)	93 (53%)	55 (32%)	26 (15%)	0	1
31	BH	147/149 (99%)	69 (47%)	50 (34%)	28 (19%)	0	0
31	DH	147/149 (99%)	68 (46%)	54 (37%)	25 (17%)	0	1
32	BI	139/141 (99%)	118 (85%)	16 (12%)	5 (4%)	5	36
32	DI	139/141 (99%)	114 (82%)	21 (15%)	4 (3%)	7	43
33	BJ	140/142 (99%)	88 (63%)	30 (21%)	22 (16%)	0	1
33	DJ	140/142 (99%)	88 (63%)	30 (21%)	22 (16%)	0	1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	BK	119/123 (97%)	75 (63%)	26 (22%)	18 (15%)	0	1
34	DK	119/123 (97%)	75 (63%)	26 (22%)	18 (15%)	0	1
35	BL	141/144 (98%)	81 (57%)	37 (26%)	23 (16%)	0	1
35	DL	141/144 (98%)	81 (57%)	37 (26%)	23 (16%)	0	1
36	BM	134/136 (98%)	77 (58%)	32 (24%)	25 (19%)	0	0
36	DM	134/136 (98%)	77 (58%)	33 (25%)	24 (18%)	0	1
37	BN	118/127 (93%)	75 (64%)	27 (23%)	16 (14%)	0	2
37	DN	118/127 (93%)	75 (64%)	27 (23%)	16 (14%)	0	2
38	BO	114/117 (97%)	85 (75%)	24 (21%)	5 (4%)	4	29
38	DO	114/117 (97%)	85 (75%)	24 (21%)	5 (4%)	4	29
39	BP	112/114 (98%)	71 (63%)	20 (18%)	21 (19%)	0	0
39	DP	112/114 (98%)	71 (63%)	20 (18%)	21 (19%)	0	0
40	BQ	115/117 (98%)	74 (64%)	28 (24%)	13 (11%)	1	4
40	DQ	115/117 (98%)	74 (64%)	28 (24%)	13 (11%)	1	4
41	BR	101/103 (98%)	64 (63%)	24 (24%)	13 (13%)	0	3
41	DR	101/103 (98%)	64 (63%)	24 (24%)	13 (13%)	0	3
42	BS	108/110 (98%)	66 (61%)	26 (24%)	16 (15%)	0	1
42	DS	108/110 (98%)	66 (61%)	26 (24%)	16 (15%)	0	1
43	BT	91/100 (91%)	54 (59%)	23 (25%)	14 (15%)	0	1
43	DT	91/100 (91%)	52 (57%)	25 (28%)	14 (15%)	0	1
44	BU	100/103 (97%)	58 (58%)	27 (27%)	15 (15%)	0	1
44	DU	100/103 (97%)	57 (57%)	28 (28%)	15 (15%)	0	1
45	BV	92/94 (98%)	74 (80%)	11 (12%)	7 (8%)	2	12
45	DV	92/94 (98%)	73 (79%)	12 (13%)	7 (8%)	2	12
46	BW	77/84 (92%)	29 (38%)	23 (30%)	25 (32%)	0	0
46	DW	77/84 (92%)	29 (38%)	22 (29%)	26 (34%)	0	0
47	BX	75/77 (97%)	43 (57%)	26 (35%)	6 (8%)	1	11
47	DX	75/77 (97%)	41 (55%)	27 (36%)	7 (9%)	1	8
48	BY	61/63 (97%)	37 (61%)	18 (30%)	6 (10%)	1	7
48	DY	61/63 (97%)	34 (56%)	21 (34%)	6 (10%)	1	7
49	BZ	56/58 (97%)	42 (75%)	11 (20%)	3 (5%)	3	24

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	DZ	56/58 (97%)	42 (75%)	11 (20%)	3 (5%)	3	24
50	B0	54/56 (96%)	35 (65%)	8 (15%)	11 (20%)	0	0
50	D0	54/56 (96%)	34 (63%)	10 (18%)	10 (18%)	0	1
51	B1	48/54 (89%)	33 (69%)	7 (15%)	8 (17%)	0	1
51	D1	48/54 (89%)	33 (69%)	6 (12%)	9 (19%)	0	0
52	B2	44/46 (96%)	26 (59%)	13 (30%)	5 (11%)	1	4
52	D2	44/46 (96%)	26 (59%)	14 (32%)	4 (9%)	1	8
53	B3	62/64 (97%)	42 (68%)	15 (24%)	5 (8%)	1	10
53	D3	62/64 (97%)	41 (66%)	17 (27%)	4 (6%)	2	17
54	B4	36/38 (95%)	21 (58%)	11 (31%)	4 (11%)	1	5
54	D4	36/38 (95%)	21 (58%)	11 (31%)	4 (11%)	1	5
All	All	11239/11910 (94%)	6961 (62%)	2802 (25%)	1476 (13%)	0	2

5 of 1476 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AB	19	THR
4	AB	22	TRP
4	AB	75	ALA
4	AB	76	SER
4	AB	91	VAL

### 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	
4	AB	180/198 (91%)	140 (78%)	40 (22%)	1	6
4	CB	180/198 (91%)	143 (79%)	37 (21%)	2	8
5	AC	170/189 (90%)	134 (79%)	36 (21%)	1	8
5	CC	170/189 (90%)	138 (81%)	32 (19%)	2	11
6	AD	172/172 (100%)	146 (85%)	26 (15%)	4	19
6	CD	172/172 (100%)	130 (76%)	42 (24%)	1	3

Continued on next page...



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	AE	113/125 (90%)	95 (84%)	18 (16%)	4	16
7	CE	113/125 (90%)	87 (77%)	26 (23%)	1	5
8	AF	87/116 (75%)	74 (85%)	13 (15%)	4	20
8	CF	87/116 (75%)	76 (87%)	11 (13%)	7	30
9	AG	123/146 (84%)	99 (80%)	24 (20%)	2	10
9	CG	123/146 (84%)	100 (81%)	23 (19%)	2	11
10	AH	104/104 (100%)	89 (86%)	15 (14%)	5	22
10	CH	104/104 (100%)	81 (78%)	23 (22%)	1	6
11	AI	105/106 (99%)	83 (79%)	22 (21%)	1	8
11	CI	105/106 (99%)	83 (79%)	22 (21%)	1	8
12	AJ	86/90 (96%)	75 (87%)	11 (13%)	6	29
12	CJ	86/90 (96%)	71 (83%)	15 (17%)	3	13
13	AK	90/98 (92%)	75 (83%)	15 (17%)	3	14
13	CK	90/98 (92%)	77 (86%)	13 (14%)	5	22
14	AL	103/103 (100%)	83 (81%)	20 (19%)	2	10
14	CL	103/103 (100%)	80 (78%)	23 (22%)	1	6
15	AM	92/95 (97%)	75 (82%)	17 (18%)	2	11
15	CM	91/95 (96%)	71 (78%)	20 (22%)	1	6
16	AN	79/83 (95%)	60 (76%)	19 (24%)	1	4
16	CN	79/83 (95%)	66 (84%)	13 (16%)	3	14
17	AO	76/76 (100%)	65 (86%)	11 (14%)	5	22
17	CO	76/76 (100%)	67 (88%)	9 (12%)	8	34
18	AP	65/65 (100%)	52 (80%)	13 (20%)	2	9
18	CP	65/65 (100%)	58 (89%)	7 (11%)	9	37
19	AQ	74/77 (96%)	60 (81%)	14 (19%)	2	11
19	CQ	74/77 (96%)	66 (89%)	8 (11%)	9	37
20	AR	48/64 (75%)	37 (77%)	11 (23%)	1	5
20	CR	48/64 (75%)	43 (90%)	5 (10%)	10	39
21	AS	70/78 (90%)	55 (79%)	15 (21%)	1	7
21	CS	70/78 (90%)	51 (73%)	19 (27%)	1	2
22	AT	65/65 (100%)	56 (86%)	9 (14%)	5	24

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	CT	65/65 (100%)	55 (85%)	10 (15%)	4	18
23	AU	44/60 (73%)	37 (84%)	7 (16%)	4	16
23	CU	44/60 (73%)	32 (73%)	12 (27%)	0	2
26	BC	216/217 (100%)	182 (84%)	34 (16%)	4	17
26	DC	216/217 (100%)	182 (84%)	34 (16%)	4	17
27	BD	164/164 (100%)	136 (83%)	28 (17%)	3	14
27	DD	164/164 (100%)	137 (84%)	27 (16%)	3	14
28	BE	165/165 (100%)	130 (79%)	35 (21%)	1	8
28	DE	165/165 (100%)	130 (79%)	35 (21%)	1	8
29	BF	149/149 (100%)	116 (78%)	33 (22%)	1	6
29	DF	149/149 (100%)	117 (78%)	32 (22%)	1	7
30	BG	137/137 (100%)	110 (80%)	27 (20%)	2	9
30	DG	137/137 (100%)	110 (80%)	27 (20%)	2	9
31	BH	114/114 (100%)	85 (75%)	29 (25%)	1	2
31	DH	114/114 (100%)	86 (75%)	28 (25%)	1	3
32	BI	109/109 (100%)	107 (98%)	2 (2%)	71	93
32	DI	109/109 (100%)	104 (95%)	5 (5%)	37	80
33	BJ	116/116 (100%)	100 (86%)	16 (14%)	5	24
33	DJ	116/116 (100%)	100 (86%)	16 (14%)	5	24
34	BK	102/104 (98%)	84 (82%)	18 (18%)	3	13
34	DK	102/104 (98%)	83 (81%)	19 (19%)	2	11
35	BL	102/103 (99%)	87 (85%)	15 (15%)	4	21
35	DL	102/103 (99%)	88 (86%)	14 (14%)	5	25
36	BM	109/109 (100%)	93 (85%)	16 (15%)	4	21
36	DM	109/109 (100%)	93 (85%)	16 (15%)	4	21
37	BN	100/103 (97%)	85 (85%)	15 (15%)	4	20
37	DN	100/103 (97%)	84 (84%)	16 (16%)	3	16
38	BO	86/87 (99%)	76 (88%)	10 (12%)	8	35
38	DO	86/87 (99%)	76 (88%)	10 (12%)	8	35
39	BP	99/99 (100%)	76 (77%)	23 (23%)	1	5
39	DP	99/99 (100%)	77 (78%)	22 (22%)	1	6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	BQ	89/89 (100%)	73 (82%)	16 (18%)	2	12
40	DQ	89/89 (100%)	73 (82%)	16 (18%)	2	12
41	BR	84/84 (100%)	67 (80%)	17 (20%)	2	9
41	DR	84/84 (100%)	67 (80%)	17 (20%)	2	9
42	BS	93/93 (100%)	79 (85%)	14 (15%)	4	19
42	DS	93/93 (100%)	79 (85%)	14 (15%)	4	19
43	BT	80/84 (95%)	65 (81%)	15 (19%)	2	11
43	DT	80/84 (95%)	64 (80%)	16 (20%)	2	9
44	BU	83/84 (99%)	69 (83%)	14 (17%)	3	14
44	DU	83/84 (99%)	70 (84%)	13 (16%)	4	17
45	BV	78/78 (100%)	67 (86%)	11 (14%)	5	23
45	DV	78/78 (100%)	67 (86%)	11 (14%)	5	23
46	BW	59/62 (95%)	49 (83%)	10 (17%)	3	14
46	DW	59/62 (95%)	48 (81%)	11 (19%)	2	11
47	BX	67/67 (100%)	56 (84%)	11 (16%)	3	15
47	DX	67/67 (100%)	57 (85%)	10 (15%)	4	20
48	BY	55/55 (100%)	43 (78%)	12 (22%)	1	7
48	DY	55/55 (100%)	43 (78%)	12 (22%)	1	7
49	BZ	48/48 (100%)	43 (90%)	5 (10%)	10	39
49	DZ	48/48 (100%)	43 (90%)	5 (10%)	10	39
50	B0	47/47 (100%)	40 (85%)	7 (15%)	4	20
50	D0	47/47 (100%)	40 (85%)	7 (15%)	4	20
51	B1	45/48 (94%)	38 (84%)	7 (16%)	4	17
51	D1	45/48 (94%)	38 (84%)	7 (16%)	4	17
52	B2	38/38 (100%)	33 (87%)	5 (13%)	6	27
52	D2	38/38 (100%)	33 (87%)	5 (13%)	6	27
53	B3	51/51 (100%)	44 (86%)	7 (14%)	5	25
53	D3	51/51 (100%)	43 (84%)	8 (16%)	4	17
54	B4	34/34 (100%)	29 (85%)	5 (15%)	4	21
54	D4	34/34 (100%)	29 (85%)	5 (15%)	4	21
All	All	9329/9696 (96%)	7688 (82%)	1641 (18%)	3	13

5 of 1641 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
45	BV	79	ARG
6	CD	170	LEU
41	DR	95	ASP
47	BX	77	TYR
4	CB	122	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 364 such sidechains are listed below:

Mol	Chain	Res	Type
45	BV	88	HIS
7	CE	11	GLN
42	DS	57	ASN
48	BY	25	GLN
4	CB	121	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1529/1542 (99%)	278 (18%)	20 (1%)
1	CA	1529/1542 (99%)	272 (17%)	19 (1%)
2	AW	16/17 (94%)	0	0
2	CW	16/17 (94%)	0	0
24	BA	116/120 (96%)	19 (16%)	2 (1%)
24	DA	116/120 (96%)	19 (16%)	2 (1%)
25	BB	2837/2904 (97%)	416 (14%)	13 (0%)
25	DB	2837/2904 (97%)	420 (14%)	17 (0%)
3	AX	5/6 (83%)	3 (60%)	0
3	CX	5/6 (83%)	3 (60%)	0
All	All	9006/9178 (98%)	1430 (15%)	73 (0%)

5 of 1430 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	8	A
1	AA	9	G
1	AA	14	U
1	AA	15	G

5 of 73 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	BB	2756	U
1	CA	366	A
25	DB	2308	G
1	CA	243	A
1	CA	428	G

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 360 ligands modelled in this entry, 360 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	AA	1530/1542 (99%)	-0.46	16 (1%) 79 31	41, 98, 164, 180	0
1	CA	1530/1542 (99%)	-0.50	5 (0%) 91 60	41, 109, 167, 180	0
2	AW	17/17 (100%)	1.09	3 (17%) 2 1	73, 87, 132, 177	0
2	CW	17/17 (100%)	-0.29	1 (5%) 22 5	63, 86, 126, 150	0
3	AX	6/6 (100%)	2.99	4 (66%) 0 0	63, 78, 113, 127	0
3	CX	6/6 (100%)	0.33	1 (16%) 2 1	76, 83, 113, 115	0
4	AB	218/240 (90%)	0.52	14 (6%) 19 4	59, 127, 169, 180	0
4	CB	218/240 (90%)	1.80	72 (33%) 1 0	67, 141, 180, 180	0
5	AC	206/232 (88%)	3.21	154 (74%) 0 0	61, 104, 153, 180	0
5	CC	206/232 (88%)	1.28	44 (21%) 1 1	69, 121, 161, 180	0
6	AD	205/205 (100%)	1.40	60 (29%) 1 1	44, 106, 149, 180	0
6	CD	205/205 (100%)	1.57	69 (33%) 1 0	67, 120, 164, 180	0
7	AE	150/166 (90%)	1.15	33 (22%) 1 1	39, 98, 148, 180	0
7	CE	150/166 (90%)	2.48	66 (44%) 1 0	46, 129, 180, 180	0
8	AF	100/135 (74%)	0.50	5 (5%) 28 6	52, 100, 148, 180	0
8	CF	100/135 (74%)	0.31	7 (7%) 16 4	33, 101, 144, 165	0
9	AG	150/178 (84%)	1.21	35 (23%) 1 1	55, 113, 167, 180	0
9	CG	150/178 (84%)	0.28	13 (8%) 10 3	71, 122, 165, 180	0
10	AH	129/129 (100%)	0.64	21 (16%) 2 1	51, 100, 143, 179	0
10	CH	129/129 (100%)	0.01	4 (3%) 47 10	37, 106, 149, 176	0
11	AI	127/129 (98%)	0.16	6 (4%) 30 6	84, 120, 166, 180	0
11	CI	127/129 (98%)	-0.06	4 (3%) 47 10	68, 128, 167, 180	0
12	AJ	98/103 (95%)	2.55	57 (58%) 0 0	56, 124, 172, 180	0
12	CJ	98/103 (95%)	1.26	25 (25%) 1 1	76, 131, 164, 180	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
13	AK	117/128 (91%)	1.69	37 (31%)	1 1	36, 91, 142, 180	0
13	CK	117/128 (91%)	0.55	11 (9%)	9 2	48, 91, 131, 159	0
14	AL	123/123 (100%)	1.61	41 (33%)	1 0	31, 80, 130, 169	0
14	CL	123/123 (100%)	1.95	49 (39%)	1 0	42, 91, 138, 172	0
15	AM	114/117 (97%)	-0.07	4 (3%)	42 9	63, 119, 165, 180	0
15	CM	113/117 (96%)	-0.23	1 (0%)	81 35	58, 121, 165, 176	0
16	AN	96/100 (96%)	2.06	39 (40%)	1 0	56, 112, 155, 180	0
16	CN	96/100 (96%)	1.54	25 (26%)	1 1	65, 124, 154, 180	0
17	AO	88/88 (100%)	0.89	16 (18%)	2 1	54, 91, 138, 180	0
17	CO	88/88 (100%)	0.56	4 (4%)	32 7	37, 96, 143, 160	0
18	AP	82/82 (100%)	0.48	5 (6%)	21 4	49, 95, 163, 180	0
18	CP	80/82 (97%)	0.50	10 (12%)	5 1	68, 113, 155, 180	0
19	AQ	80/83 (96%)	0.96	17 (21%)	1 1	54, 107, 155, 169	0
19	CQ	80/83 (96%)	0.85	12 (15%)	3 1	50, 104, 145, 155	0
20	AR	55/74 (74%)	1.22	11 (20%)	2 1	52, 98, 134, 158	0
20	CR	55/74 (74%)	0.60	7 (12%)	4 1	46, 101, 144, 157	0
21	AS	79/91 (86%)	0.13	4 (5%)	27 5	80, 133, 169, 180	0
21	CS	79/91 (86%)	0.33	3 (3%)	38 8	75, 128, 160, 180	0
22	AT	85/86 (98%)	-0.36	1 (1%)	75 27	62, 101, 151, 162	0
22	CT	85/86 (98%)	-0.26	0	100 100	65, 104, 154, 180	0
23	AU	51/70 (72%)	3.02	34 (66%)	0 0	54, 110, 154, 180	0
23	CU	51/70 (72%)	2.00	23 (45%)	1 0	63, 125, 169, 180	0
24	BA	117/120 (97%)	0.36	1 (0%)	81 35	44, 75, 109, 180	0
24	DA	117/120 (97%)	-0.45	1 (0%)	81 35	33, 66, 105, 180	0
25	BB	2841/2904 (97%)	-0.20	57 (2%)	62 18	13, 70, 147, 180	0
25	DB	2841/2904 (97%)	-0.27	37 (1%)	74 26	12, 55, 149, 180	0
26	BC	271/272 (99%)	1.68	89 (32%)	1 0	16, 66, 111, 151	0
26	DC	271/272 (99%)	1.43	62 (22%)	1 1	9, 52, 97, 153	0
27	BD	209/209 (100%)	1.91	88 (42%)	1 0	25, 83, 146, 180	0
27	DD	209/209 (100%)	0.70	12 (5%)	23 5	20, 59, 119, 166	0
28	BE	201/201 (100%)	1.11	38 (18%)	2 1	22, 78, 139, 172	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	DE	201/201 (100%)	1.66	76 (37%) 1 0	11, 76, 143, 178	0
29	BF	178/178 (100%)	-0.20	2 (1%) 77 29	49, 111, 174, 180	0
29	DF	178/178 (100%)	-0.02	0 100 100	49, 110, 166, 180	0
30	BG	176/176 (100%)	0.14	5 (2%) 50 11	47, 112, 165, 176	0
30	DG	176/176 (100%)	0.21	9 (5%) 27 5	38, 88, 155, 174	0
31	BH	149/149 (100%)	2.79	58 (38%) 1 0	52, 131, 180, 180	0
31	DH	149/149 (100%)	1.85	50 (33%) 1 0	35, 109, 150, 180	0
32	BI	141/141 (100%)	0.52	12 (8%) 11 3	110, 167, 180, 180	0
32	DI	141/141 (100%)	0.51	8 (5%) 23 5	105, 179, 180, 180	0
33	BJ	142/142 (100%)	1.22	32 (22%) 1 1	32, 86, 133, 180	0
33	DJ	142/142 (100%)	0.08	1 (0%) 84 40	19, 53, 108, 175	0
34	BK	121/123 (98%)	3.31	104 (85%) 0 0	32, 74, 148, 180	0
34	DK	121/123 (98%)	1.52	36 (29%) 1 1	27, 64, 130, 163	0
35	BL	143/144 (99%)	0.29	8 (5%) 24 5	27, 69, 121, 180	0
35	DL	143/144 (99%)	1.94	62 (43%) 1 0	17, 64, 115, 180	0
36	BM	136/136 (100%)	0.47	4 (2%) 49 11	33, 65, 132, 168	0
36	DM	136/136 (100%)	0.71	9 (6%) 18 4	11, 56, 109, 176	0
37	BN	120/127 (94%)	2.31	59 (49%) 1 0	43, 88, 131, 169	0
37	DN	120/127 (94%)	0.47	3 (2%) 54 13	19, 57, 97, 180	0
38	BO	116/117 (99%)	0.06	0 100 100	34, 77, 118, 138	0
38	DO	116/117 (99%)	-0.12	0 100 100	28, 71, 129, 157	0
39	BP	114/114 (100%)	3.15	88 (77%) 0 0	43, 84, 145, 164	0
39	DP	114/114 (100%)	1.74	47 (41%) 1 0	26, 73, 123, 174	0
40	BQ	117/117 (100%)	0.11	2 (1%) 67 20	34, 73, 135, 149	0
40	DQ	117/117 (100%)	0.39	3 (2%) 53 12	22, 53, 104, 158	0
41	BR	103/103 (100%)	0.43	4 (3%) 37 8	44, 95, 146, 177	0
41	DR	103/103 (100%)	0.16	5 (4%) 28 6	23, 72, 131, 156	0
42	BS	110/110 (100%)	2.40	69 (62%) 0 0	47, 84, 138, 180	0
42	DS	110/110 (100%)	1.22	22 (20%) 2 1	18, 53, 108, 152	0
43	BT	93/100 (93%)	1.09	16 (17%) 2 1	44, 93, 163, 180	0
43	DT	93/100 (93%)	0.72	8 (8%) 11 3	35, 72, 141, 178	0

*Continued on next page...*



Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	BU	102/103 (99%)	0.58	5 (4%) 28 6	48, 106, 162, 175	0
44	DU	102/103 (99%)	0.01	0 100 100	41, 94, 154, 180	0
45	BV	94/94 (100%)	0.13	1 (1%) 77 29	37, 84, 140, 180	0
45	DV	94/94 (100%)	0.69	7 (7%) 14 4	31, 70, 138, 156	0
46	BW	79/84 (94%)	0.60	5 (6%) 19 4	6, 53, 116, 154	0
46	DW	79/84 (94%)	0.39	2 (2%) 54 13	7, 42, 103, 180	0
47	BX	77/77 (100%)	0.80	6 (7%) 13 3	24, 63, 107, 157	0
47	DX	77/77 (100%)	1.45	22 (28%) 1 1	23, 60, 112, 152	0
48	BY	63/63 (100%)	0.25	3 (4%) 29 6	47, 108, 165, 180	0
48	DY	63/63 (100%)	-0.27	0 100 100	34, 92, 158, 180	0
49	BZ	58/58 (100%)	-0.04	0 100 100	40, 74, 124, 150	0
49	DZ	58/58 (100%)	-0.08	0 100 100	22, 58, 110, 114	0
50	B0	56/56 (100%)	1.81	22 (39%) 1 0	35, 87, 152, 180	0
50	D0	56/56 (100%)	0.42	3 (5%) 25 5	19, 56, 118, 135	0
51	B1	50/54 (92%)	0.55	4 (8%) 12 3	43, 72, 122, 140	0
51	D1	50/54 (92%)	0.14	1 (2%) 62 18	26, 76, 119, 163	0
52	B2	46/46 (100%)	1.43	10 (21%) 1 1	42, 61, 97, 162	0
52	D2	46/46 (100%)	1.69	13 (28%) 1 1	17, 47, 97, 131	0
53	B3	64/64 (100%)	0.58	4 (6%) 19 4	21, 56, 99, 136	0
53	D3	64/64 (100%)	1.44	14 (21%) 1 1	27, 49, 85, 105	0
54	B4	38/38 (100%)	0.04	0 100 100	36, 86, 126, 146	0
54	D4	38/38 (100%)	-0.09	0 100 100	44, 68, 126, 165	0
All	All	20459/21088 (97%)	0.43	2382 (11%) 5 2	6, 86, 162, 180	0

The worst 5 of 2382 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	CE	114	LEU	16.5
31	BH	124	THR	14.2
31	BH	88	GLY	13.7
7	CE	53	ARG	13.2
31	BH	129	GLU	13.1

## 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, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	AA	1626	1/1	0.44	120.20	139,139,139,139	0
55	MG	AA	1658	1/1	0.55	47.98	147,147,147,147	0
55	MG	AA	1614	1/1	0.59	47.10	174,174,174,174	0
55	MG	AA	1637	1/1	0.70	42.16	134,134,134,134	0
55	MG	CA	1646	1/1	0.47	40.64	155,155,155,155	0
55	MG	AA	1627	1/1	0.29	35.01	91,91,91,91	0
55	MG	CA	1640	1/1	0.36	33.88	138,138,138,138	0
55	MG	DB	3065	1/1	0.26	31.11	67,67,67,67	0
55	MG	DB	3058	1/1	0.33	29.80	136,136,136,136	0
55	MG	BB	3014	1/1	0.23	20.14	76,76,76,76	0
55	MG	CA	1639	1/1	0.32	12.00	99,99,99,99	0
55	MG	AA	1617	1/1	0.29	9.50	123,123,123,123	0
55	MG	DB	3052	1/1	0.82	9.03	137,137,137,137	0
55	MG	DB	3082	1/1	0.33	8.41	104,104,104,104	0
55	MG	AA	1632	1/1	0.26	7.87	106,106,106,106	0
55	MG	BB	3063	1/1	0.47	7.36	95,95,95,95	0
55	MG	DB	3032	1/1	0.58	5.37	111,111,111,111	0
55	MG	BB	3016	1/1	0.43	5.30	91,91,91,91	0
55	MG	CA	1638	1/1	0.61	4.90	102,102,102,102	0
55	MG	BB	3031	1/1	0.47	4.76	83,83,83,83	0
55	MG	AA	1652	1/1	0.19	4.07	103,103,103,103	0
55	MG	AA	1656	1/1	0.47	4.04	101,101,101,101	0
55	MG	AA	1653	1/1	0.16	4.03	84,84,84,84	0
55	MG	AA	1625	1/1	0.14	4.00	145,145,145,145	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	CA	1613	1/1	0.20	3.94	140,140,140,140	0
55	MG	DB	3034	1/1	0.30	3.81	87,87,87,87	0
55	MG	DB	3088	1/1	0.18	3.75	83,83,83,83	0
55	MG	CA	1606	1/1	0.18	3.40	139,139,139,139	0
55	MG	CA	1655	1/1	0.20	3.39	153,153,153,153	0
55	MG	AA	1628	1/1	0.23	3.08	100,100,100,100	0
55	MG	AA	1650	1/1	0.16	3.07	92,92,92,92	0
55	MG	CA	1627	1/1	0.15	2.88	122,122,122,122	0
55	MG	DB	3043	1/1	0.24	2.46	49,49,49,49	0
55	MG	AA	1643	1/1	0.21	2.44	112,112,112,112	0
55	MG	AA	1655	1/1	0.18	2.40	82,82,82,82	0
55	MG	AA	1639	1/1	0.11	2.33	126,126,126,126	0
55	MG	BB	3033	1/1	0.18	2.29	86,86,86,86	0
55	MG	BB	3093	1/1	0.56	2.24	120,120,120,120	0
55	MG	DB	3070	1/1	0.19	2.08	61,61,61,61	0
55	MG	CA	1614	1/1	0.18	1.99	171,171,171,171	0
55	MG	AA	1619	1/1	0.28	1.88	92,92,92,92	0
55	MG	DB	3109	1/1	0.23	1.67	28,28,28,28	0
55	MG	BB	3083	1/1	0.21	1.66	47,47,47,47	0
55	MG	DB	3091	1/1	0.20	1.54	39,39,39,39	0
55	MG	CA	1643	1/1	0.17	1.52	138,138,138,138	0
55	MG	DB	3095	1/1	0.17	1.41	26,26,26,26	0
55	MG	AX	101	1/1	0.39	1.41	84,84,84,84	0
55	MG	CA	1610	1/1	0.23	1.39	130,130,130,130	0
55	MG	BB	3105	1/1	0.18	1.35	64,64,64,64	0
55	MG	BB	3057	1/1	0.73	1.29	100,100,100,100	0
55	MG	AA	1649	1/1	0.12	1.14	84,84,84,84	0
55	MG	CA	1623	1/1	0.14	1.04	136,136,136,136	0
55	MG	CA	1649	1/1	0.14	1.00	100,100,100,100	0
55	MG	CA	1632	1/1	0.30	0.99	154,154,154,154	0
55	MG	CA	1618	1/1	0.12	0.94	87,87,87,87	0
55	MG	DB	3029	1/1	0.83	0.94	92,92,92,92	0
55	MG	DB	3069	1/1	0.32	0.89	48,48,48,48	0
55	MG	BB	3077	1/1	0.15	0.71	50,50,50,50	0
55	MG	CA	1634	1/1	0.15	0.67	80,80,80,80	0
55	MG	DB	3012	1/1	0.17	0.66	37,37,37,37	0
55	MG	AA	1602	1/1	0.17	0.52	83,83,83,83	0
55	MG	BB	3087	1/1	0.17	0.51	63,63,63,63	0
55	MG	BB	3118	1/1	0.46	0.34	113,113,113,113	0
55	MG	BB	3010	1/1	0.16	0.33	95,95,95,95	0
55	MG	DB	3061	1/1	0.11	0.27	97,97,97,97	0
55	MG	DB	3094	1/1	0.37	0.24	77,77,77,77	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	1647	1/1	0.27	0.22	79,79,79,79	0
55	MG	CA	1654	1/1	0.19	0.21	78,78,78,78	0
55	MG	BB	3076	1/1	0.17	0.17	56,56,56,56	0
55	MG	AA	1651	1/1	0.16	0.13	83,83,83,83	0
55	MG	BB	3027	1/1	0.14	0.08	40,40,40,40	0
55	MG	AA	1622	1/1	0.16	0.04	87,87,87,87	0
55	MG	BB	3041	1/1	0.15	-0.03	28,28,28,28	0
55	MG	CA	1656	1/1	0.26	-0.07	97,97,97,97	0
55	MG	DB	3092	1/1	0.16	-0.07	44,44,44,44	0
55	MG	DB	3054	1/1	0.17	-0.13	53,53,53,53	0
55	MG	AA	1635	1/1	0.13	-0.14	129,129,129,129	0
55	MG	AA	1606	1/1	0.13	-0.15	114,114,114,114	0
55	MG	BB	3106	1/1	0.31	-0.16	53,53,53,53	0
55	MG	CA	1635	1/1	0.39	-0.21	129,129,129,129	0
55	MG	AA	1645	1/1	0.17	-0.26	127,127,127,127	0
55	MG	CA	1621	1/1	0.10	-0.34	161,161,161,161	0
55	MG	BB	3095	1/1	0.19	-0.34	48,48,48,48	0
55	MG	BB	3110	1/1	0.12	-0.36	56,56,56,56	0
55	MG	BB	3071	1/1	0.17	-0.36	41,41,41,41	0
55	MG	AA	1660	1/1	0.38	-0.36	95,95,95,95	0
55	MG	CA	1611	1/1	0.13	-0.37	102,102,102,102	0
55	MG	CA	1637	1/1	0.15	-0.42	81,81,81,81	0
55	MG	BB	3109	1/1	0.14	-0.42	52,52,52,52	0
55	MG	BB	3112	1/1	0.23	-0.43	27,27,27,27	0
55	MG	CA	1651	1/1	0.12	-0.46	66,66,66,66	0
55	MG	CA	1653	1/1	0.14	-0.47	149,149,149,149	0
55	MG	BB	3034	1/1	0.27	-0.53	70,70,70,70	0
55	MG	DB	3119	1/1	0.14	-0.57	64,64,64,64	0
55	MG	BB	3024	1/1	0.16	-0.57	47,47,47,47	0
55	MG	BB	3060	1/1	0.16	-0.58	33,33,33,33	0
55	MG	BB	3117	1/1	0.24	-0.59	82,82,82,82	0
56	ZN	D4	401	1/1	0.12	-0.59	72,72,72,72	0
55	MG	BB	3051	1/1	0.17	-0.63	94,94,94,94	0
55	MG	AA	1621	1/1	0.11	-0.65	36,36,36,36	0
55	MG	BB	3115	1/1	0.11	-0.67	106,106,106,106	0
55	MG	AA	1630	1/1	0.10	-0.70	114,114,114,114	0
55	MG	DB	3008	1/1	0.15	-0.72	55,55,55,55	0
55	MG	DB	3093	1/1	0.12	-0.72	54,54,54,54	0
55	MG	DB	3089	1/1	0.10	-0.72	51,51,51,51	0
55	MG	DB	3023	1/1	0.09	-0.73	46,46,46,46	0
55	MG	DB	3114	1/1	0.18	-0.75	43,43,43,43	0
55	MG	AA	1618	1/1	0.11	-0.75	92,92,92,92	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BB	3046	1/1	0.10	-0.76	90,90,90,90	0
55	MG	CN	201	1/1	0.09	-0.77	104,104,104,104	0
55	MG	AA	1620	1/1	0.11	-0.78	74,74,74,74	0
55	MG	AA	1608	1/1	0.10	-0.80	113,113,113,113	0
55	MG	CA	1603	1/1	0.12	-0.80	124,124,124,124	0
55	MG	DB	3108	1/1	0.10	-0.80	36,36,36,36	0
55	MG	AA	1631	1/1	0.10	-0.81	91,91,91,91	0
55	MG	AA	1607	1/1	0.13	-0.84	93,93,93,93	0
55	MG	CA	1619	1/1	0.03	-0.84	79,79,79,79	0
55	MG	DB	3077	1/1	0.19	-0.85	57,57,57,57	0
55	MG	CA	1607	1/1	0.08	-0.86	108,108,108,108	0
55	MG	AX	102	1/1	0.18	-0.86	66,66,66,66	0
55	MG	DB	3057	1/1	0.11	-0.86	63,63,63,63	0
55	MG	CA	1608	1/1	0.12	-0.88	82,82,82,82	0
55	MG	CA	1624	1/1	0.05	-0.89	103,103,103,103	0
55	MG	CA	1641	1/1	0.10	-0.91	123,123,123,123	0
55	MG	AA	1636	1/1	0.04	-0.96	61,61,61,61	0
55	MG	BB	3099	1/1	0.12	-0.97	41,41,41,41	0
55	MG	CA	1644	1/1	0.11	-1.06	131,131,131,131	0
55	MG	BB	3012	1/1	0.12	-1.07	32,32,32,32	0
55	MG	DB	3064	1/1	0.15	-1.08	32,32,32,32	0
55	MG	AA	1646	1/1	0.23	-1.12	74,74,74,74	0
55	MG	BB	3075	1/1	0.10	-1.15	44,44,44,44	0
55	MG	BB	3080	1/1	0.12	-1.17	65,65,65,65	0
55	MG	BB	3054	1/1	0.12	-1.18	56,56,56,56	0
55	MG	AA	1638	1/1	0.11	-1.19	95,95,95,95	0
55	MG	CA	1615	1/1	0.12	-1.21	156,156,156,156	0
55	MG	AA	1640	1/1	0.10	-1.23	99,99,99,99	0
55	MG	BB	3029	1/1	0.09	-1.25	81,81,81,81	0
55	MG	DB	3030	1/1	0.14	-1.25	46,46,46,46	0
55	MG	DB	3056	1/1	0.20	-1.26	28,28,28,28	0
55	MG	DB	3099	1/1	0.07	-1.28	19,19,19,19	0
55	MG	CA	1617	1/1	0.10	-1.28	149,149,149,149	0
55	MG	DB	3113	1/1	0.09	-1.33	27,27,27,27	0
55	MG	AA	1613	1/1	0.09	-1.35	106,106,106,106	0
55	MG	BB	3094	1/1	0.12	-1.35	81,81,81,81	0
55	MG	BB	3113	1/1	0.07	-1.37	41,41,41,41	0
55	MG	BB	3111	1/1	0.10	-1.43	43,43,43,43	0
55	MG	BB	3007	1/1	0.09	-1.46	115,115,115,115	0
55	MG	AA	1615	1/1	0.07	-1.49	85,85,85,85	0
55	MG	DB	3025	1/1	0.10	-1.50	40,40,40,40	0
55	MG	CA	1609	1/1	0.10	-1.50	60,60,60,60	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BB	3042	1/1	0.13	-1.54	90,90,90,90	0
55	MG	DB	3111	1/1	0.11	-1.56	38,38,38,38	0
55	MG	AA	1624	1/1	0.09	-1.57	88,88,88,88	0
55	MG	BB	3019	1/1	0.12	-1.60	62,62,62,62	0
55	MG	BB	3005	1/1	0.11	-1.64	52,52,52,52	0
55	MG	DB	3003	1/1	0.04	-1.70	24,24,24,24	0
55	MG	DB	3112	1/1	0.16	-1.71	52,52,52,52	0
55	MG	CX	101	1/1	0.06	-1.72	73,73,73,73	0
55	MG	CA	1620	1/1	0.09	-1.74	103,103,103,103	0
55	MG	BB	3040	1/1	0.09	-1.74	64,64,64,64	0
55	MG	CA	1605	1/1	0.05	-1.75	98,98,98,98	0
55	MG	DB	3050	1/1	0.10	-1.76	51,51,51,51	0
55	MG	CA	1612	1/1	0.12	-1.77	95,95,95,95	0
55	MG	CA	1647	1/1	0.06	-1.81	109,109,109,109	0
55	MG	BB	3107	1/1	0.13	-1.81	86,86,86,86	0
55	MG	BB	3102	1/1	0.10	-1.83	71,71,71,71	0
55	MG	DB	3066	1/1	0.18	-1.83	30,30,30,30	0
55	MG	BB	3066	1/1	0.09	-1.84	51,51,51,51	0
55	MG	BB	3038	1/1	0.08	-1.84	125,125,125,125	0
55	MG	DB	3010	1/1	0.11	-1.84	20,20,20,20	0
55	MG	AA	1634	1/1	0.16	-1.86	55,55,55,55	0
55	MG	BB	3101	1/1	0.08	-1.87	50,50,50,50	0
55	MG	AA	1612	1/1	0.09	-1.87	117,117,117,117	0
55	MG	BB	3025	1/1	0.12	-1.92	63,63,63,63	0
55	MG	CA	1633	1/1	0.06	-1.93	136,136,136,136	0
55	MG	CA	1629	1/1	0.07	-1.93	94,94,94,94	0
55	MG	BB	3116	1/1	0.07	-1.93	24,24,24,24	0
55	MG	BB	3072	1/1	0.10	-1.94	58,58,58,58	0
55	MG	BB	3091	1/1	0.15	-1.95	44,44,44,44	0
55	MG	DB	3027	1/1	0.10	-1.95	43,43,43,43	0
55	MG	BB	3067	1/1	0.09	-1.96	39,39,39,39	0
55	MG	CA	1650	1/1	0.07	-1.97	103,103,103,103	0
55	MG	BB	3085	1/1	0.07	-1.97	57,57,57,57	0
55	MG	BB	3103	1/1	0.16	-1.98	38,38,38,38	0
55	MG	AA	1642	1/1	0.10	-2.00	63,63,63,63	0
55	MG	BB	3048	1/1	0.07	-2.00	38,38,38,38	0
55	MG	BB	3079	1/1	0.10	-2.01	46,46,46,46	0
55	MG	DB	3117	1/1	0.04	-2.04	26,26,26,26	0
55	MG	BB	3064	1/1	0.12	-2.05	63,63,63,63	0
55	MG	CA	1626	1/1	0.07	-2.05	154,154,154,154	0
55	MG	CA	1642	1/1	0.05	-2.06	110,110,110,110	0
55	MG	DB	3047	1/1	0.08	-2.06	36,36,36,36	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DB	3102	1/1	0.18	-2.07	67,67,67,67	0
56	ZN	B4	101	1/1	0.02	-2.08	72,72,72,72	0
55	MG	DB	3035	1/1	0.09	-2.12	27,27,27,27	0
55	MG	BB	3092	1/1	0.10	-2.16	62,62,62,62	0
55	MG	BB	3096	1/1	0.08	-2.17	49,49,49,49	0
55	MG	BB	3100	1/1	0.09	-2.19	128,128,128,128	0
55	MG	BB	3008	1/1	0.09	-2.19	63,63,63,63	0
55	MG	DB	3068	1/1	0.06	-2.21	35,35,35,35	0
55	MG	DB	3021	1/1	0.09	-2.26	50,50,50,50	0
55	MG	BB	3114	1/1	0.10	-2.26	57,57,57,57	0
55	MG	DB	3051	1/1	0.07	-2.26	48,48,48,48	0
55	MG	BB	3006	1/1	0.09	-2.27	35,35,35,35	0
55	MG	DB	3018	1/1	0.13	-2.27	32,32,32,32	0
55	MG	DB	3033	1/1	0.11	-2.30	43,43,43,43	0
55	MG	BB	3053	1/1	0.04	-2.31	43,43,43,43	0
55	MG	BB	3047	1/1	0.09	-2.32	131,131,131,131	0
55	MG	CA	1648	1/1	0.07	-2.34	119,119,119,119	0
55	MG	CA	1601	1/1	0.09	-2.38	48,48,48,48	0
55	MG	DB	3076	1/1	0.07	-2.41	49,49,49,49	0
55	MG	DB	3062	1/1	0.10	-2.41	54,54,54,54	0
55	MG	DB	3080	1/1	0.09	-2.42	29,29,29,29	0
55	MG	BB	3098	1/1	0.10	-2.42	73,73,73,73	0
55	MG	CA	1604	1/1	0.07	-2.42	58,58,58,58	0
55	MG	CA	1652	1/1	0.07	-2.44	117,117,117,117	0
55	MG	BB	3002	1/1	0.11	-2.44	31,31,31,31	0
55	MG	BB	3056	1/1	0.12	-2.46	49,49,49,49	0
55	MG	BB	3044	1/1	0.10	-2.47	62,62,62,62	0
55	MG	DB	3007	1/1	0.09	-2.47	49,49,49,49	0
55	MG	DB	3036	1/1	0.09	-2.51	36,36,36,36	0
55	MG	AA	1610	1/1	0.04	-2.55	61,61,61,61	0
55	MG	DB	3013	1/1	0.09	-2.55	62,62,62,62	0
55	MG	AA	1609	1/1	0.12	-2.58	67,67,67,67	0
55	MG	BB	3004	1/1	0.11	-2.59	65,65,65,65	0
55	MG	DB	3067	1/1	0.17	-2.60	33,33,33,33	0
55	MG	BB	3021	1/1	0.13	-2.62	45,45,45,45	0
55	MG	BB	3090	1/1	0.09	-2.62	71,71,71,71	0
55	MG	BB	3037	1/1	0.07	-2.65	56,56,56,56	0
55	MG	BB	3081	1/1	0.08	-2.67	85,85,85,85	0
55	MG	DB	3020	1/1	0.07	-2.68	25,25,25,25	0
55	MG	DB	3074	1/1	0.05	-2.70	9,9,9,9	0
55	MG	BB	3035	1/1	0.08	-2.73	40,40,40,40	0
55	MG	BB	3023	1/1	0.07	-2.77	15,15,15,15	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	CA	1631	1/1	0.10	-2.78	91,91,91,91	0
55	MG	BB	3084	1/1	0.13	-2.80	61,61,61,61	0
55	MG	DB	3118	1/1	0.06	-2.84	35,35,35,35	0
55	MG	BB	3017	1/1	0.07	-2.84	35,35,35,35	0
55	MG	DB	3116	1/1	0.06	-2.85	54,54,54,54	0
55	MG	BB	3009	1/1	0.05	-2.87	92,92,92,92	0
55	MG	BB	3011	1/1	0.09	-2.90	45,45,45,45	0
55	MG	AA	1654	1/1	0.05	-2.95	49,49,49,49	0
55	MG	BB	3028	1/1	0.11	-2.96	54,54,54,54	0
55	MG	DB	3098	1/1	0.07	-2.99	42,42,42,42	0
55	MG	BB	3088	1/1	0.09	-3.00	76,76,76,76	0
55	MG	DB	3015	1/1	0.09	-3.01	49,49,49,49	0
55	MG	DB	3107	1/1	0.09	-3.02	24,24,24,24	0
55	MG	DB	3086	1/1	0.08	-3.02	57,57,57,57	0
55	MG	DB	3011	1/1	0.09	-3.02	16,16,16,16	0
55	MG	DB	3071	1/1	0.10	-3.03	30,30,30,30	0
55	MG	BB	3082	1/1	0.12	-3.06	80,80,80,80	0
55	MG	DB	3045	1/1	0.09	-3.10	140,140,140,140	0
55	MG	AA	1659	1/1	0.07	-3.11	86,86,86,86	0
55	MG	AA	1641	1/1	0.07	-3.17	111,111,111,111	0
55	MG	DB	3103	1/1	0.04	-3.19	46,46,46,46	0
55	MG	BB	3036	1/1	0.09	-3.24	52,52,52,52	0
55	MG	BB	3045	1/1	0.07	-3.28	60,60,60,60	0
55	MG	CA	1602	1/1	0.07	-3.30	87,87,87,87	0
55	MG	DB	3085	1/1	0.05	-3.37	21,21,21,21	0
55	MG	BB	3003	1/1	0.09	-3.38	20,20,20,20	0
55	MG	DB	3006	1/1	0.08	-3.39	38,38,38,38	0
55	MG	CA	1622	1/1	0.08	-3.40	98,98,98,98	0
55	MG	BB	3049	1/1	0.06	-3.40	40,40,40,40	0
55	MG	AA	1648	1/1	0.06	-3.48	67,67,67,67	0
55	MG	BB	3104	1/1	0.08	-3.50	38,38,38,38	0
55	MG	BB	3062	1/1	0.06	-3.56	42,42,42,42	0
55	MG	DB	3090	1/1	0.08	-3.56	62,62,62,62	0
55	MG	DB	3017	1/1	0.08	-3.57	34,34,34,34	0
55	MG	CA	1616	1/1	0.06	-3.63	80,80,80,80	0
55	MG	AA	1644	1/1	0.06	-3.66	99,99,99,99	0
55	MG	BB	3050	1/1	0.08	-3.68	54,54,54,54	0
55	MG	AA	1601	1/1	0.04	-3.68	62,62,62,62	0
55	MG	DB	3024	1/1	0.05	-3.68	22,22,22,22	0
55	MG	DB	3048	1/1	0.07	-3.70	45,45,45,45	0
55	MG	BB	3070	1/1	0.08	-3.73	52,52,52,52	0
55	MG	CA	1630	1/1	0.06	-3.73	97,97,97,97	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DB	3005	1/1	0.07	-3.76	66,66,66,66	0
55	MG	BB	3022	1/1	0.06	-3.77	56,56,56,56	0
55	MG	DB	3038	1/1	0.08	-3.80	19,19,19,19	0
55	MG	DB	3014	1/1	0.04	-3.83	32,32,32,32	0
55	MG	DB	3084	1/1	0.10	-3.85	26,26,26,26	0
55	MG	BB	3074	1/1	0.07	-3.88	25,25,25,25	0
55	MG	AA	1604	1/1	0.06	-3.90	45,45,45,45	0
55	MG	BB	3018	1/1	0.07	-3.92	42,42,42,42	0
55	MG	DB	3040	1/1	0.09	-3.93	41,41,41,41	0
55	MG	DB	3105	1/1	0.11	-4.05	18,18,18,18	0
55	MG	BB	3086	1/1	0.09	-4.05	50,50,50,50	0
55	MG	BB	3026	1/1	0.11	-4.05	26,26,26,26	0
55	MG	BB	3032	1/1	0.14	-4.06	53,53,53,53	0
55	MG	DB	3044	1/1	0.07	-4.14	20,20,20,20	0
55	MG	DB	3063	1/1	0.06	-4.15	45,45,45,45	0
55	MG	DB	3083	1/1	0.11	-4.18	31,31,31,31	0
55	MG	BB	3108	1/1	0.11	-4.20	30,30,30,30	0
55	MG	BB	3013	1/1	0.07	-4.22	52,52,52,52	0
55	MG	CA	1636	1/1	0.08	-4.22	127,127,127,127	0
55	MG	DB	3097	1/1	0.07	-4.23	39,39,39,39	0
55	MG	AA	1633	1/1	0.05	-4.24	85,85,85,85	0
55	MG	DB	3055	1/1	0.04	-4.25	30,30,30,30	0
55	MG	DB	3104	1/1	0.08	-4.27	50,50,50,50	0
55	MG	BB	3020	1/1	0.27	-4.30	45,45,45,45	0
55	MG	AA	1605	1/1	0.07	-4.31	87,87,87,87	0
55	MG	DB	3087	1/1	0.08	-4.41	28,28,28,28	0
55	MG	DB	3101	1/1	0.05	-4.54	44,44,44,44	0
55	MG	DB	3100	1/1	0.05	-4.69	10,10,10,10	0
55	MG	BB	3061	1/1	0.06	-4.73	57,57,57,57	0
55	MG	DB	3041	1/1	0.05	-4.89	32,32,32,32	0
55	MG	DB	3004	1/1	0.06	-4.94	21,21,21,21	0
55	MG	BB	3097	1/1	0.06	-4.95	112,112,112,112	0
55	MG	DB	3059	1/1	0.08	-4.96	110,110,110,110	0
55	MG	DB	3002	1/1	0.10	-4.97	44,44,44,44	0
55	MG	BB	3039	1/1	0.10	-5.02	55,55,55,55	0
55	MG	BB	3073	1/1	0.06	-5.07	30,30,30,30	0
55	MG	CA	1625	1/1	0.07	-5.12	54,54,54,54	0
55	MG	AA	1629	1/1	0.07	-5.18	53,53,53,53	0
55	MG	DB	3001	1/1	0.05	-5.18	14,14,14,14	0
55	MG	DB	3016	1/1	0.05	-5.22	43,43,43,43	0
55	MG	DB	3110	1/1	0.07	-5.29	41,41,41,41	0
55	MG	DB	3028	1/1	0.05	-5.37	42,42,42,42	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DB	3009	1/1	0.04	-5.47	48,48,48,48	0
55	MG	DB	3019	1/1	0.06	-5.50	43,43,43,43	0
55	MG	DB	3026	1/1	0.07	-5.60	38,38,38,38	0
55	MG	DB	3075	1/1	0.04	-5.65	46,46,46,46	0
55	MG	BB	3001	1/1	0.07	-5.76	57,57,57,57	0
55	MG	BB	3069	1/1	0.10	-5.83	28,28,28,28	0
55	MG	DB	3073	1/1	0.08	-5.90	7,7,7,7	0
55	MG	DB	3072	1/1	0.13	-5.95	39,39,39,39	0
55	MG	DB	3060	1/1	0.06	-5.99	35,35,35,35	0
55	MG	BB	3043	1/1	0.07	-6.46	107,107,107,107	0
55	MG	DB	3081	1/1	0.05	-7.24	36,36,36,36	0
55	MG	BB	3055	1/1	0.08	-7.34	72,72,72,72	0
55	MG	DB	3049	1/1	0.12	-7.90	42,42,42,42	0
55	MG	BB	3030	1/1	0.08	-7.94	111,111,111,111	0
55	MG	DB	3022	1/1	0.06	-8.11	42,42,42,42	0
55	MG	AA	1616	1/1	0.05	-8.62	104,104,104,104	0
55	MG	CA	1628	1/1	0.07	-8.70	106,106,106,106	0
55	MG	DB	3042	1/1	0.11	-8.80	56,56,56,56	0
55	MG	AA	1603	1/1	0.05	-9.41	55,55,55,55	0
55	MG	DB	3079	1/1	0.07	-9.67	18,18,18,18	0
55	MG	BB	3015	1/1	0.08	-9.81	69,69,69,69	0
55	MG	DB	3046	1/1	0.08	-9.95	47,47,47,47	0
55	MG	DB	3037	1/1	0.08	-10.12	32,32,32,32	0
55	MG	DB	3078	1/1	0.05	-10.20	28,28,28,28	0
55	MG	DB	3031	1/1	0.04	-10.39	16,16,16,16	0
55	MG	BB	3078	1/1	0.08	-10.43	71,71,71,71	0
55	MG	BB	3058	1/1	0.06	-10.44	62,62,62,62	0
55	MG	BB	3059	1/1	0.07	-10.96	37,37,37,37	0
55	MG	BB	3052	1/1	0.05	-11.07	33,33,33,33	0
55	MG	DB	3096	1/1	0.06	-11.20	46,46,46,46	0
55	MG	DB	3106	1/1	0.06	-12.36	29,29,29,29	0
55	MG	BB	3065	1/1	0.11	-12.93	46,46,46,46	0
55	MG	AA	1657	1/1	0.06	-14.12	85,85,85,85	0
55	MG	DB	3053	1/1	0.05	-14.57	37,37,37,37	0
55	MG	BB	3089	1/1	0.05	-17.24	51,51,51,51	0
55	MG	BB	3068	1/1	0.10	-27.17	40,40,40,40	0
55	MG	CA	1645	1/1	0.11	-49.00	119,119,119,119	0
55	MG	DB	3039	1/1	0.06	-128.69	95,95,95,95	0
55	MG	AA	1611	1/1	5.42	-	148,148,148,148	0
55	MG	BJ	201	1/1	0.63	-	160,160,160,160	0
55	MG	DB	3115	1/1	0.43	-	132,132,132,132	0
55	MG	AA	1623	1/1	0.22	-	115,115,115,115	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.