



wwPDB X-ray Structure Validation Summary Report i

Jun 16, 2014 – 08:58 PM BST

PDB ID : 4V7S
Title : Crystal structure of the E. coli ribosome bound to telithromycin.
Authors : Dunkle, J.A.; Xiong, L.; Mankin, A.S.; Cate, J.H.D.
Deposited on : 2010-08-05
Resolution : 3.25 Å(reported)

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

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

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

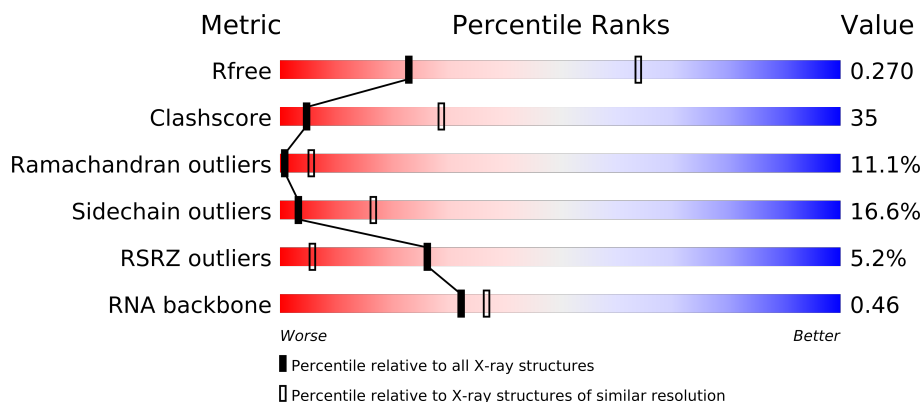
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.25 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	1085 (3.32-3.20)
Clashscore	79885	1374 (3.32-3.20)
Ramachandran outliers	78287	1348 (3.32-3.20)
Sidechain outliers	78261	1346 (3.32-3.20)
RSRZ outliers	66119	1086 (3.32-3.20)
RNA backbone	1838	1028 (3.82-2.70)

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 ≥ 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	1533	
2	AB	218	
2	CB	218	
3	AC	206	
3	CC	206	
4	AD	205	
4	CD	205	
5	AE	150	
5	CE	150	
6	AF	100	
6	CF	100	
7	AG	151	

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Mol	Chain	Length	Quality of chain
8	AH	129	
8	CH	129	
9	AI	127	
9	CI	127	
10	AJ	98	
10	CJ	98	
11	AK	117	
11	CK	117	
12	AL	123	
12	CL	123	
13	AM	114	
14	AN	100	
14	CN	100	
15	AO	88	
15	CO	88	
16	AP	82	
17	AQ	80	
17	CQ	80	
18	AR	55	
18	CR	55	
19	AS	79	
19	CS	79	
20	AT	85	
20	CT	85	
21	AU	51	
21	CU	51	
22	BA	2903	
22	DA	2903	
23	BB	118	
24	BC	271	
24	DC	271	
25	BD	209	
25	DD	209	
26	BE	201	
26	DE	201	
27	BF	177	
28	BG	176	
28	DG	176	
29	BH	149	
29	DH	149	
30	BI	141	
30	DI	141	

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Mol	Chain	Length	Quality of chain
31	BJ	142	
31	DJ	142	
32	BK	122	
32	DK	122	
33	BL	143	
33	DL	143	
34	BM	136	
34	DM	136	
35	BN	120	
35	DN	120	
36	BO	116	
36	DO	116	
37	BP	114	
37	DP	114	
38	BQ	117	
38	DQ	117	
39	BR	103	
39	DR	103	
40	BS	110	
40	DS	110	
41	BT	93	
41	DT	93	
42	BU	102	
42	DU	102	
43	BV	94	
43	DV	94	
44	BW	79	
44	DW	79	
45	BX	77	
45	DX	77	
46	BY	63	
46	DY	63	
47	BZ	58	
47	DZ	58	
48	B0	56	
48	D0	56	
49	B1	50	
49	D1	50	
50	B2	46	
50	D2	46	
51	B3	64	
51	D3	64	

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Mol	Chain	Length	Quality of chain
52	B4	38	
52	D4	38	
53	CA	1530	
54	CG	150	
55	CM	113	
56	CP	80	
57	DB	117	
58	DF	178	

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

Mol	Type	Chain	Res	Geometry	Electron density
59	MG	AA	1608	-	X
59	MG	AA	1614	-	X
59	MG	AA	1619	-	X
59	MG	AA	1621	-	X
59	MG	AA	1622	-	X
59	MG	AA	1627	-	X
59	MG	AA	1628	-	X
59	MG	AA	1636	-	X
59	MG	AA	1641	-	X
59	MG	BA	3004	-	X
59	MG	BA	3013	-	X
59	MG	BA	3014	-	X
59	MG	BA	3021	-	X
59	MG	BA	3025	-	X
59	MG	BA	3033	-	X
59	MG	BA	3034	-	X
59	MG	BA	3036	-	X
59	MG	BA	3040	-	X
59	MG	BA	3055	-	X
59	MG	BA	3056	-	X
59	MG	BA	3057	-	X
59	MG	BA	3059	-	X
59	MG	BA	3060	-	X
59	MG	BA	3062	-	X
59	MG	BA	3069	-	X
59	MG	BA	3070	-	X
59	MG	BA	3072	-	X
59	MG	BA	3074	-	X
59	MG	BA	3078	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
59	MG	BA	3083	-	X
59	MG	BA	3085	-	X
59	MG	BA	3095	-	X
59	MG	BA	3096	-	X
59	MG	BA	3099	-	X
59	MG	BA	3102	-	X
59	MG	BA	3105	-	X
59	MG	BA	3106	-	X
59	MG	BA	3110	-	X
59	MG	BA	3117	-	X
59	MG	BA	3120	-	X
59	MG	BA	3122	-	X
59	MG	BA	3129	-	X
59	MG	BA	3131	-	X
59	MG	BA	3133	-	X
59	MG	BA	3134	-	X
59	MG	BB	201	-	X
59	MG	CA	1603	-	X
59	MG	CA	1612	-	X
59	MG	CA	1614	-	X
59	MG	CA	1615	-	X
59	MG	CA	1619	-	X
59	MG	CA	1626	-	X
59	MG	CA	1627	-	X
59	MG	CA	1629	-	X
59	MG	CA	1636	-	X
59	MG	CA	1639	-	X
59	MG	CE	201	-	X
59	MG	DA	3002	-	X
59	MG	DA	3003	-	X
59	MG	DA	3005	-	X
59	MG	DA	3007	-	X
59	MG	DA	3011	-	X
59	MG	DA	3015	-	X
59	MG	DA	3016	-	X
59	MG	DA	3020	-	X
59	MG	DA	3022	-	X
59	MG	DA	3026	-	X
59	MG	DA	3028	-	X
59	MG	DA	3029	-	X
59	MG	DA	3030	-	X
59	MG	DA	3036	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
59	MG	DA	3049	-	X
59	MG	DA	3053	-	X
59	MG	DA	3057	-	X
59	MG	DA	3058	-	X
59	MG	DA	3059	-	X
59	MG	DA	3060	-	X
59	MG	DA	3062	-	X
59	MG	DA	3063	-	X
59	MG	DA	3064	-	X
59	MG	DA	3069	-	X
59	MG	DA	3074	-	X
59	MG	DA	3078	-	X
59	MG	DA	3079	-	X
59	MG	DA	3085	-	X
59	MG	DA	3086	-	X
59	MG	DA	3091	-	X
59	MG	DA	3094	-	X
59	MG	DA	3097	-	X
59	MG	DA	3098	-	X
59	MG	DA	3100	-	X
59	MG	DA	3106	-	X
59	MG	DA	3108	-	X
59	MG	DA	3109	-	X
59	MG	DA	3127	-	X
59	MG	DA	3129	-	X
59	MG	DA	3130	-	X
59	MG	DA	3132	-	X
59	MG	DC	302	-	X
59	MG	DJ	201	-	X

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 284525 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 rRNA.

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

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	218	Total	C	N	O	S	0	0	0
			1705	1081	305	312	7			
2	CB	218	Total	C	N	O	S	0	0	0
			1705	1081	305	312	7			

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0	0
			1625	1028	305	289	3			
3	CC	206	Total	C	N	O	S	0	0	0
			1625	1028	305	289	3			

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	150	Total	C	N	O	S	0	0	0
			1106	687	211	202	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	CE	150	Total	C	N	O	S	0	0	0
			1106	687	211	202	6			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	100	Total	C	N	O	S	0	0	0
			818	515	148	149	6			
6	CF	100	Total	C	N	O	S	0	0	0
			818	515	148	149	6			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	151	Total	C	N	O	S	0	0	0
			1182	735	227	216	4			

- Molecule 8 is a protein called 30S ribosomal protein S8.

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

- Molecule 9 is a protein called 30S ribosomal protein S9.

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

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	98	Total	C	N	O	S	0	0	0
			787	493	150	143	1			
10	CJ	98	Total	C	N	O	S	0	0	0
			787	493	150	143	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

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

- Molecule 12 is a protein called 30S ribosomal protein S12.

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

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	114	Total	C	N	O	S	0	0	0
			884	546	178	157	3			

- Molecule 14 is a protein called 30S ribosomal protein S14.

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

- Molecule 15 is a protein called 30S ribosomal protein S15.

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

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	80	Total	C	N	O	S	0	0	0
			649	411	121	114	3			
17	CQ	80	Total	C	N	O	S	0	0	0
			649	411	121	114	3			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AR	55	Total	C	N	O	S	0	0	0
			456	288	86	82				
18	CR	55	Total	C	N	O	S	0	0	0
			456	288	86	82				

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	79	Total	C	N	O	S	0	0	0
			638	408	120	108	2			
19	CS	79	Total	C	N	O	S	0	0	0
			638	408	120	108	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AU	51	Total	C	N	O	S	0	0	0
			426	265	86	74	1			
21	CU	51	Total	C	N	O	S	0	0	0
			426	265	86	74	1			

- Molecule 22 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	BA	2854	Total	C	N	O	P	0	0	0
			61274	27334	11279	19807	2854			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	DA	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	BC	271	Total	C	N	O	S	0	0	0
			2083	1288	423	365	7			
24	DC	271	Total	C	N	O	S	0	0	0
			2083	1288	423	365	7			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BF	177	Total	C	N	O	S	0	0	0
			1411	899	249	257	6			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BK	122	Total	C	N	O	S	0	0	0
			939	587	180	166	6			
32	DK	122	Total	C	N	O	S	0	0	0
			939	587	180	166	6			

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BN	120	Total	C	N	O	S	0	0	0
			961	593	196	167	5			
35	DN	120	Total	C	N	O	S	0	0	0
			961	593	196	167	5			

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BT	93	Total	C	N	O	S	0	0	0
			739	466	139	132	2			
41	DT	93	Total	C	N	O	S	0	0	0
			739	466	139	132	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
42	BU	102	Total	C	N	O	0	0	0
			780	492	146	142			
42	DU	102	Total	C	N	O	0	0	0
			780	492	146	142			

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	B1	50	Total	C	N	O	0	0	0
			410	263	75	72			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	D1	50	Total	C	N	O	0	0	0
			410	263	75	72			

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

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

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

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

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

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

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

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

- Molecule 54 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	CG	150	Total	C	N	O	S	0	0	0
			1175	730	226	215	4			

- Molecule 55 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	CM	113	Total	C	N	O	S	0	0	0
			877	541	177	156	3			

- Molecule 56 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	CP	80	Total	C	N	O	S	0	0	0
			639	400	126	112	1			

- Molecule 57 is a RNA chain called 5S rRNA.

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

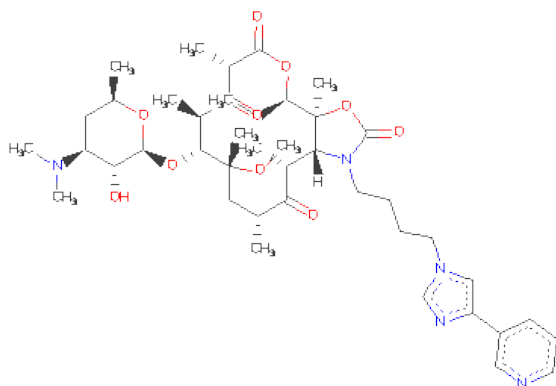
- Molecule 58 is a protein called 50S ribosomal protein L5.

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

- Molecule 59 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	BB	4	Total	Mg	0	0
			4	4		
59	BA	134	Total	Mg	0	0
			134	134		
59	CA	41	Total	Mg	0	0
			41	41		
59	DJ	1	Total	Mg	0	0
			1	1		
59	AA	43	Total	Mg	0	0
			43	43		
59	DA	133	Total	Mg	0	0
			133	133		
59	CE	1	Total	Mg	0	0
			1	1		
59	DC	2	Total	Mg	0	0
			2	2		
59	DB	1	Total	Mg	0	0
			1	1		

- Molecule 60 is TELITHROMYCIN (three-letter code: TEL) (formula: $C_{43}H_{65}N_5O_{10}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
60	BA	1	Total	C	N	O	0	0
			58	43	5	10		

- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 62 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	AA	198	Total	O	0	0
			198	198		
62	AL	1	Total	O	0	0
			1	1		
62	AN	6	Total	O	0	0
			6	6		
62	AT	2	Total	O	0	0
			2	2		
62	AU	1	Total	O	0	0
			1	1		
62	BA	598	Total	O	0	0
			598	598		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	BB	20	Total 20	O 20	0	0
62	BC	10	Total 10	O 10	0	0
62	BD	2	Total 2	O 2	0	0
62	BE	1	Total 1	O 1	0	0
62	BL	2	Total 2	O 2	0	0
62	BN	3	Total 3	O 3	0	0
62	BQ	1	Total 1	O 1	0	0
62	BR	1	Total 1	O 1	0	0
62	BT	1	Total 1	O 1	0	0
62	B2	1	Total 1	O 1	0	0
62	B3	3	Total 3	O 3	0	0
62	B4	1	Total 1	O 1	0	0
62	CA	192	Total 192	O 192	0	0
62	CE	5	Total 5	O 5	0	0
62	CI	1	Total 1	O 1	0	0
62	CL	1	Total 1	O 1	0	0
62	CN	3	Total 3	O 3	0	0
62	CT	3	Total 3	O 3	0	0
62	CU	2	Total 2	O 2	0	0
62	DA	595	Total 595	O 595	0	0
62	DB	4	Total 4	O 4	0	0

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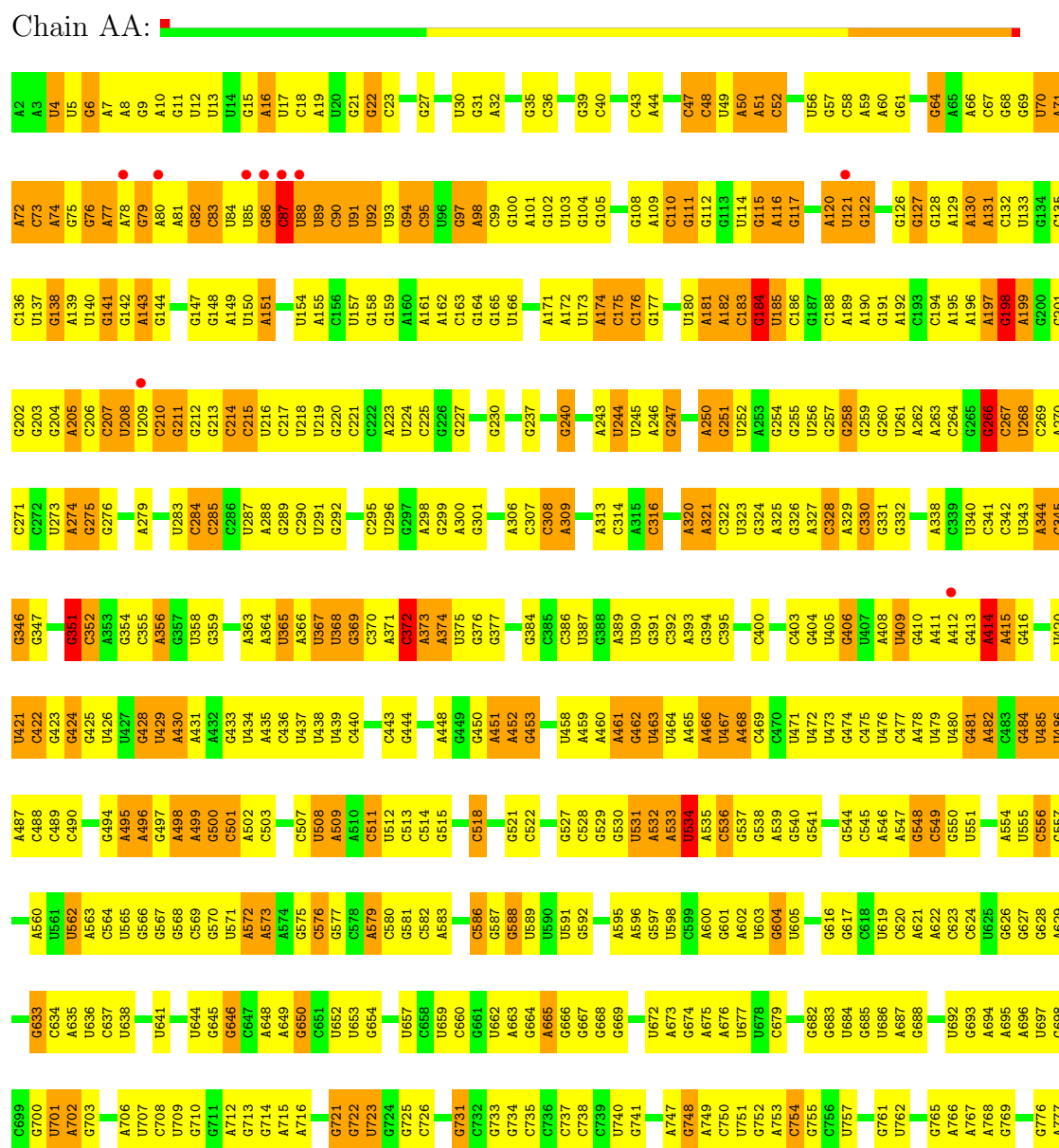
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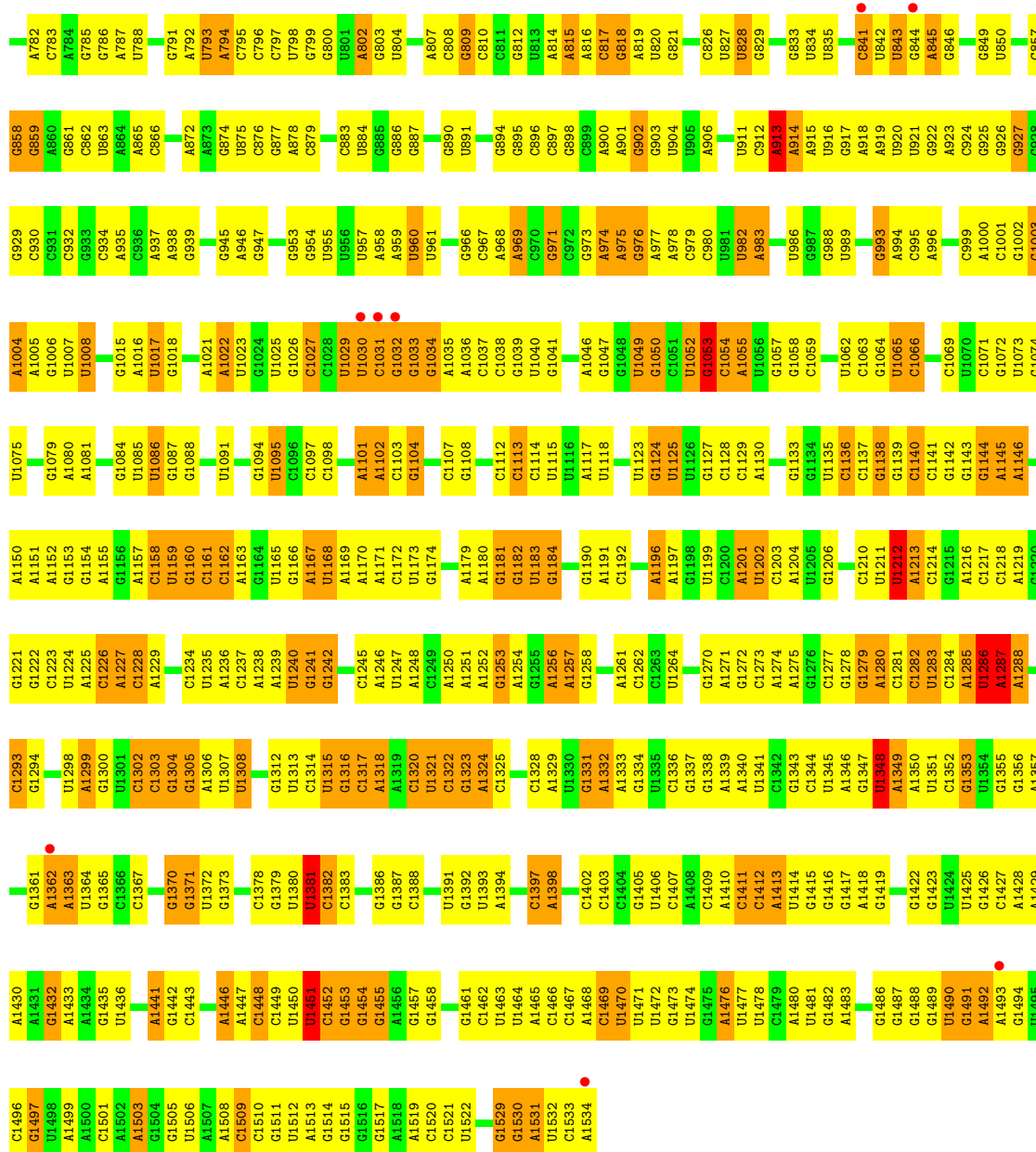
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	DC	13	Total 13	O 13	0	0
62	DD	3	Total 3	O 3	0	0
62	DE	3	Total 3	O 3	0	0
62	DJ	6	Total 6	O 6	0	0
62	DL	6	Total 6	O 6	0	0
62	DN	2	Total 2	O 2	0	0
62	DT	3	Total 3	O 3	0	0
62	DU	2	Total 2	O 2	0	0
62	DV	1	Total 1	O 1	0	0
62	D2	1	Total 1	O 1	0	0
62	D3	1	Total 1	O 1	0	0
62	D4	3	Total 3	O 3	0	0

3 Residue-property plots

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

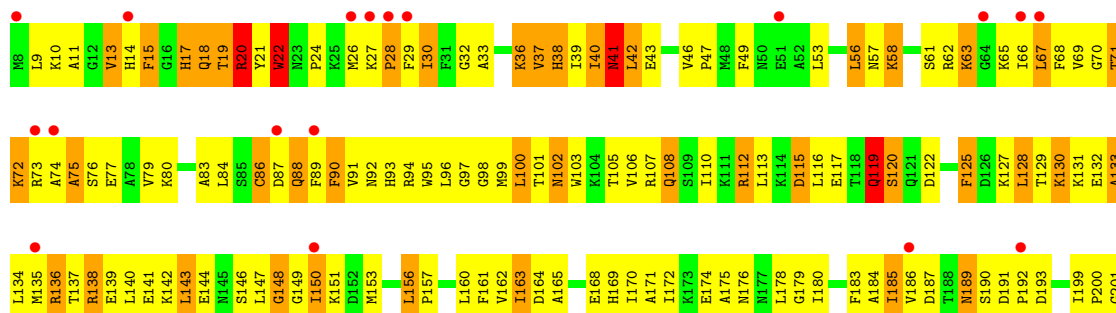
• Molecule 1: 16S rRNA





• Molecule 2: 30S ribosomal protein S2

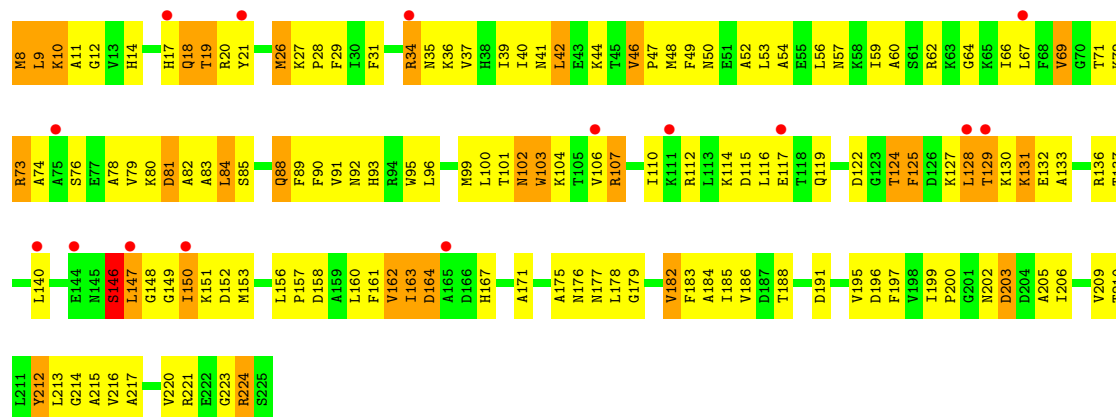
Chain AB:





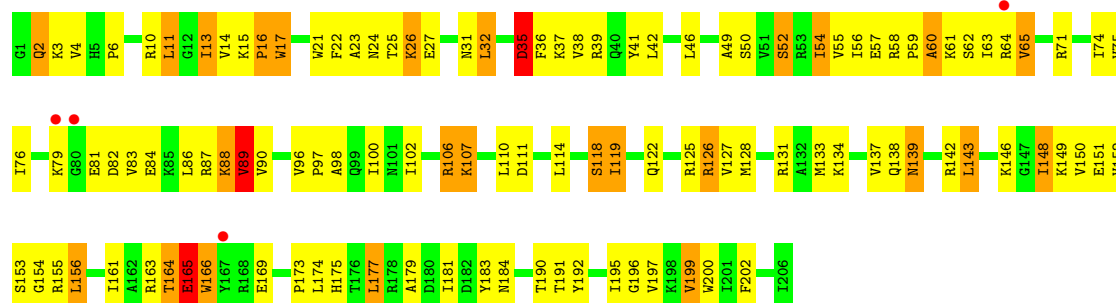
• Molecule 2: 30S ribosomal protein S2

Chain CB:



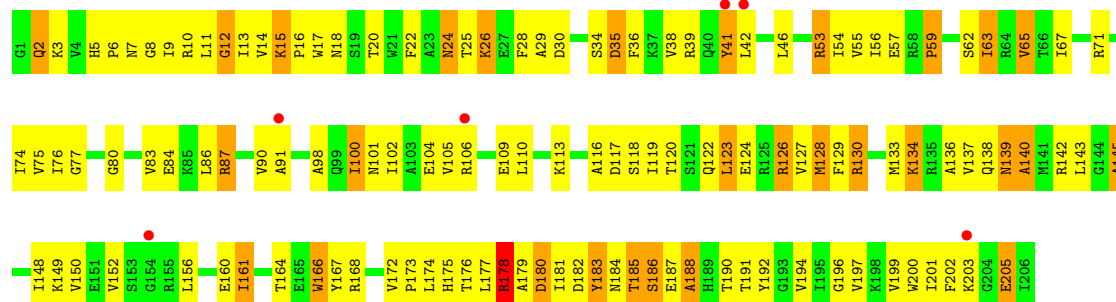
• Molecule 3: 30S ribosomal protein S3

Chain AC:



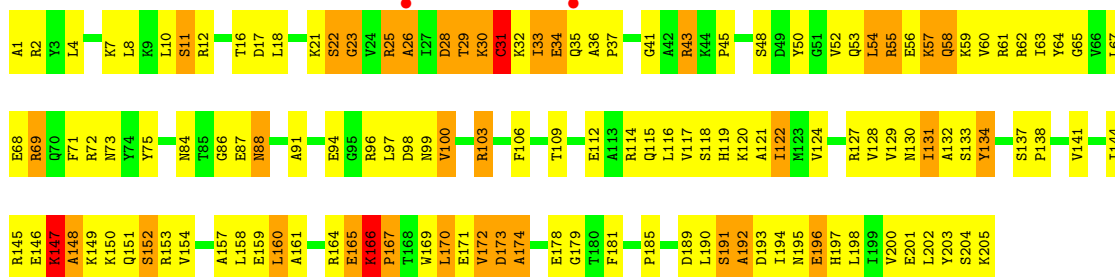
• Molecule 3: 30S ribosomal protein S3

Chain CC:



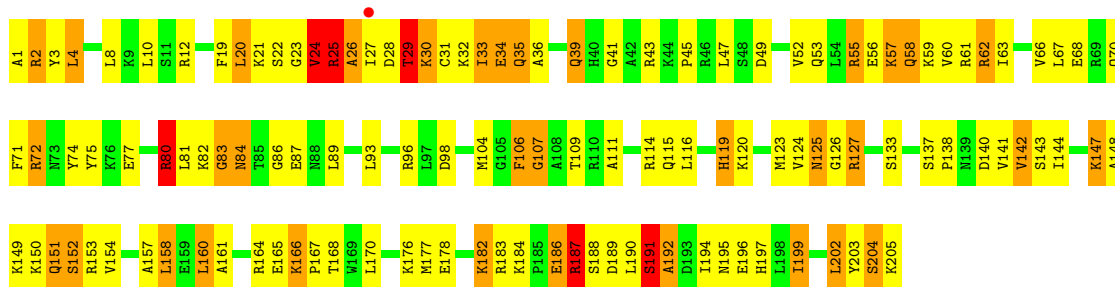
• Molecule 4: 30S ribosomal protein S4

Chain AD:



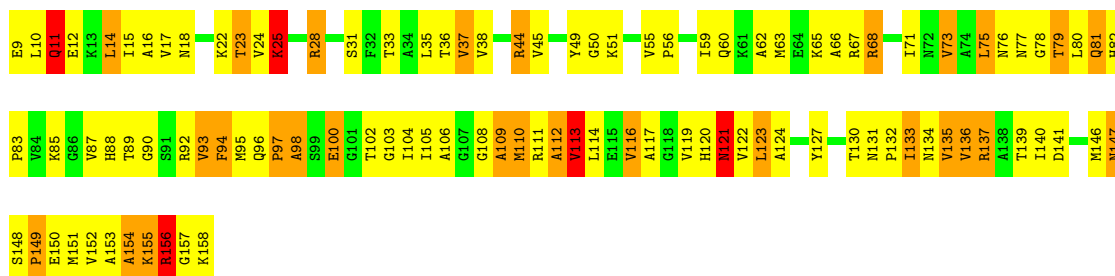
• Molecule 4: 30S ribosomal protein S4

Chain CD:



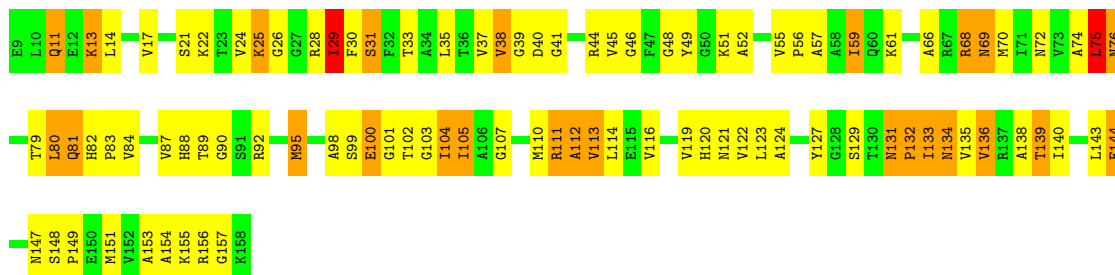
• Molecule 5: 30S ribosomal protein S5

Chain AE:



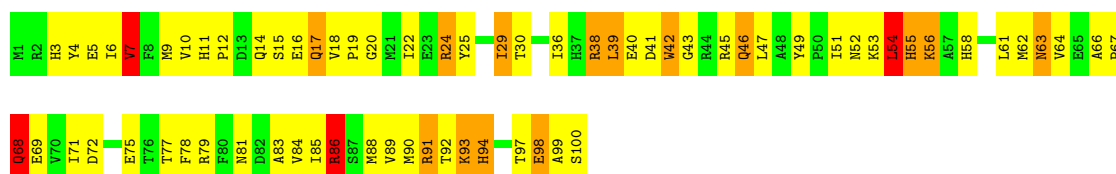
• Molecule 5: 30S ribosomal protein S5

Chain CE:



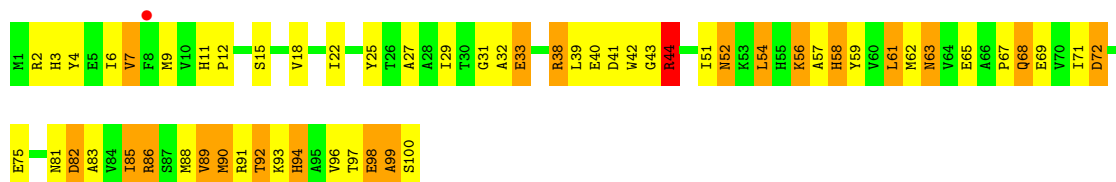
• Molecule 6: 30S ribosomal protein S6

Chain AF:



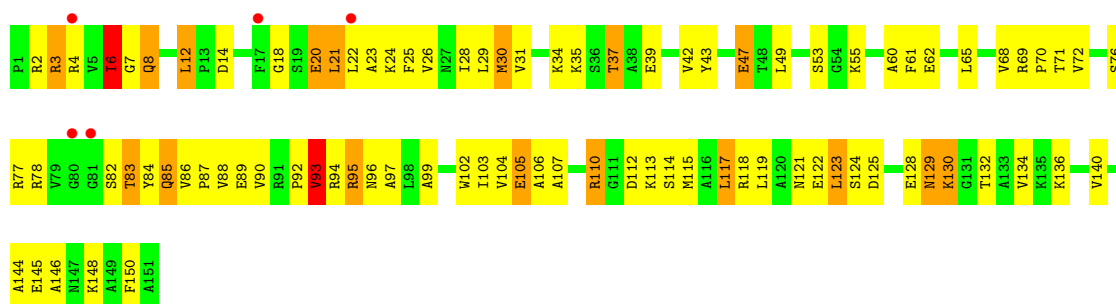
• Molecule 6: 30S ribosomal protein S6

Chain CF:



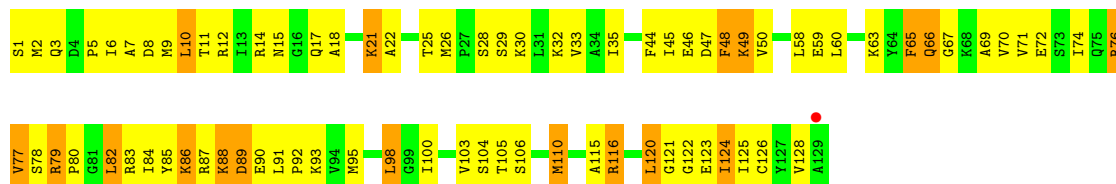
• Molecule 7: 30S ribosomal protein S7

Chain AG:



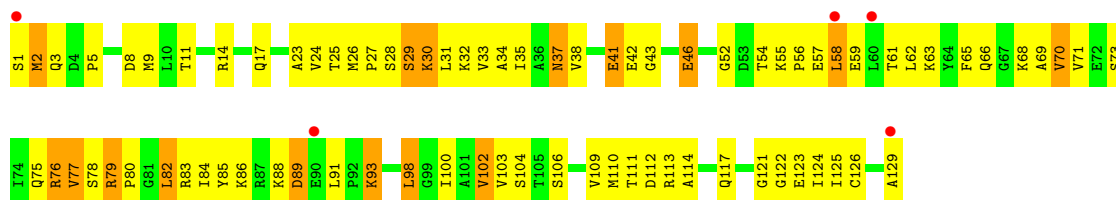
• Molecule 8: 30S ribosomal protein S8

Chain AH:



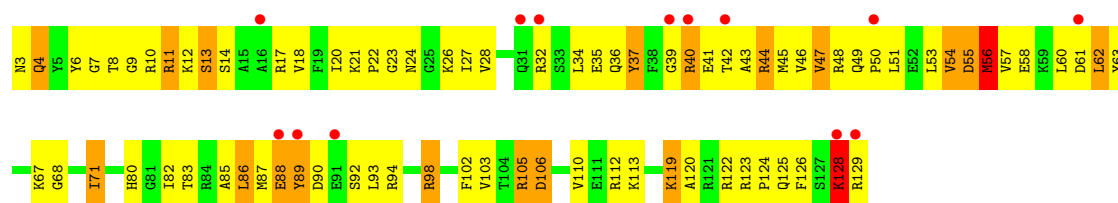
• Molecule 8: 30S ribosomal protein S8

Chain CH:



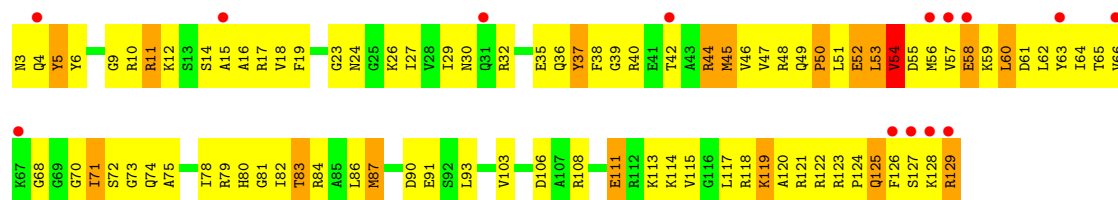
• Molecule 9: 30S ribosomal protein S9

Chain AI:



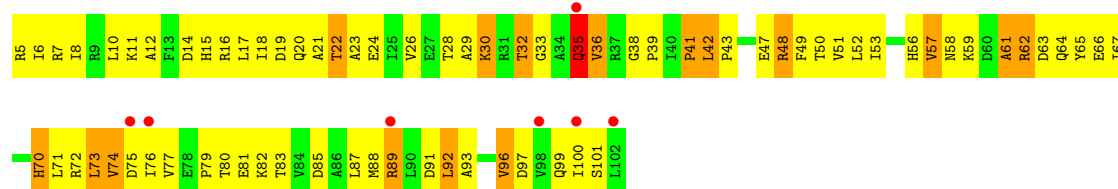
• Molecule 9: 30S ribosomal protein S9

Chain CI:



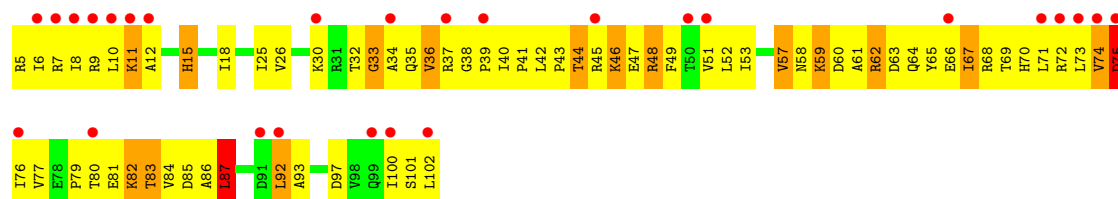
• Molecule 10: 30S ribosomal protein S10

Chain AJ:



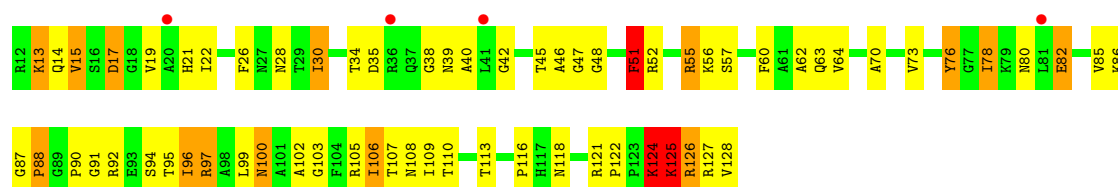
• Molecule 10: 30S ribosomal protein S10

Chain CJ:



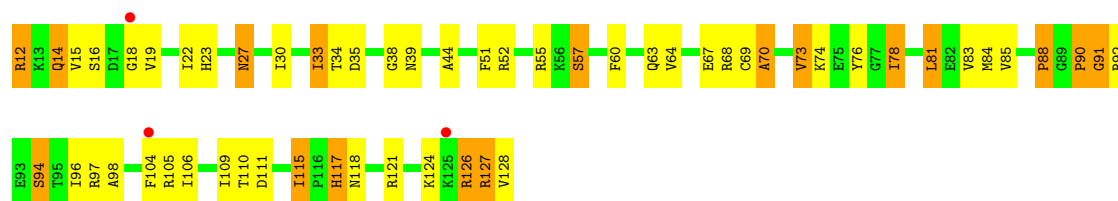
• Molecule 11: 30S ribosomal protein S11

Chain AK:



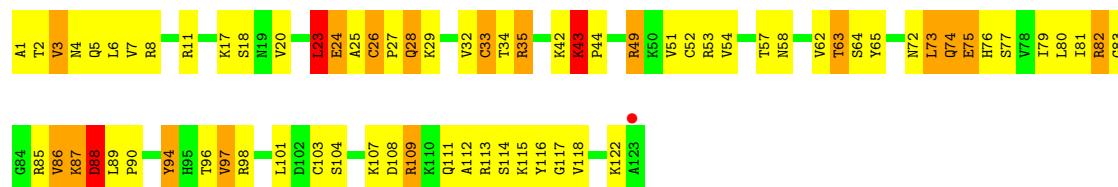
• Molecule 11: 30S ribosomal protein S11

Chain CK:



• Molecule 12: 30S ribosomal protein S12

Chain AL:



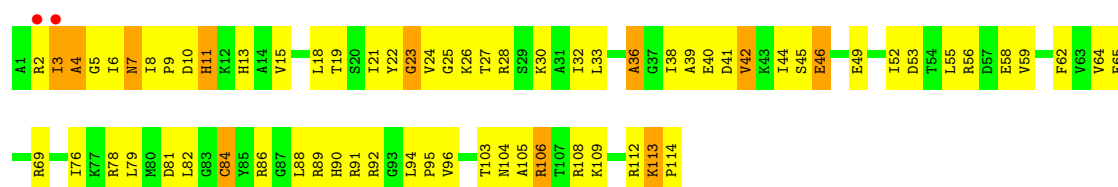
• Molecule 12: 30S ribosomal protein S12

Chain CL:



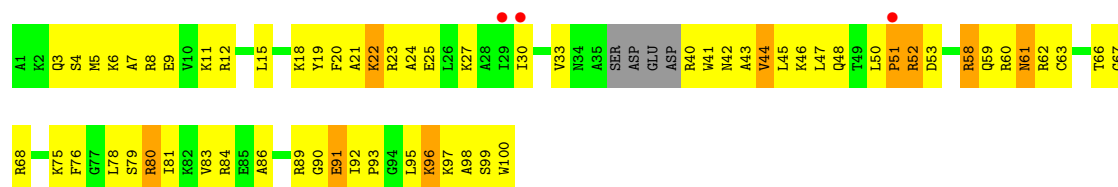
• Molecule 13: 30S ribosomal protein S13

Chain AM:



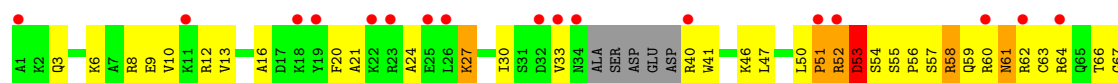
• Molecule 14: 30S ribosomal protein S14

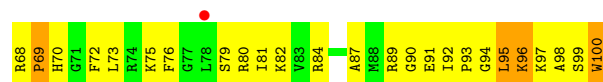
Chain AN:



• Molecule 14: 30S ribosomal protein S14

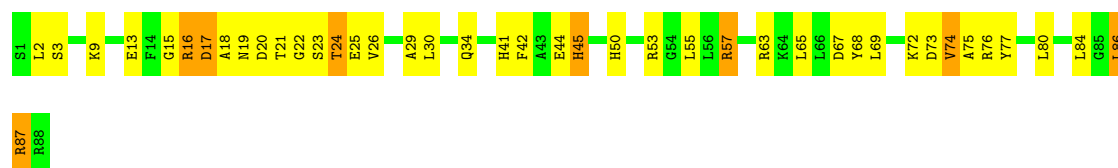
Chain CN:





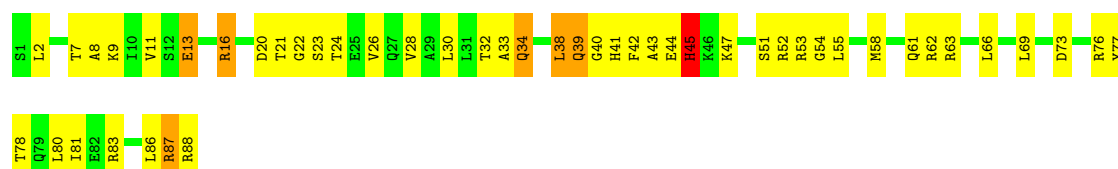
- Molecule 15: 30S ribosomal protein S15

Chain AO:



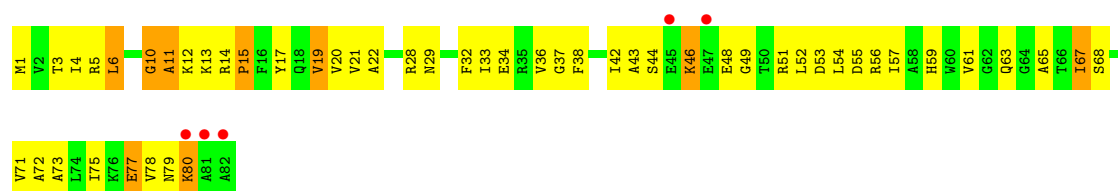
- Molecule 15: 30S ribosomal protein S15

Chain CO:



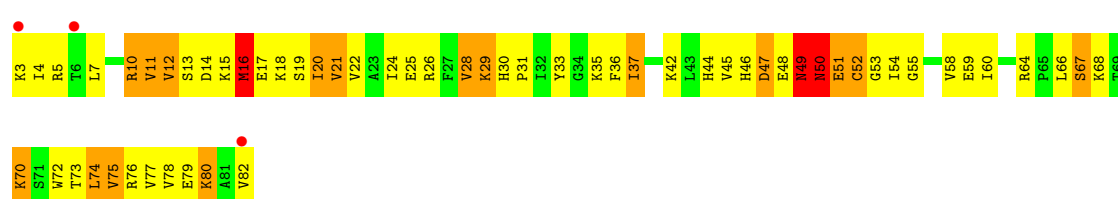
- Molecule 16: 30S ribosomal protein S16

Chain AP:



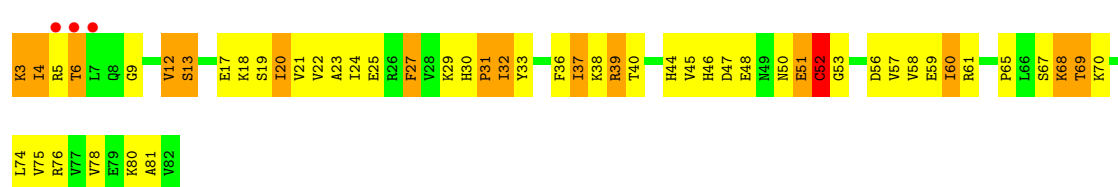
- Molecule 17: 30S ribosomal protein S17

Chain AQ:



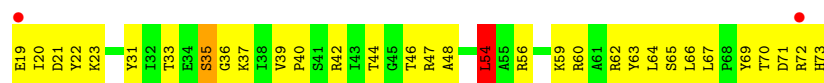
- Molecule 17: 30S ribosomal protein S17

Chain CQ:



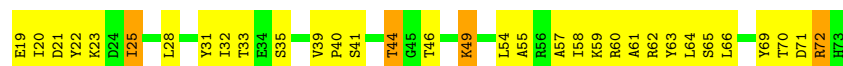
- Molecule 18: 30S ribosomal protein S18

Chain AR:



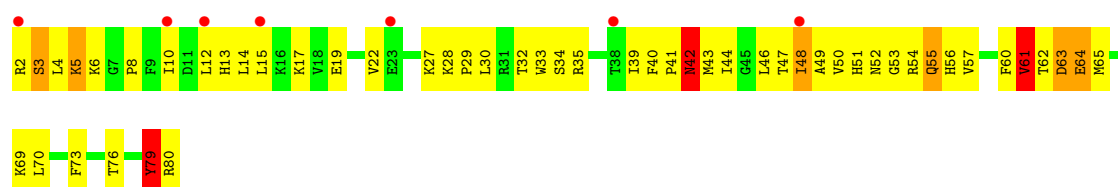
- Molecule 18: 30S ribosomal protein S18

Chain CR:



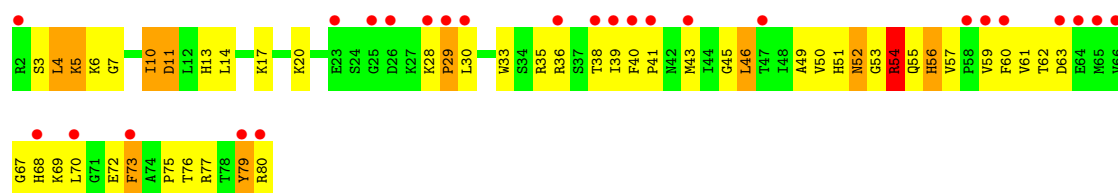
- Molecule 19: 30S ribosomal protein S19

Chain AS:



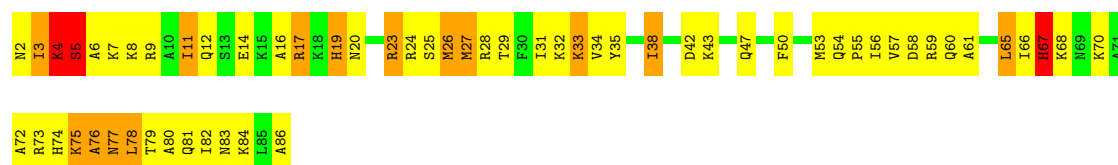
- Molecule 19: 30S ribosomal protein S19

Chain CS:



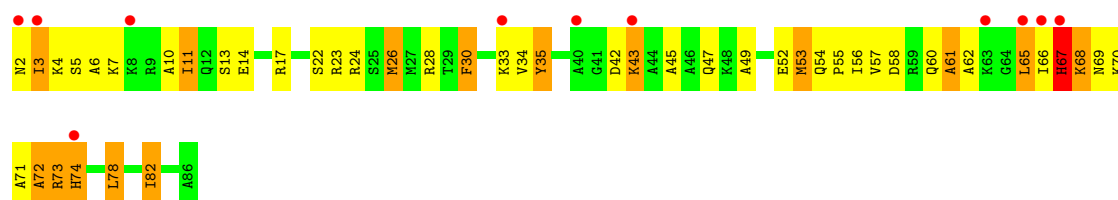
- Molecule 20: 30S ribosomal protein S20

Chain AT:



- Molecule 20: 30S ribosomal protein S20

Chain CT:

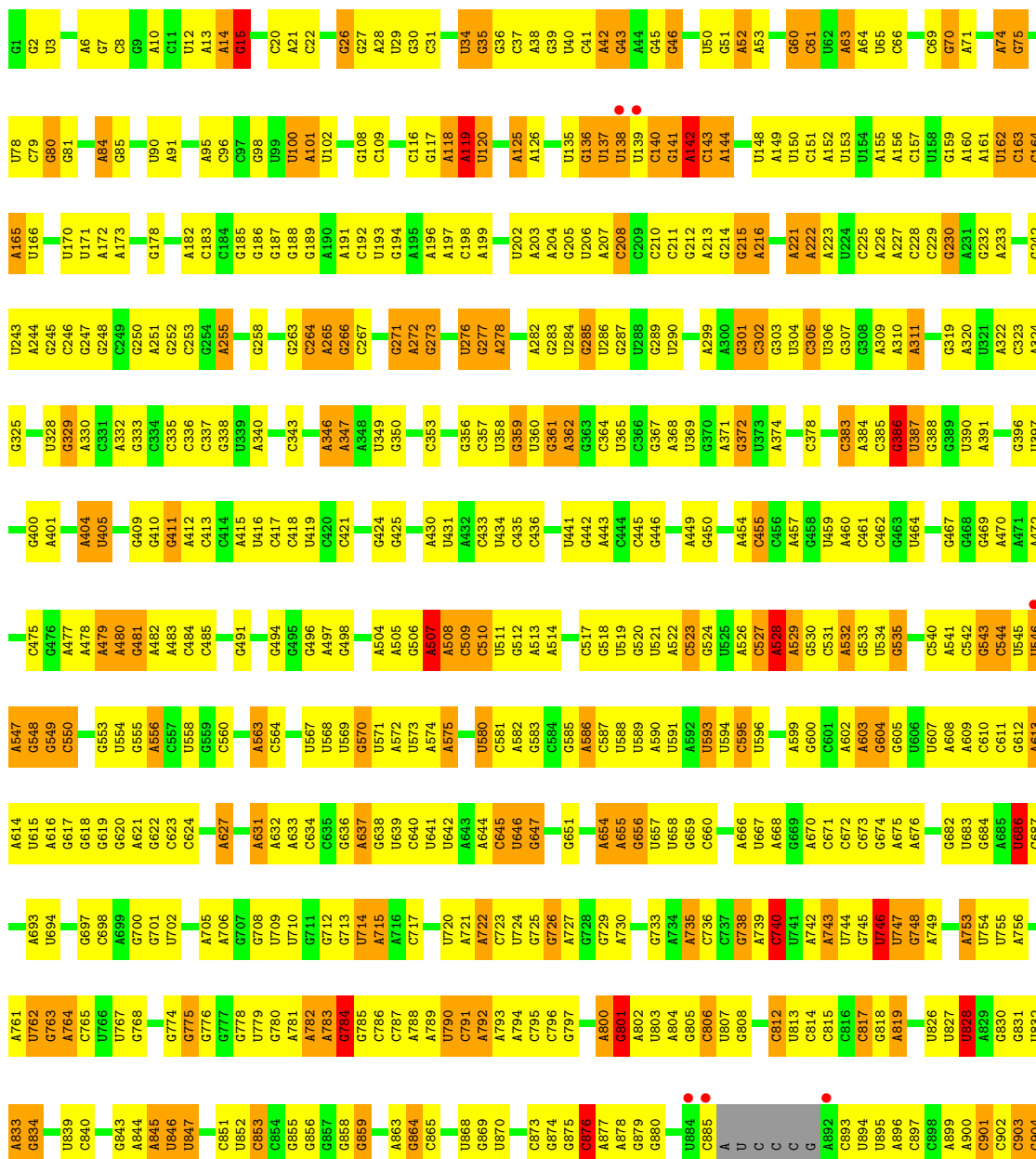


- Molecule 21: 30S ribosomal protein S21

- Chain CU: 

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- Chain BA:

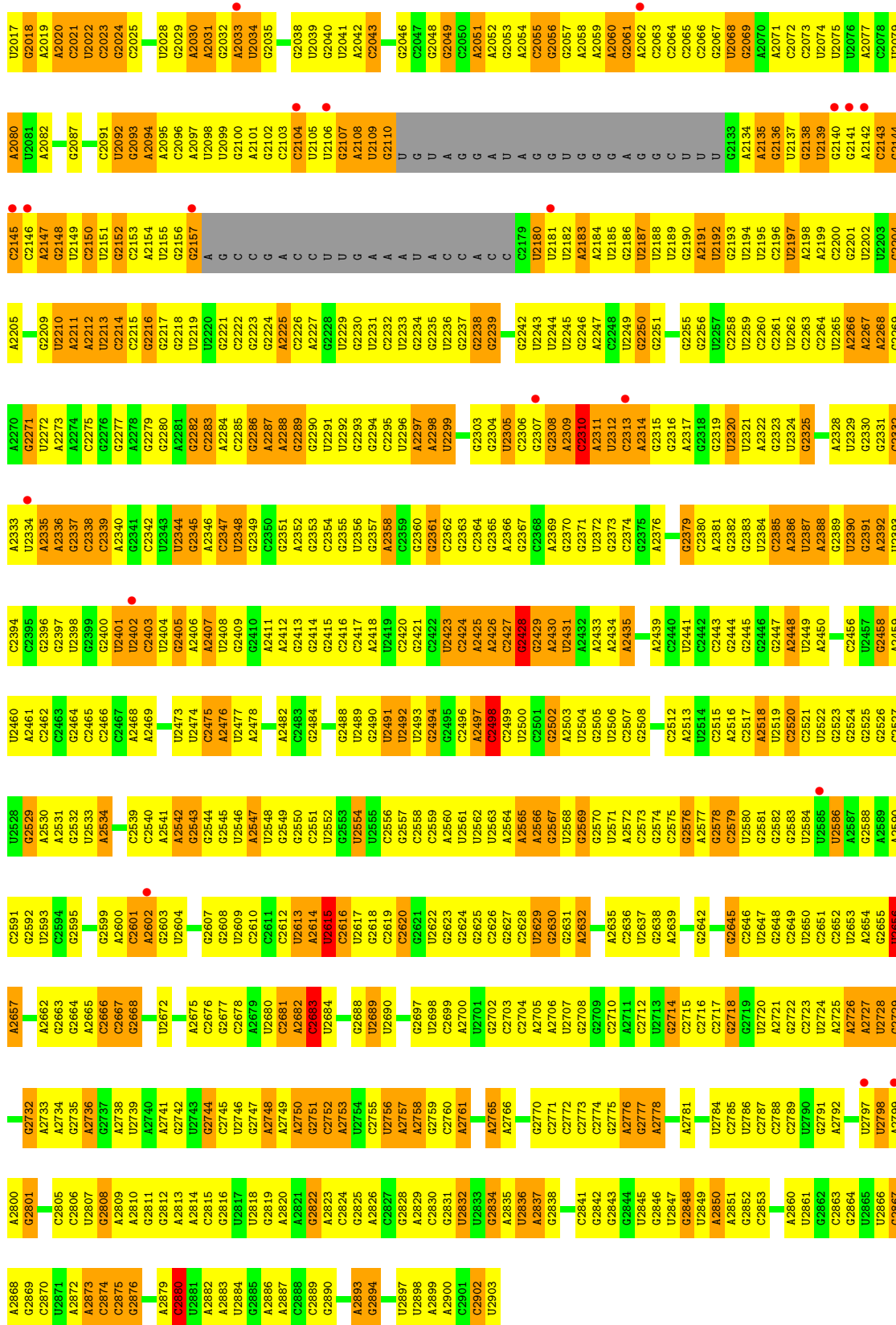


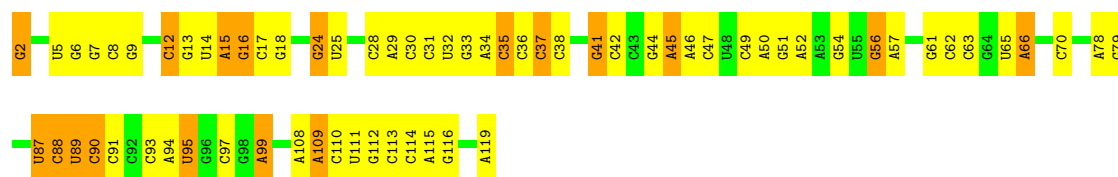
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G2024	C1947	G1867	U1796	C1728	G1649	A1571	G1483	A1419	U1340	U1267	G1177	U1108	G1042	A980	U906
C2025	G1948	C1868	G1797	U1729	A1652	A1572	U1484	A1420	G1341	A1268	C1178	C1109	C1043	A981	
U2026		G1869	U1798	C1730	A1653	G1573	U1485	G1421		A1269	C1179	G1110	C1044	C982	A910
G2027	A1952	C1870	G1799	G1731	G1654	C1574	U1486	G1422	A1347	G1271	U1180	A1111	C1045	A983	A911
U2028	A1953	C1871	G1800	G1732	A1655		U1487	G1423	C1348	G1272	U1181	G1112	A1046	A984	
G2029	G1954	A1872	G1733	G1733	A1655	C1577			C1349	U1273	G1182	U1113	G1047	C985	G942
A2030	U1955	G1873	G1734	G1734	G1656	U1578	C1493	G1426		U1274	U1183	C1114	A1048	C987	C915
A2031	U1956	C1874	A1735	A1735	G1659	U1578	A1494	A1427	U1352	A1275	U1184	G1115	A1048	C987	C916
G2032	C1957	G1875	U1736	U1736	G1659	G1581	A1495	A1428	A1353	A1276	U1185	G1116	A1050	C987	A917
A2033	G1807	A1808	G1807	G1737	G1663	C1582	A1496	G1429	A1354	G1277	U1186	G1117	A1050	C988	A918
U2034	A1808	G1877	G1738	G1738	G1664	A1583	U1497	G1430	A1355	G1278	U1187			C989	U919
G2035	A1809	A1878	A1739	A1739	A1664	U1584	C1498	A1431	G1356	G1279	U1188			A990	A920
U2041	C1961	C1879	G1740	G1740	A1665	C1585	C1499	G1432		G1280	U1189				C921
A2042					G1666	A1586	G1500	A1433	A1359	G1281	G1190	C1123	G1054	G993	C922
G2043	U1982	C1880	U1812	A1744	G1667	G1587	G1501	A1434		G1282		G1124	G1055	C994	C922
C2037	U1983	C1881	G1813	A1745	G1668	G1587	A1502	A1434	C1363	A1287	U1199	G1128	G1056	C995	C923
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A1011	A1011	C	G879	C816	U754	U686	G623	A563	A498	C432	G372	C246	G247	C185
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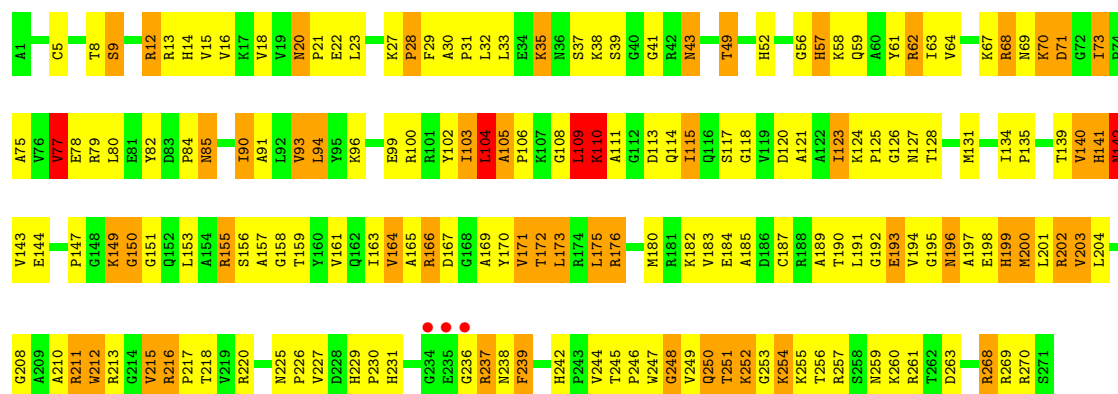
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G2006	U1937	A1858	A1789	G1724	A1655	U1589	A1525	U1458	U1391	A1328	A1265	U1198	U1132
C2007	A1938		C1790	C1656		A1590	G1526	G1459	A1392	U1329		U1199	A1133
C2008	U1939	U1865	A1791		G1659	C1592	G1527	A1460	A1393	C1330	U1267	C1200	A1134
G2010	G2010	A1866	G1792	U1729	A1593	U1594	A1528	G1461	U1394	G1331	A1268	G1136	C1135
U2011	C1941	G1867	C1793	G1730	G1660	G1595	G1529	C1462	A1395	G1332	A1269	U1203	G1137
G2012	G1942	C1868	A1794	G1731	G1661	C1596	G1530		U1396	G1333	C1270	A1204	G1138
A2013	U1943	G1869	C1795	C1732	U1662	A1596	C1531	G1465	U1397	G1334	G1271	A1205	G1139
A2014	U1944	C1870	U1796	G1733	G1663	A1597	A1532	U1466	C1398	C1335		G1206	C1140
A2015	G1945	A1871	G1797	G1734	A1664	A1598	U1534	U1468	A1336	U1273	A1274	G1207	G1141
U2016		A1872	U1798	A1735	A1665	U1599			U1400	G1337		G1208	A1141





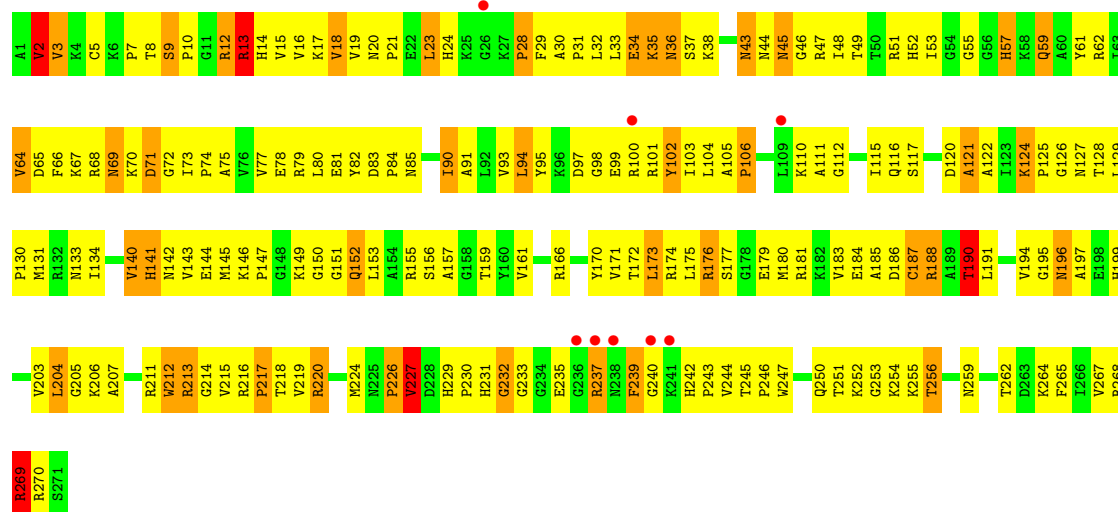
• Molecule 24: 50S ribosomal protein L2

Chain BC:



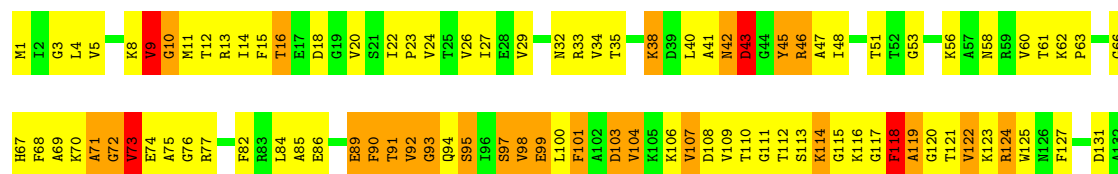
• Molecule 24: 50S ribosomal protein L2

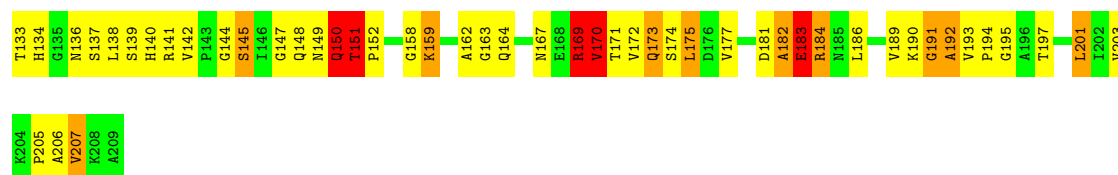
Chain DC:



• Molecule 25: 50S ribosomal protein L3

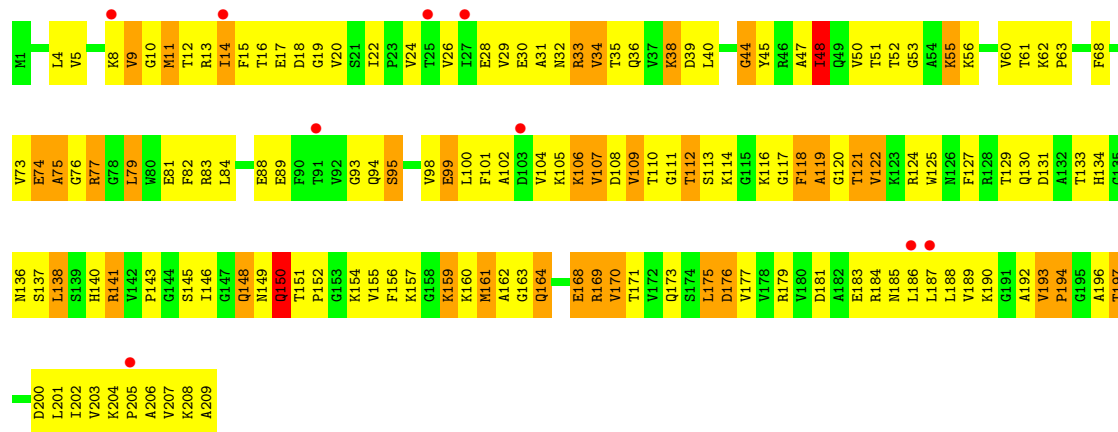
Chain BD:





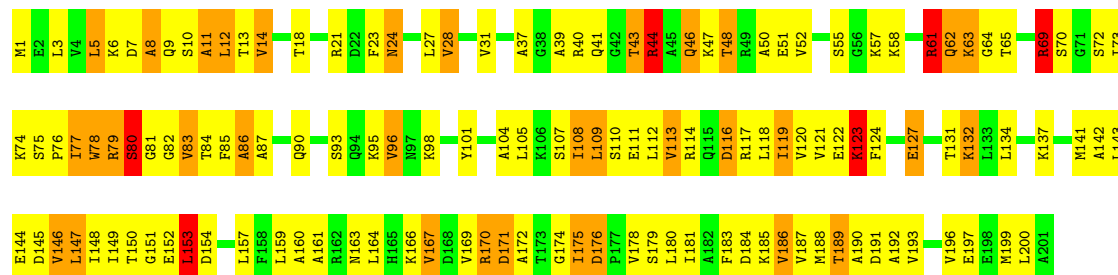
• Molecule 25: 50S ribosomal protein L3

Chain DD:



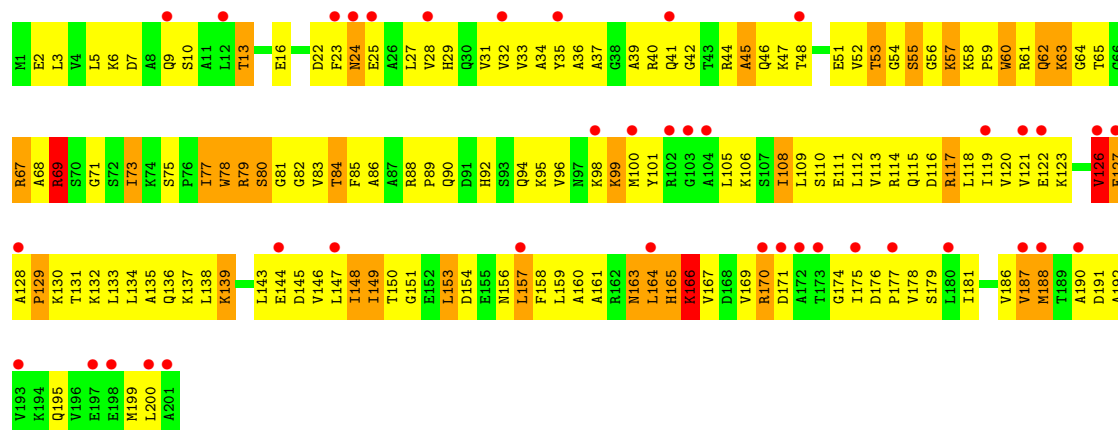
• Molecule 26: 50S ribosomal protein L4

Chain BE:

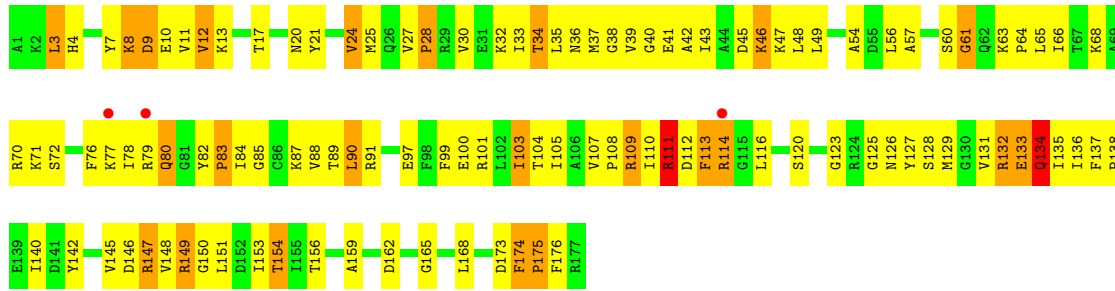


• Molecule 26: 50S ribosomal protein L4

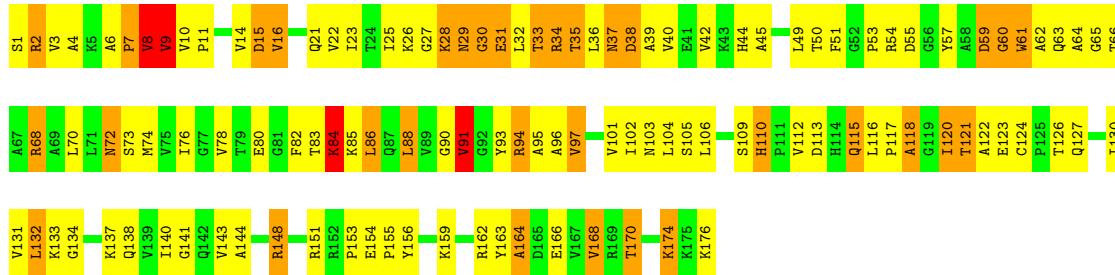
Chain DE:



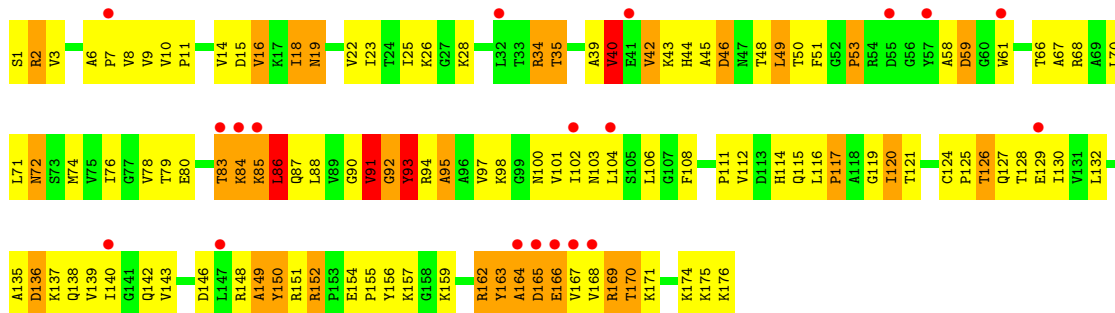
Chain BF:



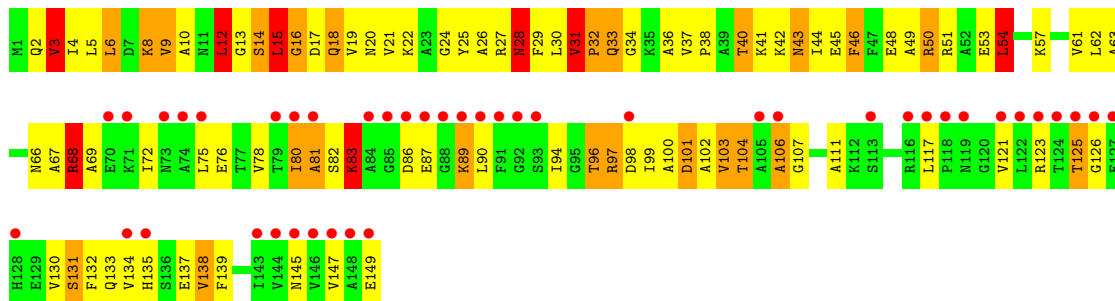
Chain BG:



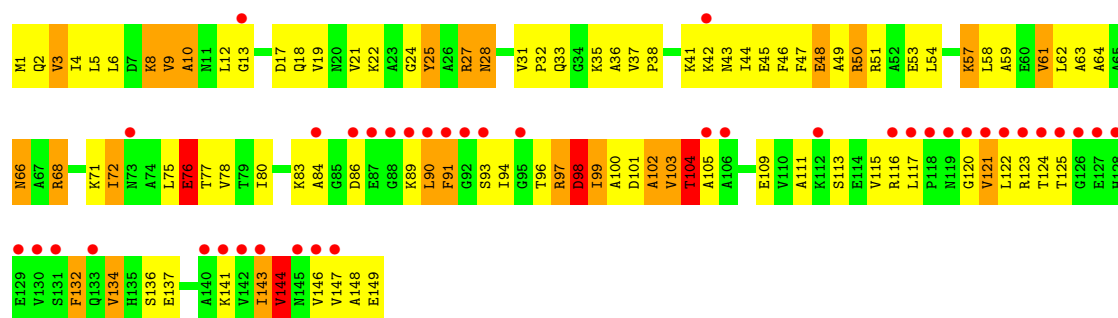
Chain DG:



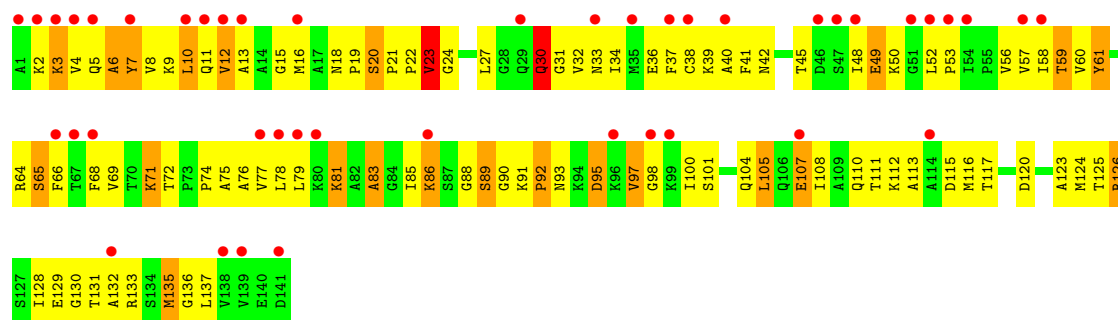
Chain BH:



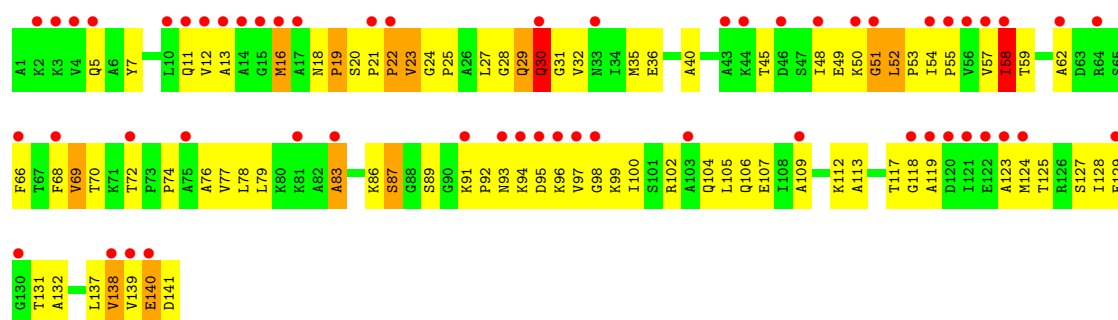
- Molecule 29: 50S ribosomal protein L9

Chain DH: 

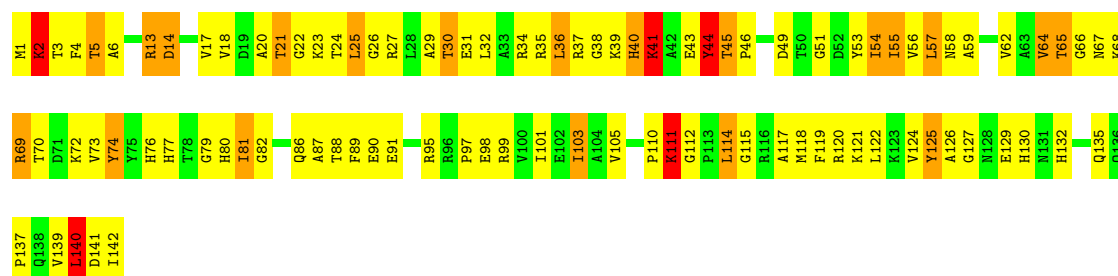
- Molecule 30: 50S ribosomal protein L11

Chain BI: 

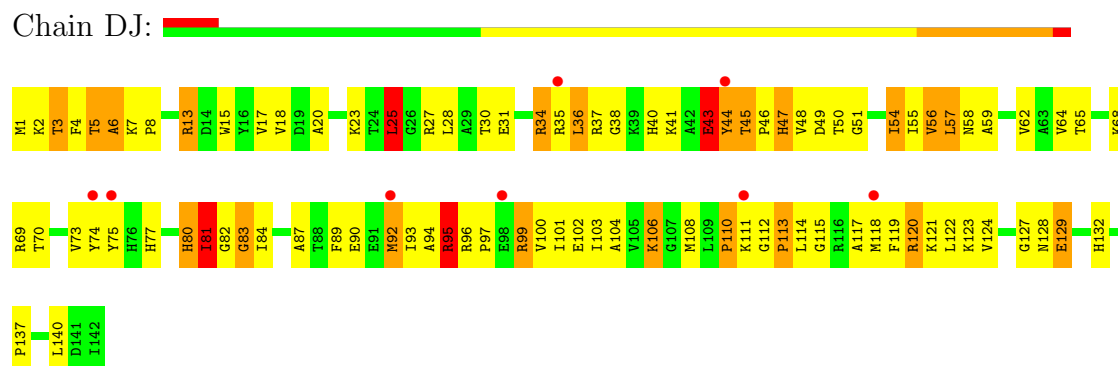
- Molecule 30: 50S ribosomal protein L11

Chain DI: 

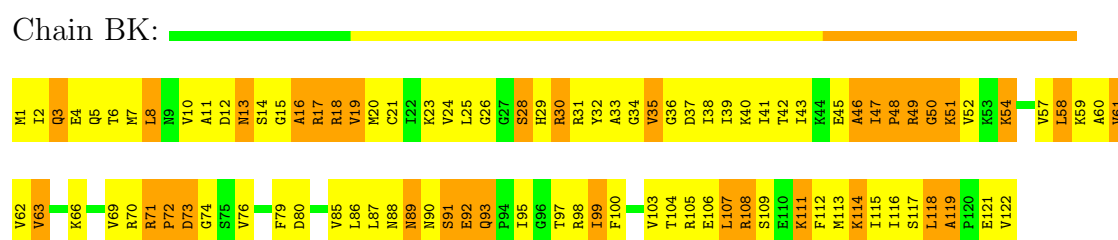
- Molecule 31: 50S ribosomal protein L13

Chain BJ: 

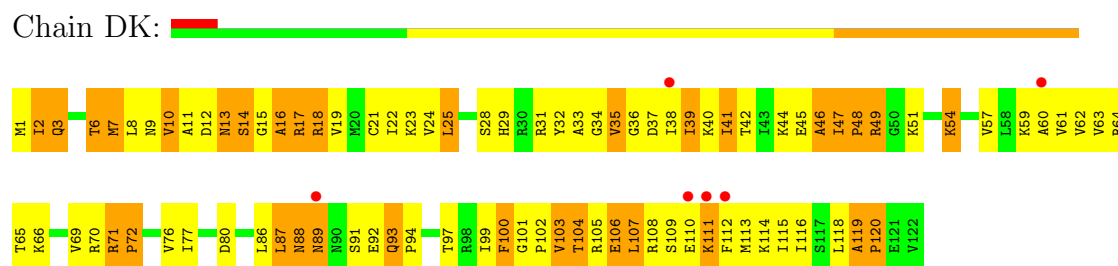
- Molecule 31: 50S ribosomal protein L13



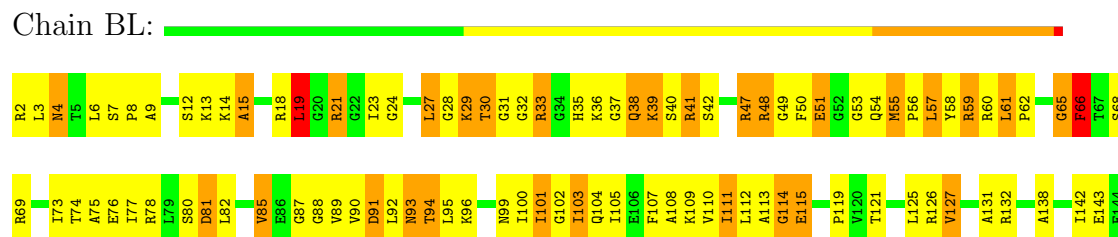
- Molecule 32: 50S ribosomal protein L14



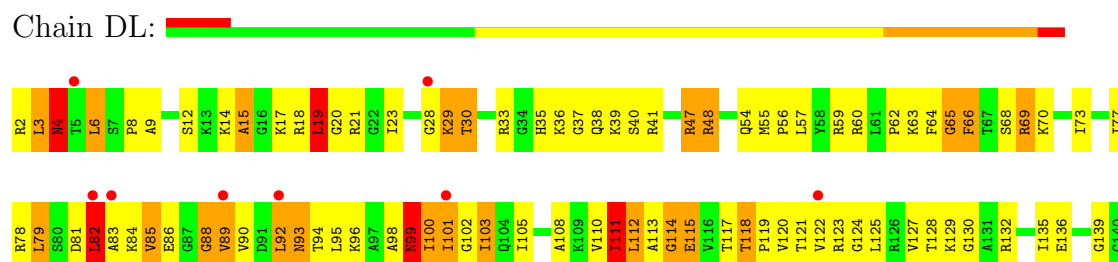
- Molecule 32: 50S ribosomal protein L14



- Molecule 33: 50S ribosomal protein L15



- Molecule 33: 50S ribosomal protein L15





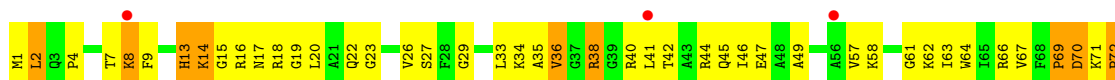
- Molecule 34: 50S ribosomal protein L16

Chain BM:



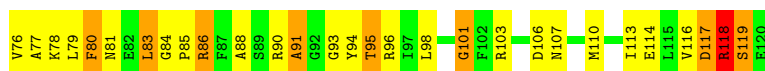
- Molecule 34: 50S ribosomal protein L16

Chain DM:



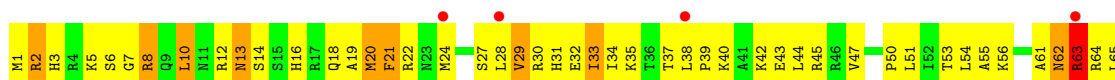
- Molecule 35: 50S ribosomal protein L17

Chain BN:



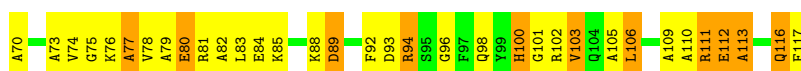
- Molecule 35: 50S ribosomal protein L17

Chain DN:



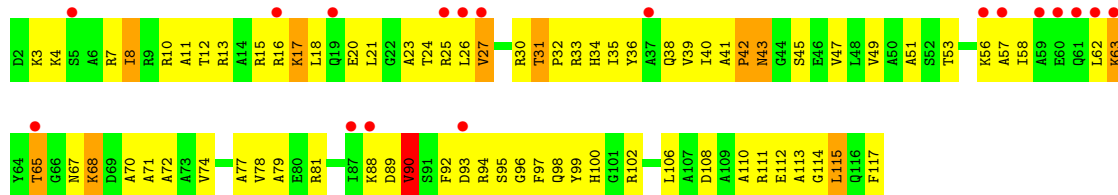
- Molecule 36: 50S ribosomal protein L18

Chain BO:



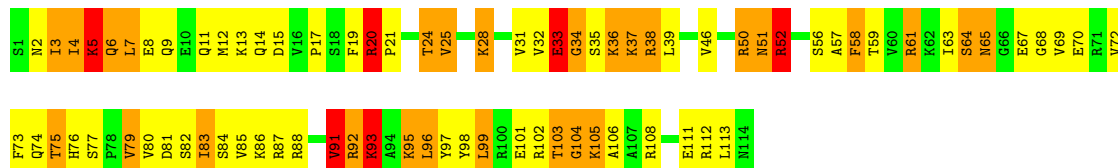
- Molecule 36: 50S ribosomal protein L18

Chain DO:



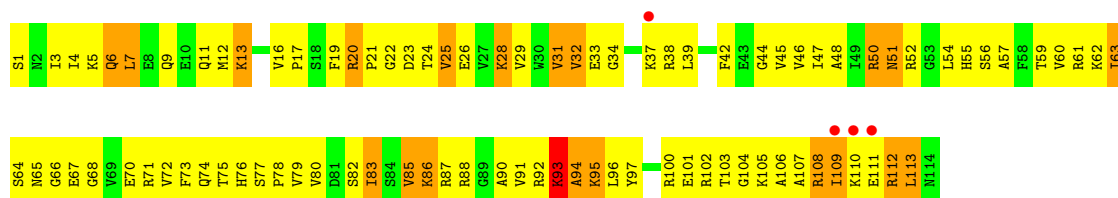
- Molecule 37: 50S ribosomal protein L19

Chain BP:



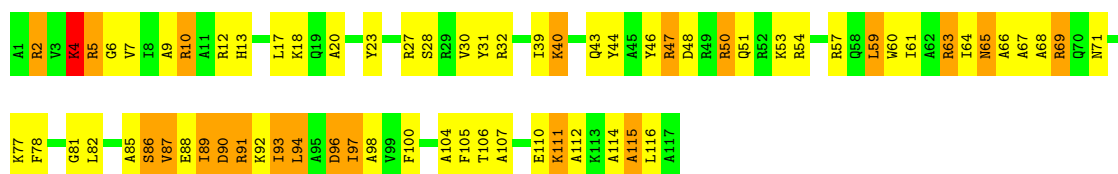
- Molecule 37: 50S ribosomal protein L19

Chain DP:



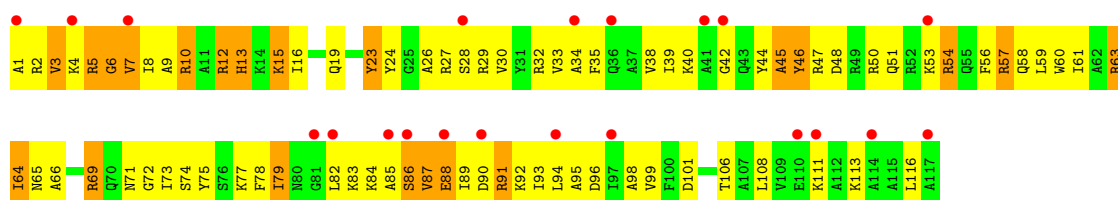
- Molecule 38: 50S ribosomal protein L20

Chain BQ:



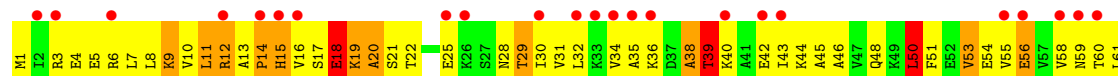
- Molecule 38: 50S ribosomal protein L20

Chain DQ:



- Molecule 39: 50S ribosomal protein L21

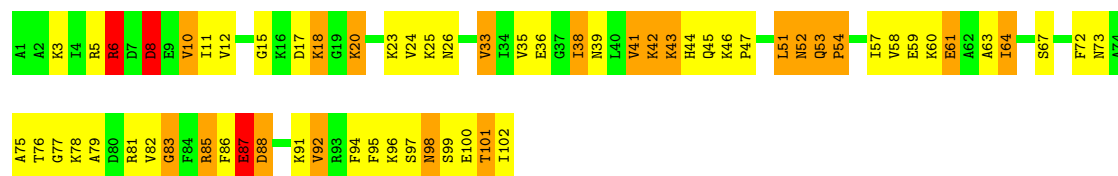
Chain BR:





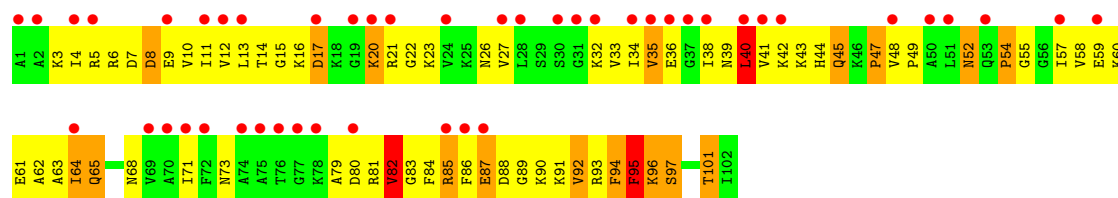
- Molecule 42: 50S ribosomal protein L24

Chain BU:



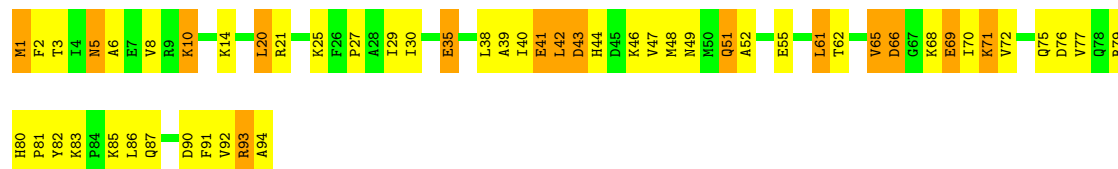
- Molecule 42: 50S ribosomal protein L24

Chain DU:



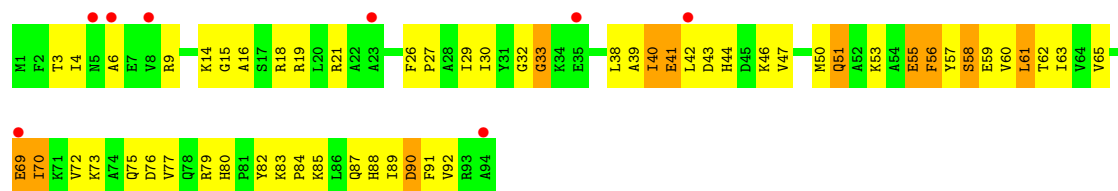
- Molecule 43: 50S ribosomal protein L25

Chain BV:



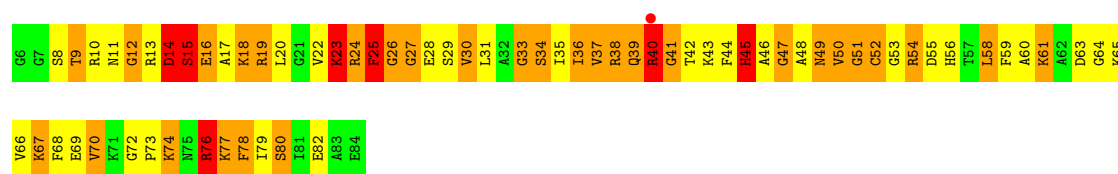
- Molecule 43: 50S ribosomal protein L25

Chain DV:



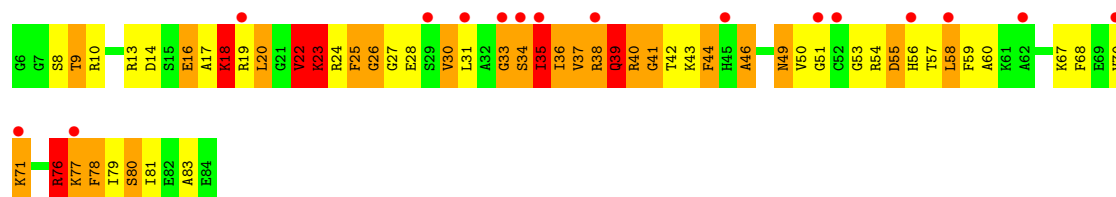
- Molecule 44: 50S ribosomal protein L27

Chain BW:



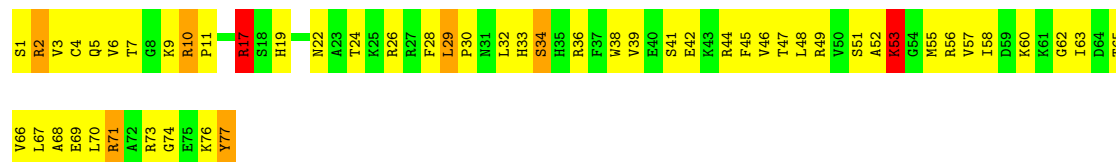
- Molecule 44: 50S ribosomal protein L27

Chain DW: 



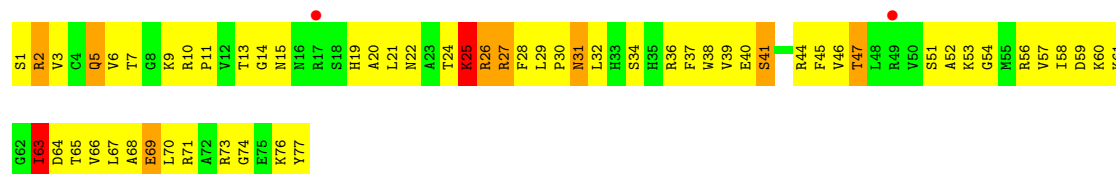
- Molecule 45: 50S ribosomal protein L28

Chain BX: 



- Molecule 45: 50S ribosomal protein L28

Chain DX: 



- Molecule 46: 50S ribosomal protein L29

Chain BY: 



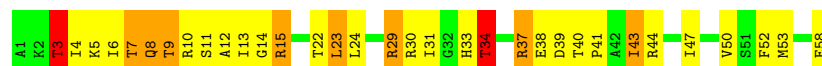
- Molecule 46: 50S ribosomal protein L29

Chain DY: 



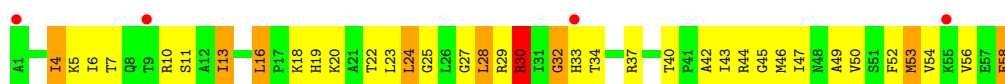
- Molecule 47: 50S ribosomal protein L30

Chain BZ: 



- Molecule 47: 50S ribosomal protein L30

Chain DZ: 



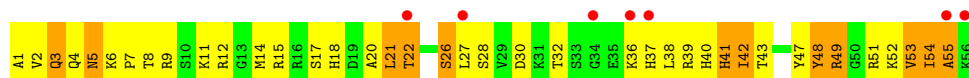
- Molecule 48: 50S ribosomal protein L32

Chain B0:



- Molecule 48: 50S ribosomal protein L32

Chain D0:



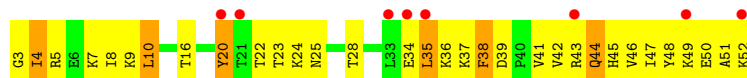
- Molecule 49: 50S ribosomal protein L33

Chain B1:



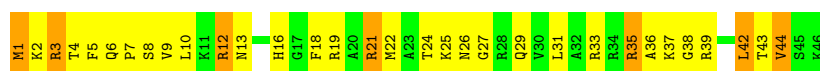
- Molecule 49: 50S ribosomal protein L33

Chain D1:



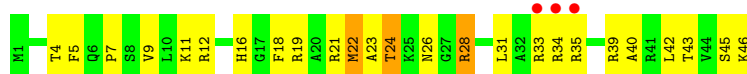
- Molecule 50: 50S ribosomal protein L34

Chain B2:



- Molecule 50: 50S ribosomal protein L34

Chain D2:



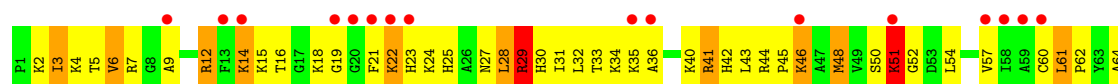
- Molecule 51: 50S ribosomal protein L35

Chain B3:



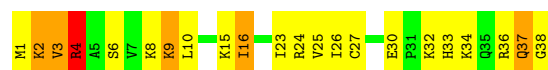
- Molecule 51: 50S ribosomal protein L35

Chain D3:



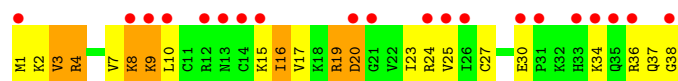
- Molecule 52: 50S ribosomal protein L36

Chain B4:



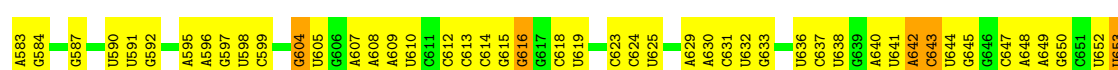
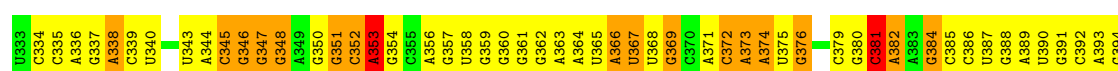
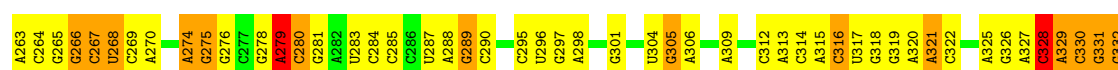
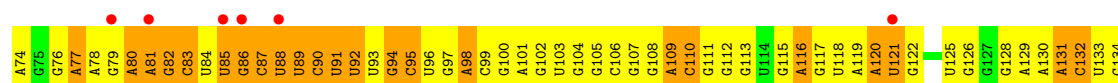
- Molecule 52: 50S ribosomal protein L36

Chain D4:

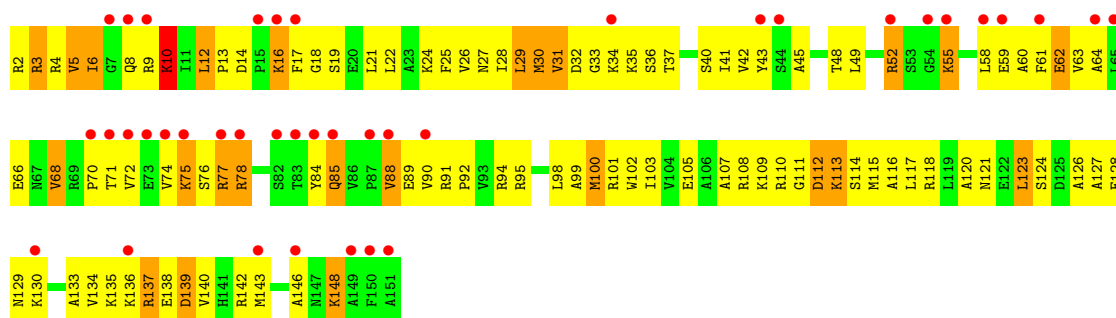


- Molecule 53: 16S rRNA

Chain CA:

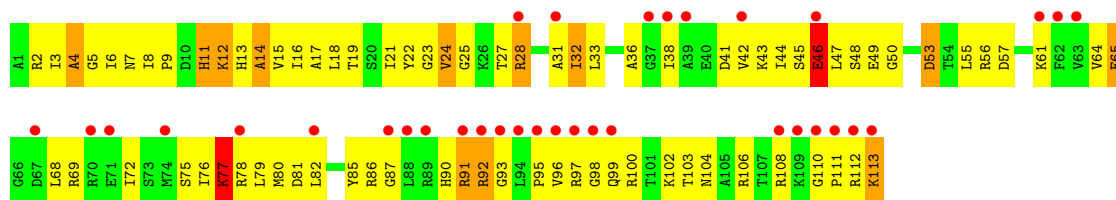






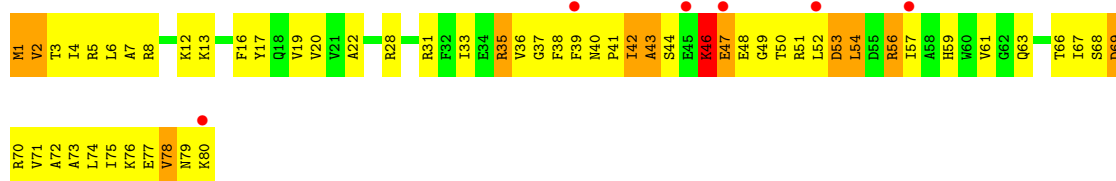
- Molecule 55: 30S ribosomal protein S13

Chain CM:



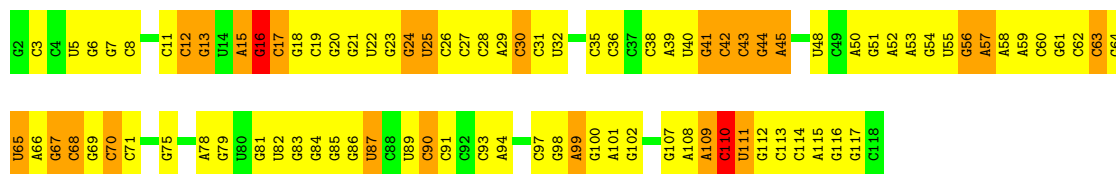
- Molecule 56: 30S ribosomal protein S16

Chain CP:



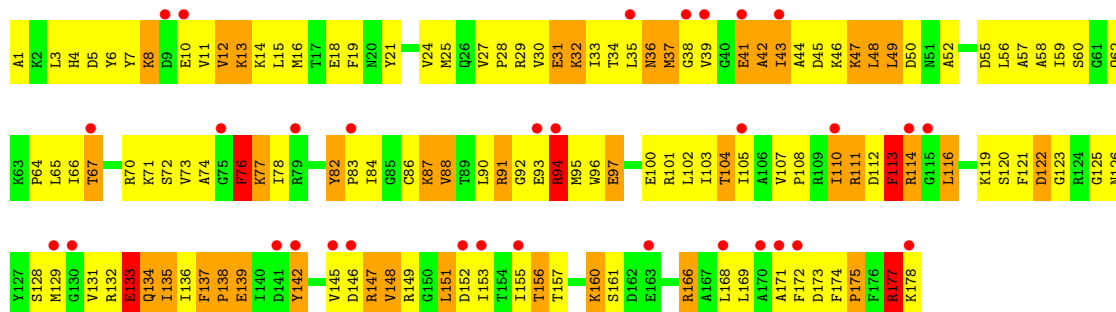
- Molecule 57: 5S rRNA

Chain DB:



- Molecule 58: 50S ribosomal protein L5

Chain DF:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.76Å 433.27Å 618.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	85.22 – 3.25 85.13 – 3.25	Depositor EDS
% Data completeness (in resolution range)	85.8 (85.22-3.25) 85.6 (85.13-3.25)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 3.26Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.193 , 0.245 0.227 , 0.270	Depositor DCC
R_{free} test set	15235 reflections (2.06%)	DCC
Wilson B-factor (Å ²)	60.4	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 33.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	1 of 801754 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	284525	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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, TEL, 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	0.45	2/36834 (0.0%)	0.87	33/57462 (0.1%)
2	AB	0.34	1/1736 (0.1%)	0.52	1/2338 (0.0%)
2	CB	0.30	1/1736 (0.1%)	0.58	4/2338 (0.2%)
3	AC	0.28	0/1652	0.50	0/2225
3	CC	0.25	0/1652	0.44	0/2225
4	AD	0.32	0/1665	0.53	0/2227
4	CD	0.39	0/1665	0.61	0/2227
5	AE	0.45	1/1119 (0.1%)	0.66	2/1504 (0.1%)
5	CE	0.36	0/1119	0.58	0/1504
6	AF	0.31	0/836	0.49	0/1128
6	CF	0.30	0/836	0.50	0/1128
7	AG	0.25	0/1196	0.45	0/1602
8	AH	0.33	0/989	0.55	0/1326
8	CH	0.30	0/989	0.52	0/1326
9	AI	0.26	0/1034	0.48	0/1375
9	CI	0.23	0/1034	0.43	0/1375
10	AJ	0.28	0/797	0.48	0/1077
10	CJ	0.24	0/797	0.47	0/1077
11	AK	0.30	0/893	0.53	0/1205
11	CK	0.28	0/893	0.52	0/1205
12	AL	0.38	0/969	0.69	1/1300 (0.1%)
12	CL	0.36	0/969	0.58	0/1300
13	AM	0.25	0/893	0.47	0/1193
14	AN	0.28	0/785	0.50	0/1043
14	CN	0.23	0/780	0.39	0/1036
15	AO	0.29	0/722	0.48	0/964
15	CO	0.39	1/722 (0.1%)	0.48	0/964
16	AP	0.31	0/659	0.51	0/884
17	AQ	0.40	0/658	0.62	0/881
17	CQ	0.34	0/658	0.52	0/881
18	AR	0.31	0/463	0.50	0/621
18	CR	0.31	0/463	0.47	0/621

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	AS	0.25	0/653	0.45	0/877
19	CS	0.21	0/653	0.42	0/877
20	AT	0.37	0/671	0.56	0/888
20	CT	0.28	0/671	0.50	0/888
21	AU	0.29	0/431	0.46	0/570
21	CU	0.34	0/431	0.59	0/570
22	BA	0.77	9/68626 (0.0%)	1.12	282/107056 (0.3%)
22	DA	0.39	1/68314 (0.0%)	0.86	83/106569 (0.1%)
23	BB	0.68	0/2828	1.04	4/4410 (0.1%)
24	BC	0.48	0/2122	0.73	1/2852 (0.0%)
24	DC	0.31	0/2122	0.54	0/2852
25	BD	0.55	0/1586	0.78	1/2134 (0.0%)
25	DD	0.31	0/1586	0.58	0/2134
26	BE	0.45	0/1571	0.68	1/2113 (0.0%)
26	DE	0.26	0/1571	0.48	0/2113
27	BF	0.34	0/1435	0.53	0/1926
28	BG	0.39	0/1343	0.62	0/1816
28	DG	0.24	0/1343	0.47	0/1816
29	BH	0.33	0/1122	0.52	0/1515
29	DH	0.38	1/1122 (0.1%)	0.52	0/1515
30	BI	0.23	0/1046	0.47	0/1410
30	DI	0.21	0/1046	0.42	0/1410
31	BJ	0.58	0/1152	0.84	1/1551 (0.1%)
31	DJ	0.29	0/1152	0.57	1/1551 (0.1%)
32	BK	0.55	0/948	0.80	0/1268
32	DK	0.35	0/948	0.57	0/1268
33	BL	0.46	0/1054	0.79	1/1403 (0.1%)
33	DL	0.27	0/1054	0.53	0/1403
34	BM	0.54	0/1093	0.73	0/1460
34	DM	0.30	0/1093	0.50	0/1460
35	BN	0.51	0/974	0.75	0/1301
35	DN	0.28	0/974	0.51	0/1301
36	BO	0.43	0/902	0.66	0/1209
36	DO	0.24	0/902	0.43	0/1209
37	BP	0.51	0/929	0.74	0/1242
37	DP	0.32	0/929	0.50	0/1242
38	BQ	0.61	0/960	0.78	0/1278
38	DQ	0.29	0/960	0.47	0/1278
39	BR	0.63	1/829 (0.1%)	0.79	0/1107
39	DR	0.29	0/829	0.51	0/1107
40	BS	0.57	0/864	0.78	0/1156
40	DS	0.28	0/864	0.52	0/1156
41	BT	0.45	0/745	0.70	0/994

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
41	DT	0.24	0/745	0.48	0/994
42	BU	0.43	0/788	0.70	0/1051
42	DU	0.24	0/788	0.46	0/1051
43	BV	0.44	0/766	0.61	0/1025
43	DV	0.25	0/766	0.43	0/1025
44	BW	0.61	0/603	0.89	0/797
44	DW	0.29	0/603	0.51	0/797
45	BX	0.41	0/635	0.70	0/848
45	DX	0.29	0/635	0.56	0/848
46	BY	0.37	0/510	0.64	0/677
46	DY	0.23	0/510	0.44	0/677
47	BZ	0.52	0/453	0.83	0/605
47	DZ	0.28	0/453	0.51	0/605
48	B0	0.48	0/450	0.73	0/599
48	D0	0.29	0/450	0.50	0/599
49	B1	0.38	0/417	0.62	0/554
49	D1	0.27	0/417	0.46	0/554
50	B2	0.53	0/380	0.78	0/498
50	D2	0.27	0/380	0.49	0/498
51	B3	0.49	0/513	0.70	0/676
51	D3	0.29	0/513	0.53	0/676
52	B4	0.53	0/303	0.70	0/397
52	D4	0.45	0/303	0.50	0/397
53	CA	0.41	2/36762 (0.0%)	0.83	32/57350 (0.1%)
54	CG	0.23	0/1188	0.44	0/1591
55	CM	0.20	0/885	0.40	0/1181
56	CP	0.29	0/649	0.53	0/870
57	DB	0.36	1/2803 (0.0%)	0.81	2/4371 (0.0%)
58	DF	0.23	0/1444	0.53	3/1937 (0.2%)
All	All	0.51	21/306773 (0.0%)	0.86	453/458565 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
25	BD	0	1
35	BN	0	1
51	B3	0	1
All	All	0	3

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2092	U	O3'-P	-13.97	1.44	1.61
22	DA	2197	U	O3'-P	-13.44	1.45	1.61
53	CA	1396	A	O3'-P	-13.34	1.45	1.61
22	BA	1142	A	N9-C4	-9.96	1.31	1.37
57	DB	107	G	O3'-P	-9.89	1.49	1.61

The worst 5 of 453 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	783	A	C5-N7-C8	-11.37	98.22	103.90
22	BA	974	G	C5-N7-C8	-11.01	98.79	104.30
22	BA	974	G	C4-C5-N7	10.99	115.20	110.80
2	CB	146	SER	O-C-N	-10.79	105.44	122.70
22	BA	2499	C	N1-C2-O2	-10.28	112.73	118.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
51	B3	29	ARG	Peptide
25	BD	9	VAL	Peptide
35	BN	101	GLY	Peptide

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	32895	0	16553	1232	1
2	AB	1705	0	1732	183	0
2	CB	1705	0	1732	151	0
3	AC	1625	0	1699	109	0
3	CC	1625	0	1699	128	0
4	AD	1643	0	1710	145	0
4	CD	1643	0	1710	157	0
5	AE	1106	0	1148	148	0
5	CE	1106	0	1148	101	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	AF	818	0	808	87	0
6	CF	818	0	808	67	0
7	AG	1182	0	1240	86	0
8	AH	979	0	1034	99	0
8	CH	979	0	1034	92	0
9	AI	1022	0	1070	84	0
9	CI	1022	0	1070	107	0
10	AJ	787	0	828	78	0
10	CJ	787	0	828	91	0
11	AK	877	0	887	91	0
11	CK	877	0	887	71	0
12	AL	955	0	1019	90	0
12	CL	955	0	1019	100	0
13	AM	884	0	944	73	0
14	AN	774	0	827	69	0
14	CN	769	0	822	77	0
15	AO	714	0	737	46	0
15	CO	714	0	737	52	0
16	AP	649	0	666	50	0
17	AQ	649	0	691	71	0
17	CQ	649	0	691	66	0
18	AR	456	0	478	30	0
18	CR	456	0	478	39	0
19	AS	638	0	665	59	0
19	CS	638	0	665	65	0
20	AT	665	0	714	81	0
20	CT	665	0	714	45	0
21	AU	426	0	449	80	0
21	CU	426	0	449	80	0
22	BA	61274	0	30819	1937	6
22	DA	60995	0	30679	3516	8
23	BB	2529	0	1281	73	0
24	BC	2083	0	2157	217	0
24	DC	2083	0	2157	215	0
25	BD	1565	0	1616	196	1
25	DD	1565	0	1616	189	0
26	BE	1552	0	1619	151	0
26	DE	1552	0	1619	180	0
27	BF	1411	0	1447	135	0
28	BG	1323	0	1374	146	0
28	DG	1323	0	1374	126	0
29	BH	1111	0	1148	102	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	DH	1111	0	1148	96	0
30	BI	1032	0	1088	112	0
30	DI	1032	0	1088	65	0
31	BJ	1129	0	1162	156	0
31	DJ	1129	0	1162	140	0
32	BK	939	0	1012	121	0
32	DK	939	0	1012	109	0
33	BL	1045	0	1117	130	1
33	DL	1045	0	1117	128	0
34	BM	1074	0	1157	90	0
34	DM	1074	0	1157	94	0
35	BN	961	0	1000	89	0
35	DN	961	0	1000	122	0
36	BO	892	0	923	74	0
36	DO	892	0	923	79	0
37	BP	917	0	965	141	0
37	DP	917	0	965	121	0
38	BQ	947	0	1022	127	0
38	DQ	947	0	1022	121	0
39	BR	816	0	839	116	0
39	DR	816	0	839	93	0
40	BS	857	0	922	74	0
40	DS	857	0	922	60	0
41	BT	739	0	807	112	0
41	DT	739	0	807	99	0
42	BU	780	0	834	54	0
42	DU	780	0	834	92	0
43	BV	753	0	780	66	0
43	DV	753	0	780	60	0
44	BW	596	0	610	204	0
44	DW	596	0	610	115	0
45	BX	625	0	655	56	0
45	DX	625	0	655	75	0
46	BY	509	0	543	50	0
46	DY	509	0	543	63	0
47	BZ	449	0	491	33	0
47	DZ	449	0	491	40	1
48	B0	444	0	461	30	0
48	D0	444	0	461	57	0
49	B1	410	0	440	33	0
49	D1	410	0	440	36	0
50	B2	377	0	418	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	D2	377	0	418	42	0
51	B3	504	0	574	47	0
51	D3	504	0	574	57	0
52	B4	302	0	340	30	0
52	D4	302	0	342	27	0
53	CA	32831	0	16521	1619	0
54	CG	1175	0	1230	131	0
55	CM	877	0	937	91	0
56	CP	639	0	656	61	0
57	DB	2507	0	1270	159	0
58	DF	1420	0	1460	184	0
59	AA	43	0	0	0	0
59	BA	134	0	0	0	0
59	BB	4	0	0	0	0
59	CA	41	0	0	0	0
59	CE	1	0	0	0	0
59	DA	133	0	0	0	0
59	DB	1	0	0	0	0
59	DC	2	0	0	0	0
59	DJ	1	0	0	0	0
60	BA	58	0	64	8	0
61	B4	1	0	0	0	0
61	D4	1	0	0	0	0
62	AA	198	0	0	5	0
62	AL	1	0	0	0	0
62	AN	6	0	0	1	0
62	AT	2	0	0	0	0
62	AU	1	0	0	0	0
62	B2	1	0	0	0	0
62	B3	3	0	0	0	0
62	B4	1	0	0	0	0
62	BA	598	0	0	29	0
62	BB	20	0	0	1	0
62	BC	10	0	0	0	0
62	BD	2	0	0	0	0
62	BE	1	0	0	0	0
62	BL	2	0	0	1	0
62	BN	3	0	0	1	0
62	BQ	1	0	0	0	0
62	BR	1	0	0	0	0
62	BT	1	0	0	1	0
62	CA	192	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	CE	5	0	0	1	0
62	CI	1	0	0	0	0
62	CL	1	0	0	0	0
62	CN	3	0	0	0	0
62	CT	3	0	0	0	0
62	CU	2	0	0	0	0
62	D2	1	0	0	1	0
62	D3	1	0	0	0	0
62	D4	3	0	0	0	0
62	DA	595	0	0	28	0
62	DB	4	0	0	0	0
62	DC	13	0	0	1	0
62	DD	3	0	0	1	0
62	DE	3	0	0	0	0
62	DJ	6	0	0	0	0
62	DL	6	0	0	1	0
62	DN	2	0	0	0	0
62	DT	3	0	0	0	0
62	DU	2	0	0	0	0
62	DV	1	0	0	0	0
All	All	284525	0	190904	16341	9

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 35.

The worst 5 of 16341 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
53:CA:1157:A:H4'	53:CA:1158:C:O5'	1.38	1.20
22:DA:1808:A:H3'	22:DA:1809:A:H8	1.05	1.20
53:CA:120:A:C3'	53:CA:121:U:H5''	1.73	1.19
22:DA:2091:C:OP2	22:DA:2092:U:H3'	1.39	1.18
22:BA:900:A:C2'	22:BA:901:C:H5'	1.74	1.17

The worst 5 of 9 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
22:BA:138:U:O4	22:DA:305:C:OP1[3_545]	1.58	0.62
22:BA:138:U:O4	22:DA:305:C:P[3_545]	1.90	0.30
1:AA:416:G:OP1	22:DA:2139:U:O4'[4_455]	1.91	0.29
25:BD:181:ASP:OD1	22:DA:2903:U:O4[2_454]	1.97	0.23
22:BA:138:U:C4	22:DA:304:U:O3'[3_545]	1.98	0.22

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	
2	AB	216/218 (99%)	132 (61%)	52 (24%)	32 (15%)	0	2
2	CB	216/218 (99%)	155 (72%)	46 (21%)	15 (7%)	2	17
3	AC	204/206 (99%)	156 (76%)	32 (16%)	16 (8%)	1	13
3	CC	204/206 (99%)	147 (72%)	37 (18%)	20 (10%)	1	8
4	AD	203/205 (99%)	138 (68%)	37 (18%)	28 (14%)	0	3
4	CD	203/205 (99%)	140 (69%)	43 (21%)	20 (10%)	1	8
5	AE	148/150 (99%)	105 (71%)	23 (16%)	20 (14%)	0	3
5	CE	148/150 (99%)	112 (76%)	21 (14%)	15 (10%)	1	8
6	AF	98/100 (98%)	73 (74%)	13 (13%)	12 (12%)	1	4
6	CF	98/100 (98%)	65 (66%)	24 (24%)	9 (9%)	1	9
7	AG	149/151 (99%)	111 (74%)	32 (22%)	6 (4%)	5	36
8	AH	127/129 (98%)	92 (72%)	28 (22%)	7 (6%)	3	25
8	CH	127/129 (98%)	94 (74%)	22 (17%)	11 (9%)	1	11
9	AI	125/127 (98%)	89 (71%)	26 (21%)	10 (8%)	1	13
9	CI	125/127 (98%)	89 (71%)	25 (20%)	11 (9%)	1	10
10	AJ	96/98 (98%)	70 (73%)	13 (14%)	13 (14%)	0	3
10	CJ	96/98 (98%)	55 (57%)	28 (29%)	13 (14%)	0	3
11	AK	115/117 (98%)	85 (74%)	20 (17%)	10 (9%)	1	11
11	CK	115/117 (98%)	89 (77%)	19 (16%)	7 (6%)	2	22
12	AL	121/123 (98%)	88 (73%)	22 (18%)	11 (9%)	1	10
12	CL	121/123 (98%)	86 (71%)	27 (22%)	8 (7%)	2	19
13	AM	112/114 (98%)	88 (79%)	13 (12%)	11 (10%)	1	8
14	AN	92/100 (92%)	60 (65%)	20 (22%)	12 (13%)	0	3
14	CN	91/100 (91%)	59 (65%)	27 (30%)	5 (6%)	3	25
15	AO	86/88 (98%)	59 (69%)	23 (27%)	4 (5%)	4	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	CO	86/88 (98%)	67 (78%)	16 (19%)	3 (4%)	6	41
16	AP	80/82 (98%)	58 (72%)	14 (18%)	8 (10%)	1	8
17	AQ	78/80 (98%)	51 (65%)	15 (19%)	12 (15%)	0	2
17	CQ	78/80 (98%)	62 (80%)	8 (10%)	8 (10%)	1	7
18	AR	53/55 (96%)	46 (87%)	5 (9%)	2 (4%)	5	38
18	CR	53/55 (96%)	42 (79%)	11 (21%)	0	100	100
19	AS	77/79 (98%)	58 (75%)	10 (13%)	9 (12%)	1	5
19	CS	77/79 (98%)	46 (60%)	24 (31%)	7 (9%)	1	10
20	AT	83/85 (98%)	58 (70%)	19 (23%)	6 (7%)	2	16
20	CT	83/85 (98%)	63 (76%)	12 (14%)	8 (10%)	1	9
21	AU	49/51 (96%)	25 (51%)	15 (31%)	9 (18%)	0	1
21	CU	49/51 (96%)	22 (45%)	8 (16%)	19 (39%)	0	0
24	BC	269/271 (99%)	203 (76%)	40 (15%)	26 (10%)	1	8
24	DC	269/271 (99%)	183 (68%)	54 (20%)	32 (12%)	1	4
25	BD	207/209 (99%)	148 (72%)	31 (15%)	28 (14%)	0	3
25	DD	207/209 (99%)	136 (66%)	40 (19%)	31 (15%)	0	2
26	BE	199/201 (99%)	149 (75%)	32 (16%)	18 (9%)	1	10
26	DE	199/201 (99%)	125 (63%)	46 (23%)	28 (14%)	0	2
27	BF	175/177 (99%)	130 (74%)	30 (17%)	15 (9%)	1	11
28	BG	174/176 (99%)	118 (68%)	32 (18%)	24 (14%)	0	3
28	DG	174/176 (99%)	102 (59%)	41 (24%)	31 (18%)	0	1
29	BH	147/149 (99%)	67 (46%)	52 (35%)	28 (19%)	0	1
29	DH	147/149 (99%)	76 (52%)	53 (36%)	18 (12%)	1	4
30	BI	139/141 (99%)	84 (60%)	41 (30%)	14 (10%)	1	8
30	DI	139/141 (99%)	84 (60%)	38 (27%)	17 (12%)	1	4
31	BJ	140/142 (99%)	103 (74%)	26 (19%)	11 (8%)	1	13
31	DJ	140/142 (99%)	96 (69%)	29 (21%)	15 (11%)	1	6
32	BK	120/122 (98%)	88 (73%)	12 (10%)	20 (17%)	0	1
32	DK	120/122 (98%)	82 (68%)	18 (15%)	20 (17%)	0	1
33	BL	141/143 (99%)	103 (73%)	28 (20%)	10 (7%)	2	16
33	DL	141/143 (99%)	80 (57%)	41 (29%)	20 (14%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	BM	134/136 (98%)	100 (75%)	21 (16%)	13 (10%)	1	8
34	DM	134/136 (98%)	95 (71%)	27 (20%)	12 (9%)	1	10
35	BN	118/120 (98%)	92 (78%)	14 (12%)	12 (10%)	1	7
35	DN	118/120 (98%)	70 (59%)	36 (30%)	12 (10%)	1	7
36	BO	114/116 (98%)	88 (77%)	17 (15%)	9 (8%)	1	13
36	DO	114/116 (98%)	81 (71%)	26 (23%)	7 (6%)	2	22
37	BP	112/114 (98%)	74 (66%)	21 (19%)	17 (15%)	0	2
37	DP	112/114 (98%)	64 (57%)	29 (26%)	19 (17%)	0	1
38	BQ	115/117 (98%)	90 (78%)	17 (15%)	8 (7%)	2	17
38	DQ	115/117 (98%)	83 (72%)	20 (17%)	12 (10%)	1	7
39	BR	101/103 (98%)	80 (79%)	14 (14%)	7 (7%)	2	17
39	DR	101/103 (98%)	71 (70%)	18 (18%)	12 (12%)	1	4
40	BS	108/110 (98%)	84 (78%)	17 (16%)	7 (6%)	2	19
40	DS	108/110 (98%)	74 (68%)	25 (23%)	9 (8%)	1	12
41	BT	91/93 (98%)	49 (54%)	26 (29%)	16 (18%)	0	1
41	DT	91/93 (98%)	48 (53%)	28 (31%)	15 (16%)	0	1
42	BU	100/102 (98%)	67 (67%)	17 (17%)	16 (16%)	0	2
42	DU	100/102 (98%)	51 (51%)	28 (28%)	21 (21%)	0	1
43	BV	92/94 (98%)	80 (87%)	11 (12%)	1 (1%)	21	74
43	DV	92/94 (98%)	64 (70%)	21 (23%)	7 (8%)	2	15
44	BW	77/79 (98%)	28 (36%)	22 (29%)	27 (35%)	0	0
44	DW	77/79 (98%)	33 (43%)	23 (30%)	21 (27%)	0	0
45	BX	75/77 (97%)	62 (83%)	9 (12%)	4 (5%)	3	26
45	DX	75/77 (97%)	50 (67%)	17 (23%)	8 (11%)	1	6
46	BY	61/63 (97%)	44 (72%)	11 (18%)	6 (10%)	1	8
46	DY	61/63 (97%)	44 (72%)	12 (20%)	5 (8%)	1	12
47	BZ	56/58 (97%)	47 (84%)	7 (12%)	2 (4%)	5	40
47	DZ	56/58 (97%)	34 (61%)	17 (30%)	5 (9%)	1	10
48	B0	54/56 (96%)	41 (76%)	9 (17%)	4 (7%)	2	15
48	D0	54/56 (96%)	40 (74%)	8 (15%)	6 (11%)	1	5
49	B1	48/50 (96%)	39 (81%)	5 (10%)	4 (8%)	1	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	D1	48/50 (96%)	36 (75%)	8 (17%)	4 (8%)	1	12
50	B2	44/46 (96%)	36 (82%)	6 (14%)	2 (4%)	4	32
50	D2	44/46 (96%)	29 (66%)	11 (25%)	4 (9%)	1	10
51	B3	62/64 (97%)	50 (81%)	7 (11%)	5 (8%)	1	13
51	D3	62/64 (97%)	39 (63%)	18 (29%)	5 (8%)	1	13
52	B4	36/38 (95%)	29 (81%)	3 (8%)	4 (11%)	1	5
52	D4	36/38 (95%)	23 (64%)	8 (22%)	5 (14%)	0	3
54	CG	148/150 (99%)	100 (68%)	36 (24%)	12 (8%)	1	13
55	CM	111/113 (98%)	64 (58%)	35 (32%)	12 (11%)	1	6
56	CP	78/80 (98%)	50 (64%)	18 (23%)	10 (13%)	0	3
58	DF	176/178 (99%)	98 (56%)	46 (26%)	32 (18%)	0	1
All	All	11238/11447 (98%)	7713 (69%)	2283 (20%)	1242 (11%)	1	5

5 of 1242 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	18	GLN
2	AB	20	ARG
2	AB	33	ALA
2	AB	40	ILE
2	AB	72	LYS

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	180/180 (100%)	141 (78%)	39 (22%)	1	7
2	CB	180/180 (100%)	152 (84%)	28 (16%)	4	19
3	AC	170/170 (100%)	142 (84%)	28 (16%)	3	17
3	CC	170/170 (100%)	151 (89%)	19 (11%)	9	38
4	AD	172/172 (100%)	145 (84%)	27 (16%)	4	19
4	CD	172/172 (100%)	135 (78%)	37 (22%)	1	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	AE	113/113 (100%)	86 (76%)	27 (24%)	1	4
5	CE	113/113 (100%)	90 (80%)	23 (20%)	2	9
6	AF	87/87 (100%)	73 (84%)	14 (16%)	3	18
6	CF	87/87 (100%)	74 (85%)	13 (15%)	4	22
7	AG	124/124 (100%)	106 (86%)	18 (14%)	5	24
8	AH	104/104 (100%)	89 (86%)	15 (14%)	5	24
8	CH	104/104 (100%)	91 (88%)	13 (12%)	7	32
9	AI	105/105 (100%)	83 (79%)	22 (21%)	1	8
9	CI	105/105 (100%)	91 (87%)	14 (13%)	6	28
10	AJ	86/86 (100%)	74 (86%)	12 (14%)	5	25
10	CJ	86/86 (100%)	75 (87%)	11 (13%)	6	30
11	AK	90/90 (100%)	75 (83%)	15 (17%)	3	16
11	CK	90/90 (100%)	78 (87%)	12 (13%)	6	28
12	AL	103/103 (100%)	85 (82%)	18 (18%)	3	14
12	CL	103/103 (100%)	86 (84%)	17 (16%)	3	17
13	AM	92/92 (100%)	87 (95%)	5 (5%)	31	76
14	AN	79/83 (95%)	75 (95%)	4 (5%)	33	77
14	CN	79/83 (95%)	69 (87%)	10 (13%)	6	31
15	AO	76/76 (100%)	70 (92%)	6 (8%)	18	59
15	CO	76/76 (100%)	70 (92%)	6 (8%)	18	59
16	AP	65/65 (100%)	58 (89%)	7 (11%)	9	39
17	AQ	74/74 (100%)	57 (77%)	17 (23%)	1	5
17	CQ	74/74 (100%)	60 (81%)	14 (19%)	2	11
18	AR	48/48 (100%)	45 (94%)	3 (6%)	25	70
18	CR	48/48 (100%)	43 (90%)	5 (10%)	10	41
19	AS	70/70 (100%)	62 (89%)	8 (11%)	8	37
19	CS	70/70 (100%)	63 (90%)	7 (10%)	11	43
20	AT	65/65 (100%)	49 (75%)	16 (25%)	1	3
20	CT	65/65 (100%)	51 (78%)	14 (22%)	1	8
21	AU	44/44 (100%)	34 (77%)	10 (23%)	1	6
21	CU	44/44 (100%)	36 (82%)	8 (18%)	2	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	BC	216/216 (100%)	167 (77%)	49 (23%)	1	6
24	DC	216/216 (100%)	189 (88%)	27 (12%)	7	32
25	BD	164/164 (100%)	134 (82%)	30 (18%)	2	12
25	DD	164/164 (100%)	144 (88%)	20 (12%)	7	33
26	BE	165/165 (100%)	122 (74%)	43 (26%)	1	2
26	DE	165/165 (100%)	147 (89%)	18 (11%)	9	39
27	BF	148/148 (100%)	130 (88%)	18 (12%)	7	33
28	BG	137/137 (100%)	105 (77%)	32 (23%)	1	5
28	DG	137/137 (100%)	119 (87%)	18 (13%)	6	29
29	BH	114/114 (100%)	96 (84%)	18 (16%)	4	19
29	DH	114/114 (100%)	96 (84%)	18 (16%)	4	19
30	BI	109/109 (100%)	91 (84%)	18 (16%)	3	17
30	DI	109/109 (100%)	102 (94%)	7 (6%)	25	69
31	BJ	116/116 (100%)	88 (76%)	28 (24%)	1	4
31	DJ	116/116 (100%)	100 (86%)	16 (14%)	5	26
32	BK	103/103 (100%)	81 (79%)	22 (21%)	1	8
32	DK	103/103 (100%)	83 (81%)	20 (19%)	2	10
33	BL	102/102 (100%)	76 (74%)	26 (26%)	1	3
33	DL	102/102 (100%)	85 (83%)	17 (17%)	3	16
34	BM	109/109 (100%)	87 (80%)	22 (20%)	2	9
34	DM	109/109 (100%)	96 (88%)	13 (12%)	8	35
35	BN	100/100 (100%)	82 (82%)	18 (18%)	2	13
35	DN	100/100 (100%)	85 (85%)	15 (15%)	4	21
36	BO	86/86 (100%)	69 (80%)	17 (20%)	2	10
36	DO	86/86 (100%)	77 (90%)	9 (10%)	10	41
37	BP	99/99 (100%)	73 (74%)	26 (26%)	1	2
37	DP	99/99 (100%)	89 (90%)	10 (10%)	11	42
38	BQ	89/89 (100%)	71 (80%)	18 (20%)	2	9
38	DQ	89/89 (100%)	74 (83%)	15 (17%)	3	16
39	BR	84/84 (100%)	70 (83%)	14 (17%)	3	16
39	DR	84/84 (100%)	71 (84%)	13 (16%)	4	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	BS	93/93 (100%)	74 (80%)	19 (20%)	2	9
40	DS	93/93 (100%)	79 (85%)	14 (15%)	4	21
41	BT	80/80 (100%)	61 (76%)	19 (24%)	1	4
41	DT	80/80 (100%)	73 (91%)	7 (9%)	14	52
42	BU	83/83 (100%)	66 (80%)	17 (20%)	2	9
42	DU	83/83 (100%)	74 (89%)	9 (11%)	9	39
43	BV	78/78 (100%)	59 (76%)	19 (24%)	1	3
43	DV	78/78 (100%)	68 (87%)	10 (13%)	6	30
44	BW	59/59 (100%)	41 (70%)	18 (30%)	0	1
44	DW	59/59 (100%)	42 (71%)	17 (29%)	0	2
45	BX	67/67 (100%)	54 (81%)	13 (19%)	2	10
45	DX	67/67 (100%)	58 (87%)	9 (13%)	6	28
46	BY	55/55 (100%)	41 (74%)	14 (26%)	1	3
46	DY	55/55 (100%)	52 (94%)	3 (6%)	30	75
47	BZ	48/48 (100%)	33 (69%)	15 (31%)	0	1
47	DZ	48/48 (100%)	40 (83%)	8 (17%)	3	16
48	B0	47/47 (100%)	39 (83%)	8 (17%)	3	16
48	D0	47/47 (100%)	39 (83%)	8 (17%)	3	16
49	B1	45/45 (100%)	37 (82%)	8 (18%)	2	14
49	D1	45/45 (100%)	41 (91%)	4 (9%)	14	51
50	B2	38/38 (100%)	29 (76%)	9 (24%)	1	4
50	D2	38/38 (100%)	33 (87%)	5 (13%)	6	29
51	B3	51/51 (100%)	44 (86%)	7 (14%)	5	27
51	D3	51/51 (100%)	40 (78%)	11 (22%)	1	7
52	B4	34/34 (100%)	28 (82%)	6 (18%)	3	14
52	D4	34/34 (100%)	29 (85%)	5 (15%)	4	23
54	CG	123/123 (100%)	102 (83%)	21 (17%)	3	16
55	CM	91/91 (100%)	80 (88%)	11 (12%)	7	34
56	CP	65/65 (100%)	57 (88%)	8 (12%)	7	33
58	DF	149/149 (100%)	123 (83%)	26 (17%)	3	15
All	All	9331/9339 (100%)	7786 (83%)	1545 (17%)	3	16

5 of 1545 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
39	BR	20	VAL
50	B2	9	VAL
39	DR	58	VAL
40	BS	48	LYS
44	BW	14	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 331 such sidechains are listed below:

Mol	Chain	Res	Type
41	BT	91	GLN
3	CC	31	ASN
42	DU	44	HIS
43	BV	44	HIS
47	BZ	33	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1532/1533 (99%)	363 (23%)	63 (4%)
22	BA	2850/2903 (98%)	554 (19%)	87 (3%)
22	DA	2837/2903 (97%)	869 (30%)	183 (6%)
23	BB	117/118 (99%)	19 (16%)	0
53	CA	1529/1530 (99%)	445 (29%)	81 (5%)
57	DB	116/117 (99%)	33 (28%)	7 (6%)
All	All	8981/9104 (98%)	2283 (25%)	421 (4%)

5 of 2283 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	6	G
1	AA	9	G
1	AA	22	G
1	AA	32	A

5 of 421 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
53	CA	512	U

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Mol	Chain	Res	Type
22	DA	52	A
22	DA	2492	U
53	CA	701	U
53	CA	1142	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 363 ligands modelled in this entry, 362 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
60	TEL	BA	3135	-	62,62,62	2.16	12 (19%)	92,92,92	3.76	39 (42%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	TEL	BA	3135	-	2/2/19/19	0/73/108/108	0/5/5/5

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	BA	3135	TEL	O16-C10	10.25	1.37	1.21
60	BA	3135	TEL	C10-N6	8.03	1.51	1.35
60	BA	3135	TEL	O5-C10	4.27	1.42	1.35
60	BA	3135	TEL	O9-C4	-3.86	1.39	1.46
60	BA	3135	TEL	O45-C50	-3.31	1.38	1.44

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	BA	3135	TEL	C3-N6-C10	-15.53	93.00	111.97
60	BA	3135	TEL	C7-C3-N6	13.09	135.56	112.50
60	BA	3135	TEL	O5-C10-N6	-10.28	101.29	109.87
60	BA	3135	TEL	O5-C10-O16	-9.27	110.75	122.49
60	BA	3135	TEL	C1-C2-C3	-7.76	107.96	116.79

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
60	BA	3135	TEL	C3
60	BA	3135	TEL	C21

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1533/1533 (100%)	-0.50	17 (1%) 77 30	31, 83, 185, 422	0
2	AB	218/218 (100%)	0.89	19 (8%) 10 3	67, 161, 222, 300	0
2	CB	218/218 (100%)	0.93	15 (6%) 17 4	76, 168, 231, 274	0
3	AC	206/206 (100%)	0.34	4 (1%) 64 19	53, 101, 156, 201	0
3	CC	206/206 (100%)	0.48	6 (2%) 49 11	76, 138, 202, 264	0
4	AD	205/205 (100%)	0.12	2 (0%) 79 32	48, 93, 168, 305	0
4	CD	205/205 (100%)	-0.14	1 (0%) 88 48	26, 60, 114, 257	0
5	AE	150/150 (100%)	0.09	0 100 100	38, 76, 150, 231	0
5	CE	150/150 (100%)	0.06	0 100 100	34, 85, 143, 282	0
6	AF	100/100 (100%)	0.13	0 100 100	52, 100, 147, 188	0
6	CF	100/100 (100%)	0.11	1 (1%) 79 32	69, 109, 169, 214	0
7	AG	151/151 (100%)	0.36	5 (3%) 44 10	77, 131, 195, 217	0
8	AH	129/129 (100%)	0.18	1 (0%) 83 37	45, 82, 133, 191	0
8	CH	129/129 (100%)	0.37	5 (3%) 37 8	60, 101, 151, 212	0
9	AI	127/127 (100%)	0.68	13 (10%) 7 2	64, 137, 207, 266	0
9	CI	127/127 (100%)	0.94	14 (11%) 6 2	98, 168, 246, 283	0
10	AJ	98/98 (100%)	0.52	7 (7%) 16 4	65, 111, 196, 260	0
10	CJ	98/98 (100%)	1.51	27 (27%) 1 1	94, 178, 248, 272	0
11	AK	117/117 (100%)	0.44	4 (3%) 43 10	45, 108, 190, 238	0
11	CK	117/117 (100%)	0.38	3 (2%) 53 13	49, 112, 169, 192	0
12	AL	123/123 (100%)	-0.06	1 (0%) 83 37	24, 62, 106, 208	0
12	CL	123/123 (100%)	0.22	2 (1%) 68 22	37, 73, 124, 211	0
13	AM	114/114 (100%)	0.24	2 (1%) 65 20	86, 135, 206, 262	0
14	AN	96/100 (96%)	0.38	3 (3%) 47 11	58, 105, 187, 274	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
14	CN	95/100 (95%)	1.19	18 (18%) 2 1	95, 187, 280, 335	0
15	AO	88/88 (100%)	-0.15	0 100 100	43, 81, 124, 170	0
15	CO	88/88 (100%)	0.01	0 100 100	57, 107, 153, 265	0
16	AP	82/82 (100%)	0.41	5 (6%) 21 5	56, 80, 166, 241	0
17	AQ	80/80 (100%)	0.34	3 (3%) 38 8	44, 78, 145, 219	0
17	CQ	80/80 (100%)	0.54	3 (3%) 38 8	57, 106, 146, 163	0
18	AR	55/55 (100%)	0.14	2 (3%) 41 9	60, 88, 151, 212	0
18	CR	55/55 (100%)	0.00	0 100 100	55, 88, 179, 249	0
19	AS	79/79 (100%)	0.86	7 (8%) 10 3	96, 137, 193, 233	0
19	CS	79/79 (100%)	1.66	26 (32%) 1 1	183, 316, 391, 403	0
20	AT	85/85 (100%)	0.02	0 100 100	47, 84, 131, 157	0
20	CT	85/85 (100%)	0.89	11 (12%) 4 2	66, 115, 191, 210	0
21	AU	51/51 (100%)	1.50	13 (25%) 1 1	96, 152, 206, 217	0
21	CU	51/51 (100%)	0.58	4 (7%) 13 4	66, 117, 183, 253	0
22	BA	2854/2903 (98%)	-0.46	27 (0%) 81 36	5, 32, 160, 403	0
22	DA	2841/2903 (97%)	0.39	86 (3%) 48 11	53, 122, 250, 469	0
23	BB	118/118 (100%)	-0.50	0 100 100	13, 44, 74, 101	0
24	BC	271/271 (100%)	-0.14	3 (1%) 77 30	12, 42, 93, 209	0
24	DC	271/271 (100%)	0.43	8 (2%) 48 11	59, 93, 144, 185	0
25	BD	209/209 (100%)	-0.23	0 100 100	4, 26, 73, 178	0
25	DD	209/209 (100%)	0.64	9 (4%) 34 7	58, 109, 173, 246	0
26	BE	201/201 (100%)	-0.21	0 100 100	5, 43, 103, 156	0
26	DE	201/201 (100%)	1.23	40 (19%) 2 1	65, 192, 378, 459	0
27	BF	177/177 (100%)	0.25	3 (1%) 67 21	27, 75, 156, 242	0
28	BG	176/176 (100%)	0.03	0 100 100	22, 62, 121, 186	0
28	DG	176/176 (100%)	1.02	19 (10%) 6 2	100, 185, 264, 328	0
29	BH	149/149 (100%)	1.53	43 (28%) 1 1	49, 179, 279, 375	0
29	DH	149/149 (100%)	1.52	40 (26%) 1 1	93, 184, 287, 326	0
30	BI	141/141 (100%)	1.75	43 (30%) 1 1	136, 253, 308, 367	0
30	DI	141/141 (100%)	1.96	56 (39%) 1 0	167, 294, 351, 377	0
31	BJ	142/142 (100%)	-0.30	0 100 100	7, 23, 64, 143	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
31	DJ	142/142 (100%)	0.69	8 (5%) 24 5	52, 106, 159, 195	0
32	BK	122/122 (100%)	-0.22	0 100 100	10, 31, 80, 254	0
32	DK	122/122 (100%)	0.79	6 (4%) 28 6	57, 91, 150, 229	0
33	BL	143/143 (100%)	-0.20	0 100 100	7, 38, 75, 111	0
33	DL	143/143 (100%)	0.78	10 (6%) 16 4	69, 149, 262, 337	0
34	BM	136/136 (100%)	-0.26	0 100 100	6, 29, 76, 120	0
34	DM	136/136 (100%)	0.50	4 (2%) 49 11	46, 107, 161, 204	0
35	BN	120/120 (100%)	-0.31	0 100 100	9, 25, 46, 155	0
35	DN	120/120 (100%)	0.88	13 (10%) 6 2	73, 124, 194, 293	0
36	BO	116/116 (100%)	-0.08	0 100 100	24, 44, 83, 116	0
36	DO	116/116 (100%)	1.05	18 (15%) 3 2	113, 162, 224, 259	0
37	BP	114/114 (100%)	-0.12	0 100 100	11, 41, 104, 161	0
37	DP	114/114 (100%)	0.55	4 (3%) 42 9	63, 105, 164, 195	0
38	BQ	117/117 (100%)	-0.38	0 100 100	4, 20, 47, 206	0
38	DQ	117/117 (100%)	1.01	21 (17%) 2 1	67, 108, 191, 312	0
39	BR	103/103 (100%)	-0.28	1 (0%) 79 32	5, 30, 80, 109	0
39	DR	103/103 (100%)	1.33	24 (23%) 1 1	80, 138, 239, 291	0
40	BS	110/110 (100%)	-0.30	1 (0%) 81 36	6, 21, 61, 178	0
40	DS	110/110 (100%)	1.45	24 (21%) 1 1	70, 133, 241, 285	0
41	BT	93/93 (100%)	0.13	1 (1%) 77 30	23, 51, 121, 235	0
41	DT	93/93 (100%)	1.71	32 (34%) 1 0	110, 202, 299, 369	0
42	BU	102/102 (100%)	0.03	0 100 100	19, 55, 136, 246	0
42	DU	102/102 (100%)	2.02	46 (45%) 1 0	122, 287, 418, 543	0
43	BV	94/94 (100%)	-0.11	0 100 100	13, 43, 85, 124	0
43	DV	94/94 (100%)	0.89	8 (8%) 11 3	100, 144, 196, 226	0
44	BW	79/79 (100%)	0.05	1 (1%) 74 27	10, 36, 110, 208	0
44	DW	79/79 (100%)	1.37	16 (20%) 1 1	87, 141, 230, 253	0
45	BX	77/77 (100%)	-0.15	0 100 100	15, 46, 88, 135	0
45	DX	77/77 (100%)	0.75	2 (2%) 53 13	67, 118, 172, 239	0
46	BY	63/63 (100%)	0.03	2 (3%) 45 10	34, 75, 134, 210	0
46	DY	63/63 (100%)	0.87	7 (11%) 6 2	130, 305, 419, 450	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
47	BZ	58/58 (100%)	-0.22	0 100 100	6, 24, 74, 116	0
47	DZ	58/58 (100%)	0.55	4 (6%) 17 4	86, 123, 190, 236	0
48	B0	56/56 (100%)	-0.41	0 100 100	3, 22, 75, 168	0
48	D0	56/56 (100%)	1.06	7 (12%) 5 2	66, 132, 242, 278	0
49	B1	50/50 (100%)	0.13	0 100 100	30, 50, 98, 178	0
49	D1	50/50 (100%)	1.15	8 (16%) 3 1	98, 155, 211, 275	0
50	B2	46/46 (100%)	-0.33	0 100 100	13, 27, 51, 183	0
50	D2	46/46 (100%)	0.84	3 (6%) 18 5	78, 118, 155, 203	0
51	B3	64/64 (100%)	-0.26	0 100 100	9, 27, 46, 71	0
51	D3	64/64 (100%)	1.28	16 (25%) 1 1	90, 125, 198, 250	0
52	B4	38/38 (100%)	0.20	0 100 100	28, 49, 87, 112	0
52	D4	38/38 (100%)	2.16	20 (52%) 0 0	78, 141, 210, 225	0
53	CA	1530/1530 (100%)	-0.06	32 (2%) 60 17	38, 100, 272, 376	0
54	CG	150/150 (100%)	1.31	39 (26%) 1 1	118, 209, 283, 333	0
55	CM	113/113 (100%)	1.52	34 (30%) 1 1	196, 344, 437, 471	0
56	CP	80/80 (100%)	0.59	6 (7%) 14 4	59, 91, 145, 249	0
57	DB	117/117 (100%)	0.01	0 100 100	95, 167, 229, 249	0
58	DF	178/178 (100%)	1.30	32 (17%) 2 1	135, 220, 279, 350	0
All	All	20431/20551 (99%)	0.23	1071 (5%) 26 6	3, 97, 258, 543	0

The worst 5 of 1071 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	BA	2179	C	10.3
29	DH	123	ARG	10.0
29	DH	124	THR	9.8
19	CS	29	PRO	9.4
29	DH	105	ALA	9.1

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
59	MG	AA	1627	1/1	0.35	381.00	137,137,137,137	0
59	MG	DA	3063	1/1	2.19	117.48	213,213,213,213	0
59	MG	BB	201	1/1	0.20	117.00	228,228,228,228	0
59	MG	DA	3058	1/1	0.29	81.50	202,202,202,202	0
59	MG	BA	3129	1/1	1.03	69.83	243,243,243,243	0
59	MG	DA	3132	1/1	0.97	68.71	185,185,185,185	0
59	MG	BA	3025	1/1	0.56	59.76	165,165,165,165	0
59	MG	BA	3055	1/1	0.39	59.56	215,215,215,215	0
59	MG	DA	3091	1/1	0.41	46.75	154,154,154,154	0
59	MG	DA	3109	1/1	0.46	44.56	184,184,184,184	0
59	MG	DA	3016	1/1	1.39	44.47	214,214,214,214	0
59	MG	DA	3108	1/1	0.82	43.09	212,212,212,212	0
59	MG	DA	3003	1/1	0.92	37.74	229,229,229,229	0
59	MG	DJ	201	1/1	1.02	35.72	312,312,312,312	0
59	MG	DA	3020	1/1	0.60	35.60	240,240,240,240	0
59	MG	DA	3074	1/1	0.82	35.31	247,247,247,247	0
59	MG	DA	3127	1/1	0.99	35.16	228,228,228,228	0
59	MG	DA	3098	1/1	0.32	35.00	151,151,151,151	0
59	MG	DA	3060	1/1	0.71	28.47	198,198,198,198	0
59	MG	AA	1619	1/1	0.64	25.42	209,209,209,209	0
59	MG	BA	3034	1/1	0.25	25.20	197,197,197,197	0
59	MG	DA	3079	1/1	0.89	24.53	200,200,200,200	0
59	MG	CA	1614	1/1	0.76	23.75	245,245,245,245	0
59	MG	AA	1628	1/1	0.35	21.38	136,136,136,136	0
59	MG	CA	1627	1/1	1.35	20.26	237,237,237,237	0
59	MG	BA	3056	1/1	0.39	18.43	219,219,219,219	0
59	MG	DA	3015	1/1	0.70	17.40	176,176,176,176	0
59	MG	BA	3060	1/1	0.29	17.24	188,188,188,188	0
59	MG	BA	3072	1/1	0.22	17.19	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
59	MG	DA	3002	1/1	0.75	16.88	225,225,225,225	0
59	MG	DA	3026	1/1	1.05	16.78	258,258,258,258	0
59	MG	CA	1612	1/1	0.41	16.15	113,113,113,113	0
59	MG	BA	3117	1/1	0.26	15.75	173,173,173,173	0
59	MG	DA	3036	1/1	0.52	15.53	222,222,222,222	0
59	MG	BA	3036	1/1	0.34	14.45	187,187,187,187	0
59	MG	DA	3049	1/1	0.55	14.02	192,192,192,192	0
59	MG	BA	3074	1/1	0.16	14.00	85,85,85,85	0
59	MG	BA	3059	1/1	0.35	13.64	129,129,129,129	0
59	MG	DA	3106	1/1	0.71	12.98	316,316,316,316	0
59	MG	DA	3064	1/1	0.69	12.18	280,280,280,280	0
59	MG	DA	3130	1/1	3.25	11.70	280,280,280,280	0
59	MG	CA	1603	1/1	0.30	11.35	177,177,177,177	0
59	MG	CA	1626	1/1	0.38	10.25	196,196,196,196	0
59	MG	CA	1619	1/1	0.26	10.22	210,210,210,210	0
59	MG	DA	3086	1/1	0.41	9.93	84,84,84,84	0
59	MG	BA	3133	1/1	0.24	9.70	146,146,146,146	0
59	MG	BA	3122	1/1	0.59	9.61	155,155,155,155	0
59	MG	BA	3021	1/1	0.28	9.37	158,158,158,158	0
59	MG	BA	3096	1/1	0.18	9.00	93,93,93,93	0
59	MG	BA	3069	1/1	0.22	8.99	136,136,136,136	0
59	MG	DA	3069	1/1	0.64	8.69	233,233,233,233	0
59	MG	CA	1615	1/1	0.28	8.24	170,170,170,170	0
59	MG	DA	3029	1/1	0.90	8.23	142,142,142,142	0
59	MG	DA	3007	1/1	0.43	7.92	248,248,248,248	0
59	MG	CA	1639	1/1	0.21	7.75	161,161,161,161	0
59	MG	DA	3011	1/1	0.44	7.57	145,145,145,145	0
59	MG	DA	3085	1/1	0.42	6.73	132,132,132,132	0
59	MG	DA	3062	1/1	0.61	6.02	213,213,213,213	0
59	MG	BA	3131	1/1	0.40	5.91	184,184,184,184	0
59	MG	AA	1636	1/1	0.24	5.86	199,199,199,199	0
59	MG	BA	3134	1/1	0.34	5.83	196,196,196,196	0
59	MG	BA	3014	1/1	0.20	5.73	44,44,44,44	0
59	MG	DA	3005	1/1	0.37	5.61	284,284,284,284	0
59	MG	BA	3057	1/1	0.16	5.46	147,147,147,147	0
59	MG	DA	3059	1/1	0.30	5.43	197,197,197,197	0
59	MG	DA	3078	1/1	0.27	5.40	182,182,182,182	0
59	MG	BA	3106	1/1	0.22	5.35	5,5,5,5	0
59	MG	DA	3053	1/1	0.25	5.23	98,98,98,98	0
59	MG	AA	1614	1/1	0.21	5.17	156,156,156,156	0
59	MG	BA	3110	1/1	0.21	4.43	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
59	MG	BA	3102	1/1	0.20	4.39	9,9,9,9	0
59	MG	AA	1621	1/1	0.17	4.34	143,143,143,143	0
59	MG	BA	3120	1/1	0.19	4.26	3,3,3,3	0
59	MG	AA	1641	1/1	0.20	4.03	148,148,148,148	0
59	MG	BA	3013	1/1	0.19	4.01	1,1,1,1	0
59	MG	BA	3070	1/1	0.21	3.92	135,135,135,135	0
59	MG	BA	3004	1/1	0.25	3.87	156,156,156,156	0
59	MG	CA	1636	1/1	0.27	3.52	119,119,119,119	0
59	MG	BA	3083	1/1	0.17	3.50	37,37,37,37	0
59	MG	DA	3097	1/1	0.36	3.44	137,137,137,137	0
59	MG	DC	302	1/1	0.31	3.37	159,159,159,159	0
59	MG	BA	3033	1/1	0.18	3.28	14,14,14,14	0
59	MG	CE	201	1/1	0.27	3.10	132,132,132,132	0
59	MG	DA	3030	1/1	0.32	3.02	104,104,104,104	0
59	MG	BA	3099	1/1	0.20	2.99	8,8,8,8	0
59	MG	BA	3040	1/1	0.17	2.90	13,13,13,13	0
59	MG	BA	3078	1/1	0.17	2.67	31,31,31,31	0
59	MG	BA	3095	1/1	0.20	2.62	117,117,117,117	0
59	MG	DA	3022	1/1	0.34	2.54	173,173,173,173	0
59	MG	BA	3085	1/1	0.18	2.53	124,124,124,124	0
59	MG	BA	3105	1/1	0.17	2.45	27,27,27,27	0
59	MG	DA	3028	1/1	0.65	2.38	222,222,222,222	0
59	MG	AA	1608	1/1	0.20	2.36	47,47,47,47	0
59	MG	AA	1622	1/1	0.20	2.29	40,40,40,40	0
59	MG	BA	3062	1/1	0.20	2.29	5,5,5,5	0
59	MG	DA	3094	1/1	0.26	2.18	134,134,134,134	0
59	MG	DA	3100	1/1	0.31	2.13	105,105,105,105	0
59	MG	CA	1629	1/1	0.24	2.03	126,126,126,126	0
59	MG	DA	3123	1/1	0.28	1.99	183,183,183,183	0
59	MG	DA	3129	1/1	0.60	1.93	210,210,210,210	0
59	MG	CA	1624	1/1	0.25	1.92	128,128,128,128	0
59	MG	DA	3045	1/1	0.24	1.88	160,160,160,160	0
59	MG	BA	3019	1/1	0.17	1.87	13,13,13,13	0
59	MG	DA	3014	1/1	0.36	1.82	133,133,133,133	0
59	MG	DA	3087	1/1	0.28	1.75	152,152,152,152	0
59	MG	BA	3028	1/1	0.20	1.71	49,49,49,49	0
59	MG	BA	3037	1/1	0.16	1.70	24,24,24,24	0
59	MG	DA	3057	1/1	0.60	1.68	185,185,185,185	0
59	MG	DA	3081	1/1	0.29	1.63	78,78,78,78	0
60	TEL	BA	3135	58/58	0.22	1.49	0,23,68,74	0
59	MG	CA	1625	1/1	0.17	1.47	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
59	MG	CA	1618	1/1	0.24	1.47	146,146,146,146	0
59	MG	DA	3033	1/1	0.32	1.42	132,132,132,132	0
59	MG	BA	3015	1/1	0.16	1.42	95,95,95,95	0
59	MG	BA	3009	1/1	0.17	1.40	38,38,38,38	0
59	MG	DA	3133	1/1	0.35	1.39	198,198,198,198	0
59	MG	BA	3007	1/1	0.15	1.37	104,104,104,104	0
59	MG	CA	1606	1/1	0.16	1.27	54,54,54,54	0
59	MG	DA	3013	1/1	0.36	1.27	189,189,189,189	0
59	MG	BA	3039	1/1	0.16	1.24	8,8,8,8	0
59	MG	BA	3073	1/1	0.16	1.04	17,17,17,17	0
59	MG	AA	1630	1/1	0.23	0.93	189,189,189,189	0
59	MG	DC	301	1/1	0.24	0.93	155,155,155,155	0
59	MG	BA	3018	1/1	0.14	0.92	44,44,44,44	0
59	MG	DA	3125	1/1	0.38	0.85	152,152,152,152	0
59	MG	CA	1630	1/1	0.26	0.75	126,126,126,126	0
59	MG	BA	3008	1/1	0.16	0.72	12,12,12,12	0
59	MG	DA	3047	1/1	0.20	0.71	142,142,142,142	0
59	MG	CA	1620	1/1	0.15	0.67	164,164,164,164	0
59	MG	BA	3041	1/1	0.16	0.62	21,21,21,21	0
59	MG	BA	3051	1/1	0.17	0.60	24,24,24,24	0
59	MG	BA	3011	1/1	0.23	0.48	126,126,126,126	0
59	MG	DA	3004	1/1	0.19	0.46	122,122,122,122	0
59	MG	DA	3075	1/1	0.28	0.45	172,172,172,172	0
59	MG	BA	3048	1/1	0.16	0.42	101,101,101,101	0
59	MG	DA	3050	1/1	0.28	0.39	160,160,160,160	0
59	MG	DA	3099	1/1	0.19	0.36	164,164,164,164	0
59	MG	CA	1607	1/1	0.19	0.33	134,134,134,134	0
59	MG	BA	3022	1/1	0.16	0.31	5,5,5,5	0
59	MG	BA	3061	1/1	0.16	0.27	11,11,11,11	0
59	MG	DA	3126	1/1	0.22	0.27	112,112,112,112	0
59	MG	DA	3027	1/1	0.27	0.24	157,157,157,157	0
59	MG	AA	1618	1/1	0.17	0.23	87,87,87,87	0
59	MG	DA	3105	1/1	0.23	0.22	61,61,61,61	0
59	MG	DA	3076	1/1	0.25	0.20	149,149,149,149	0
59	MG	BA	3109	1/1	0.15	0.14	112,112,112,112	0
59	MG	BA	3107	1/1	0.16	0.13	12,12,12,12	0
59	MG	DA	3128	1/1	0.34	0.12	116,116,116,116	0
59	MG	AA	1631	1/1	0.15	0.01	168,168,168,168	0
59	MG	BA	3030	1/1	0.17	-0.04	9,9,9,9	0
59	MG	BA	3064	1/1	0.14	-0.07	5,5,5,5	0
59	MG	DA	3110	1/1	0.36	-0.12	146,146,146,146	0
59	MG	BA	3126	1/1	0.14	-0.26	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	BA	3111	1/1	0.15	-0.31	38,38,38,38	0
59	MG	CA	1616	1/1	0.28	-0.33	203,203,203,203	0
59	MG	DA	3082	1/1	0.19	-0.35	132,132,132,132	0
59	MG	CA	1621	1/1	0.17	-0.35	50,50,50,50	0
59	MG	DA	3083	1/1	0.22	-0.37	204,204,204,204	0
59	MG	AA	1642	1/1	0.14	-0.37	36,36,36,36	0
59	MG	BA	3090	1/1	0.11	-0.38	120,120,120,120	0
59	MG	AA	1638	1/1	0.17	-0.40	47,47,47,47	0
59	MG	DA	3043	1/1	0.30	-0.43	179,179,179,179	0
59	MG	DA	3102	1/1	0.22	-0.46	87,87,87,87	0
59	MG	BA	3103	1/1	0.15	-0.49	21,21,21,21	0
59	MG	BA	3089	1/1	0.11	-0.50	95,95,95,95	0
59	MG	AA	1617	1/1	0.18	-0.54	147,147,147,147	0
59	MG	DA	3019	1/1	0.20	-0.56	192,192,192,192	0
59	MG	AA	1637	1/1	0.13	-0.57	96,96,96,96	0
59	MG	CA	1635	1/1	0.16	-0.61	201,201,201,201	0
59	MG	BA	3130	1/1	0.14	-0.64	108,108,108,108	0
59	MG	AA	1635	1/1	0.13	-0.71	73,73,73,73	0
59	MG	BA	3114	1/1	0.15	-0.72	8,8,8,8	0
59	MG	DA	3018	1/1	0.16	-0.72	125,125,125,125	0
59	MG	AA	1633	1/1	0.11	-0.73	62,62,62,62	0
59	MG	AA	1624	1/1	0.13	-0.76	102,102,102,102	0
59	MG	AA	1620	1/1	0.11	-0.82	126,126,126,126	0
59	MG	DA	3120	1/1	0.21	-0.85	91,91,91,91	0
59	MG	DA	3006	1/1	0.11	-0.86	176,176,176,176	0
59	MG	CA	1632	1/1	0.10	-0.88	65,65,65,65	0
59	MG	BA	3042	1/1	0.12	-0.91	16,16,16,16	0
59	MG	DA	3084	1/1	0.16	-0.91	201,201,201,201	0
59	MG	BA	3077	1/1	0.13	-0.92	38,38,38,38	0
59	MG	CA	1631	1/1	0.13	-0.92	160,160,160,160	0
59	MG	BA	3084	1/1	0.16	-0.92	3,3,3,3	0
59	MG	BA	3124	1/1	0.14	-0.96	33,33,33,33	0
59	MG	BA	3053	1/1	0.15	-0.98	6,6,6,6	0
59	MG	AA	1639	1/1	0.12	-0.98	109,109,109,109	0
59	MG	DA	3103	1/1	0.17	-0.99	76,76,76,76	0
59	MG	BA	3119	1/1	0.07	-1.00	47,47,47,47	0
59	MG	DA	3031	1/1	0.20	-1.00	76,76,76,76	0
59	MG	CA	1623	1/1	0.15	-1.02	121,121,121,121	0
59	MG	CA	1611	1/1	0.18	-1.03	111,111,111,111	0
59	MG	CA	1617	1/1	0.11	-1.06	214,214,214,214	0
59	MG	AA	1610	1/1	0.08	-1.07	201,201,201,201	0
59	MG	DA	3115	1/1	0.20	-1.10	126,126,126,126	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
59	MG	AA	1605	1/1	0.13	-1.11	52,52,52,52	0
59	MG	CA	1628	1/1	0.15	-1.13	165,165,165,165	0
59	MG	DA	3025	1/1	0.20	-1.16	104,104,104,104	0
59	MG	DA	3067	1/1	0.21	-1.18	64,64,64,64	0
59	MG	CA	1608	1/1	0.17	-1.18	44,44,44,44	0
59	MG	BA	3029	1/1	0.13	-1.26	52,52,52,52	0
59	MG	DA	3048	1/1	0.16	-1.26	95,95,95,95	0
59	MG	BA	3063	1/1	0.13	-1.27	12,12,12,12	0
59	MG	DA	3046	1/1	0.21	-1.27	125,125,125,125	0
59	MG	BA	3079	1/1	0.14	-1.30	11,11,11,11	0
59	MG	DA	3111	1/1	0.18	-1.33	179,179,179,179	0
59	MG	DA	3044	1/1	0.18	-1.40	92,92,92,92	0
59	MG	BA	3100	1/1	0.12	-1.41	85,85,85,85	0
59	MG	DA	3012	1/1	0.19	-1.42	41,41,41,41	0
59	MG	CA	1637	1/1	0.11	-1.45	170,170,170,170	0
59	MG	BA	3081	1/1	0.14	-1.50	92,92,92,92	0
59	MG	CA	1622	1/1	0.11	-1.52	190,190,190,190	0
59	MG	DA	3077	1/1	0.17	-1.52	123,123,123,123	0
59	MG	BA	3098	1/1	0.12	-1.54	26,26,26,26	0
59	MG	BB	203	1/1	0.12	-1.59	34,34,34,34	0
59	MG	BA	3125	1/1	0.13	-1.59	16,16,16,16	0
59	MG	DA	3096	1/1	0.14	-1.66	93,93,93,93	0
59	MG	BA	3001	1/1	0.12	-1.67	117,117,117,117	0
59	MG	AA	1616	1/1	0.14	-1.72	106,106,106,106	0
59	MG	CA	1640	1/1	0.15	-1.74	80,80,80,80	0
59	MG	BA	3123	1/1	0.14	-1.79	11,11,11,11	0
59	MG	DA	3093	1/1	0.15	-1.80	234,234,234,234	0
59	MG	DA	3095	1/1	0.19	-1.80	122,122,122,122	0
59	MG	CA	1605	1/1	0.13	-1.81	32,32,32,32	0
59	MG	DA	3116	1/1	0.13	-1.84	54,54,54,54	0
59	MG	DA	3072	1/1	0.16	-1.86	131,131,131,131	0
59	MG	DA	3009	1/1	0.14	-1.87	100,100,100,100	0
59	MG	DA	3071	1/1	0.18	-1.92	74,74,74,74	0
59	MG	CA	1633	1/1	0.14	-1.94	138,138,138,138	0
59	MG	DA	3104	1/1	0.16	-1.94	33,33,33,33	0
59	MG	DA	3080	1/1	0.11	-1.95	152,152,152,152	0
59	MG	AA	1604	1/1	0.09	-1.98	121,121,121,121	0
59	MG	DA	3037	1/1	0.10	-2.00	97,97,97,97	0
59	MG	DA	3008	1/1	0.17	-2.02	112,112,112,112	0
59	MG	BA	3017	1/1	0.10	-2.05	33,33,33,33	0
59	MG	AA	1629	1/1	0.11	-2.06	84,84,84,84	0
59	MG	BA	3027	1/1	0.15	-2.07	119,119,119,119	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
59	MG	DA	3112	1/1	0.14	-2.09	80,80,80,80	0
59	MG	BA	3052	1/1	0.15	-2.12	46,46,46,46	0
59	MG	BA	3116	1/1	0.13	-2.15	71,71,71,71	0
59	MG	CA	1602	1/1	0.15	-2.15	145,145,145,145	0
59	MG	BA	3104	1/1	0.16	-2.16	13,13,13,13	0
59	MG	DA	3024	1/1	0.20	-2.17	100,100,100,100	0
59	MG	DA	3113	1/1	0.11	-2.22	121,121,121,121	0
59	MG	BA	3049	1/1	0.13	-2.23	6,6,6,6	0
61	ZN	D4	101	1/1	0.10	-2.27	157,157,157,157	0
59	MG	AA	1609	1/1	0.12	-2.39	54,54,54,54	0
59	MG	CA	1641	1/1	0.11	-2.40	82,82,82,82	0
59	MG	DA	3092	1/1	0.25	-2.42	119,119,119,119	0
59	MG	DA	3089	1/1	0.18	-2.42	100,100,100,100	0
59	MG	DA	3131	1/1	0.16	-2.45	91,91,91,91	0
59	MG	BA	3065	1/1	0.11	-2.46	20,20,20,20	0
59	MG	AA	1643	1/1	0.11	-2.46	43,43,43,43	0
59	MG	AA	1602	1/1	0.12	-2.49	152,152,152,152	0
59	MG	AA	1606	1/1	0.10	-2.50	72,72,72,72	0
59	MG	DA	3119	1/1	0.12	-2.50	67,67,67,67	0
59	MG	DA	3107	1/1	0.21	-2.53	91,91,91,91	0
59	MG	AA	1615	1/1	0.08	-2.56	128,128,128,128	0
59	MG	DA	3032	1/1	0.18	-2.59	131,131,131,131	0
59	MG	CA	1613	1/1	0.15	-2.61	107,107,107,107	0
59	MG	DA	3065	1/1	0.18	-2.61	77,77,77,77	0
59	MG	BA	3121	1/1	0.11	-2.67	35,35,35,35	0
59	MG	BA	3112	1/1	0.08	-2.68	41,41,41,41	0
59	MG	AA	1623	1/1	0.08	-2.68	89,89,89,89	0
59	MG	DA	3070	1/1	0.14	-2.69	60,60,60,60	0
59	MG	AA	1634	1/1	0.09	-2.75	62,62,62,62	0
59	MG	DA	3061	1/1	0.11	-2.78	131,131,131,131	0
59	MG	CA	1609	1/1	0.14	-2.87	97,97,97,97	0
59	MG	DA	3017	1/1	0.13	-2.88	51,51,51,51	0
59	MG	AA	1603	1/1	0.12	-2.89	131,131,131,131	0
59	MG	BA	3071	1/1	0.11	-2.90	7,7,7,7	0
59	MG	BA	3132	1/1	0.13	-2.92	1,1,1,1	0
59	MG	BA	3047	1/1	0.08	-2.93	151,151,151,151	0
59	MG	DA	3042	1/1	0.18	-2.94	99,99,99,99	0
61	ZN	B4	101	1/1	0.09	-2.95	118,118,118,118	0
59	MG	DA	3052	1/1	0.12	-2.99	56,56,56,56	0
59	MG	BA	3045	1/1	0.14	-3.00	30,30,30,30	0
59	MG	DA	3068	1/1	0.14	-3.04	67,67,67,67	0
59	MG	DA	3117	1/1	0.19	-3.11	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	BA	3118	1/1	0.13	-3.12	23,23,23,23	0
59	MG	BA	3086	1/1	0.13	-3.19	134,134,134,134	0
59	MG	DA	3073	1/1	0.06	-3.26	148,148,148,148	0
59	MG	BA	3005	1/1	0.11	-3.29	75,75,75,75	0
59	MG	DA	3088	1/1	0.17	-3.32	170,170,170,170	0
59	MG	DA	3118	1/1	0.10	-3.39	59,59,59,59	0
59	MG	DA	3124	1/1	0.17	-3.49	70,70,70,70	0
59	MG	DA	3021	1/1	0.15	-3.55	83,83,83,83	0
59	MG	CA	1610	1/1	0.06	-3.60	151,151,151,151	0
59	MG	AA	1612	1/1	0.09	-3.64	85,85,85,85	0
59	MG	CA	1601	1/1	0.10	-3.67	120,120,120,120	0
59	MG	DA	3054	1/1	0.15	-3.72	70,70,70,70	0
59	MG	DA	3121	1/1	0.14	-3.75	122,122,122,122	0
59	MG	CA	1638	1/1	0.09	-3.85	141,141,141,141	0
59	MG	BB	204	1/1	0.07	-3.92	23,23,23,23	0
59	MG	DA	3051	1/1	0.12	-3.93	91,91,91,91	0
59	MG	BA	3092	1/1	0.07	-3.97	70,70,70,70	0
59	MG	AA	1625	1/1	0.08	-4.00	64,64,64,64	0
59	MG	BA	3127	1/1	0.13	-4.00	2,2,2,2	0
59	MG	AA	1601	1/1	0.07	-4.09	77,77,77,77	0
59	MG	BA	3128	1/1	0.11	-4.11	15,15,15,15	0
59	MG	BA	3076	1/1	0.09	-4.13	119,119,119,119	0
59	MG	DB	201	1/1	0.10	-4.27	88,88,88,88	0
59	MG	BA	3068	1/1	0.10	-4.57	151,151,151,151	0
59	MG	BA	3024	1/1	0.11	-4.58	18,18,18,18	0
59	MG	DA	3035	1/1	0.14	-4.59	79,79,79,79	0
59	MG	BB	202	1/1	0.06	-4.62	64,64,64,64	0
59	MG	BA	3023	1/1	0.10	-4.63	16,16,16,16	0
59	MG	BA	3108	1/1	0.10	-4.67	83,83,83,83	0
59	MG	AA	1613	1/1	0.08	-4.76	50,50,50,50	0
59	MG	CA	1634	1/1	0.10	-4.78	74,74,74,74	0
59	MG	BA	3044	1/1	0.06	-4.85	43,43,43,43	0
59	MG	DA	3056	1/1	0.17	-4.87	72,72,72,72	0
59	MG	DA	3039	1/1	0.16	-4.92	79,79,79,79	0
59	MG	DA	3001	1/1	0.08	-4.93	149,149,149,149	0
59	MG	BA	3002	1/1	0.09	-5.03	85,85,85,85	0
59	MG	BA	3050	1/1	0.08	-5.03	33,33,33,33	0
59	MG	BA	3012	1/1	0.13	-5.04	1,1,1,1	0
59	MG	BA	3058	1/1	0.04	-5.23	47,47,47,47	0
59	MG	BA	3087	1/1	0.11	-5.31	36,36,36,36	0
59	MG	BA	3097	1/1	0.10	-5.44	33,33,33,33	0
59	MG	BA	3031	1/1	0.11	-5.48	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	BA	3067	1/1	0.12	-5.48	17,17,17,17	0
59	MG	AA	1611	1/1	0.07	-5.56	60,60,60,60	0
59	MG	DA	3040	1/1	0.15	-5.59	65,65,65,65	0
59	MG	BA	3035	1/1	0.09	-5.66	5,5,5,5	0
59	MG	BA	3088	1/1	0.09	-5.69	62,62,62,62	0
59	MG	DA	3066	1/1	0.13	-5.87	61,61,61,61	0
59	MG	BA	3075	1/1	0.05	-5.93	26,26,26,26	0
59	MG	BA	3046	1/1	0.09	-5.99	12,12,12,12	0
59	MG	BA	3115	1/1	0.10	-6.00	7,7,7,7	0
59	MG	BA	3113	1/1	0.09	-6.10	138,138,138,138	0
59	MG	BA	3006	1/1	0.08	-6.18	31,31,31,31	0
59	MG	BA	3038	1/1	0.10	-6.44	12,12,12,12	0
59	MG	BA	3003	1/1	0.10	-6.50	58,58,58,58	0
59	MG	BA	3082	1/1	0.11	-6.51	109,109,109,109	0
59	MG	BA	3020	1/1	0.10	-6.57	11,11,11,11	0
59	MG	BA	3066	1/1	0.10	-6.66	21,21,21,21	0
59	MG	BA	3016	1/1	0.09	-6.79	4,4,4,4	0
59	MG	DA	3023	1/1	0.12	-6.80	111,111,111,111	0
59	MG	DA	3034	1/1	0.16	-6.90	78,78,78,78	0
59	MG	DA	3090	1/1	0.11	-7.00	78,78,78,78	0
59	MG	AA	1632	1/1	0.07	-7.32	90,90,90,90	0
59	MG	BA	3080	1/1	0.04	-7.46	26,26,26,26	0
59	MG	BA	3101	1/1	0.06	-7.63	18,18,18,18	0
59	MG	DA	3122	1/1	0.14	-7.68	94,94,94,94	0
59	MG	CA	1604	1/1	0.05	-7.78	57,57,57,57	0
59	MG	DA	3101	1/1	0.12	-8.04	75,75,75,75	0
59	MG	DA	3055	1/1	0.11	-8.31	72,72,72,72	0
59	MG	AA	1607	1/1	0.09	-8.33	105,105,105,105	0
59	MG	AA	1640	1/1	0.05	-8.33	84,84,84,84	0
59	MG	BA	3032	1/1	0.12	-8.46	25,25,25,25	0
59	MG	DA	3041	1/1	0.12	-8.73	110,110,110,110	0
59	MG	DA	3038	1/1	0.13	-8.91	203,203,203,203	0
59	MG	BA	3043	1/1	0.06	-9.09	18,18,18,18	0
59	MG	DA	3114	1/1	0.08	-9.52	147,147,147,147	0
59	MG	BA	3010	1/1	0.07	-9.88	17,17,17,17	0
59	MG	BA	3091	1/1	0.07	-10.75	49,49,49,49	0
59	MG	BA	3093	1/1	0.07	-13.77	35,35,35,35	0
59	MG	BA	3026	1/1	0.07	-15.26	32,32,32,32	0
59	MG	AA	1626	1/1	0.10	-19.65	52,52,52,52	0
59	MG	BA	3054	1/1	0.10	-24.19	58,58,58,58	0
59	MG	BA	3094	1/1	0.05	-35.95	22,22,22,22	0
59	MG	DA	3010	1/1	0.62	-	195,195,195,195	0

6.5 Other polymers ⓘ

There are no such residues in this entry.