



wwPDB X-ray Structure Validation Summary Report

Jul 24, 2014 – 05:14 PM EDT

PDB ID : 4U1U
Title : Crystal structure of the E. coli ribosome bound to quinupristin.
Authors : Noeske, J.; Huang, J.; Olivier, N.B.; Giacobbe, R.A.; Zambrowski, M.; Cate, J.H.D.
Deposited on : 2014-04-23
Resolution : 2.95 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>

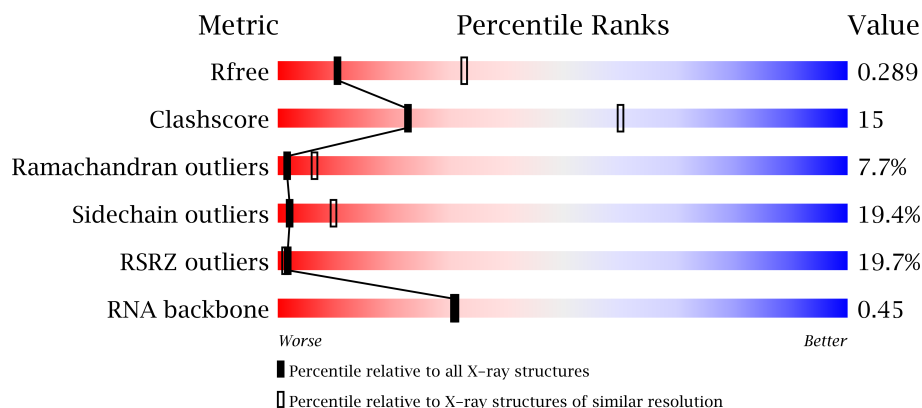
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.16 November 2013
Xtriage (Phenix)	:	dev-1439
EDS	:	stable23489
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)	:	stable23489

1 Overall quality at a glance

The reported resolution of this entry is 2.95 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	1587 (3.00-2.92)
Clashscore	79885	2029 (3.00-2.92)
Ramachandran outliers	78287	1955 (3.00-2.92)
Sidechain outliers	78261	1958 (3.00-2.92)
RSRZ outliers	66119	1588 (3.00-2.92)
RNA backbone	1838	1019 (3.46-2.46)

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	1539	
1	CA	1539	
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	

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Mol	Chain	Length	Quality of chain
6	CF	100	
7	AG	151	
7	CG	151	
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	
13	CM	114	
14	AN	100	
14	CN	100	
15	AO	88	
15	CO	88	
16	AP	82	
16	CP	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	119	
23	DB	119	
24	BC	271	
24	DC	271	
25	BD	209	
25	DD	209	
26	BE	201	
26	DE	201	
27	BF	177	

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Mol	Chain	Length	Quality of chain
27	DF	177	
28	BG	176	
28	DG	176	
29	BH	149	
29	DH	149	
30	BI	141	
30	DI	141	
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	76	
44	DW	76	
45	BX	77	
45	DX	77	
46	BY	63	
46	DY	63	
47	BZ	58	
47	DZ	58	
48	B0	56	

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Mol	Chain	Length	Quality of chain
48	D0	56	
49	B1	50	
49	D1	50	
50	B2	46	
50	D2	46	
51	B3	64	
51	D3	64	
52	B4	38	
52	D4	38	
53	B5	228	
54	B6	8	
54	D6	8	

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

Mol	Type	Chain	Res	Geometry	Electron density
55	MG	AA	1614	-	X
55	MG	AA	1619	-	X
55	MG	AA	1622	-	X
55	MG	AA	1626	-	X
55	MG	AA	1627	-	X
55	MG	AA	1637	-	X
55	MG	AA	1644	-	X
55	MG	AA	1646	-	X
55	MG	AA	1648	-	X
55	MG	AA	1649	-	X
55	MG	AA	1651	-	X
55	MG	AA	1652	-	X
55	MG	AA	1653	-	X
55	MG	AA	1654	-	X
55	MG	AA	1657	-	X
55	MG	AA	1659	-	X
55	MG	AA	1660	-	X
55	MG	AA	1661	-	X
55	MG	AA	1662	-	X
55	MG	AA	1666	-	X
55	MG	AA	1667	-	X
55	MG	AA	1668	-	X
55	MG	AA	1669	-	X
55	MG	AA	1670	-	X
55	MG	AM	201	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
55	MG	BA	3015	-	X
55	MG	BA	3019	-	X
55	MG	BA	3025	-	X
55	MG	BA	3030	-	X
55	MG	BA	3033	-	X
55	MG	BA	3037	-	X
55	MG	BA	3040	-	X
55	MG	BA	3046	-	X
55	MG	BA	3055	-	X
55	MG	BA	3057	-	X
55	MG	BA	3060	-	X
55	MG	BA	3061	-	X
55	MG	BA	3067	-	X
55	MG	BA	3070	-	X
55	MG	BA	3072	-	X
55	MG	BA	3083	-	X
55	MG	BA	3098	-	X
55	MG	BA	3102	-	X
55	MG	BA	3106	-	X
55	MG	BA	3108	-	X
55	MG	BA	3113	-	X
55	MG	BA	3114	-	X
55	MG	BA	3116	-	X
55	MG	BA	3119	-	X
55	MG	BA	3126	-	X
55	MG	BA	3128	-	X
55	MG	BA	3130	-	X
55	MG	BA	3133	-	X
55	MG	BA	3137	-	X
55	MG	BA	3138	-	X
55	MG	BA	3139	-	X
55	MG	BA	3140	-	X
55	MG	BA	3141	-	X
55	MG	BA	3142	-	X
55	MG	BA	3143	-	X
55	MG	BA	3144	-	X
55	MG	BA	3145	-	X
55	MG	BA	3146	-	X
55	MG	BA	3147	-	X
55	MG	BA	3148	-	X
55	MG	BA	3150	-	X
55	MG	BA	3151	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
55	MG	BA	3152	-	X
55	MG	BA	3153	-	X
55	MG	BA	3154	-	X
55	MG	BA	3155	-	X
55	MG	BA	3156	-	X
55	MG	BA	3157	-	X
55	MG	BA	3160	-	X
55	MG	BA	3161	-	X
55	MG	BA	3162	-	X
55	MG	BA	3164	-	X
55	MG	BA	3166	-	X
55	MG	BA	3168	-	X
55	MG	BA	3170	-	X
55	MG	BA	3178	-	X
55	MG	BA	3179	-	X
55	MG	BA	3180	-	X
55	MG	BA	3181	-	X
55	MG	BA	3182	-	X
55	MG	BA	3186	-	X
55	MG	BA	3188	-	X
55	MG	BA	3190	-	X
55	MG	BA	3191	-	X
55	MG	BB	204	-	X
55	MG	CA	1605	-	X
55	MG	CA	1608	-	X
55	MG	CA	1609	-	X
55	MG	CA	1615	-	X
55	MG	CA	1623	-	X
55	MG	CA	1625	-	X
55	MG	CA	1628	-	X
55	MG	CA	1633	-	X
55	MG	CA	1637	-	X
55	MG	CA	1638	-	X
55	MG	CA	1640	-	X
55	MG	CA	1641	-	X
55	MG	CA	1642	-	X
55	MG	CA	1643	-	X
55	MG	CA	1644	-	X
55	MG	CA	1647	-	X
55	MG	CA	1648	-	X
55	MG	CA	1650	-	X
55	MG	CA	1653	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
55	MG	CA	1654	-	X
55	MG	CA	1655	-	X
55	MG	DA	3002	-	X
55	MG	DA	3004	-	X
55	MG	DA	3005	-	X
55	MG	DA	3007	-	X
55	MG	DA	3008	-	X
55	MG	DA	3013	-	X
55	MG	DA	3015	-	X
55	MG	DA	3016	-	X
55	MG	DA	3020	-	X
55	MG	DA	3025	-	X
55	MG	DA	3027	-	X
55	MG	DA	3029	-	X
55	MG	DA	3031	-	X
55	MG	DA	3034	-	X
55	MG	DA	3041	-	X
55	MG	DA	3054	-	X
55	MG	DA	3055	-	X
55	MG	DA	3056	-	X
55	MG	DA	3057	-	X
55	MG	DA	3059	-	X
55	MG	DA	3060	-	X
55	MG	DA	3061	-	X
55	MG	DA	3070	-	X
55	MG	DA	3071	-	X
55	MG	DA	3076	-	X
55	MG	DA	3084	-	X
55	MG	DA	3088	-	X
55	MG	DA	3091	-	X
55	MG	DA	3092	-	X
55	MG	DA	3094	-	X
55	MG	DA	3098	-	X
55	MG	DA	3109	-	X
55	MG	DA	3110	-	X
55	MG	DA	3119	-	X
55	MG	DA	3124	-	X
55	MG	DA	3131	-	X
55	MG	DA	3133	-	X
55	MG	DA	3137	-	X
55	MG	DA	3138	-	X
55	MG	DA	3139	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
55	MG	DA	3140	-	X
55	MG	DA	3142	-	X
55	MG	DA	3148	-	X
55	MG	DA	3149	-	X
55	MG	DA	3150	-	X
55	MG	DA	3151	-	X
55	MG	DA	3153	-	X
55	MG	DA	3155	-	X
55	MG	DA	3157	-	X
55	MG	DA	3160	-	X
55	MG	DA	3162	-	X
55	MG	DA	3163	-	X
55	MG	DA	3165	-	X

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 288328 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	1538	Total	C	N	O	P	0	0	0
			32995	14716	6050	10691	1538			
1	CA	1539	Total	C	N	O	P	0	0	0
			33015	14725	6052	10699	1539			

- 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			
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			
7	CG	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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			
13	CM	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	96	Total	C	N	O	S	0	0	0
			774	483	160	128	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
			710	437	143	129	1			
15	CO	88	Total	C	N	O	S	0	0	0
			710	437	143	129	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			
16	CP	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	0	0	0
			456	288	86	82			
18	CR	55	Total	C	N	O	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	2897	Total	C	N	O	P	0	0	0
			62195	27745	11446	20107	2897			
22	DA	2897	Total	C	N	O	P	0	0	0
			62195	27745	11446	20107	2897			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	BB	119	Total	C	N	O	P	0	0	0
			2549	1135	466	829	119			
23	DB	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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			
27	DF	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
			1110	699	197	213	1			
29	DH	149	Total	C	N	O	S	0	0	0
			1110	699	197	213	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			
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	0	0	0
			892	552	178	162			
36	DO	116	Total	C	N	O	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	S	0	0	0
			780	492	146	142				

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
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	76	Total	C	N	O	S	0	0	0
			580	359	117	103	1			
44	DW	75	Total	C	N	O	S	0	0	0
			569	353	113	102	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 509	C 313	N 99	O 95	S 2	0	0	0
46	DY	63	Total 509	C 313	N 99	O 95	S 2	0	0	0

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

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

- 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			
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 protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
53	B5	191	Total	C	N	O	0	0	1
			1142	691	221	230			

- Molecule 54 is a protein called Quinupristin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B6	8	Total	C	N	O	S	0	0	0
			73	53	9	10	1			
54	D6	8	Total	C	N	O	S	0	0	0
			73	53	9	10	1			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	BB	4	Total	Mg	0	0
			4	4		
55	BA	195	Total	Mg	0	0
			195	195		
55	CA	55	Total	Mg	0	0
			55	55		
55	DQ	1	Total	Mg	0	0
			1	1		
55	CM	1	Total	Mg	0	0
			1	1		
55	AA	71	Total	Mg	0	0
			71	71		
55	DA	167	Total	Mg	0	0
			167	167		
55	DB	3	Total	Mg	0	0
			3	3		
55	AM	1	Total	Mg	0	0
			1	1		

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

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

- Molecule 57 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	AA	194	Total O 194 194	0	0
57	AL	1	Total O 1 1	0	0
57	AN	5	Total O 5 5	0	0
57	AT	2	Total O 2 2	0	0
57	AU	1	Total O 1 1	0	0
57	BA	619	Total O 619 619	0	0
57	BB	13	Total O 13 13	0	0
57	BC	8	Total O 8 8	0	0
57	BD	3	Total O 3 3	0	0
57	BE	3	Total O 3 3	0	0
57	BF	1	Total O 1 1	0	0
57	BG	1	Total O 1 1	0	0
57	BL	5	Total O 5 5	0	0
57	BN	5	Total O 5 5	0	0
57	BS	1	Total O 1 1	0	0
57	BV	1	Total O 1 1	0	0
57	B2	1	Total O 1 1	0	0
57	B3	3	Total O 3 3	0	0
57	B4	2	Total O 2 2	0	0
57	CA	189	Total O 189 189	0	0
57	CL	1	Total O 1 1	0	0
57	CN	3	Total O 3 3	0	0

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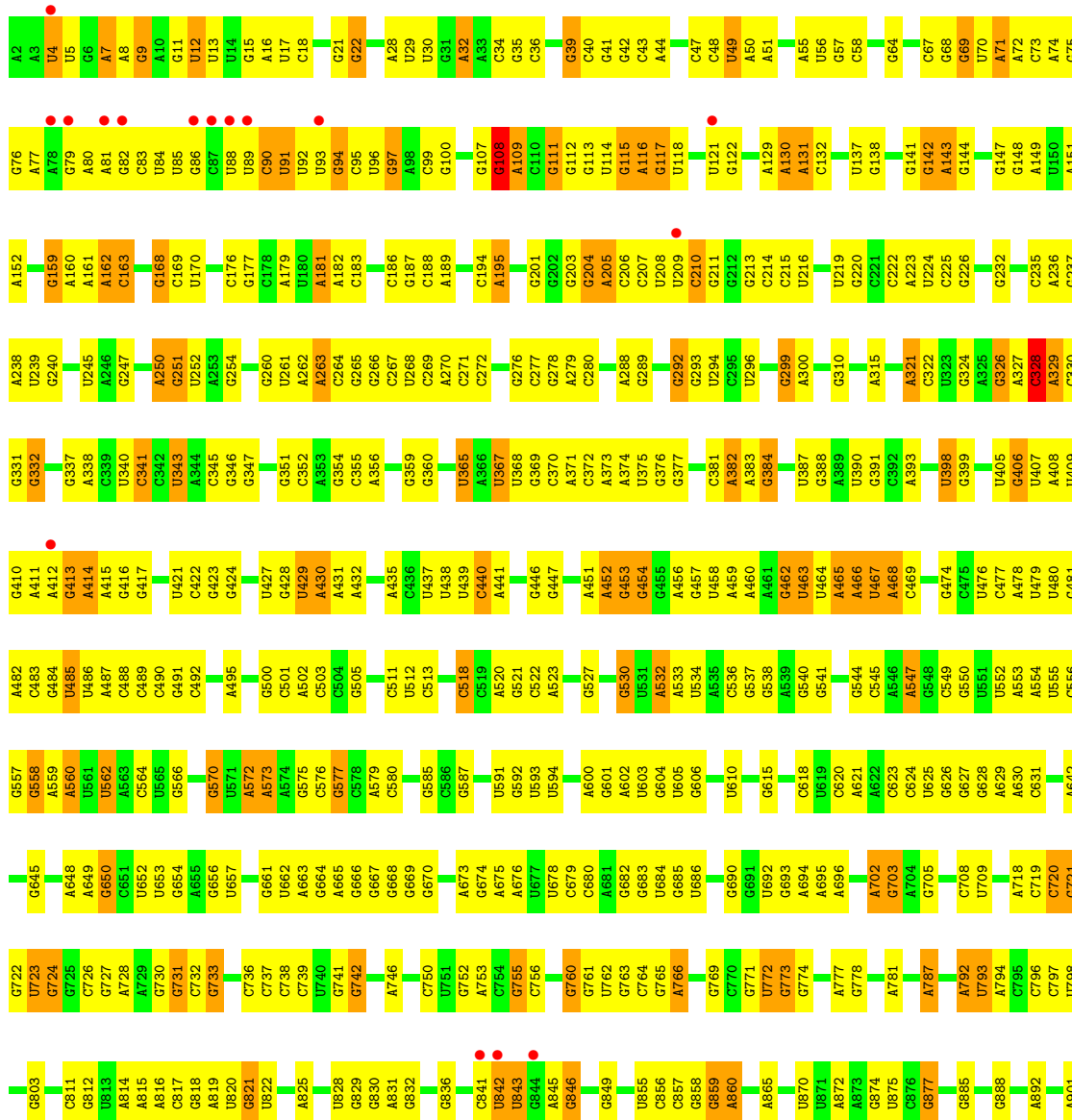
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57	CU	1	Total 1	O 1	0	0
57	DA	612	Total 612	O 612	0	0
57	DB	13	Total 13	O 13	0	0
57	DC	7	Total 7	O 7	0	0
57	DD	4	Total 4	O 4	0	0
57	DE	4	Total 4	O 4	0	0
57	DL	4	Total 4	O 4	0	0
57	DN	1	Total 1	O 1	0	0
57	DQ	2	Total 2	O 2	0	0
57	DT	3	Total 3	O 3	0	0
57	DV	1	Total 1	O 1	0	0
57	D0	1	Total 1	O 1	0	0
57	D2	2	Total 2	O 2	0	0
57	D3	1	Total 1	O 1	0	0
57	D4	1	Total 1	O 1	0	0

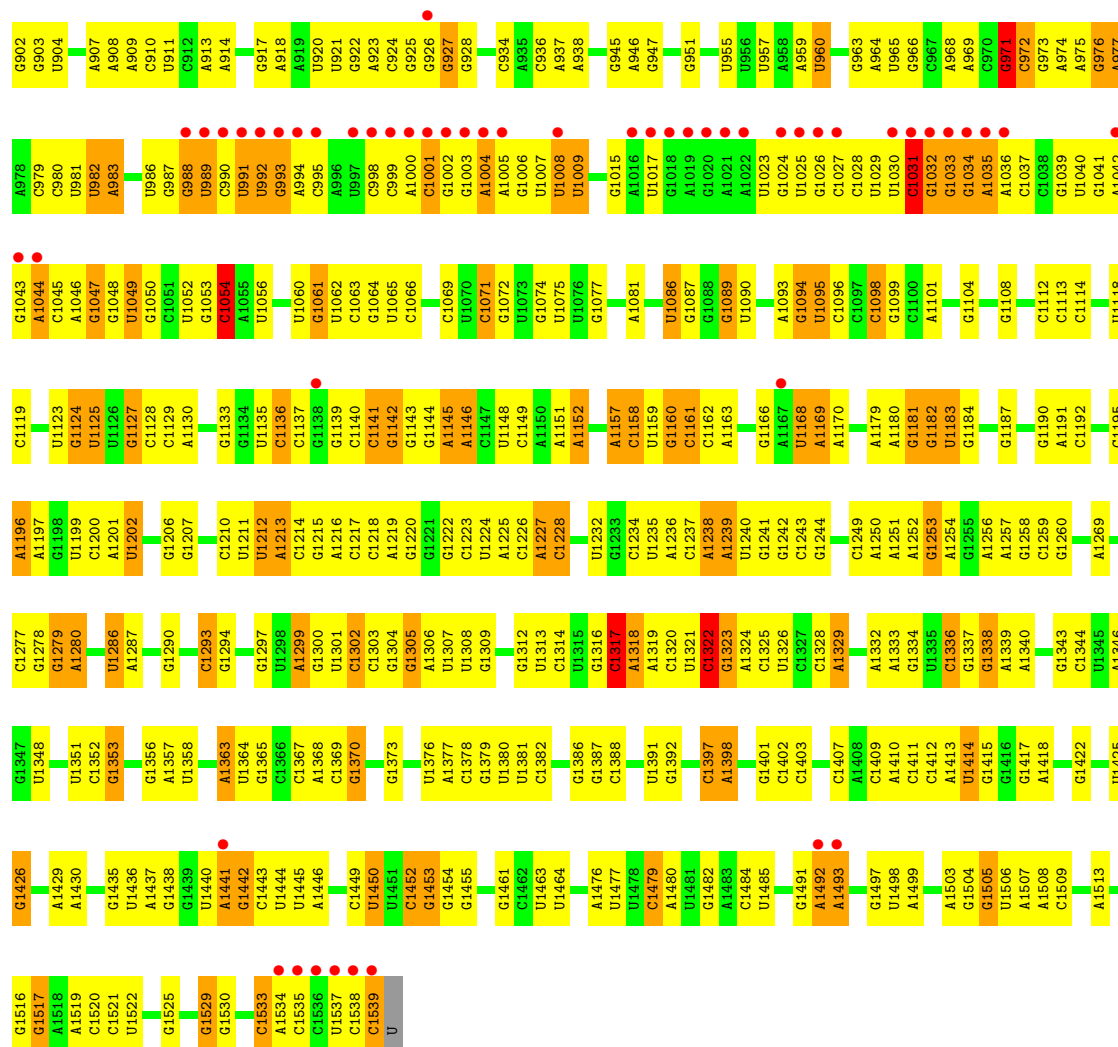
3 Residue-property plots

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

• Molecule 1: 16S rRNA

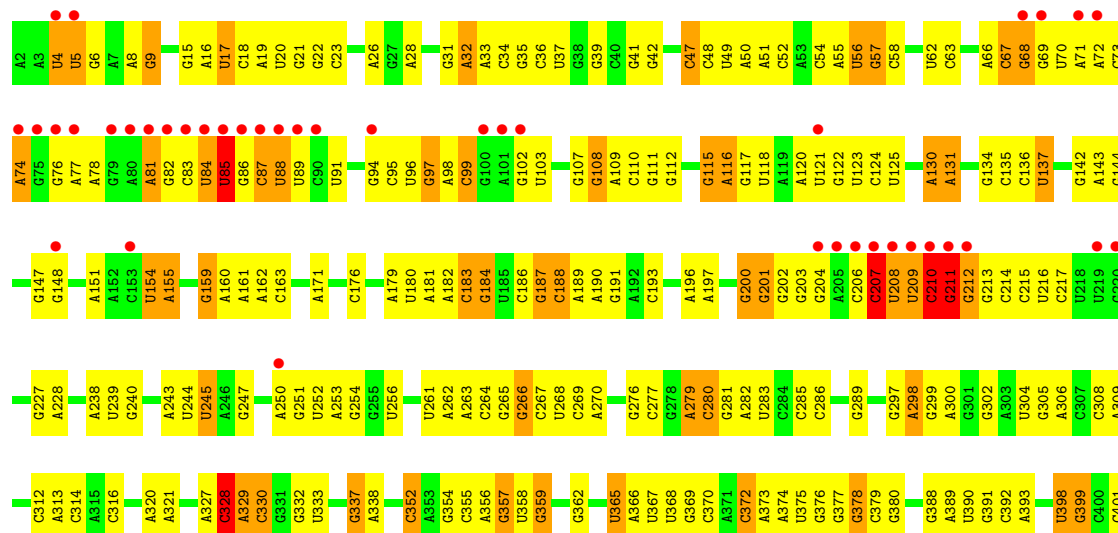
Chain AA: 





• Molecule 1: 16S rRNA

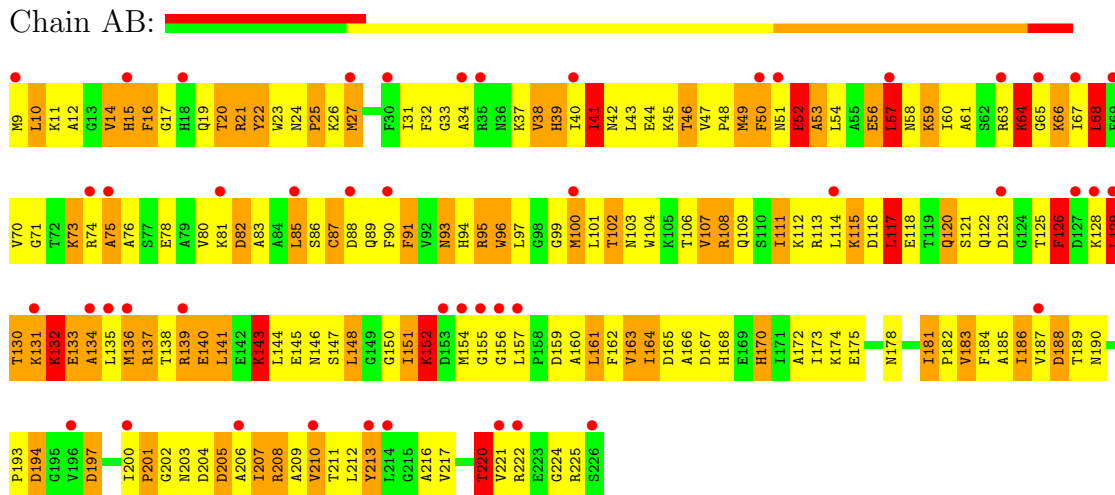
Chain CA:



U1490	G1404	G1331	G1270	G1133	G1053	C990	A914	A816	A729	A642	C545	U480	G402
G1491	A1408	A1332	A1271	G1134	G1054	U991	A915	C817	G730	C643	A546	G481	C403
A1492	C1409	G1333	G1272	U1136	C1055	U992	U920	G818	C731	C645	A547	A482	G404
A1493	G1409	G1273	C1273	C1136	U1055	A994	U921	U820	C732	U645	G548	C483	U405
G1494	A1410	A1212	A1274	C1137	U1056	C995	G922	G821	G733	U649	C549	G484	G406
G1497	C1411	A1213	G1275	G1138	U1060	A996	U926	U822	G734	C650	G550	U485	U407
U1498	G1412	G1338	G1276	G1139	U1061	U997	G926	U827	C735	U651	U551	U486	A408
A1499	A1413	A1339	G1277	C1141	U1062	C998	U927	C823	C736	C651	U552	U487	U409
A1500	G1415	C1342	G1278	G1142	U1063	C999	G929	U827	C737	U652	A553	C488	G410
C1501	G1416	G1343	A1280	G1143	G1064	A1000	C930	U828	C738	U653	A554	C489	A411
A1502	G1417	C1344	G1281	G1144	U1065	C1001	C931	U828	C739	U654	U555	C490	A412
A1503	A1418	U1345	G1282	A1145	C1066	G1002	C932	G833	U740	U654	C556	G491	G413
G1504	G1419	A1346	G1283	A1146	A1067	G1003	G933	U834	G741	A663	G557	C492	C418
G1505	A1431	G1347	C1284	C1147	U1068	A1004	C934	U835	G746	G664	G558	A493	C418
U1506	A1432	A1285	G1285	U1148	C1069	A1005	A935	U835	A746	A665	A559	G494	U421
A1507	G1433	A1349	U1286	C1149	U1070	G1006	U938	C940	A747	A666	A560	A495	C422
A1508	A1434	A1350	A1287	A1150	C1071	U1007	G939	C941	G748	U667	U561	A496	G423
C1509	G1435	U1351	A1288	A1151	U1072	U1008	C940	U842	A749	U672	U562	G497	G424
		G1352	A1288	A1152	U1073	U1009	G941	U843	C750	A673	C564	A499	G425
		A1357	A1288	G1153	G1077	C1011	G942	A845	U751	G674	U565	G500	G426
		U1291	A1288	G1154	U1077	A1012	G943	G846	C752	A675	G566	C501	U427
		G1292	G1230	G1155	G1077	A1013	G944	G847	A753	G676	G567	A502	G428
		C1293	G1231	G1156	G1077	G1013	G945	G848	C754	U677	G568	C503	U429
		G1294	U1232	G1157	A1080	G1013	G946	C948	G755	G569	C504	G504	A430
		U1295	G1233	A1158	A1081	A1016	U950	C966	C756	G682	G505	G505	A436
		C1296	C1234	C1159	A1082	U1017	U951	C967	U757	G683	A572	A509	U437
		U1297	U1235	G1160	U1083	G1018	U952	C968	A574	A687	A573	A510	U438
		G1298	A1236	C1161	U1084	A1019	G953	U855	G760	C575	C575	C511	U439
		A1299	C1237	G1162	U1085	G1020	G954	C957	G765	C689	A579	U512	C440
		G1300	A1238	G1163	U1086	A1021	U955	C958	A766	G690	C580	C514	A441
		U1301	U1239	A1166	U1087	A1022	U956	G959	C777	U692	C582	U516	G445
		C1302	G1240	A1167	U1087	U1023	U957	C960	A695	G682	G585	C517	A451
		G1303	C1241	A1168	U1088	G1024	A958	C968	A790	G701	C586	C518	A452
		U1304	G1242	A1169	U1088	U1025	U959	C969	G791	A702	C586	C519	G453
		G1305	C1243	A1170	U1089	G1026	U960	G974	A792	G703	G604	A520	G454
		A1306	U1244	G1175	U1095	U1027	U965	C971	C795	A704	U605	G521	U458
		U1307	C1245	A1176	U1096	C1028	U966	C982	C795	G705	G606	A523	A459
		G1308	A1246	A1177	U1097	U1029	U967	C983	U706	U707	A607	G524	G462
		U1309	U1247	A1178	U1098	U1030	U968	C984	C708	C708	A608	G527	U463
		G1310	A1248	A1179	U1099	C1031	U969	C985	U709	C709	A609	G527	U464
		A1311	C1249	G1180	U1100	G1032	C970	C986	U801	C618	G530	U531	A465
		G1312	A1250	G1181	U1101	G1033	C971	C987	G803	C620	U619	A532	U466
		U1313	A1251	G1182	G1108	G1034	C972	C988	U804	A621	C621	A533	A468
		C1314	U1252	U1183	G1109	A1035	G973	C989	C805	A622	U534	U534	C469
		G1315	G1253	G1184	C1112	U1036	A974	C990	C806	C623	A535	A535	C470
		U1316	A1254	A1191	C1113	G1037	A975	C991	U798	C624	G536	G537	U473
		C1317	U1255	C1192	C1114	U1038	A976	C992	G799	U625	C624	G537	U474
		A1318	A1256	G1193	U1118	G1039	A977	C993	U800	U626	U626	U538	C475
		G1319	A1257	G1194	C1119	U1040	A978	C994	U801	U627	U627	A539	U476
		C1320	G1260	A1196	U1120	U1041	U979	C995	G806	U628	U628	G540	C477
		U1321	A1261	G1197	U1121	A1042	U980	C996	C807	U629	U629	U543	A478
		G1322	C1262	U1198	U1122	G1043	U981	C997	C808	U630	U630	G544	U479
		A1323	G1263	C1200	G1124	A1044	U982	C998	C809	C719	C624	G544	U479
		G1324	U1264	A1201	U1125	C1045	U983	C999	C810	C720	U625	G544	U479
		A1325	A1265	U1202	U1126	A1046	C984	C999	C811	G721	U625	G544	U479
		U1326	G1266	U1203	U1127	G1047	C985	C999	C812	G722	U625	G544	U479
		C1327	G1267	C1203	U1128	G1048	C986	C999	U813	G724	U625	G544	U479
		G1328	U1268	U1204	U1129	U1049	C987	C999	U814	G724	U625	G544	U479
		A1329	G1269	U1205	U1130	G1050	C988	C999	A815	A728	U625	G544	U479
		C1403		G1206	C1132		U989	C910					

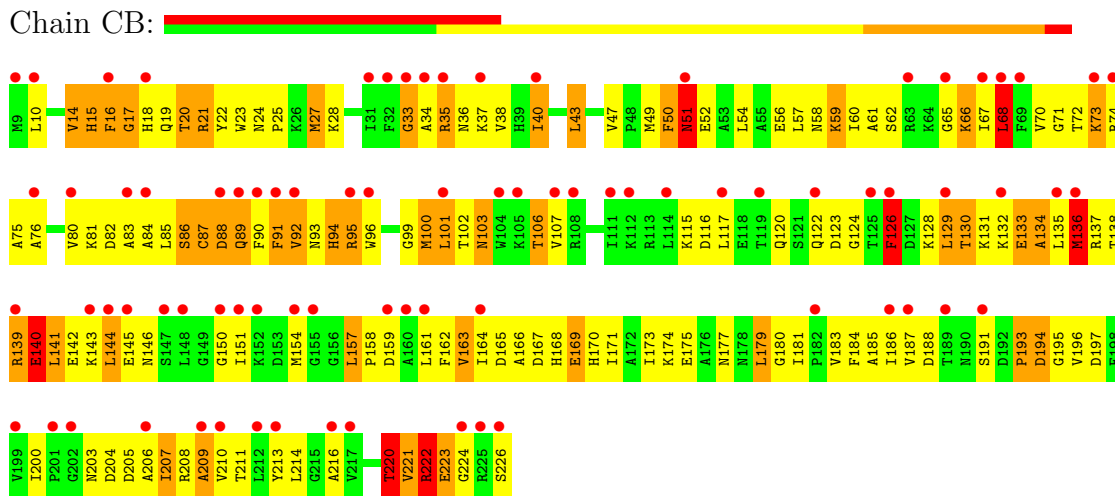
- Molecule 2: 30S ribosomal protein S2

Chain AB:



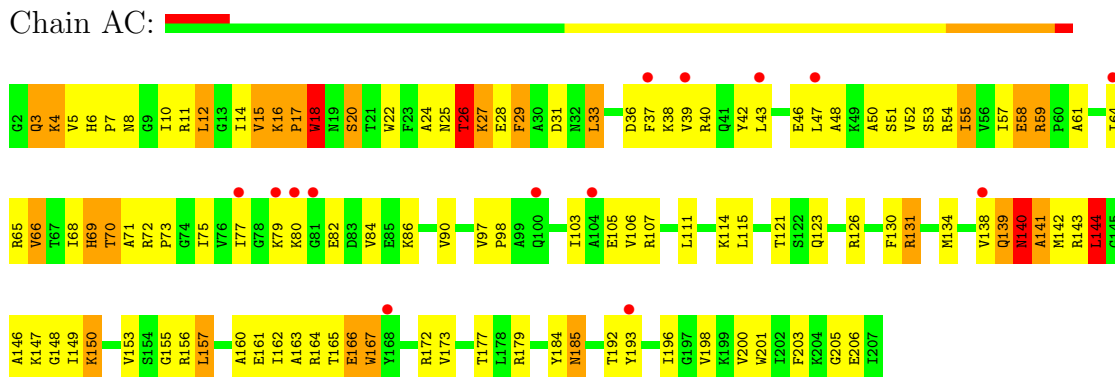
- Molecule 2: 30S ribosomal protein S2

Chain CB:



- Molecule 3: 30S ribosomal protein S3

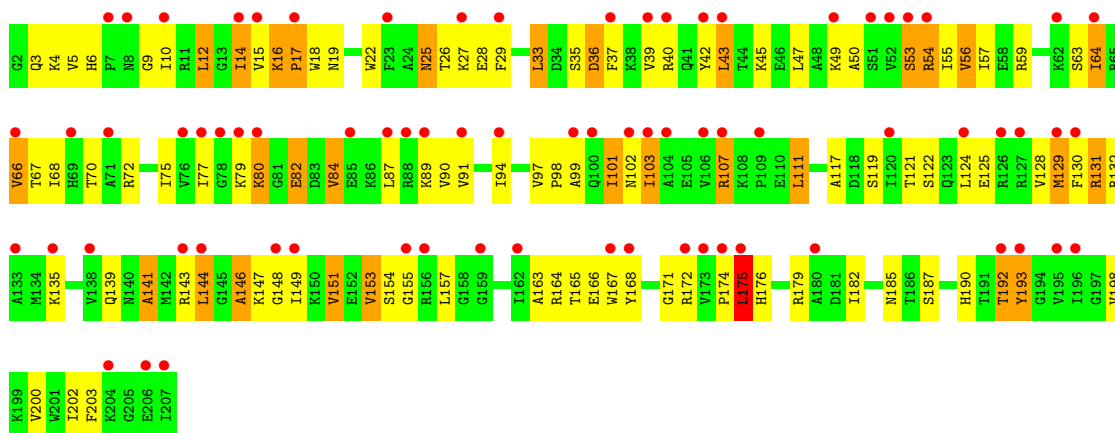
Chain AC:



- Molecule 3: 30S ribosomal protein S3

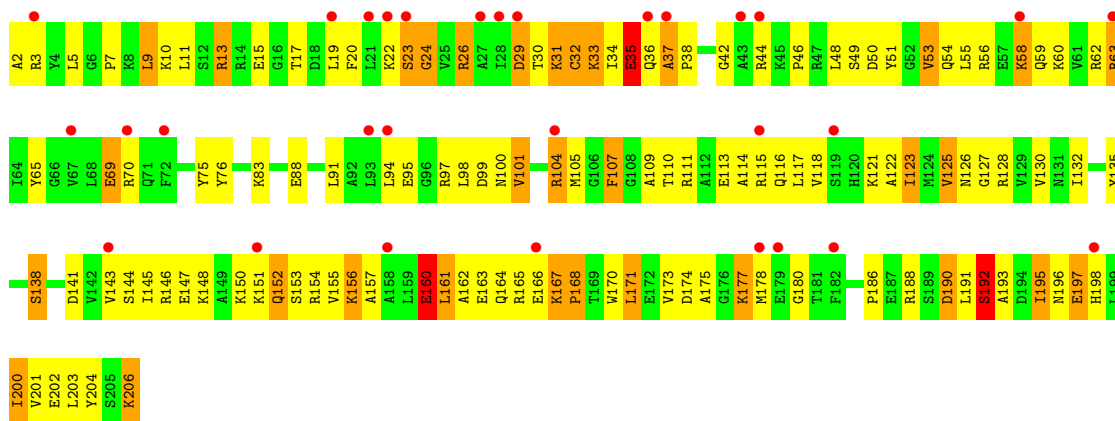
Chain CC:





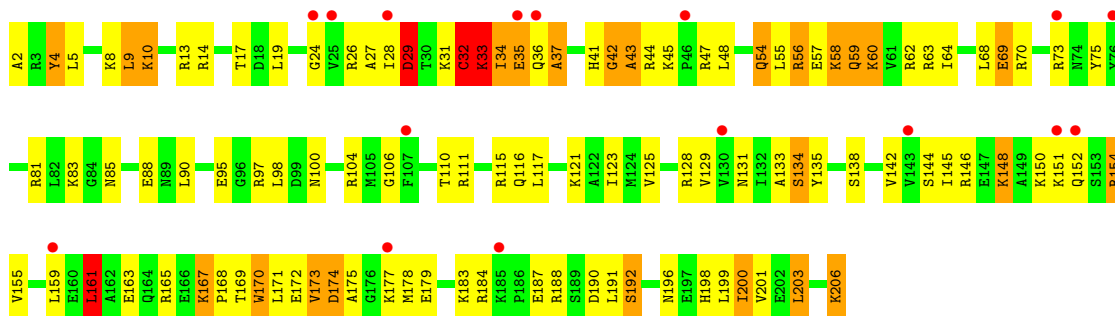
• Molecule 4: 30S ribosomal protein S4

Chain AD:



• Molecule 4: 30S ribosomal protein S4

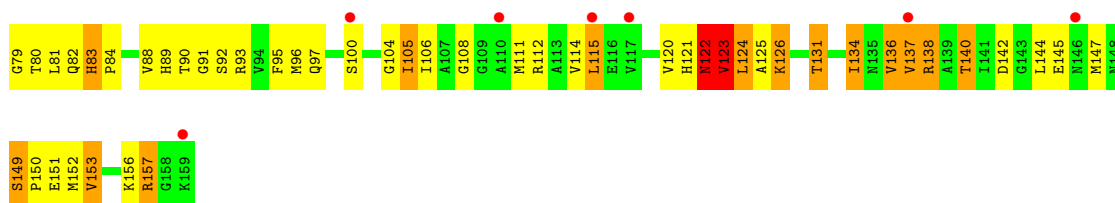
Chain CD:



• Molecule 5: 30S ribosomal protein S5

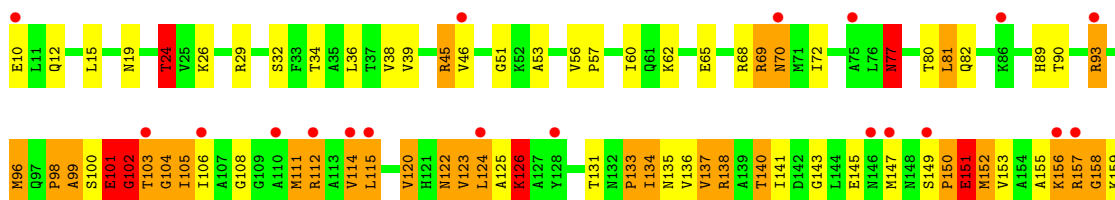
Chain AE:





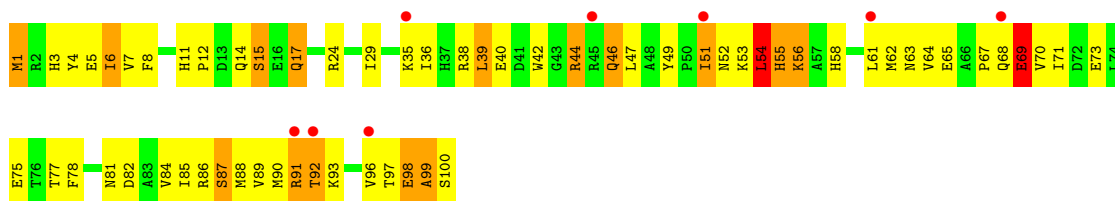
• Molecule 5: 30S ribosomal protein S5

Chain CE:



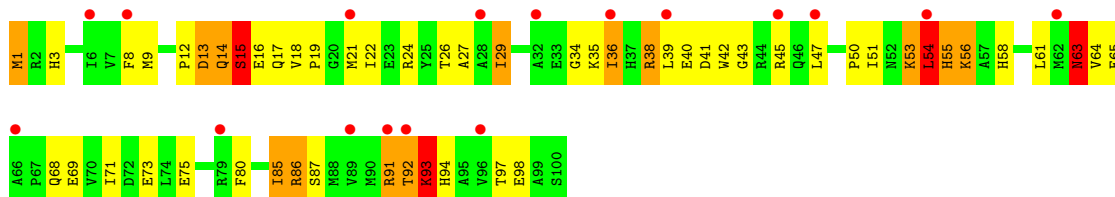
• Molecule 6: 30S ribosomal protein S6

Chain AF:



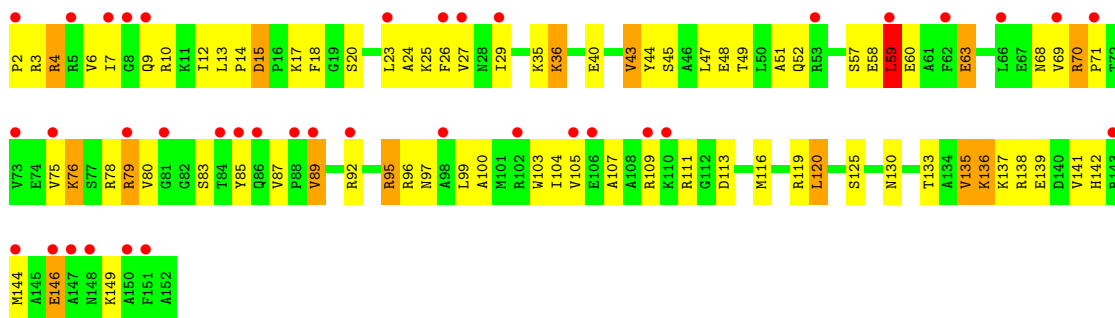
• Molecule 6: 30S ribosomal protein S6

Chain CF:



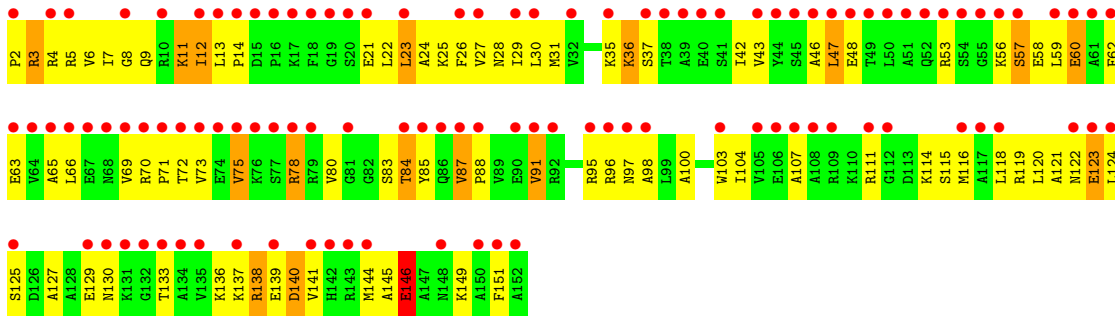
• Molecule 7: 30S ribosomal protein S7

Chain AG:

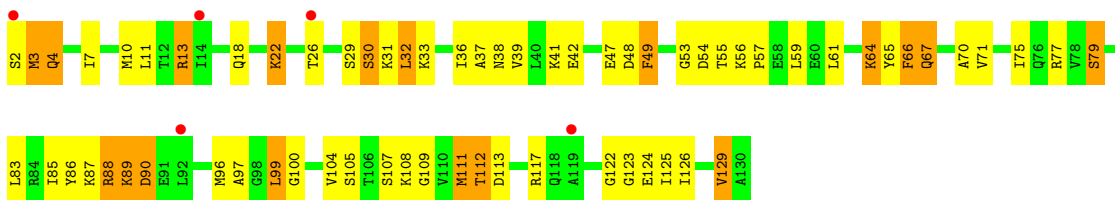


• Molecule 7: 30S ribosomal protein S7

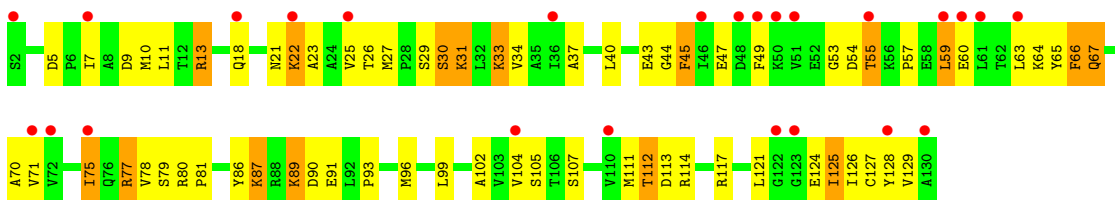
Government	Percentage
Current government	85%
Previous government	15%



- Molecule 8: 30S ribosomal protein S8

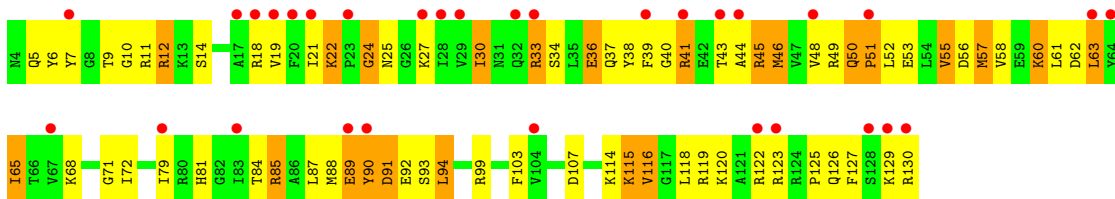


- Molecule 8: 30S ribosomal protein S8



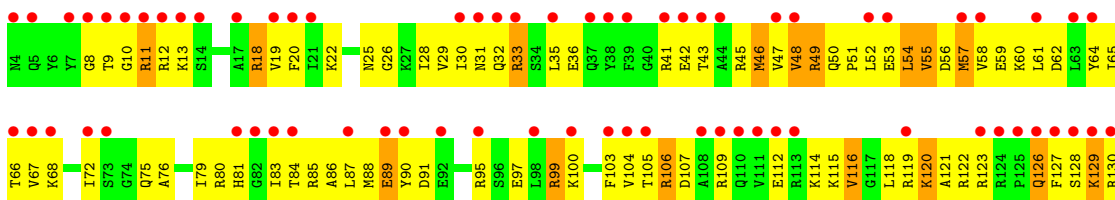
- Molecule 9: 30S ribosomal protein S9

Age Group	Percentage
18-24	15%
25-34	25%
35-44	40%
45-54	20%
55-64	0%
65-74	0%
75-84	0%
85+	0%

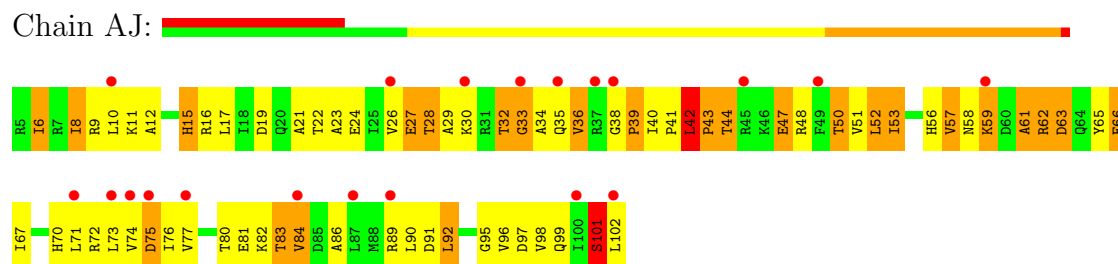


- Molecule 9: 30S ribosomal protein S9

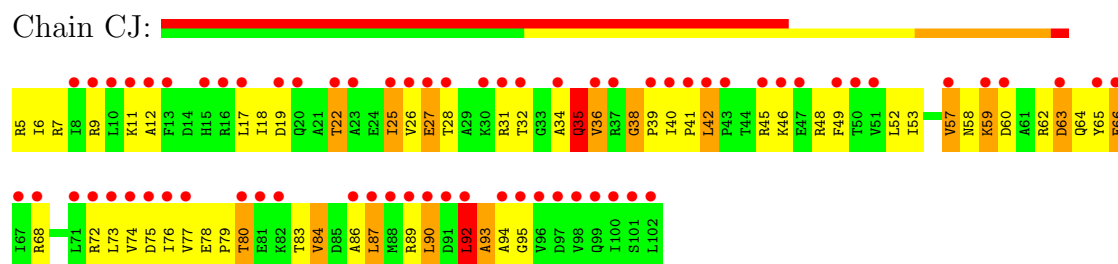
Age Group	Percentage
18-24	35%
25-34	25%
35-44	20%
45-54	15%
55-64	5%



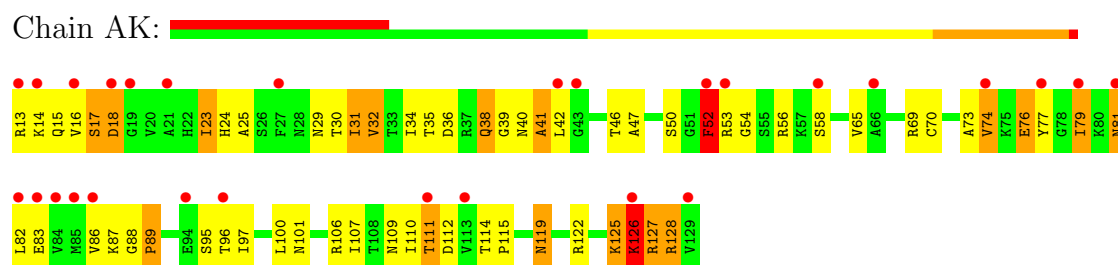
- Molecule 10: 30S ribosomal protein S10



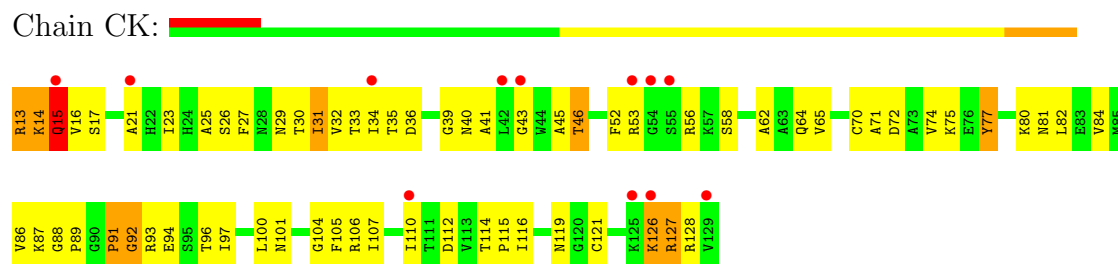
- Molecule 10: 30S ribosomal protein S10



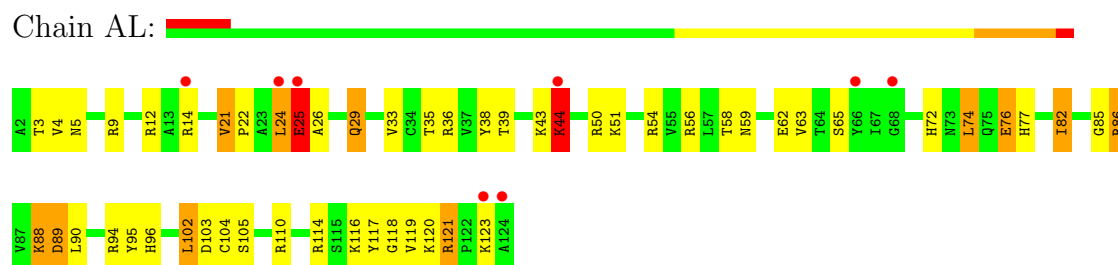
- Molecule 11: 30S ribosomal protein S11



- Molecule 11: 30S ribosomal protein S11

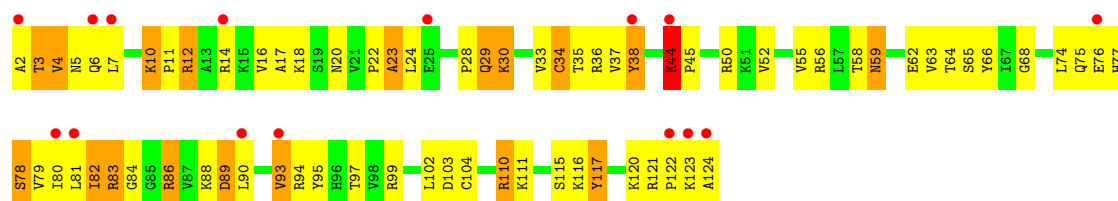


- Molecule 12: 30S ribosomal protein S12



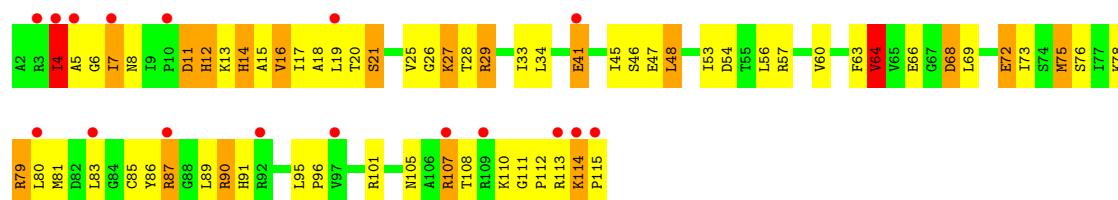
- Molecule 12: 30S ribosomal protein S12

Chain CL:



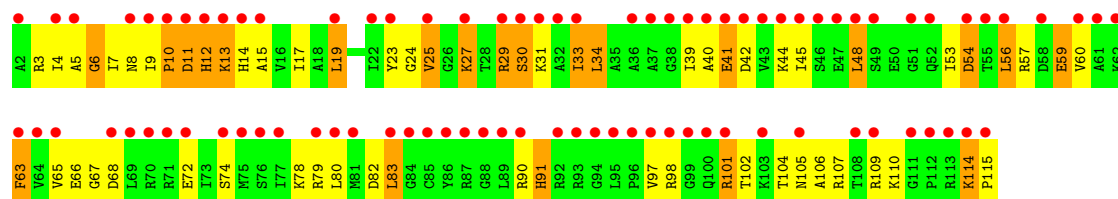
- Molecule 13: 30S ribosomal protein S13

Chain AM:



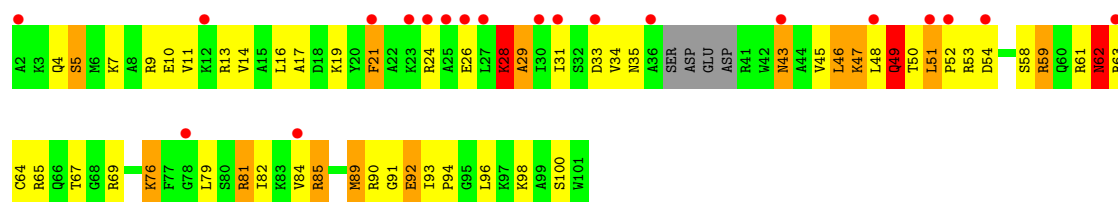
- Molecule 13: 30S ribosomal protein S13

Chain CM:



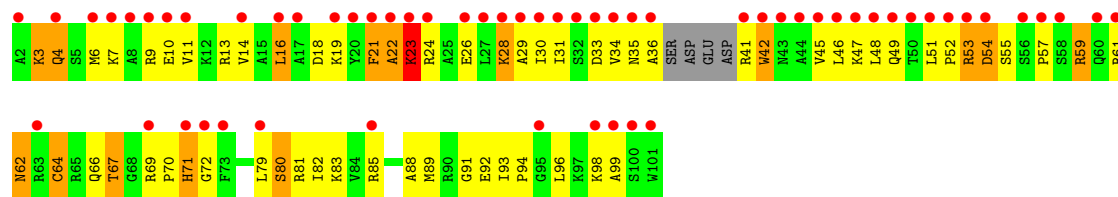
- Molecule 14: 30S ribosomal protein S14

Chain AN:



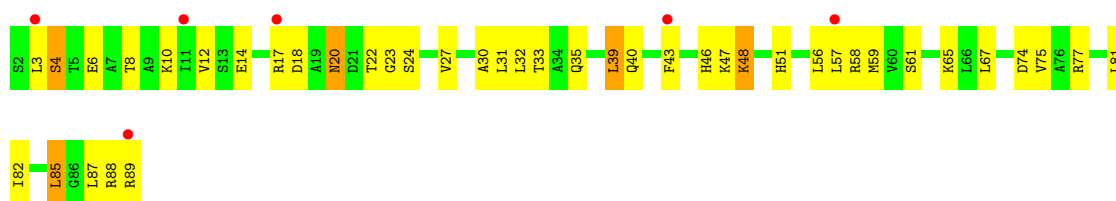
- Molecule 14: 30S ribosomal protein S14

Chain CN:



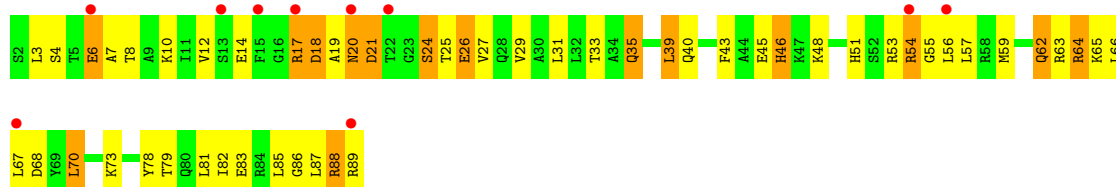
- Molecule 15: 30S ribosomal protein S15

Chain AO:



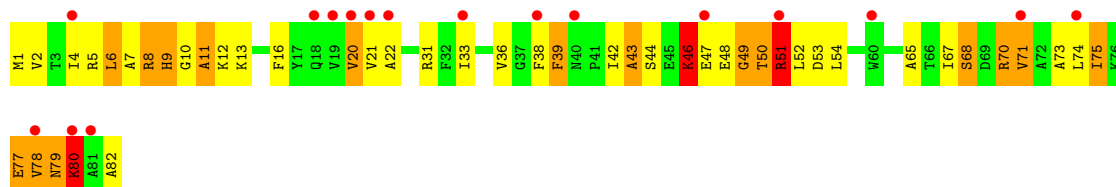
• Molecule 15: 30S ribosomal protein S15

Chain CO:



• Molecule 16: 30S ribosomal protein S16

Chain AP:



• Molecule 16: 30S ribosomal protein S16

Chain CP:



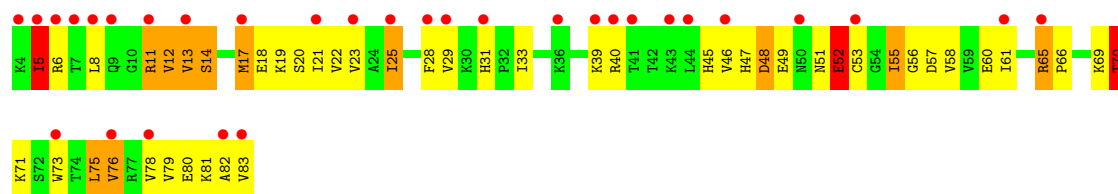
• Molecule 17: 30S ribosomal protein S17

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

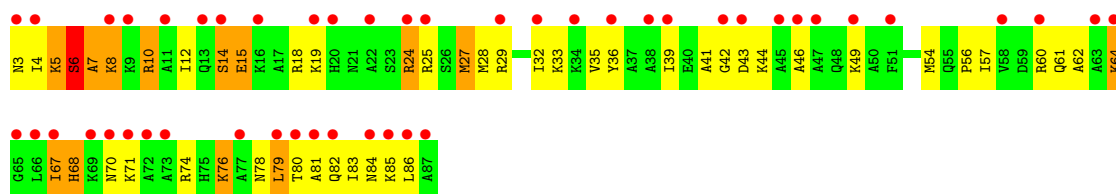
Chain CS:

• Molecule 20: 30S ribosomal protein S20

Chain AT:

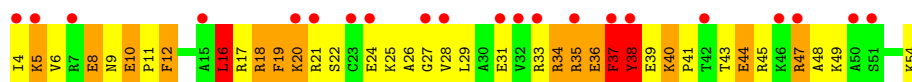
• Molecule 20: 30S ribosomal protein S20

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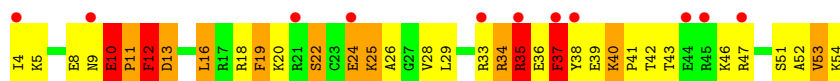
- Molecule 21: 30S ribosomal protein S21

Chain AU:



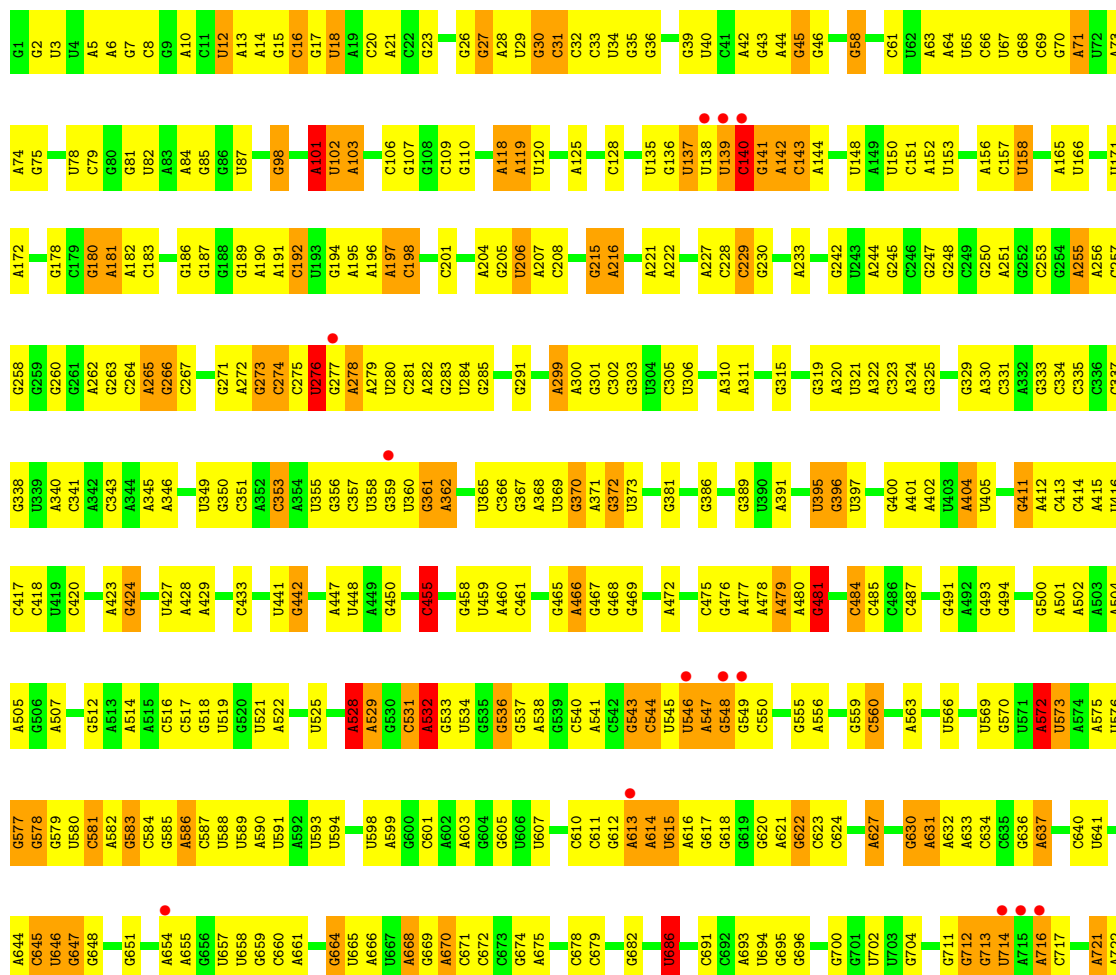
- Molecule 21: 30S ribosomal protein S21

Chain CU:

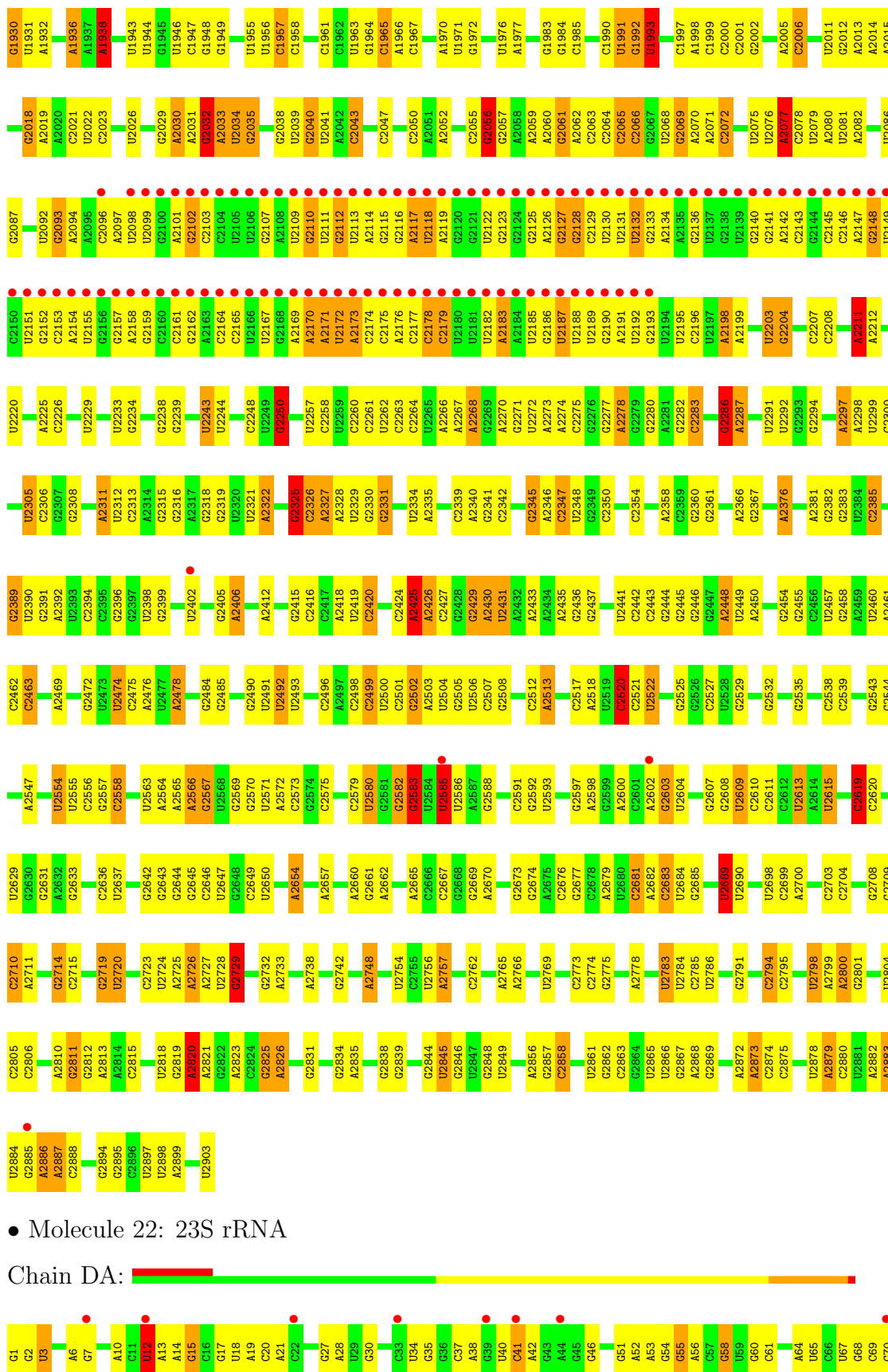


- Molecule 22: 23S rRNA

Chain BA:



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G1949	A1618	C1774	A1617	U1513	A1427	A1368	G1280	U1199	U1035		G954	C869	G797	G726
G1850	G1691	G1776	G1619	A1514	C1428	A1369	G1281	C1200	C1114	A1046	G956	U871	G801	G728
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U1852	U1693	U1693	U1624	A1523	A1431	G1364	A1287	A1205	G1125	G1051	U958	A878	U803	A730
A1853	C1694	C1694	A1432	U1523	G1432	A1365	G1287	G1206	G1052	A959	A960	C879	A804	A731
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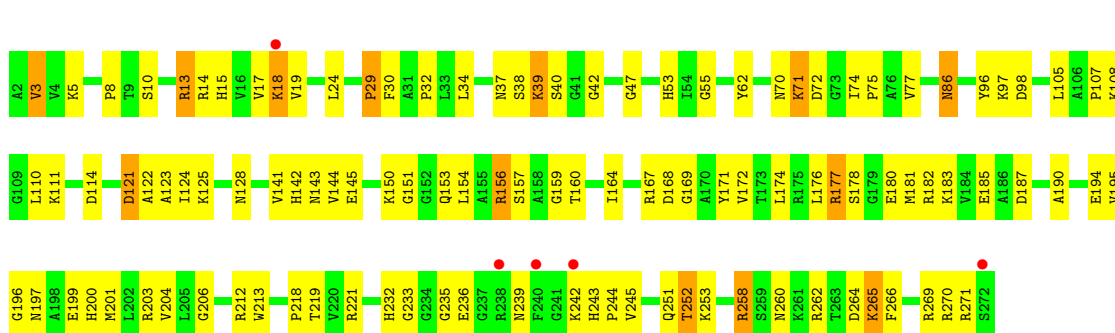


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G1935	A1936	A1937	A1938					C1947	G1948		U1951	U1952	U1953	U1954	U1955	A2031	C2032	A2033	U2034		C1961	U1962	U1963	G1964	C1965	U1966	C1967	G1968	U1969				U1970	U1971	U1972	G1973	C1974	C2055	G2056	U1976	U1977	U1978			U1981	G1992	U1993	C2004	C2066	G2069	A2070	A2071	C2072	C2073	C2001			G2004	A2005	C2006	U2007	A2080	G2152	C2153	A2154	U2155	U2156
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G1854	U1855	A1856	G1857	U1858	U1859	U1860	G1861			C1868	U1869	C1870	A1871	U1872	G1873	C1874	U1875	U1876	G1877	G1878	U1879	U1880	C1881	U1882		G1888	C1895	U1896	G1897		A1900	U1901	C1902	G1903			C1904	C1905			U1911	U1912	A1913	C1914	U1915	U1916	U1917	U1918			U1923	C2000	C2001			G2004	A2005	C2006	U200								



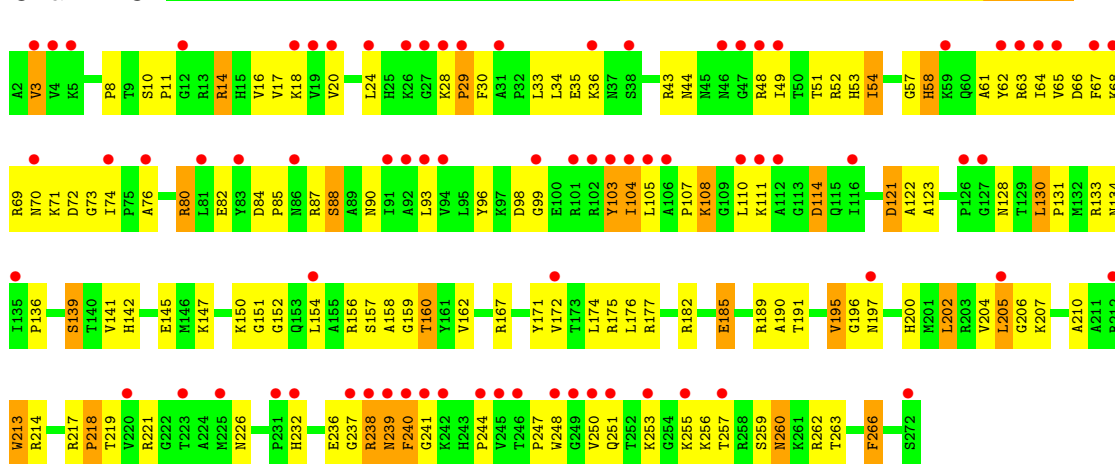
- Molecule 24: 50S ribosomal protein L2

Chain BC:



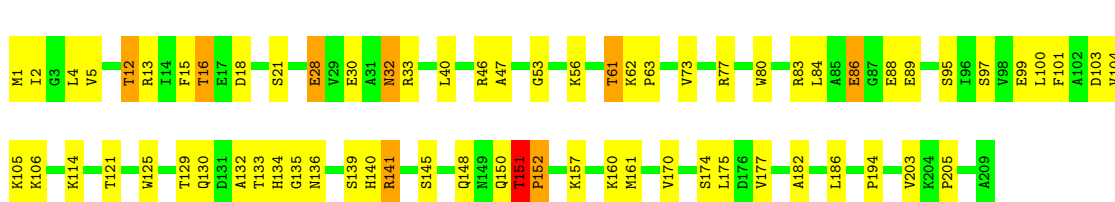
- Molecule 24: 50S ribosomal protein L2

Chain DC:



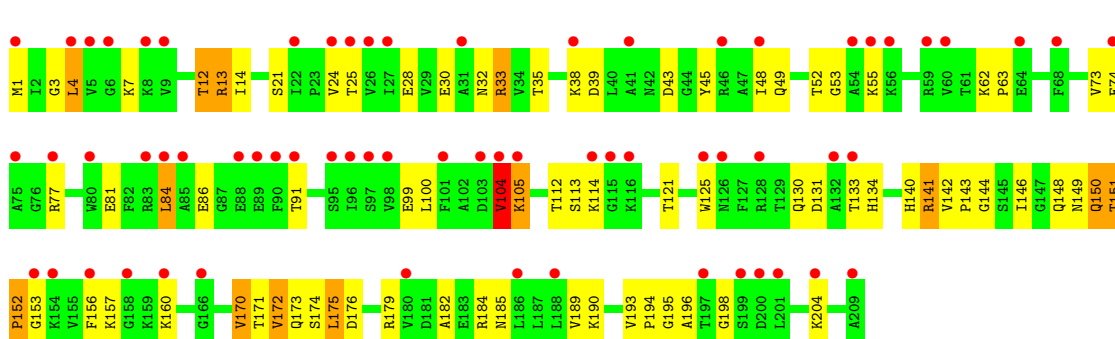
- Molecule 25: 50S ribosomal protein L3

Chain BD:



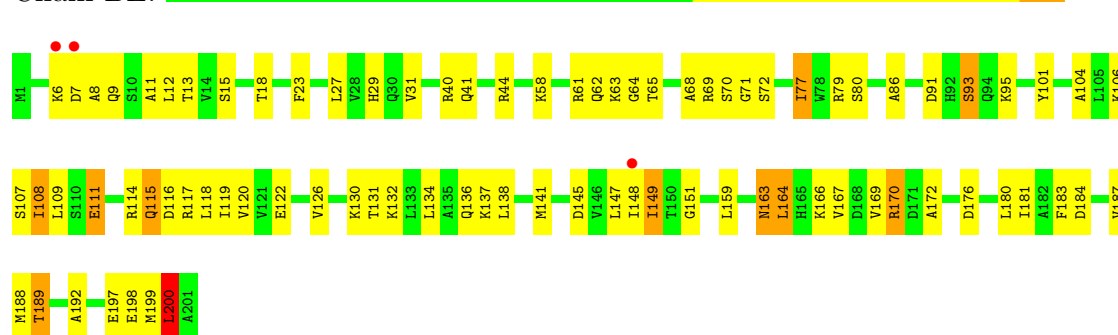
- Molecule 25: 50S ribosomal protein L3

Chain DD:



- Molecule 26: 50S ribosomal protein L4

Chain BE:



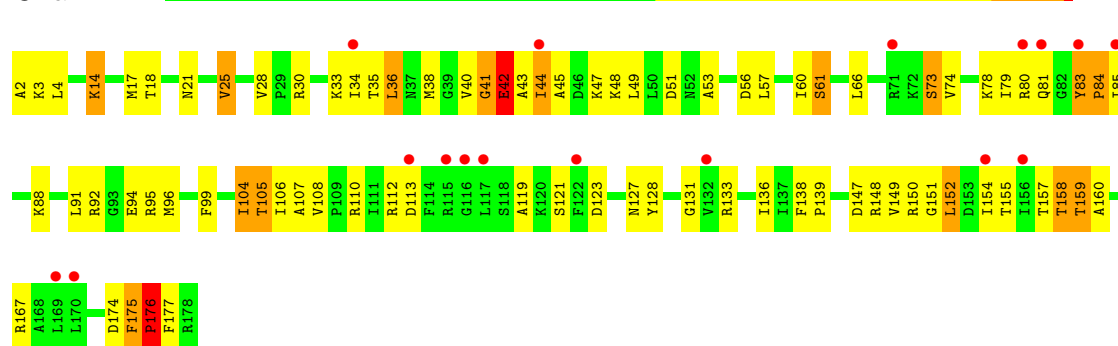
- Molecule 26: 50S ribosomal protein L4

Chain DE:



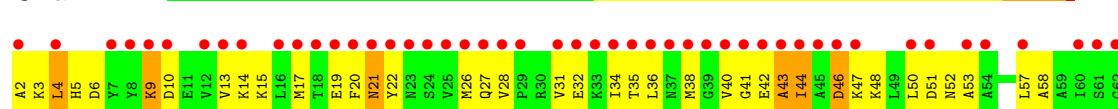
- Molecule 27: 50S ribosomal protein L5

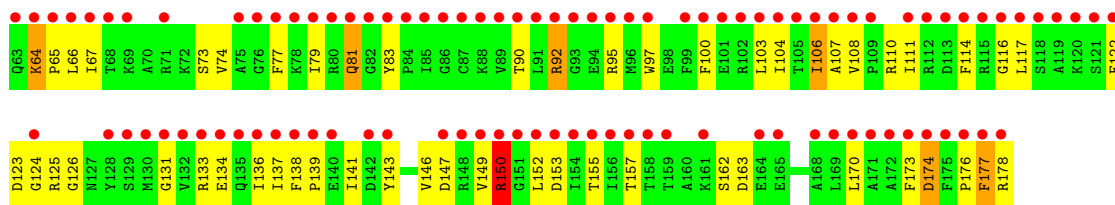
Chain BF:



- Molecule 27: 50S ribosomal protein L5

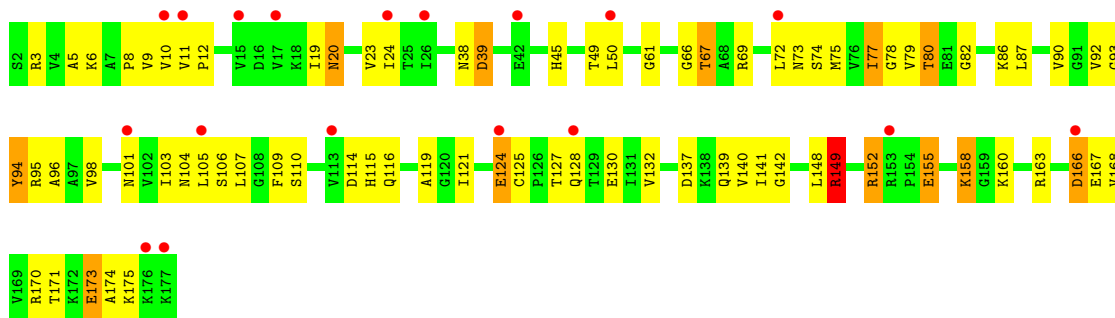
Chain DF:





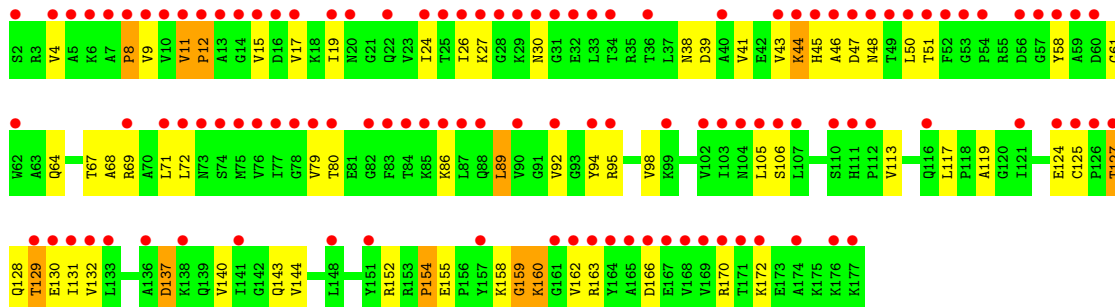
• Molecule 28: 50S ribosomal protein L6

Chain BG:



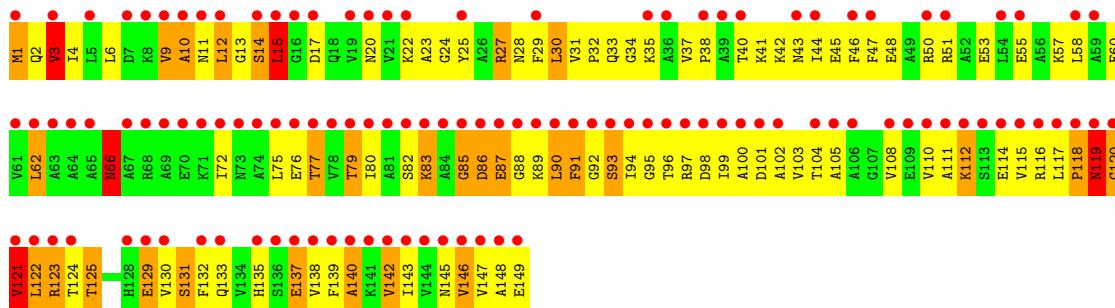
• Molecule 28: 50S ribosomal protein L6

Chain DG:



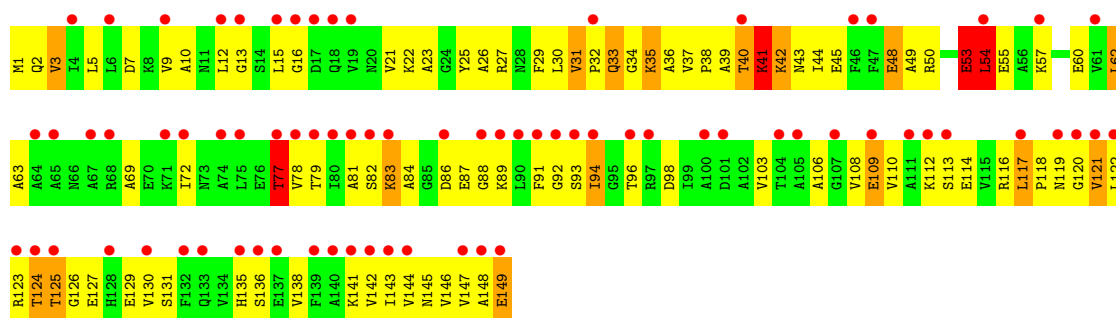
• Molecule 29: 50S ribosomal protein L9

Chain BH:



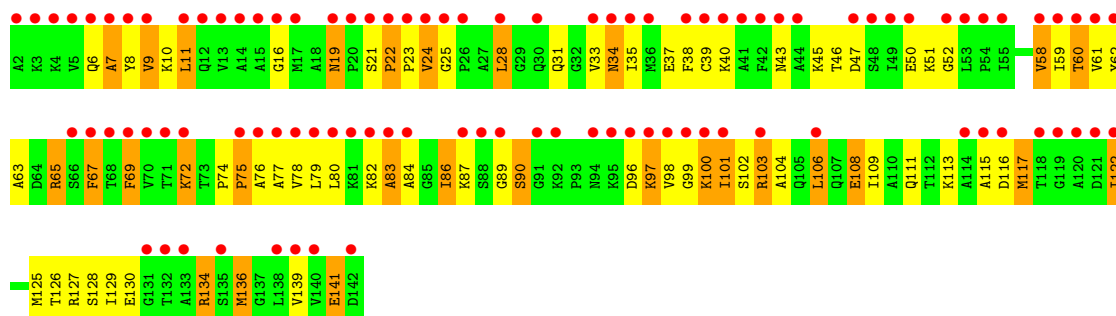
• Molecule 29: 50S ribosomal protein L9

Chain DH:



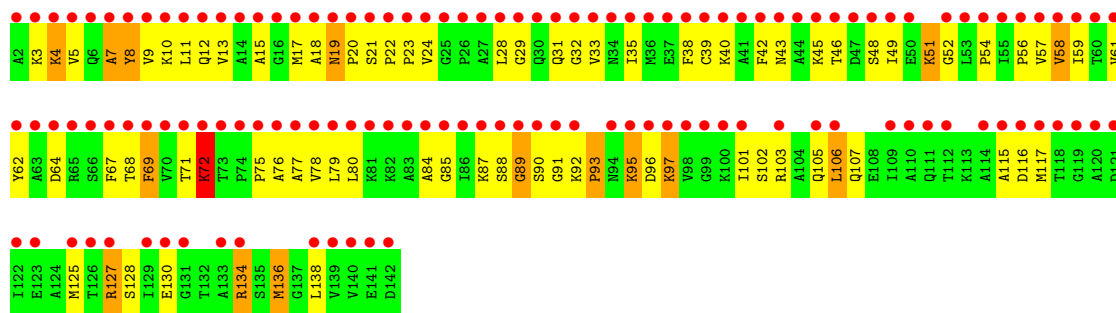
- Molecule 30: 50S ribosomal protein L11

Chain BI:



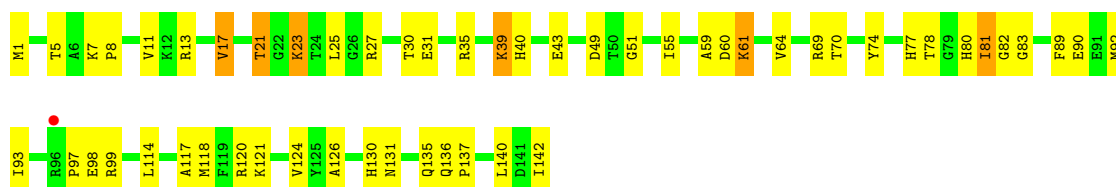
- Molecule 30: 50S ribosomal protein L11

Chain DI:



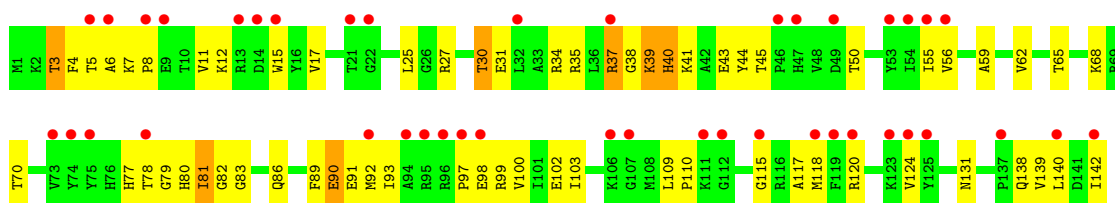
- Molecule 31: 50S ribosomal protein L13

Chain BJ:



- Molecule 31: 50S ribosomal protein L13

Chain DJ:



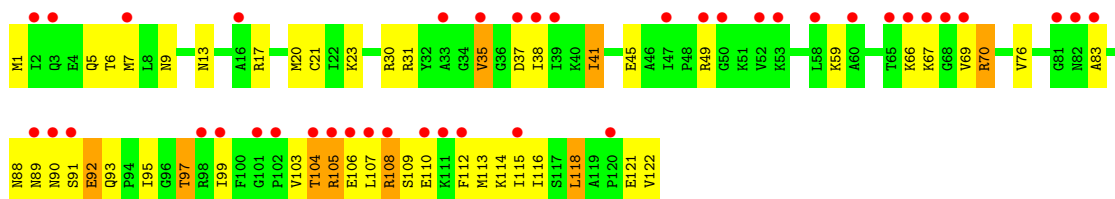
• Molecule 32: 50S ribosomal protein L14

Chain BK:



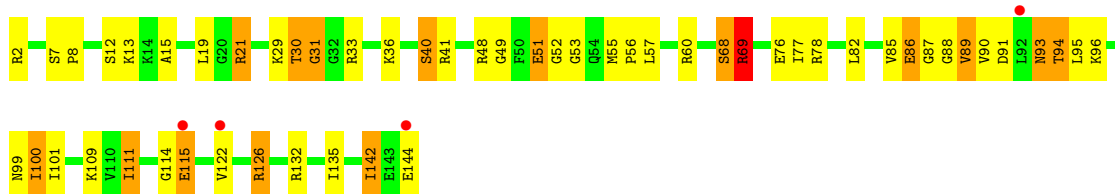
• Molecule 32: 50S ribosomal protein L14

Chain DK:



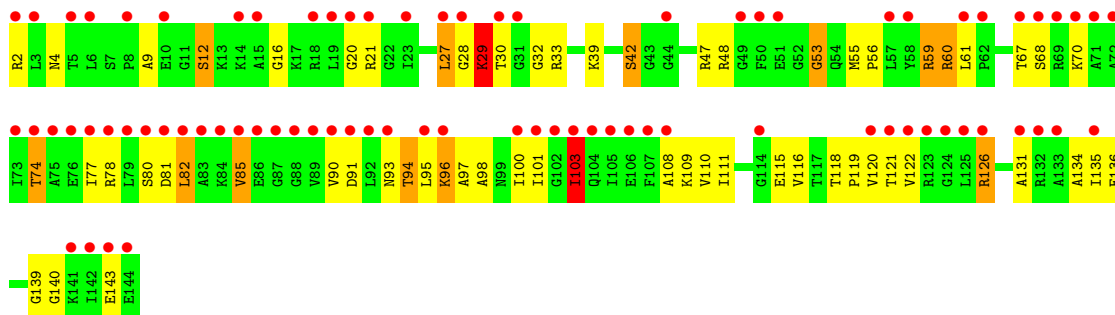
• Molecule 33: 50S ribosomal protein L15

Chain BL:



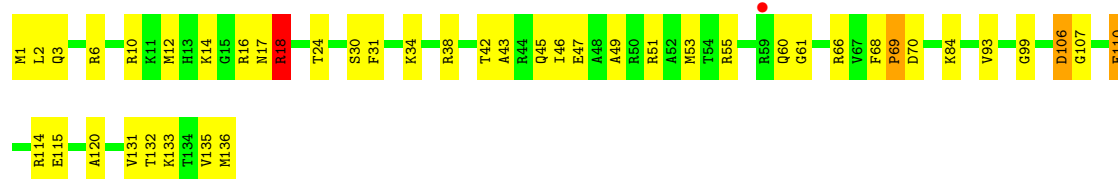
• Molecule 33: 50S ribosomal protein L15

Chain DL:



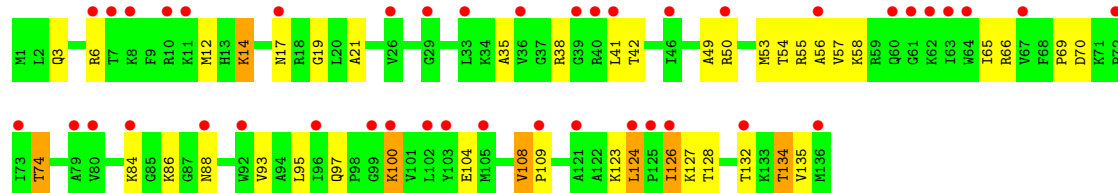
• Molecule 34: 50S ribosomal protein L16

Chain BM:



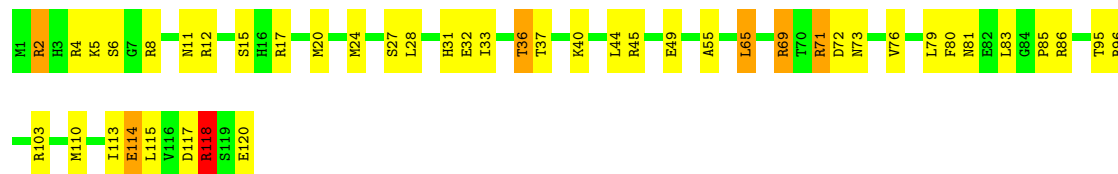
- Molecule 34: 50S ribosomal protein L16

Chain DM:



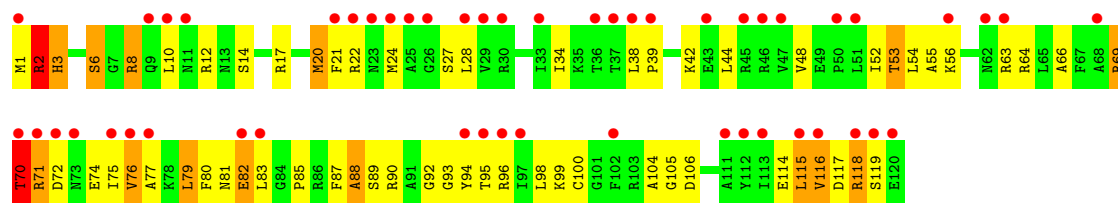
- Molecule 35: 50S ribosomal protein L17

Chain BN:



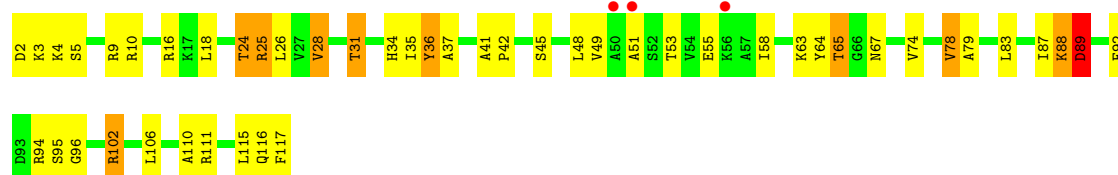
- Molecule 35: 50S ribosomal protein L17

Chain DN:



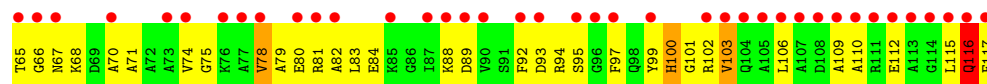
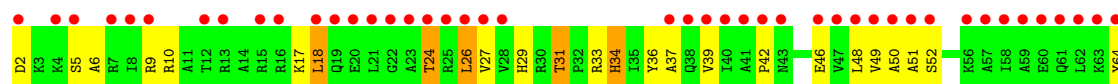
- Molecule 36: 50S ribosomal protein L18

Chain BO:



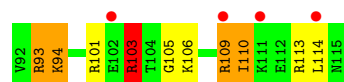
- Molecule 36: 50S ribosomal protein L18

Chain DO:



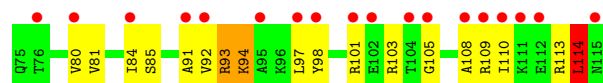
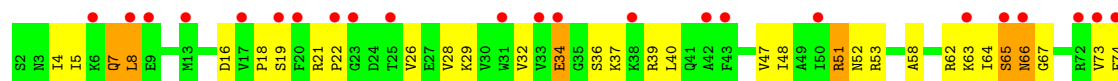
• Molecule 37: 50S ribosomal protein L19

Chain BP:



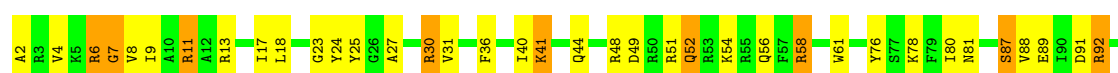
• Molecule 37: 50S ribosomal protein L19

Chain DP:



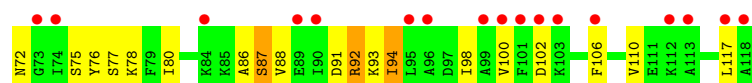
• Molecule 38: 50S ribosomal protein L20

Chain BQ:



• Molecule 38: 50S ribosomal protein L20

Chain DQ:



• Molecule 39: 50S ribosomal protein L21

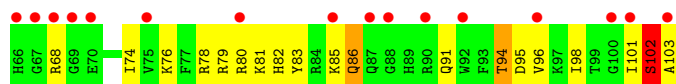
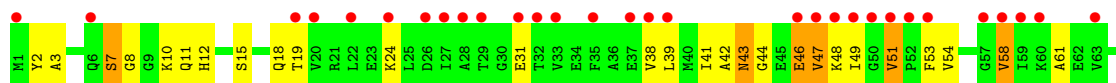
Chain BR:





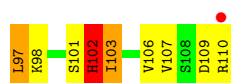
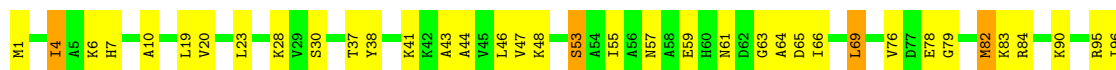
- Molecule 39: 50S ribosomal protein L21

Chain DR:



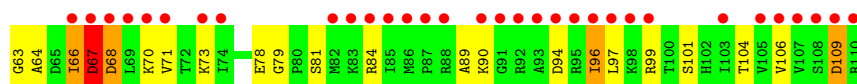
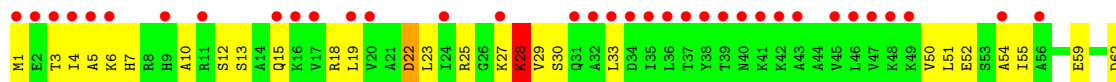
- Molecule 40: 50S ribosomal protein L22

Chain BS:



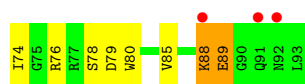
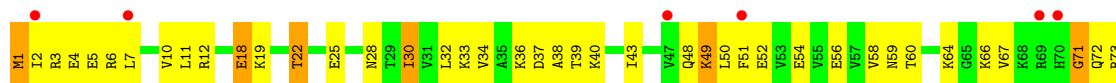
- Molecule 40: 50S ribosomal protein L22

Chain DS:



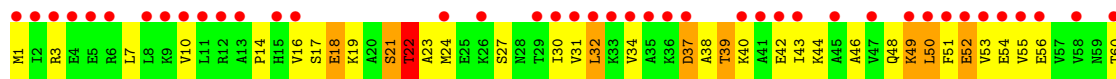
- Molecule 41: 50S ribosomal protein L23

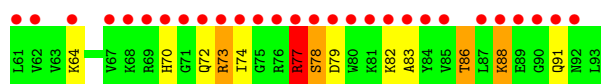
Chain BT:



- Molecule 41: 50S ribosomal protein L23

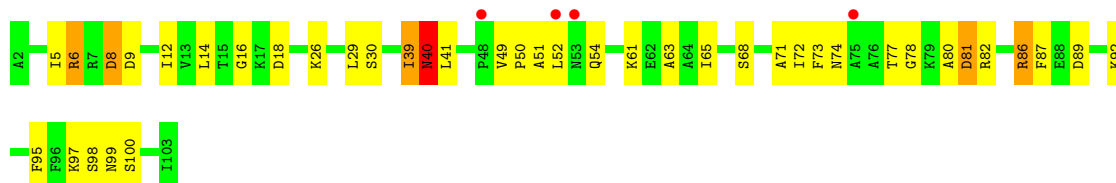
Chain DT:





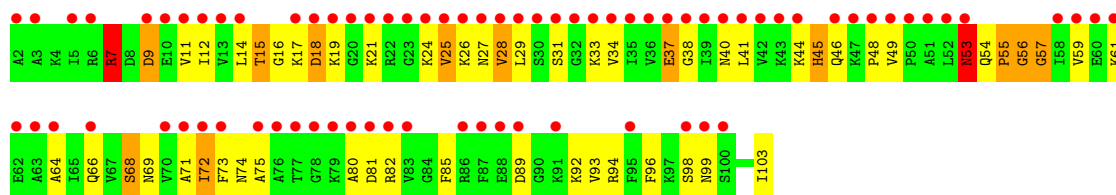
- Molecule 42: 50S ribosomal protein L24

Chain BU:



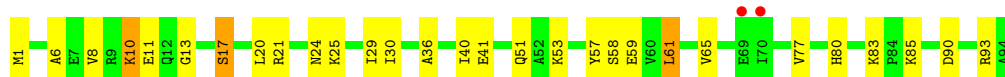
- Molecule 42: 50S ribosomal protein L24

Chain DU:



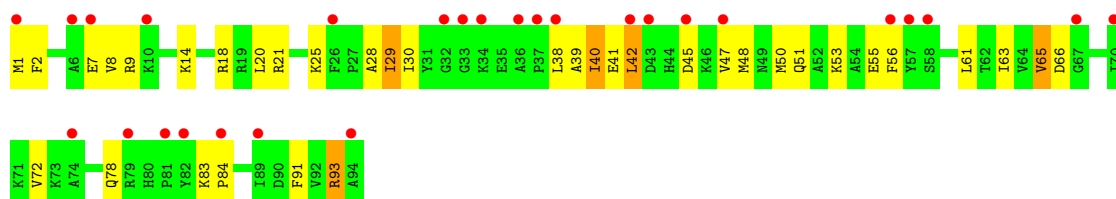
- Molecule 43: 50S ribosomal protein L25

Chain BV:



- Molecule 43: 50S ribosomal protein L25

Chain DV:



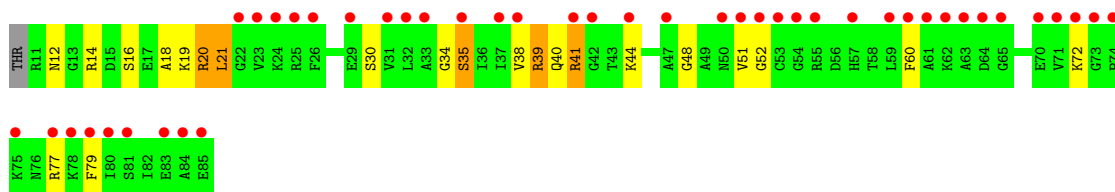
- Molecule 44: 50S ribosomal protein L27

Chain BW:



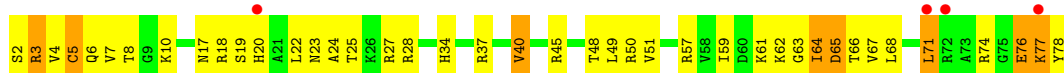
- Molecule 44: 50S ribosomal protein L27

Chain DW:



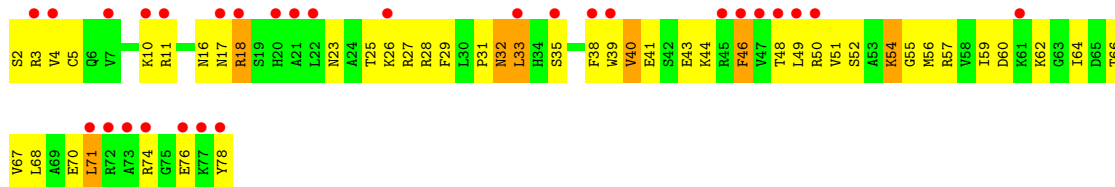
- Molecule 45: 50S ribosomal protein L28

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:



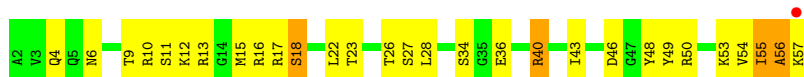
- Molecule 47: 50S ribosomal protein L30

Chain DZ:



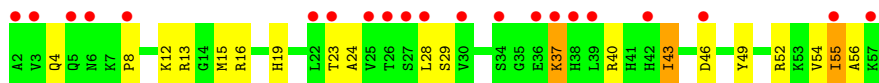
- Molecule 48: 50S ribosomal protein L32

Chain B0:



- Molecule 48: 50S ribosomal protein L32

Chain D0:



- Molecule 49: 50S ribosomal protein L33

Chain B1:



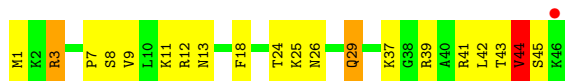
- Molecule 49: 50S ribosomal protein L33

Chain D1:



- Molecule 50: 50S ribosomal protein L34

Chain B2:



- Molecule 50: 50S ribosomal protein L34

Chain D2:



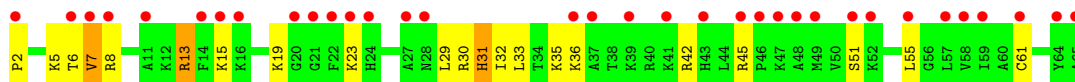
- Molecule 51: 50S ribosomal protein L35

Chain B3:



- Molecule 51: 50S ribosomal protein L35

Chain D3:



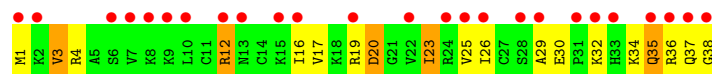
- Molecule 52: 50S ribosomal protein L36

Chain B4: 



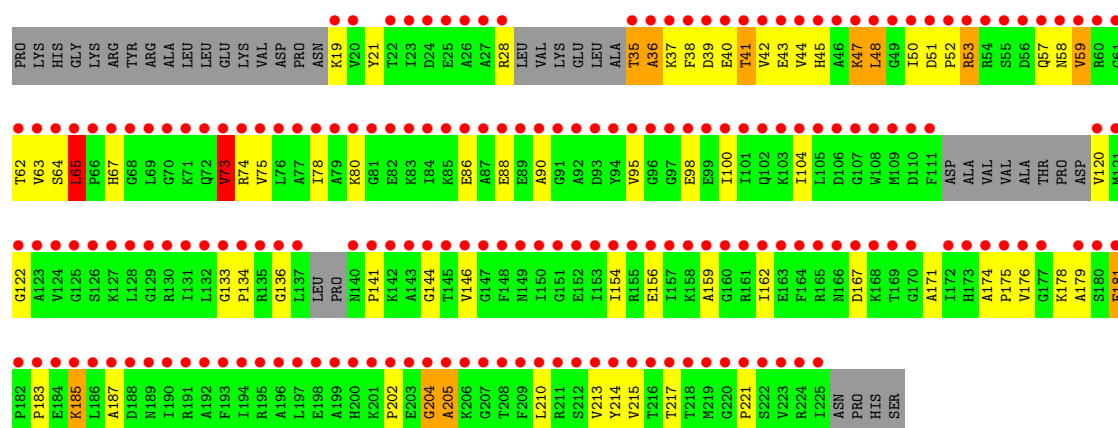
- Molecule 52: 50S ribosomal protein L36

Chain D4: 



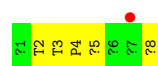
- Molecule 53: 50S ribosomal protein L1

Chain B5: 



- Molecule 54: Quinupristin

Chain B6: 



- Molecule 54: Quinupristin

Chain D6: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.08Å 432.73Å 631.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.68 – 2.95 68.68 – 2.95	Depositor EDS
% Data completeness (in resolution range)	93.2 (68.68-2.95) 93.2 (68.68-2.95)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.96Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.248 , 0.282 0.255 , 0.289	Depositor DCC
R_{free} test set	4515 reflections (0.41%)	DCC
Wilson B-factor (Å ²)	54.4	Xtriage
Anisotropy	0.520	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 15.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 1118451 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	288328	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.49% 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, DBB, MG, 004, MHV, MHW, MHT, MHU

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	0.44	0/36944	1.04	74/57632 (0.1%)
1	CA	0.39	0/36966	0.99	74/57666 (0.1%)
2	AB	0.36	0/1736	0.72	1/2338 (0.0%)
2	CB	0.33	0/1736	0.70	0/2338
3	AC	0.35	0/1652	0.65	2/2225 (0.1%)
3	CC	0.32	0/1652	0.58	1/2225 (0.0%)
4	AD	0.35	0/1665	0.68	0/2227
4	CD	0.38	0/1665	0.71	1/2227 (0.0%)
5	AE	0.38	0/1119	0.74	0/1504
5	CE	0.37	0/1119	0.73	0/1504
6	AF	0.39	0/836	0.71	2/1128 (0.2%)
6	CF	0.34	0/836	0.68	0/1128
7	AG	0.32	0/1196	0.59	0/1602
7	CG	0.31	0/1196	0.56	0/1602
8	AH	0.36	0/989	0.67	0/1326
8	CH	0.30	0/989	0.59	0/1326
9	AI	0.32	0/1034	0.65	1/1375 (0.1%)
9	CI	0.32	0/1034	0.64	0/1375
10	AJ	0.35	0/797	0.65	0/1077
10	CJ	0.30	0/797	0.66	2/1077 (0.2%)
11	AK	0.35	0/893	0.63	0/1205
11	CK	0.32	0/893	0.63	0/1205
12	AL	0.39	0/969	0.69	0/1300
12	CL	0.35	0/969	0.72	0/1300
13	AM	0.33	0/893	0.69	0/1193
13	CM	0.33	0/893	0.65	0/1193
14	AN	0.31	0/785	0.66	0/1043
14	CN	0.29	0/785	0.57	0/1043
15	AO	0.31	0/718	0.61	0/959
15	CO	0.30	0/718	0.61	0/959
16	AP	0.39	0/659	0.72	1/884 (0.1%)
16	CP	0.33	0/659	0.59	0/884

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.37	0/658	0.72	1/881 (0.1%)
17	CQ	0.38	0/658	0.63	0/881
18	AR	0.31	0/463	0.60	0/621
18	CR	0.30	0/463	0.57	0/621
19	AS	0.32	0/653	0.63	0/877
19	CS	0.33	0/653	0.59	0/877
20	AT	0.36	0/671	0.64	0/888
20	CT	0.32	0/671	0.62	0/888
21	AU	0.43	0/431	0.75	0/570
21	CU	0.45	0/431	0.78	0/570
22	BA	0.68	6/69659 (0.0%)	1.32	534/108672 (0.5%)
22	DA	0.38	0/69659	0.99	76/108672 (0.1%)
23	BB	0.62	1/2850 (0.0%)	1.22	7/4444 (0.2%)
23	DB	0.32	0/2828	0.92	2/4410 (0.0%)
24	BC	0.45	0/2122	0.71	0/2852
24	DC	0.34	0/2122	0.62	0/2852
25	BD	0.50	0/1586	0.74	1/2134 (0.0%)
25	DD	0.32	0/1586	0.59	0/2134
26	BE	0.42	0/1571	0.70	0/2113
26	DE	0.34	0/1571	0.62	1/2113 (0.0%)
27	BF	0.37	0/1435	0.63	0/1926
27	DF	0.30	0/1435	0.56	0/1926
28	BG	0.39	0/1343	0.69	1/1816 (0.1%)
28	DG	0.31	0/1343	0.55	0/1816
29	BH	0.36	0/1121	0.66	1/1515 (0.1%)
29	DH	0.35	0/1121	0.56	0/1515
30	BI	0.38	0/1046	0.69	0/1410
30	DI	0.35	0/1046	0.67	0/1410
31	BJ	0.49	0/1152	0.70	0/1551
31	DJ	0.31	0/1152	0.59	0/1551
32	BK	0.51	0/948	0.73	0/1268
32	DK	0.34	0/948	0.58	0/1268
33	BL	0.45	0/1054	0.80	2/1403 (0.1%)
33	DL	0.32	0/1054	0.62	0/1403
34	BM	0.48	0/1093	0.73	1/1460 (0.1%)
34	DM	0.30	0/1093	0.57	0/1460
35	BN	0.47	0/974	0.77	0/1301
35	DN	0.33	0/974	0.59	0/1301
36	BO	0.43	0/902	0.66	0/1209
36	DO	0.29	0/902	0.53	0/1209
37	BP	0.47	0/929	0.72	1/1242 (0.1%)
37	DP	0.32	0/929	0.59	1/1242 (0.1%)
38	BQ	0.56	0/960	0.73	0/1278

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DQ	0.32	0/960	0.53	0/1278
39	BR	0.53	0/829	0.82	1/1107 (0.1%)
39	DR	0.34	0/829	0.66	0/1107
40	BS	0.71	2/864 (0.2%)	0.89	2/1156 (0.2%)
40	DS	0.33	0/864	0.63	0/1156
41	BT	0.45	0/745	0.70	0/994
41	DT	0.33	0/745	0.61	0/994
42	BU	0.43	0/788	0.72	0/1051
42	DU	0.37	0/788	0.61	0/1051
43	BV	0.40	0/766	0.67	1/1025 (0.1%)
43	DV	0.28	0/766	0.54	0/1025
44	BW	0.52	0/587	0.69	0/776
44	DW	0.29	0/576	0.54	0/762
45	BX	0.39	0/635	0.67	0/848
45	DX	0.32	0/635	0.61	0/848
46	BY	0.39	0/510	0.76	0/677
46	DY	0.32	0/510	0.64	0/677
47	BZ	0.52	0/453	0.74	0/605
47	DZ	0.30	0/453	0.56	0/605
48	B0	0.52	0/450	0.75	0/599
48	D0	0.31	0/450	0.61	0/599
49	B1	0.44	0/417	0.69	0/554
49	D1	0.32	0/417	0.56	0/554
50	B2	0.48	0/380	0.80	0/498
50	D2	0.30	0/380	0.58	0/498
51	B3	0.43	0/513	0.71	0/676
51	D3	0.29	0/513	0.49	0/676
52	B4	0.52	0/303	0.66	0/397
52	D4	0.37	0/303	0.58	0/397
53	B5	0.32	0/1145	0.69	1/1556 (0.1%)
54	B6	1.71	0/13	2.43	1/15 (6.7%)
54	D6	1.45	0/13	2.67	2/15 (13.3%)
All	All	0.47	9/310652 (0.0%)	1.01	796/464396 (0.2%)

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
2	CB	0	1
5	AE	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
5	CE	0	2
6	CF	0	1
11	AK	0	1
11	CK	0	1
12	CL	0	2
21	AU	0	2
21	CU	0	1
25	BD	0	1
25	DD	0	1
26	BE	0	1
40	BS	0	1
All	All	0	16

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	984	A	N9-C4	-9.06	1.32	1.37
22	BA	1142	A	N9-C4	-8.98	1.32	1.37
40	BS	102	HIS	CB-CG	-6.45	1.38	1.50
22	BA	1936	A	N9-C4	-5.92	1.34	1.37
23	BB	99	A	N9-C4	-5.46	1.34	1.37

The worst 5 of 796 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	984	A	C2-N3-C4	-12.57	104.31	110.60
1	AA	1054	C	O5'-P-OP2	-12.23	94.69	105.70
22	BA	1936	A	C2-N3-C4	-10.65	105.28	110.60
25	BD	151	THR	C-N-CD	-10.63	97.20	120.60
22	BA	1142	A	C2-N3-C4	-10.48	105.36	110.60

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	AE	123	VAL	Peptide
11	AK	126	LYS	Peptide
21	AU	39	GLU	Peptide
21	AU	8	GLU	Peptide
25	BD	151	THR	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	32995	0	16607	608	14
1	CA	33015	0	16616	645	0
2	AB	1705	0	1732	135	0
2	CB	1705	0	1732	109	0
3	AC	1625	0	1696	75	0
3	CC	1625	0	1696	67	0
4	AD	1643	0	1707	93	0
4	CD	1643	0	1707	74	0
5	AE	1106	0	1148	60	0
5	CE	1106	0	1148	72	0
6	AF	818	0	808	37	0
6	CF	818	0	808	35	0
7	AG	1182	0	1238	47	0
7	CG	1182	0	1238	49	0
8	AH	979	0	1031	38	0
8	CH	979	0	1031	43	0
9	AI	1022	0	1070	51	0
9	CI	1022	0	1070	64	0
10	AJ	787	0	828	60	0
10	CJ	787	0	828	44	0
11	AK	877	0	887	54	0
11	CK	877	0	887	39	0
12	AL	955	0	1016	38	0
12	CL	955	0	1016	48	0
13	AM	884	0	941	49	0
13	CM	884	0	941	40	0
14	AN	774	0	824	44	0
14	CN	774	0	824	44	0
15	AO	710	0	728	20	0
15	CO	710	0	728	38	0
16	AP	649	0	666	34	0
16	CP	649	0	666	30	0
17	AQ	649	0	691	30	0
17	CQ	649	0	691	33	0
18	AR	456	0	478	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	CR	456	0	478	25	0
19	AS	638	0	665	32	0
19	CS	638	0	665	31	0
20	AT	665	0	714	31	0
20	CT	665	0	714	34	0
21	AU	426	0	449	39	0
21	CU	426	0	449	29	0
22	BA	62195	0	31280	1058	0
22	DA	62195	0	31280	1193	1
23	BB	2549	0	1291	19	0
23	DB	2529	0	1281	44	0
24	BC	2083	0	2154	76	0
24	DC	2083	0	2154	94	0
25	BD	1565	0	1616	48	0
25	DD	1565	0	1616	55	0
26	BE	1552	0	1619	47	0
26	DE	1552	0	1619	63	0
27	BF	1411	0	1444	51	0
27	DF	1411	0	1444	50	0
28	BG	1323	0	1371	44	0
28	DG	1323	0	1371	39	0
29	BH	1110	0	1145	196	0
29	DH	1110	0	1148	91	13
30	BI	1032	0	1085	52	0
30	DI	1032	0	1085	54	0
31	BJ	1129	0	1162	28	0
31	DJ	1129	0	1162	48	0
32	BK	939	0	1012	30	0
32	DK	939	0	1012	29	0
33	BL	1045	0	1117	38	0
33	DL	1045	0	1117	46	0
34	BM	1074	0	1157	30	0
34	DM	1074	0	1157	20	0
35	BN	961	0	1000	35	0
35	DN	961	0	1000	47	0
36	BO	892	0	923	25	0
36	DO	892	0	923	42	0
37	BP	917	0	962	39	0
37	DP	917	0	962	34	0
38	BQ	947	0	1019	35	0
38	DQ	947	0	1019	44	0
39	BR	816	0	839	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	DR	816	0	839	34	0
40	BS	857	0	922	34	0
40	DS	857	0	922	25	0
41	BT	739	0	807	27	0
41	DT	739	0	807	27	0
42	BU	780	0	831	18	0
42	DU	780	0	831	44	0
43	BV	753	0	780	14	0
43	DV	753	0	780	27	0
44	BW	580	0	594	14	0
44	DW	569	0	581	18	0
45	BX	625	0	652	29	0
45	DX	625	0	652	46	0
46	BY	509	0	543	25	0
46	DY	509	0	543	24	0
47	BZ	449	0	488	7	0
47	DZ	449	0	488	15	0
48	B0	444	0	458	20	0
48	D0	444	0	458	16	0
49	B1	410	0	440	15	0
49	D1	410	0	440	14	0
50	B2	377	0	418	13	0
50	D2	377	0	418	14	0
51	B3	504	0	572	18	0
51	D3	504	0	572	17	0
52	B4	302	0	341	15	0
52	D4	302	0	340	12	0
53	B5	1142	0	865	27	0
54	B6	73	0	64	5	0
54	D6	73	0	64	7	0
55	AA	71	0	0	0	0
55	AM	1	0	0	0	0
55	BA	195	0	0	0	0
55	BB	4	0	0	0	0
55	CA	55	0	0	0	0
55	CM	1	0	0	0	0
55	DA	167	0	0	0	0
55	DB	3	0	0	0	0
55	DQ	1	0	0	0	0
56	B4	1	0	0	0	0
56	D4	1	0	0	0	0
57	AA	194	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	AL	1	0	0	0	0
57	AN	5	0	0	1	0
57	AT	2	0	0	0	0
57	AU	1	0	0	1	0
57	B2	1	0	0	0	0
57	B3	3	0	0	0	0
57	B4	2	0	0	0	0
57	BA	619	0	0	59	0
57	BB	13	0	0	1	0
57	BC	8	0	0	1	0
57	BD	3	0	0	2	0
57	BE	3	0	0	0	0
57	BF	1	0	0	1	0
57	BG	1	0	0	0	0
57	BL	5	0	0	1	0
57	BN	5	0	0	1	0
57	BS	1	0	0	0	0
57	BV	1	0	0	0	0
57	CA	189	0	0	10	0
57	CL	1	0	0	0	0
57	CN	3	0	0	0	0
57	CT	4	0	0	0	0
57	CU	1	0	0	1	0
57	D0	1	0	0	0	0
57	D2	2	0	0	1	0
57	D3	1	0	0	0	0
57	D4	1	0	0	0	0
57	DA	612	0	0	63	0
57	DB	13	0	0	0	0
57	DC	7	0	0	1	0
57	DD	4	0	0	1	0
57	DE	4	0	0	0	0
57	DL	4	0	0	0	0
57	DN	1	0	0	0	0
57	DQ	2	0	0	0	0
57	DT	3	0	0	0	0
57	DV	1	0	0	0	0
All	All	288328	0	192913	6784	14

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 15.

The worst 5 of 6784 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
29:BH:83:LYS:HD2	1:CA:55:A:O2'	1.21	1.29
29:BH:117:LEU:O	29:BH:121:VAL:HG23	1.34	1.22
29:BH:117:LEU:O	29:BH:121:VAL:CG2	1.95	1.14
29:BH:123:ARG:O	29:BH:124:THR:CG2	2.01	1.09
29:BH:97:ARG:HD2	1:CA:369:G:O2'	1.51	1.09

The worst 5 of 14 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)
1:AA:368:U:OP2	29:DH:123:ARG:NE[4_455]	1.50	0.70
1:AA:55:A:N1	29:DH:91:PHE:CE1[4_455]	1.60	0.60
1:AA:55:A:N3	29:DH:91:PHE:CZ[4_455]	1.66	0.54
1:AA:55:A:C2	29:DH:91:PHE:CE1[4_455]	1.70	0.50
1:AA:55:A:C2	29:DH:91:PHE:CZ[4_455]	1.71	0.49

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%)	130 (60%)	40 (18%)	46 (21%)	0	0
2	CB	216/218 (99%)	134 (62%)	47 (22%)	35 (16%)	0	1
3	AC	204/206 (99%)	158 (78%)	30 (15%)	16 (8%)	1	6
3	CC	204/206 (99%)	156 (76%)	33 (16%)	15 (7%)	2	7
4	AD	203/205 (99%)	150 (74%)	29 (14%)	24 (12%)	1	2
4	CD	203/205 (99%)	152 (75%)	29 (14%)	22 (11%)	1	3
5	AE	148/150 (99%)	112 (76%)	20 (14%)	16 (11%)	1	3
5	CE	148/150 (99%)	103 (70%)	20 (14%)	25 (17%)	0	1
6	AF	98/100 (98%)	72 (74%)	15 (15%)	11 (11%)	1	2
6	CF	98/100 (98%)	69 (70%)	14 (14%)	15 (15%)	0	1
7	AG	149/151 (99%)	110 (74%)	30 (20%)	9 (6%)	2	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	CG	149/151 (99%)	118 (79%)	22 (15%)	9 (6%)	2	12
8	AH	127/129 (98%)	94 (74%)	26 (20%)	7 (6%)	3	14
8	CH	127/129 (98%)	103 (81%)	17 (13%)	7 (6%)	3	14
9	AI	125/127 (98%)	96 (77%)	20 (16%)	9 (7%)	2	7
9	CI	125/127 (98%)	97 (78%)	20 (16%)	8 (6%)	2	10
10	AJ	96/98 (98%)	67 (70%)	12 (12%)	17 (18%)	0	1
10	CJ	96/98 (98%)	70 (73%)	14 (15%)	12 (12%)	1	2
11	AK	115/117 (98%)	90 (78%)	16 (14%)	9 (8%)	1	6
11	CK	115/117 (98%)	85 (74%)	21 (18%)	9 (8%)	1	6
12	AL	121/123 (98%)	96 (79%)	19 (16%)	6 (5%)	3	17
12	CL	121/123 (98%)	97 (80%)	13 (11%)	11 (9%)	1	5
13	AM	112/114 (98%)	85 (76%)	16 (14%)	11 (10%)	1	4
13	CM	112/114 (98%)	82 (73%)	19 (17%)	11 (10%)	1	4
14	AN	92/100 (92%)	61 (66%)	20 (22%)	11 (12%)	1	2
14	CN	92/100 (92%)	61 (66%)	15 (16%)	16 (17%)	0	1
15	AO	86/88 (98%)	65 (76%)	18 (21%)	3 (4%)	6	27
15	CO	86/88 (98%)	68 (79%)	14 (16%)	4 (5%)	4	19
16	AP	80/82 (98%)	49 (61%)	15 (19%)	16 (20%)	0	0
16	CP	80/82 (98%)	59 (74%)	17 (21%)	4 (5%)	3	17
17	AQ	78/80 (98%)	57 (73%)	11 (14%)	10 (13%)	0	2
17	CQ	78/80 (98%)	53 (68%)	17 (22%)	8 (10%)	1	3
18	AR	53/55 (96%)	45 (85%)	4 (8%)	4 (8%)	2	7
18	CR	53/55 (96%)	40 (76%)	8 (15%)	5 (9%)	1	4
19	AS	77/79 (98%)	55 (71%)	14 (18%)	8 (10%)	1	3
19	CS	77/79 (98%)	61 (79%)	13 (17%)	3 (4%)	5	23
20	AT	83/85 (98%)	66 (80%)	12 (14%)	5 (6%)	2	12
20	CT	83/85 (98%)	68 (82%)	9 (11%)	6 (7%)	2	7
21	AU	49/51 (96%)	29 (59%)	9 (18%)	11 (22%)	0	0
21	CU	49/51 (96%)	29 (59%)	6 (12%)	14 (29%)	0	0
24	BC	269/271 (99%)	217 (81%)	41 (15%)	11 (4%)	4	22
24	DC	269/271 (99%)	209 (78%)	42 (16%)	18 (7%)	2	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	BD	207/209 (99%)	183 (88%)	19 (9%)	5 (2%)	9	40
25	DD	207/209 (99%)	173 (84%)	29 (14%)	5 (2%)	9	40
26	BE	199/201 (99%)	171 (86%)	22 (11%)	6 (3%)	7	32
26	DE	199/201 (99%)	157 (79%)	29 (15%)	13 (6%)	2	9
27	BF	175/177 (99%)	144 (82%)	23 (13%)	8 (5%)	4	19
27	DF	175/177 (99%)	146 (83%)	17 (10%)	12 (7%)	2	8
28	BG	174/176 (99%)	147 (84%)	15 (9%)	12 (7%)	2	8
28	DG	174/176 (99%)	138 (79%)	25 (14%)	11 (6%)	2	10
29	BH	147/149 (99%)	89 (60%)	37 (25%)	21 (14%)	0	1
29	DH	147/149 (99%)	100 (68%)	32 (22%)	15 (10%)	1	3
30	BI	139/141 (99%)	78 (56%)	37 (27%)	24 (17%)	0	1
30	DI	139/141 (99%)	80 (58%)	44 (32%)	15 (11%)	1	3
31	BJ	140/142 (99%)	124 (89%)	11 (8%)	5 (4%)	5	26
31	DJ	140/142 (99%)	123 (88%)	15 (11%)	2 (1%)	16	58
32	BK	120/122 (98%)	98 (82%)	13 (11%)	9 (8%)	2	7
32	DK	120/122 (98%)	100 (83%)	14 (12%)	6 (5%)	3	17
33	BL	141/143 (99%)	109 (77%)	20 (14%)	12 (8%)	1	5
33	DL	141/143 (99%)	105 (74%)	29 (21%)	7 (5%)	3	17
34	BM	134/136 (98%)	117 (87%)	15 (11%)	2 (2%)	15	56
34	DM	134/136 (98%)	112 (84%)	19 (14%)	3 (2%)	10	43
35	BN	118/120 (98%)	96 (81%)	21 (18%)	1 (1%)	27	74
35	DN	118/120 (98%)	97 (82%)	11 (9%)	10 (8%)	1	5
36	BO	114/116 (98%)	95 (83%)	15 (13%)	4 (4%)	6	27
36	DO	114/116 (98%)	96 (84%)	14 (12%)	4 (4%)	6	27
37	BP	112/114 (98%)	98 (88%)	9 (8%)	5 (4%)	4	20
37	DP	112/114 (98%)	91 (81%)	16 (14%)	5 (4%)	4	20
38	BQ	115/117 (98%)	107 (93%)	3 (3%)	5 (4%)	4	21
38	DQ	115/117 (98%)	108 (94%)	6 (5%)	1 (1%)	25	71
39	BR	101/103 (98%)	86 (85%)	8 (8%)	7 (7%)	2	8
39	DR	101/103 (98%)	77 (76%)	20 (20%)	4 (4%)	5	22
40	BS	108/110 (98%)	100 (93%)	5 (5%)	3 (3%)	8	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	DS	108/110 (98%)	89 (82%)	14 (13%)	5 (5%)	4	19
41	BT	91/93 (98%)	70 (77%)	13 (14%)	8 (9%)	1	5
41	DT	91/93 (98%)	70 (77%)	9 (10%)	12 (13%)	0	2
42	BU	100/102 (98%)	80 (80%)	12 (12%)	8 (8%)	1	6
42	DU	100/102 (98%)	73 (73%)	17 (17%)	10 (10%)	1	3
43	BV	92/94 (98%)	85 (92%)	6 (6%)	1 (1%)	21	66
43	DV	92/94 (98%)	82 (89%)	8 (9%)	2 (2%)	10	43
44	BW	74/76 (97%)	67 (90%)	7 (10%)	0	100	100
44	DW	73/76 (96%)	65 (89%)	6 (8%)	2 (3%)	8	36
45	BX	75/77 (97%)	72 (96%)	1 (1%)	2 (3%)	8	36
45	DX	75/77 (97%)	64 (85%)	9 (12%)	2 (3%)	8	36
46	BY	61/63 (97%)	40 (66%)	12 (20%)	9 (15%)	0	1
46	DY	61/63 (97%)	49 (80%)	8 (13%)	4 (7%)	2	9
47	BZ	56/58 (97%)	52 (93%)	4 (7%)	0	100	100
47	DZ	56/58 (97%)	53 (95%)	1 (2%)	2 (4%)	5	26
48	B0	54/56 (96%)	46 (85%)	5 (9%)	3 (6%)	3	14
48	D0	54/56 (96%)	41 (76%)	11 (20%)	2 (4%)	5	25
49	B1	48/50 (96%)	38 (79%)	6 (12%)	4 (8%)	1	5
49	D1	48/50 (96%)	37 (77%)	8 (17%)	3 (6%)	2	10
50	B2	44/46 (96%)	39 (89%)	3 (7%)	2 (4%)	4	20
50	D2	44/46 (96%)	38 (86%)	4 (9%)	2 (4%)	4	20
51	B3	62/64 (97%)	56 (90%)	5 (8%)	1 (2%)	14	54
51	D3	62/64 (97%)	54 (87%)	7 (11%)	1 (2%)	14	54
52	B4	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
52	D4	36/38 (95%)	33 (92%)	1 (3%)	2 (6%)	3	14
53	B5	183/228 (80%)	94 (51%)	54 (30%)	35 (19%)	0	0
54	B6	2/8 (25%)	2 (100%)	0	0	100	100
54	D6	2/8 (25%)	2 (100%)	0	0	100	100
All	All	11422/11688 (98%)	8887 (78%)	1654 (14%)	881 (8%)	1	6

5 of 881 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	16	PHE
2	AB	22	TYR
2	AB	34	ALA
2	AB	64	LYS
2	AB	73	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%)	113 (63%)	67 (37%)	0	1
2	CB	180/180 (100%)	129 (72%)	51 (28%)	0	2
3	AC	170/170 (100%)	132 (78%)	38 (22%)	1	6
3	CC	170/170 (100%)	131 (77%)	39 (23%)	1	5
4	AD	172/172 (100%)	129 (75%)	43 (25%)	1	3
4	CD	172/172 (100%)	138 (80%)	34 (20%)	2	9
5	AE	113/113 (100%)	85 (75%)	28 (25%)	1	3
5	CE	113/113 (100%)	85 (75%)	28 (25%)	1	3
6	AF	87/87 (100%)	64 (74%)	23 (26%)	1	3
6	CF	87/87 (100%)	63 (72%)	24 (28%)	0	2
7	AG	124/124 (100%)	94 (76%)	30 (24%)	1	4
7	CG	124/124 (100%)	91 (73%)	33 (27%)	1	3
8	AH	104/104 (100%)	79 (76%)	25 (24%)	1	4
8	CH	104/104 (100%)	83 (80%)	21 (20%)	2	8
9	AI	105/105 (100%)	74 (70%)	31 (30%)	0	2
9	CI	105/105 (100%)	77 (73%)	28 (27%)	1	3
10	AJ	86/86 (100%)	64 (74%)	22 (26%)	1	3
10	CJ	86/86 (100%)	67 (78%)	19 (22%)	1	6
11	AK	90/90 (100%)	66 (73%)	24 (27%)	1	3
11	CK	90/90 (100%)	69 (77%)	21 (23%)	1	5
12	AL	103/103 (100%)	84 (82%)	19 (18%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	CL	103/103 (100%)	78 (76%)	25 (24%)	1	4
13	AM	92/92 (100%)	74 (80%)	18 (20%)	2	9
13	CM	92/92 (100%)	70 (76%)	22 (24%)	1	4
14	AN	79/83 (95%)	61 (77%)	18 (23%)	1	5
14	CN	79/83 (95%)	68 (86%)	11 (14%)	5	21
15	AO	75/76 (99%)	59 (79%)	16 (21%)	1	7
15	CO	75/76 (99%)	57 (76%)	18 (24%)	1	4
16	AP	65/65 (100%)	52 (80%)	13 (20%)	2	9
16	CP	65/65 (100%)	49 (75%)	16 (25%)	1	4
17	AQ	74/74 (100%)	52 (70%)	22 (30%)	0	2
17	CQ	74/74 (100%)	53 (72%)	21 (28%)	0	2
18	AR	48/48 (100%)	41 (85%)	7 (15%)	5	19
18	CR	48/48 (100%)	39 (81%)	9 (19%)	2	11
19	AS	70/70 (100%)	57 (81%)	13 (19%)	2	11
19	CS	70/70 (100%)	55 (79%)	15 (21%)	1	7
20	AT	65/65 (100%)	46 (71%)	19 (29%)	0	2
20	CT	65/65 (100%)	48 (74%)	17 (26%)	1	3
21	AU	44/44 (100%)	27 (61%)	17 (39%)	0	1
21	CU	44/44 (100%)	32 (73%)	12 (27%)	0	3
24	BC	216/216 (100%)	190 (88%)	26 (12%)	7	28
24	DC	216/216 (100%)	180 (83%)	36 (17%)	3	14
25	BD	164/164 (100%)	147 (90%)	17 (10%)	10	35
25	DD	164/164 (100%)	144 (88%)	20 (12%)	7	27
26	BE	165/165 (100%)	138 (84%)	27 (16%)	3	14
26	DE	165/165 (100%)	133 (81%)	32 (19%)	2	10
27	BF	148/148 (100%)	121 (82%)	27 (18%)	2	11
27	DF	148/148 (100%)	118 (80%)	30 (20%)	2	8
28	BG	137/137 (100%)	117 (85%)	20 (15%)	5	19
28	DG	137/137 (100%)	123 (90%)	14 (10%)	11	36
29	BH	114/114 (100%)	88 (77%)	26 (23%)	1	5
29	DH	114/114 (100%)	88 (77%)	26 (23%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	BI	109/109 (100%)	86 (79%)	23 (21%)	1	7
30	DI	109/109 (100%)	84 (77%)	25 (23%)	1	5
31	BJ	116/116 (100%)	103 (89%)	13 (11%)	9	31
31	DJ	116/116 (100%)	102 (88%)	14 (12%)	7	28
32	BK	103/103 (100%)	93 (90%)	10 (10%)	12	40
32	DK	103/103 (100%)	90 (87%)	13 (13%)	7	25
33	BL	102/102 (100%)	85 (83%)	17 (17%)	3	14
33	DL	102/102 (100%)	81 (79%)	21 (21%)	2	7
34	BM	109/109 (100%)	97 (89%)	12 (11%)	9	32
34	DM	109/109 (100%)	97 (89%)	12 (11%)	9	32
35	BN	100/100 (100%)	87 (87%)	13 (13%)	6	24
35	DN	100/100 (100%)	83 (83%)	17 (17%)	3	13
36	BO	86/86 (100%)	64 (74%)	22 (26%)	1	3
36	DO	86/86 (100%)	72 (84%)	14 (16%)	3	15
37	BP	99/99 (100%)	88 (89%)	11 (11%)	9	32
37	DP	99/99 (100%)	80 (81%)	19 (19%)	2	10
38	BQ	89/89 (100%)	74 (83%)	15 (17%)	3	13
38	DQ	89/89 (100%)	76 (85%)	13 (15%)	5	19
39	BR	84/84 (100%)	73 (87%)	11 (13%)	6	24
39	DR	84/84 (100%)	70 (83%)	14 (17%)	3	14
40	BS	93/93 (100%)	78 (84%)	15 (16%)	3	15
40	DS	93/93 (100%)	77 (83%)	16 (17%)	3	13
41	BT	80/80 (100%)	68 (85%)	12 (15%)	4	18
41	DT	80/80 (100%)	66 (82%)	14 (18%)	3	12
42	BU	83/83 (100%)	68 (82%)	15 (18%)	2	11
42	DU	83/83 (100%)	64 (77%)	19 (23%)	1	5
43	BV	78/78 (100%)	66 (85%)	12 (15%)	4	17
43	DV	78/78 (100%)	67 (86%)	11 (14%)	5	20
44	BW	57/58 (98%)	53 (93%)	4 (7%)	21	60
44	DW	56/58 (97%)	49 (88%)	7 (12%)	7	26
45	BX	67/67 (100%)	55 (82%)	12 (18%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	DX	67/67 (100%)	55 (82%)	12 (18%)	2	12
46	BY	55/55 (100%)	48 (87%)	7 (13%)	6	25
46	DY	55/55 (100%)	43 (78%)	12 (22%)	1	6
47	BZ	48/48 (100%)	43 (90%)	5 (10%)	10	35
47	DZ	48/48 (100%)	38 (79%)	10 (21%)	2	7
48	B0	47/47 (100%)	40 (85%)	7 (15%)	4	18
48	D0	47/47 (100%)	42 (89%)	5 (11%)	10	34
49	B1	45/45 (100%)	38 (84%)	7 (16%)	4	16
49	D1	45/45 (100%)	39 (87%)	6 (13%)	6	23
50	B2	38/38 (100%)	32 (84%)	6 (16%)	4	16
50	D2	38/38 (100%)	32 (84%)	6 (16%)	4	16
51	B3	51/51 (100%)	46 (90%)	5 (10%)	12	39
51	D3	51/51 (100%)	46 (90%)	5 (10%)	12	39
52	B4	34/34 (100%)	30 (88%)	4 (12%)	8	29
52	D4	34/34 (100%)	28 (82%)	6 (18%)	3	12
53	B5	61/180 (34%)	48 (79%)	13 (21%)	1	7
54	B6	2/2 (100%)	2 (100%)	0	100	100
54	D6	2/2 (100%)	2 (100%)	0	100	100
All	All	9390/9522 (99%)	7570 (81%)	1820 (19%)	2	10

5 of 1820 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
42	BU	81	ASP
4	CD	138	SER
39	DR	43	ASN
45	BX	48	THR
2	CB	68	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
45	BX	34	HIS
3	CC	176	HIS
41	DT	59	ASN

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Mol	Chain	Res	Type
2	CB	18	HIS
2	CB	51	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1537/1539 (99%)	357 (23%)	0
1	CA	1538/1539 (99%)	337 (21%)	0
22	BA	2895/2903 (99%)	563 (19%)	0
22	DA	2895/2903 (99%)	643 (22%)	0
23	BB	118/119 (99%)	23 (19%)	0
23	DB	117/119 (98%)	25 (21%)	0
All	All	9100/9122 (99%)	1948 (21%)	0

5 of 1948 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	5	U
1	AA	7	A
1	AA	9	G
1	AA	13	U

There are no RNA pucker outliers to report.

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

10 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
54	MHW	B6	1	54	9,9,10	1.73	1 (11%)	8,11,13	2.41	2 (25%)
54	DBB	B6	3	54	5,5,6	7.75	2 (40%)	3,5,7	2.55	2 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	MHU	B6	5	54	15,15,16	4.38	3 (20%)	16,19,21	1.21	2 (12%)
54	MHV	B6	6	54	9,9,10	5.47	2 (22%)	9,11,13	3.63	5 (55%)
54	004	B6	7	54	10,10,11	6.14	2 (20%)	10,12,14	10.28	5 (50%)
54	MHW	D6	1	54	9,9,10	1.77	1 (11%)	8,11,13	3.27	4 (50%)
54	DBB	D6	3	54	5,5,6	8.12	2 (40%)	3,5,7	2.09	2 (66%)
54	MHU	D6	5	54	15,15,16	4.75	4 (26%)	16,19,21	1.30	1 (6%)
54	MHV	D6	6	54	9,9,10	5.12	1 (11%)	9,11,13	3.53	5 (55%)
54	004	D6	7	54	10,10,11	6.25	2 (20%)	10,12,14	17.37	1 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	MHW	B6	1	54	-	0/0/2/4	0/1/1/1
54	DBB	B6	3	54	-	0/2/4/6	0/0/0/0
54	MHU	B6	5	54	-	0/10/12/14	0/1/1/1
54	MHV	B6	6	54	-	0/0/12/14	0/1/1/1
54	004	B6	7	54	-	0/4/6/8	0/1/1/1
54	MHW	D6	1	54	-	0/0/2/4	0/1/1/1
54	DBB	D6	3	54	-	0/2/4/6	0/0/0/0
54	MHU	D6	5	54	-	0/10/12/14	0/1/1/1
54	MHV	D6	6	54	-	0/0/12/14	0/1/1/1
54	004	D6	7	54	-	0/4/6/8	0/1/1/1

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	D6	7	004	O-C	19.57	1.24	1.11
54	B6	7	004	O-C	17.65	1.23	1.11
54	D6	3	DBB	O-C	17.44	1.23	1.11
54	D6	5	MHU	O-C	16.99	1.23	1.11
54	B6	3	DBB	O-C	16.18	1.22	1.11

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	D6	7	004	C-CA-N	54.90	119.48	113.27
54	B6	7	004	C-CA-N	31.66	116.85	113.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	D6	6	MHV	CD2-CE-N	-8.87	90.50	110.04
54	B6	6	MHV	CD2-CE-N	-8.09	92.22	110.04
54	D6	1	MHW	CD-CE-N	6.83	134.92	123.42

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 500 ligands modelled in this entry, 500 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1538/1539 (99%)	0.31	67 (4%) 33 16	15, 50, 134, 177	0
1	CA	1539/1539 (100%)	0.71	170 (11%) 6 4	29, 71, 143, 177	0
2	AB	218/218 (100%)	1.11	47 (21%) 1 1	39, 71, 98, 131	0
2	CB	218/218 (100%)	1.62	80 (36%) 1 0	55, 80, 108, 126	0
3	AC	206/206 (100%)	0.41	14 (6%) 17 9	36, 56, 81, 95	0
3	CC	206/206 (100%)	1.68	74 (35%) 1 0	52, 73, 93, 114	0
4	AD	205/205 (100%)	0.93	30 (14%) 3 2	33, 55, 80, 109	0
4	CD	205/205 (100%)	0.46	16 (7%) 13 7	23, 40, 75, 93	0
5	AE	150/150 (100%)	0.52	10 (6%) 17 10	32, 49, 82, 111	0
5	CE	150/150 (100%)	0.71	19 (12%) 4 2	35, 56, 83, 105	0
6	AF	100/100 (100%)	0.40	8 (8%) 12 6	34, 55, 75, 85	0
6	CF	100/100 (100%)	0.92	17 (17%) 2 2	44, 72, 97, 105	0
7	AG	151/151 (100%)	1.26	38 (25%) 1 1	48, 73, 96, 107	0
7	CG	151/151 (100%)	3.42	108 (71%) 0 0	75, 92, 105, 113	0
8	AH	129/129 (100%)	0.36	5 (3%) 37 18	28, 47, 71, 80	0
8	CH	129/129 (100%)	1.05	25 (19%) 2 1	46, 63, 83, 90	0
9	AI	127/127 (100%)	1.25	31 (24%) 1 1	42, 68, 96, 115	0
9	CI	127/127 (100%)	2.48	69 (54%) 0 0	64, 87, 106, 131	0
10	AJ	98/98 (100%)	1.19	20 (20%) 1 1	42, 62, 93, 120	0
10	CJ	98/98 (100%)	3.57	68 (69%) 0 0	66, 89, 108, 122	0
11	AK	117/117 (100%)	1.09	28 (23%) 1 1	29, 61, 88, 106	0
11	CK	117/117 (100%)	0.63	12 (10%) 7 4	35, 63, 82, 91	0
12	AL	123/123 (100%)	0.56	8 (6%) 18 10	23, 36, 72, 102	0
12	CL	123/123 (100%)	0.94	15 (12%) 5 3	38, 50, 80, 102	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å²)		Q<0.9	
13	AM	114/114 (100%)	0.70	17 (14%)	3	2	43, 66, 91, 105	0
13	CM	114/114 (100%)	3.70	86 (75%)	0	0	80, 98, 113, 118	0
14	AN	96/100 (96%)	0.99	20 (20%)	1	1	39, 56, 93, 108	0
14	CN	96/100 (96%)	3.18	59 (61%)	0	0	60, 88, 106, 119	0
15	AO	88/88 (100%)	0.55	6 (6%)	17	9	31, 49, 66, 99	0
15	CO	88/88 (100%)	0.87	10 (11%)	6	3	42, 62, 84, 108	0
16	AP	82/82 (100%)	1.03	17 (20%)	1	1	35, 46, 80, 103	0
16	CP	82/82 (100%)	1.85	28 (34%)	1	0	43, 61, 87, 105	0
17	AQ	80/80 (100%)	0.82	14 (17%)	2	2	30, 55, 85, 123	0
17	CQ	80/80 (100%)	1.75	31 (38%)	1	0	42, 69, 97, 108	0
18	AR	55/55 (100%)	0.76	6 (10%)	6	4	38, 51, 76, 113	0
18	CR	55/55 (100%)	1.10	12 (21%)	1	1	40, 54, 83, 113	0
19	AS	79/79 (100%)	1.02	13 (16%)	2	2	45, 66, 92, 97	0
19	CS	79/79 (100%)	4.27	59 (74%)	0	0	79, 98, 113, 126	0
20	AT	85/85 (100%)	0.84	9 (10%)	7	4	35, 48, 74, 115	0
20	CT	85/85 (100%)	2.69	47 (55%)	0	0	52, 69, 91, 98	0
21	AU	51/51 (100%)	1.79	21 (41%)	1	0	49, 70, 92, 105	0
21	CU	51/51 (100%)	1.31	11 (21%)	1	1	43, 67, 92, 107	0
22	BA	2897/2903 (99%)	0.58	139 (4%)	29	15	3, 18, 128, 196	0
22	DA	2897/2903 (99%)	0.92	323 (11%)	6	3	42, 82, 142, 182	0
23	BB	119/119 (100%)	-0.03	0	100	100	6, 26, 52, 94	0
23	DB	118/119 (99%)	0.64	10 (8%)	11	6	68, 109, 131, 143	0
24	BC	271/271 (100%)	0.08	5 (1%)	65	29	8, 24, 44, 65	0
24	DC	271/271 (100%)	1.50	77 (28%)	1	1	40, 60, 76, 84	0
25	BD	209/209 (100%)	0.09	0	100	100	4, 15, 42, 69	0
25	DD	209/209 (100%)	1.62	65 (31%)	1	0	47, 64, 83, 99	0
26	BE	201/201 (100%)	0.08	3 (1%)	70	32	4, 27, 54, 95	0
26	DE	201/201 (100%)	2.40	109 (54%)	0	0	38, 76, 96, 108	0
27	BF	177/177 (100%)	0.49	17 (9%)	8	4	23, 44, 86, 104	0
27	DF	177/177 (100%)	4.16	145 (81%)	0	0	79, 97, 113, 125	0
28	BG	176/176 (100%)	0.56	18 (10%)	7	4	21, 39, 66, 95	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DG	176/176 (100%)	2.71	113 (64%) 0 0	66, 85, 103, 117	0
29	BH	149/149 (100%)	4.78	115 (77%) 0 0	25, 102, 121, 129	0
29	DH	149/149 (100%)	2.47	75 (50%) 0 0	25, 92, 107, 115	0
30	BI	141/141 (100%)	4.09	97 (68%) 0 0	80, 104, 120, 136	0
30	DI	141/141 (100%)	6.16	128 (90%) 0 0	91, 110, 121, 124	0
31	BJ	142/142 (100%)	-0.04	1 (0%) 84 44	5, 12, 32, 54	0
31	DJ	142/142 (100%)	1.43	42 (29%) 1 1	49, 64, 80, 96	0
32	BK	122/122 (100%)	-0.07	2 (1%) 68 32	7, 16, 40, 68	0
32	DK	122/122 (100%)	1.59	41 (33%) 1 0	47, 60, 81, 95	0
33	BL	143/143 (100%)	0.16	4 (2%) 50 22	4, 26, 49, 80	0
33	DL	143/143 (100%)	2.76	79 (55%) 0 0	45, 72, 90, 111	0
34	BM	136/136 (100%)	-0.04	1 (0%) 84 44	6, 16, 34, 93	0
34	DM	136/136 (100%)	1.47	42 (30%) 1 0	40, 64, 82, 110	0
35	BN	120/120 (100%)	-0.02	0 100 100	7, 13, 25, 70	0
35	DN	120/120 (100%)	2.19	50 (41%) 1 0	50, 71, 88, 109	0
36	BO	116/116 (100%)	0.21	3 (2%) 53 24	18, 29, 52, 59	0
36	DO	116/116 (100%)	3.38	83 (71%) 0 0	64, 86, 100, 113	0
37	BP	114/114 (100%)	0.13	4 (3%) 42 19	10, 22, 49, 73	0
37	DP	114/114 (100%)	1.57	41 (35%) 1 0	51, 66, 84, 91	0
38	BQ	117/117 (100%)	-0.00	0 100 100	3, 8, 21, 57	0
38	DQ	117/117 (100%)	1.69	47 (40%) 1 0	46, 65, 79, 83	0
39	BR	103/103 (100%)	-0.07	1 (0%) 79 38	4, 15, 37, 64	0
39	DR	103/103 (100%)	2.10	46 (44%) 1 0	49, 72, 86, 96	0
40	BS	110/110 (100%)	0.04	1 (0%) 81 39	4, 9, 27, 89	0
40	DS	110/110 (100%)	2.72	67 (60%) 0 0	53, 69, 89, 97	0
41	BT	93/93 (100%)	0.76	9 (9%) 8 4	15, 28, 83, 100	0
41	DT	93/93 (100%)	3.82	69 (74%) 0 0	60, 79, 102, 111	0
42	BU	102/102 (100%)	0.22	4 (3%) 37 18	15, 32, 62, 95	0
42	DU	102/102 (100%)	4.48	76 (74%) 0 0	61, 82, 103, 109	0
43	BV	94/94 (100%)	0.04	2 (2%) 60 27	11, 24, 48, 59	0
43	DV	94/94 (100%)	1.34	27 (28%) 1 1	60, 78, 93, 98	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BW	76/76 (100%)	0.18	2 (2%) 53 24	10, 17, 37, 56	0
44	DW	75/76 (98%)	2.58	44 (58%) 0 0	49, 75, 86, 107	0
45	BX	77/77 (100%)	0.23	4 (5%) 26 13	11, 28, 53, 81	0
45	DX	77/77 (100%)	1.81	29 (37%) 1 0	49, 66, 84, 89	0
46	BY	63/63 (100%)	0.63	5 (7%) 13 7	21, 42, 71, 93	0
46	DY	63/63 (100%)	2.37	31 (49%) 1 0	63, 86, 95, 104	0
47	BZ	58/58 (100%)	0.01	0 100 100	7, 11, 34, 40	0
47	DZ	58/58 (100%)	1.48	23 (39%) 1 0	50, 69, 82, 89	0
48	B0	56/56 (100%)	-0.06	1 (1%) 65 29	4, 14, 38, 77	0
48	D0	56/56 (100%)	2.21	21 (37%) 1 0	49, 69, 90, 106	0
49	B1	50/50 (100%)	0.27	2 (4%) 36 17	19, 33, 61, 95	0
49	D1	50/50 (100%)	2.25	24 (48%) 1 0	63, 79, 91, 103	0
50	B2	46/46 (100%)	0.15	1 (2%) 59 26	8, 14, 22, 97	0
50	D2	46/46 (100%)	2.26	20 (43%) 1 0	47, 64, 78, 100	0
51	B3	64/64 (100%)	0.20	1 (1%) 68 32	10, 16, 26, 37	0
51	D3	64/64 (100%)	2.17	34 (53%) 0 0	53, 67, 79, 83	0
52	B4	38/38 (100%)	0.52	1 (2%) 53 24	13, 23, 38, 60	0
52	D4	38/38 (100%)	3.45	25 (65%) 0 0	56, 71, 84, 96	0
53	B5	191/228 (83%)	7.72	188 (98%) 0 0	71, 107, 119, 133	0
54	B6	8/8 (100%)	-0.18	1 (12%) 5 2	6, 8, 11, 16	0
54	D6	8/8 (100%)	1.33	3 (37%) 1 0	41, 44, 50, 55	0
All	All	20750/20810 (99%)	1.15	4086 (19%) 2 1	3, 61, 117, 196	0

The worst 5 of 4086 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
30	DI	2	ALA	27.2
29	BH	96	THR	26.6
22	BA	2184	A	24.7
53	B5	111	PHE	24.1
22	BA	2104	C	23.5

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

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
54	004	B6	7	10/11	0.29	4.68	3,6,7,10	0
54	MHW	D6	1	9/10	0.35	4.28	49,54,56,59	0
54	MHW	B6	1	9/10	0.20	2.62	12,14,18,21	0
54	MHU	D6	5	15/16	0.37	1.94	37,42,54,56	0
54	MHU	B6	5	15/16	0.23	1.57	0,5,18,21	0
54	DBB	D6	3	6/7	0.34	0.31	37,40,41,43	0
54	DBB	B6	3	6/7	0.23	0.04	6,8,10,15	0
54	004	D6	7	10/11	0.20	-0.16	38,42,48,48	0
54	MHV	D6	6	9/10	0.16	-0.97	39,40,42,43	0
54	MHV	B6	6	9/10	0.16	-1.70	2,6,13,14	0

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
55	MG	CA	1637	1/1	0.42	139.12	51,51,51,51	0
55	MG	DA	3060	1/1	1.19	127.71	61,61,61,61	0
55	MG	BA	3147	1/1	0.42	113.23	13,13,13,13	0
55	MG	CA	1655	1/1	0.58	88.08	44,44,44,44	0
55	MG	BA	3190	1/1	0.24	83.00	33,33,33,33	0
55	MG	DA	3155	1/1	0.74	65.62	44,44,44,44	0
55	MG	DA	3076	1/1	0.34	50.67	48,48,48,48	0
55	MG	BA	3139	1/1	0.36	50.34	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3098	1/1	0.57	49.88	63,63,63,63	0
55	MG	BA	3102	1/1	0.39	47.29	23,23,23,23	0
55	MG	DA	3061	1/1	0.98	47.07	53,53,53,53	0
55	MG	CA	1654	1/1	0.16	47.00	26,26,26,26	0
55	MG	BA	3178	1/1	0.60	45.74	20,20,20,20	0
55	MG	AA	1657	1/1	0.72	41.02	40,40,40,40	0
55	MG	BA	3142	1/1	0.40	38.22	15,15,15,15	0
55	MG	AA	1659	1/1	0.60	34.50	34,34,34,34	0
55	MG	BA	3061	1/1	0.49	32.77	55,55,55,55	0
55	MG	CA	1633	1/1	0.45	32.41	54,54,54,54	0
55	MG	DA	3131	1/1	1.02	32.26	71,71,71,71	0
55	MG	BA	3060	1/1	0.40	31.28	33,33,33,33	0
55	MG	BA	3138	1/1	0.40	29.01	4,4,4,4	0
55	MG	AA	1627	1/1	0.34	26.87	43,43,43,43	0
55	MG	BA	3040	1/1	0.45	25.94	7,7,7,7	0
55	MG	DA	3025	1/1	0.49	25.78	49,49,49,49	0
55	MG	AA	1644	1/1	0.30	25.60	32,32,32,32	0
55	MG	AA	1614	1/1	0.43	23.32	53,53,53,53	0
55	MG	BA	3137	1/1	0.43	21.66	4,4,4,4	0
55	MG	DA	3119	1/1	0.58	21.45	68,68,68,68	0
55	MG	BA	3126	1/1	0.28	20.65	7,7,7,7	0
55	MG	AA	1648	1/1	0.31	20.62	38,38,38,38	0
55	MG	BA	3119	1/1	0.32	20.31	21,21,21,21	0
55	MG	DA	3142	1/1	0.31	19.88	38,38,38,38	0
55	MG	DA	3057	1/1	0.65	19.25	54,54,54,54	0
55	MG	CA	1650	1/1	0.47	18.40	40,40,40,40	0
55	MG	DA	3016	1/1	0.46	18.05	53,53,53,53	0
55	MG	BA	3015	1/1	0.38	17.55	52,52,52,52	0
55	MG	AA	1669	1/1	0.47	17.35	43,43,43,43	0
55	MG	BA	3179	1/1	0.45	17.09	39,39,39,39	0
55	MG	DA	3002	1/1	0.44	16.63	52,52,52,52	0
55	MG	DA	3054	1/1	0.31	16.58	44,44,44,44	0
55	MG	CA	1628	1/1	0.43	15.60	64,64,64,64	0
55	MG	AA	1653	1/1	0.29	15.55	24,24,24,24	0
55	MG	DA	3138	1/1	0.74	15.47	41,41,41,41	0
55	MG	DA	3092	1/1	0.48	15.25	62,62,62,62	0
55	MG	BA	3106	1/1	0.32	14.97	0,0,0,0	0
55	MG	BA	3186	1/1	0.35	14.59	18,18,18,18	0
55	MG	DA	3088	1/1	0.36	14.55	51,51,51,51	0
55	MG	DA	3015	1/1	0.66	14.50	56,56,56,56	0
55	MG	BA	3098	1/1	0.37	14.29	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3055	1/1	0.51	14.17	53,53,53,53	0
55	MG	BA	3025	1/1	0.25	12.63	40,40,40,40	0
55	MG	AA	1654	1/1	0.31	12.38	40,40,40,40	0
55	MG	BB	204	1/1	0.26	12.33	4,4,4,4	0
55	MG	BA	3141	1/1	0.42	12.28	4,4,4,4	0
55	MG	DA	3041	1/1	0.39	11.56	53,53,53,53	0
55	MG	BA	3146	1/1	0.25	11.52	23,23,23,23	0
55	MG	DA	3084	1/1	0.30	11.49	56,56,56,56	0
55	MG	DA	3157	1/1	0.37	11.41	47,47,47,47	0
55	MG	DA	3153	1/1	0.50	11.27	52,52,52,52	0
55	MG	CA	1642	1/1	0.25	11.04	27,27,27,27	0
55	MG	AA	1670	1/1	0.32	10.81	26,26,26,26	0
55	MG	BA	3170	1/1	0.28	10.69	35,35,35,35	0
55	MG	BA	3145	1/1	0.21	10.63	15,15,15,15	0
55	MG	BA	3083	1/1	0.24	10.47	32,32,32,32	0
55	MG	DA	3110	1/1	0.39	10.30	57,57,57,57	0
55	MG	BA	3160	1/1	0.28	10.26	7,7,7,7	0
55	MG	BA	3140	1/1	0.19	10.16	14,14,14,14	0
55	MG	BA	3164	1/1	0.42	9.91	21,21,21,21	0
55	MG	DA	3140	1/1	0.44	9.74	37,37,37,37	0
55	MG	DA	3137	1/1	0.44	9.70	42,42,42,42	0
55	MG	CA	1644	1/1	0.29	9.48	32,32,32,32	0
55	MG	AA	1646	1/1	0.20	9.36	44,44,44,44	0
55	MG	BA	3116	1/1	0.31	8.98	11,11,11,11	0
55	MG	BA	3168	1/1	0.32	8.48	18,18,18,18	0
55	MG	AA	1661	1/1	0.25	8.36	22,22,22,22	0
55	MG	AA	1667	1/1	0.27	8.31	37,37,37,37	0
55	MG	BA	3148	1/1	0.25	8.27	16,16,16,16	0
55	MG	DA	3091	1/1	0.60	8.16	71,71,71,71	0
55	MG	BA	3181	1/1	0.20	7.90	14,14,14,14	0
55	MG	BA	3019	1/1	0.23	7.80	3,3,3,3	0
55	MG	DA	3162	1/1	0.33	7.78	46,46,46,46	0
55	MG	DA	3027	1/1	0.45	7.63	51,51,51,51	0
55	MG	BA	3113	1/1	0.32	7.61	10,10,10,10	0
55	MG	AA	1649	1/1	0.26	7.61	27,27,27,27	0
55	MG	BA	3033	1/1	0.25	7.50	4,4,4,4	0
55	MG	BA	3150	1/1	0.23	7.26	42,42,42,42	0
55	MG	AA	1622	1/1	0.26	6.89	21,21,21,21	0
55	MG	DA	3163	1/1	0.33	6.89	51,51,51,51	0
55	MG	BA	3157	1/1	0.24	6.85	26,26,26,26	0
55	MG	CA	1605	1/1	0.37	6.75	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3133	1/1	0.62	6.61	57,57,57,57	0
55	MG	BA	3143	1/1	0.28	6.56	7,7,7,7	0
55	MG	BA	3055	1/1	0.25	6.44	23,23,23,23	0
55	MG	AA	1666	1/1	0.24	6.41	30,30,30,30	0
55	MG	CA	1625	1/1	0.21	6.30	25,25,25,25	0
55	MG	DA	3020	1/1	0.37	6.28	42,42,42,42	0
55	MG	CA	1608	1/1	0.32	6.02	50,50,50,50	0
55	MG	BA	3108	1/1	0.28	5.53	1,1,1,1	0
55	MG	CA	1623	1/1	0.30	5.44	40,40,40,40	0
55	MG	DA	3165	1/1	0.36	5.38	34,34,34,34	0
55	MG	BA	3162	1/1	0.19	5.33	21,21,21,21	0
55	MG	DA	3109	1/1	0.24	5.33	37,37,37,37	0
55	MG	BA	3070	1/1	0.22	5.29	9,9,9,9	0
55	MG	BA	3128	1/1	0.21	5.24	9,9,9,9	0
55	MG	AA	1660	1/1	0.21	5.21	40,40,40,40	0
55	MG	DA	3034	1/1	0.24	5.11	56,56,56,56	0
55	MG	BA	3182	1/1	0.19	5.09	22,22,22,22	0
55	MG	CA	1647	1/1	0.20	4.91	24,24,24,24	0
55	MG	DA	3013	1/1	0.37	4.91	45,45,45,45	0
55	MG	CA	1653	1/1	0.29	4.87	47,47,47,47	0
55	MG	BA	3030	1/1	0.28	4.69	10,10,10,10	0
55	MG	DA	3160	1/1	0.34	4.62	35,35,35,35	0
55	MG	DA	3005	1/1	0.22	4.60	66,66,66,66	0
55	MG	DA	3149	1/1	0.28	4.56	36,36,36,36	0
55	MG	AA	1668	1/1	0.20	4.50	18,18,18,18	0
55	MG	BA	3154	1/1	0.21	4.43	29,29,29,29	0
55	MG	BA	3144	1/1	0.22	4.43	25,25,25,25	0
55	MG	DA	3139	1/1	0.34	4.36	31,31,31,31	0
55	MG	DA	3094	1/1	0.27	4.31	59,59,59,59	0
55	MG	BA	3156	1/1	0.23	4.28	12,12,12,12	0
55	MG	AA	1619	1/1	0.27	4.19	43,43,43,43	0
55	MG	DA	3059	1/1	0.32	4.19	53,53,53,53	0
55	MG	BA	3130	1/1	0.23	4.15	4,4,4,4	0
55	MG	BA	3133	1/1	0.43	3.94	40,40,40,40	0
55	MG	DA	3056	1/1	0.27	3.94	51,51,51,51	0
55	MG	DA	3151	1/1	0.40	3.84	45,45,45,45	0
55	MG	CA	1641	1/1	0.87	3.83	46,46,46,46	0
55	MG	AA	1651	1/1	0.23	3.77	32,32,32,32	0
55	MG	DA	3029	1/1	0.30	3.60	41,41,41,41	0
55	MG	DA	3031	1/1	0.30	3.60	50,50,50,50	0
55	MG	CA	1615	1/1	0.21	3.55	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
55	MG	BA	3161	1/1	0.22	3.53	24,24,24,24	0
55	MG	BA	3166	1/1	0.19	3.46	25,25,25,25	0
55	MG	DA	3070	1/1	0.33	3.39	58,58,58,58	0
55	MG	BA	3188	1/1	0.18	3.36	27,27,27,27	0
55	MG	BA	3153	1/1	0.31	3.18	2,2,2,2	0
55	MG	AM	201	1/1	0.34	3.12	29,29,29,29	0
55	MG	BA	3180	1/1	0.24	3.10	25,25,25,25	0
55	MG	AA	1652	1/1	0.20	3.10	43,43,43,43	0
55	MG	BA	3057	1/1	0.22	3.04	20,20,20,20	0
55	MG	DA	3004	1/1	0.29	2.97	64,64,64,64	0
55	MG	BA	3046	1/1	0.22	2.89	8,8,8,8	0
55	MG	CA	1609	1/1	0.21	2.87	58,58,58,58	0
55	MG	AA	1626	1/1	0.20	2.86	26,26,26,26	0
55	MG	CA	1638	1/1	0.18	2.85	55,55,55,55	0
55	MG	DA	3008	1/1	0.42	2.81	51,51,51,51	0
55	MG	BA	3037	1/1	0.22	2.79	2,2,2,2	0
55	MG	BA	3191	1/1	0.20	2.64	35,35,35,35	0
55	MG	CA	1640	1/1	0.21	2.50	23,23,23,23	0
55	MG	CA	1648	1/1	0.22	2.43	42,42,42,42	0
55	MG	DA	3007	1/1	0.26	2.38	54,54,54,54	0
55	MG	BA	3151	1/1	0.20	2.36	31,31,31,31	0
55	MG	BA	3155	1/1	0.27	2.28	15,15,15,15	0
55	MG	BA	3072	1/1	0.19	2.26	4,4,4,4	0
55	MG	BA	3114	1/1	0.19	2.26	19,19,19,19	0
55	MG	DA	3148	1/1	0.25	2.21	45,45,45,45	0
55	MG	DA	3071	1/1	0.25	2.14	59,59,59,59	0
55	MG	CA	1643	1/1	0.27	2.14	44,44,44,44	0
55	MG	DA	3124	1/1	0.29	2.12	59,59,59,59	0
55	MG	BA	3152	1/1	0.21	2.12	11,11,11,11	0
55	MG	BA	3067	1/1	0.20	2.11	5,5,5,5	0
55	MG	AA	1662	1/1	0.24	2.10	41,41,41,41	0
55	MG	AA	1637	1/1	0.18	2.07	18,18,18,18	0
55	MG	DA	3150	1/1	0.21	2.06	42,42,42,42	0
55	MG	BA	3175	1/1	0.17	1.93	27,27,27,27	0
55	MG	AA	1608	1/1	0.21	1.90	24,24,24,24	0
55	MG	DA	3040	1/1	0.27	1.90	57,57,57,57	0
55	MG	DA	3006	1/1	0.39	1.84	64,64,64,64	0
55	MG	DA	3090	1/1	0.20	1.83	58,58,58,58	0
55	MG	BA	3125	1/1	0.20	1.81	8,8,8,8	0
55	MG	BA	3109	1/1	0.21	1.75	9,9,9,9	0
55	MG	AA	1610	1/1	0.17	1.66	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3043	1/1	0.22	1.63	54,54,54,54	0
55	MG	BA	3159	1/1	0.18	1.60	19,19,19,19	0
55	MG	CM	201	1/1	0.35	1.55	46,46,46,46	0
55	MG	DA	3116	1/1	0.18	1.52	51,51,51,51	0
55	MG	DA	3083	1/1	0.27	1.49	61,61,61,61	0
55	MG	BA	3122	1/1	0.22	1.41	2,2,2,2	0
55	MG	CA	1620	1/1	0.12	1.40	46,46,46,46	0
55	MG	BA	3115	1/1	0.21	1.39	35,35,35,35	0
55	MG	DA	3112	1/1	0.25	1.37	52,52,52,52	0
55	MG	BA	3107	1/1	0.19	1.36	6,6,6,6	0
55	MG	DA	3047	1/1	0.27	1.19	66,66,66,66	0
55	MG	DA	3033	1/1	0.22	1.14	45,45,45,45	0
55	MG	BA	3194	1/1	0.16	1.06	28,28,28,28	0
55	MG	BA	3124	1/1	0.21	1.03	21,21,21,21	0
55	MG	BA	3163	1/1	0.19	0.99	27,27,27,27	0
55	MG	BA	3045	1/1	0.19	0.99	13,13,13,13	0
55	MG	AA	1647	1/1	0.18	0.94	39,39,39,39	0
55	MG	BA	3086	1/1	0.21	0.90	9,9,9,9	0
55	MG	DA	3141	1/1	0.21	0.90	28,28,28,28	0
55	MG	CA	1606	1/1	0.28	0.86	52,52,52,52	0
55	MG	BA	3012	1/1	0.22	0.82	4,4,4,4	0
55	MG	BA	3053	1/1	0.18	0.77	4,4,4,4	0
55	MG	DA	3089	1/1	0.23	0.77	58,58,58,58	0
55	MG	AA	1630	1/1	0.19	0.71	49,49,49,49	0
55	MG	DA	3063	1/1	0.19	0.67	41,41,41,41	0
55	MG	DA	3046	1/1	0.23	0.61	53,53,53,53	0
55	MG	AA	1643	1/1	0.13	0.56	19,19,19,19	0
55	MG	AA	1663	1/1	0.16	0.55	35,35,35,35	0
55	MG	DA	3045	1/1	0.20	0.54	53,53,53,53	0
55	MG	DA	3099	1/1	0.24	0.53	53,53,53,53	0
55	MG	BA	3062	1/1	0.20	0.52	3,3,3,3	0
55	MG	BA	3042	1/1	0.17	0.49	6,6,6,6	0
55	MG	CA	1603	1/1	0.16	0.49	44,44,44,44	0
55	MG	BA	3063	1/1	0.19	0.45	0,0,0,0	0
55	MG	AA	1623	1/1	0.14	0.44	42,42,42,42	0
55	MG	AA	1624	1/1	0.17	0.44	39,39,39,39	0
55	MG	DA	3135	1/1	0.26	0.41	47,47,47,47	0
55	MG	AA	1664	1/1	0.17	0.37	36,36,36,36	0
55	MG	DA	3102	1/1	0.20	0.29	45,45,45,45	0
55	MG	BA	3093	1/1	0.15	0.24	16,16,16,16	0
55	MG	BA	3104	1/1	0.19	0.24	1,1,1,1	0
55	MG	DA	3114	1/1	0.30	0.16	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	3076	1/1	0.19	0.14	17,17,17,17	0
55	MG	DA	3108	1/1	0.18	0.12	35,35,35,35	0
55	MG	BA	3032	1/1	0.18	0.11	8,8,8,8	0
55	MG	BA	3105	1/1	0.19	0.10	4,4,4,4	0
55	MG	AA	1632	1/1	0.14	0.10	40,40,40,40	0
55	MG	CA	1611	1/1	0.17	0.09	55,55,55,55	0
55	MG	DA	3146	1/1	0.18	0.07	35,35,35,35	0
55	MG	AA	1641	1/1	0.17	0.02	20,20,20,20	0
55	MG	BA	3169	1/1	0.11	0.00	24,24,24,24	0
55	MG	AA	1634	1/1	0.17	-0.01	36,36,36,36	0
55	MG	AA	1645	1/1	0.15	-0.03	39,39,39,39	0
55	MG	BA	3184	1/1	0.15	-0.04	23,23,23,23	0
55	MG	DA	3159	1/1	0.17	-0.06	39,39,39,39	0
55	MG	DA	3001	1/1	0.19	-0.10	43,43,43,43	0
55	MG	CA	1627	1/1	0.16	-0.12	59,59,59,59	0
55	MG	BA	3047	1/1	0.13	-0.15	34,34,34,34	0
55	MG	DA	3143	1/1	0.26	-0.15	46,46,46,46	0
55	MG	AA	1605	1/1	0.15	-0.16	32,32,32,32	0
55	MG	AA	1671	1/1	0.19	-0.17	35,35,35,35	0
55	MG	BA	3165	1/1	0.15	-0.19	2,2,2,2	0
55	MG	BA	3097	1/1	0.20	-0.19	6,6,6,6	0
55	MG	BA	3044	1/1	0.16	-0.21	20,20,20,20	0
56	ZN	B4	101	1/1	0.20	-0.25	131,131,131,131	0
55	MG	CA	1646	1/1	0.12	-0.28	40,40,40,40	0
55	MG	CA	1631	1/1	0.27	-0.28	62,62,62,62	0
55	MG	DA	3125	1/1	0.17	-0.30	51,51,51,51	0
55	MG	DA	3018	1/1	0.20	-0.31	57,57,57,57	0
55	MG	DA	3019	1/1	0.16	-0.33	47,47,47,47	0
55	MG	AA	1617	1/1	0.19	-0.35	44,44,44,44	0
55	MG	DA	3048	1/1	0.20	-0.35	51,51,51,51	0
55	MG	AA	1655	1/1	0.14	-0.35	34,34,34,34	0
55	MG	BA	3112	1/1	0.17	-0.37	11,11,11,11	0
55	MG	DA	3087	1/1	0.14	-0.37	51,51,51,51	0
55	MG	AA	1635	1/1	0.15	-0.38	37,37,37,37	0
55	MG	CA	1618	1/1	0.16	-0.39	28,28,28,28	0
55	MG	BA	3185	1/1	0.15	-0.40	11,11,11,11	0
55	MG	CA	1645	1/1	0.15	-0.43	41,41,41,41	0
55	MG	AA	1636	1/1	0.20	-0.44	26,26,26,26	0
55	MG	BA	3171	1/1	0.16	-0.47	29,29,29,29	0
55	MG	DA	3068	1/1	0.16	-0.51	52,52,52,52	0
55	MG	CA	1649	1/1	0.14	-0.52	35,35,35,35	0
55	MG	DA	3011	1/1	0.21	-0.55	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	3132	1/1	0.17	-0.55	27,27,27,27	0
55	MG	DA	3096	1/1	0.18	-0.56	52,52,52,52	0
55	MG	AA	1650	1/1	0.17	-0.60	35,35,35,35	0
55	MG	DA	3121	1/1	0.18	-0.62	41,41,41,41	0
55	MG	DA	3105	1/1	0.17	-0.64	37,37,37,37	0
55	MG	BA	3158	1/1	0.15	-0.65	20,20,20,20	0
55	MG	CA	1630	1/1	0.26	-0.65	66,66,66,66	0
55	MG	BA	3041	1/1	0.13	-0.66	11,11,11,11	0
55	MG	AA	1607	1/1	0.16	-0.68	33,33,33,33	0
55	MG	AA	1601	1/1	0.13	-0.72	49,49,49,49	0
55	MG	DA	3103	1/1	0.14	-0.72	48,48,48,48	0
55	MG	DA	3023	1/1	0.18	-0.76	35,35,35,35	0
55	MG	BA	3004	1/1	0.15	-0.78	33,33,33,33	0
55	MG	DA	3107	1/1	0.14	-0.79	49,49,49,49	0
55	MG	BA	3082	1/1	0.18	-0.79	15,15,15,15	0
55	MG	DA	3081	1/1	0.17	-0.80	43,43,43,43	0
55	MG	AA	1665	1/1	0.18	-0.81	34,34,34,34	0
55	MG	DA	3024	1/1	0.16	-0.81	45,45,45,45	0
55	MG	BA	3195	1/1	0.12	-0.82	20,20,20,20	0
55	MG	CA	1604	1/1	0.16	-0.83	70,70,70,70	0
55	MG	BA	3187	1/1	0.16	-0.84	28,28,28,28	0
55	MG	DA	3036	1/1	0.14	-0.89	61,61,61,61	0
55	MG	DA	3122	1/1	0.17	-0.93	42,42,42,42	0
55	MG	CA	1636	1/1	0.23	-0.94	79,79,79,79	0
55	MG	BA	3049	1/1	0.15	-0.95	9,9,9,9	0
55	MG	DA	3123	1/1	0.18	-0.96	47,47,47,47	0
55	MG	BA	3013	1/1	0.17	-0.99	0,0,0,0	0
55	MG	BA	3134	1/1	0.17	-1.00	8,8,8,8	0
55	MG	DA	3158	1/1	0.14	-1.00	55,55,55,55	0
55	MG	BA	3088	1/1	0.15	-1.12	32,32,32,32	0
55	MG	DA	3022	1/1	0.13	-1.14	54,54,54,54	0
55	MG	DA	3030	1/1	0.15	-1.16	44,44,44,44	0
55	MG	CA	1639	1/1	0.13	-1.17	34,34,34,34	0
55	MG	DA	3167	1/1	0.12	-1.18	59,59,59,59	0
55	MG	DA	3053	1/1	0.16	-1.19	43,43,43,43	0
55	MG	DA	3115	1/1	0.17	-1.20	58,58,58,58	0
55	MG	CA	1651	1/1	0.13	-1.20	48,48,48,48	0
55	MG	DA	3132	1/1	0.11	-1.21	45,45,45,45	0
55	MG	CA	1614	1/1	0.08	-1.22	44,44,44,44	0
55	MG	DA	3012	1/1	0.15	-1.24	40,40,40,40	0
55	MG	BA	3039	1/1	0.18	-1.25	1,1,1,1	0
55	MG	BB	201	1/1	0.11	-1.32	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3072	1/1	0.15	-1.32	42,42,42,42	0
55	MG	AA	1604	1/1	0.10	-1.34	45,45,45,45	0
55	MG	DA	3147	1/1	0.13	-1.35	49,49,49,49	0
55	MG	DA	3035	1/1	0.15	-1.35	38,38,38,38	0
55	MG	AA	1620	1/1	0.11	-1.36	44,44,44,44	0
55	MG	DA	3039	1/1	0.14	-1.38	53,53,53,53	0
55	MG	AA	1656	1/1	0.12	-1.38	37,37,37,37	0
55	MG	BA	3100	1/1	0.14	-1.40	6,6,6,6	0
55	MG	BA	3120	1/1	0.15	-1.42	7,7,7,7	0
55	MG	DA	3136	1/1	0.13	-1.43	57,57,57,57	0
55	MG	BA	3059	1/1	0.17	-1.46	16,16,16,16	0
55	MG	AA	1658	1/1	0.10	-1.46	33,33,33,33	0
55	MG	DA	3079	1/1	0.12	-1.47	62,62,62,62	0
55	MG	DA	3062	1/1	0.13	-1.47	44,44,44,44	0
55	MG	BA	3034	1/1	0.16	-1.48	18,18,18,18	0
55	MG	DA	3086	1/1	0.14	-1.50	53,53,53,53	0
55	MG	DA	3113	1/1	0.16	-1.51	42,42,42,42	0
55	MG	BA	3071	1/1	0.15	-1.51	11,11,11,11	0
55	MG	CA	1613	1/1	0.14	-1.53	19,19,19,19	0
55	MG	AA	1638	1/1	0.13	-1.54	51,51,51,51	0
55	MG	DA	3074	1/1	0.11	-1.55	41,41,41,41	0
55	MG	BA	3064	1/1	0.17	-1.57	2,2,2,2	0
55	MG	DA	3154	1/1	0.11	-1.58	45,45,45,45	0
55	MG	BA	3036	1/1	0.16	-1.59	19,19,19,19	0
55	MG	BA	3189	1/1	0.16	-1.60	3,3,3,3	0
56	ZN	D4	101	1/1	0.04	-1.62	79,79,79,79	0
55	MG	DA	3126	1/1	0.15	-1.65	57,57,57,57	0
55	MG	BA	3192	1/1	0.17	-1.67	15,15,15,15	0
55	MG	DA	3152	1/1	0.12	-1.70	41,41,41,41	0
55	MG	BA	3121	1/1	0.07	-1.71	22,22,22,22	0
55	MG	DA	3077	1/1	0.08	-1.74	59,59,59,59	0
55	MG	BA	3193	1/1	0.13	-1.77	12,12,12,12	0
55	MG	CA	1624	1/1	0.13	-1.79	33,33,33,33	0
55	MG	BA	3074	1/1	0.08	-1.81	20,20,20,20	0
55	MG	CA	1632	1/1	0.14	-1.84	54,54,54,54	0
55	MG	DA	3118	1/1	0.16	-1.84	45,45,45,45	0
55	MG	DB	202	1/1	0.05	-1.85	42,42,42,42	0
55	MG	AA	1642	1/1	0.12	-1.85	24,24,24,24	0
55	MG	DA	3104	1/1	0.13	-1.95	54,54,54,54	0
55	MG	BA	3022	1/1	0.15	-1.97	3,3,3,3	0
55	MG	DA	3130	1/1	0.12	-1.99	51,51,51,51	0
55	MG	DA	3166	1/1	0.17	-2.00	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	3167	1/1	0.13	-2.03	28,28,28,28	0
55	MG	CA	1617	1/1	0.15	-2.07	35,35,35,35	0
55	MG	BA	3021	1/1	0.16	-2.08	1,1,1,1	0
55	MG	DQ	201	1/1	0.21	-2.08	32,32,32,32	0
55	MG	DA	3042	1/1	0.12	-2.08	49,49,49,49	0
55	MG	AA	1618	1/1	0.11	-2.24	35,35,35,35	0
55	MG	DA	3156	1/1	0.13	-2.25	30,30,30,30	0
55	MG	BA	3023	1/1	0.14	-2.29	15,15,15,15	0
55	MG	BA	3077	1/1	0.08	-2.30	26,26,26,26	0
55	MG	DA	3049	1/1	0.09	-2.30	49,49,49,49	0
55	MG	BA	3103	1/1	0.11	-2.38	9,9,9,9	0
55	MG	DA	3161	1/1	0.11	-2.45	42,42,42,42	0
55	MG	AA	1629	1/1	0.11	-2.47	43,43,43,43	0
55	MG	DA	3085	1/1	0.10	-2.48	42,42,42,42	0
55	MG	DA	3026	1/1	0.12	-2.52	53,53,53,53	0
55	MG	DA	3128	1/1	0.09	-2.55	57,57,57,57	0
55	MG	DB	203	1/1	0.06	-2.55	56,56,56,56	0
55	MG	DA	3037	1/1	0.10	-2.58	45,45,45,45	0
55	MG	BA	3024	1/1	0.13	-2.61	7,7,7,7	0
55	MG	AA	1615	1/1	0.12	-2.62	46,46,46,46	0
55	MG	AA	1631	1/1	0.13	-2.64	42,42,42,42	0
55	MG	BA	3099	1/1	0.12	-2.64	3,3,3,3	0
55	MG	BA	3149	1/1	0.12	-2.66	1,1,1,1	0
55	MG	BA	3069	1/1	0.05	-2.66	39,39,39,39	0
55	MG	BA	3123	1/1	0.14	-2.68	18,18,18,18	0
55	MG	BA	3031	1/1	0.14	-2.69	8,8,8,8	0
55	MG	BA	3006	1/1	0.11	-2.69	20,20,20,20	0
55	MG	DA	3021	1/1	0.11	-2.72	38,38,38,38	0
55	MG	DA	3078	1/1	0.10	-2.75	64,64,64,64	0
55	MG	DA	3095	1/1	0.10	-2.75	49,49,49,49	0
55	MG	DA	3100	1/1	0.08	-2.79	43,43,43,43	0
55	MG	BA	3075	1/1	0.14	-2.80	15,15,15,15	0
55	MG	CA	1635	1/1	0.14	-2.81	76,76,76,76	0
55	MG	DA	3134	1/1	0.10	-2.88	34,34,34,34	0
55	MG	BA	3176	1/1	0.12	-2.90	24,24,24,24	0
55	MG	BA	3085	1/1	0.15	-2.90	7,7,7,7	0
55	MG	AA	1639	1/1	0.06	-2.93	51,51,51,51	0
55	MG	BA	3052	1/1	0.14	-2.94	8,8,8,8	0
55	MG	DA	3069	1/1	0.08	-2.94	63,63,63,63	0
55	MG	DA	3014	1/1	0.09	-2.97	43,43,43,43	0
55	MG	DA	3101	1/1	0.11	-2.97	40,40,40,40	0
55	MG	DA	3145	1/1	0.09	-2.99	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3097	1/1	0.08	-3.02	44,44,44,44	0
55	MG	DA	3106	1/1	0.15	-3.04	56,56,56,56	0
55	MG	CA	1612	1/1	0.05	-3.04	30,30,30,30	0
55	MG	AA	1616	1/1	0.07	-3.05	42,42,42,42	0
55	MG	BA	3177	1/1	0.09	-3.08	24,24,24,24	0
55	MG	DA	3066	1/1	0.10	-3.11	39,39,39,39	0
55	MG	BA	3129	1/1	0.15	-3.20	5,5,5,5	0
55	MG	DA	3075	1/1	0.10	-3.21	48,48,48,48	0
55	MG	DA	3067	1/1	0.09	-3.28	49,49,49,49	0
55	MG	BA	3017	1/1	0.13	-3.28	6,6,6,6	0
55	MG	DA	3064	1/1	0.08	-3.29	38,38,38,38	0
55	MG	BA	3079	1/1	0.11	-3.31	28,28,28,28	0
55	MG	BA	3066	1/1	0.13	-3.32	6,6,6,6	0
55	MG	CA	1621	1/1	0.10	-3.33	53,53,53,53	0
55	MG	DA	3010	1/1	0.10	-3.36	48,48,48,48	0
55	MG	DA	3164	1/1	0.14	-3.40	47,47,47,47	0
55	MG	DA	3127	1/1	0.12	-3.40	47,47,47,47	0
55	MG	CA	1629	1/1	0.09	-3.43	63,63,63,63	0
55	MG	BA	3136	1/1	0.12	-3.43	24,24,24,24	0
55	MG	CA	1616	1/1	0.11	-3.44	29,29,29,29	0
55	MG	BA	3081	1/1	0.15	-3.53	1,1,1,1	0
55	MG	DA	3009	1/1	0.10	-3.64	57,57,57,57	0
55	MG	BA	3078	1/1	0.07	-3.66	33,33,33,33	0
55	MG	BA	3092	1/1	0.08	-3.68	20,20,20,20	0
55	MG	BA	3018	1/1	0.10	-3.70	27,27,27,27	0
55	MG	DB	201	1/1	0.06	-3.77	69,69,69,69	0
55	MG	CA	1610	1/1	0.09	-3.77	47,47,47,47	0
55	MG	DA	3028	1/1	0.09	-3.78	50,50,50,50	0
55	MG	BA	3056	1/1	0.12	-3.78	10,10,10,10	0
55	MG	BA	3008	1/1	0.11	-3.86	9,9,9,9	0
55	MG	CA	1601	1/1	0.10	-3.90	33,33,33,33	0
55	MG	CA	1602	1/1	0.10	-3.90	61,61,61,61	0
55	MG	BA	3068	1/1	0.16	-3.90	6,6,6,6	0
55	MG	BA	3183	1/1	0.12	-3.91	24,24,24,24	0
55	MG	BA	3050	1/1	0.10	-4.07	11,11,11,11	0
55	MG	BA	3003	1/1	0.11	-4.07	20,20,20,20	0
55	MG	AA	1612	1/1	0.13	-4.10	24,24,24,24	0
55	MG	DA	3117	1/1	0.06	-4.20	49,49,49,49	0
55	MG	BA	3001	1/1	0.08	-4.23	10,10,10,10	0
55	MG	DA	3120	1/1	0.08	-4.24	49,49,49,49	0
55	MG	DA	3038	1/1	0.09	-4.31	42,42,42,42	0
55	MG	AA	1633	1/1	0.09	-4.36	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	1640	1/1	0.05	-4.40	39,39,39,39	0
55	MG	BB	203	1/1	0.08	-4.48	10,10,10,10	0
55	MG	DA	3111	1/1	0.13	-4.54	42,42,42,42	0
55	MG	BA	3016	1/1	0.09	-4.72	17,17,17,17	0
55	MG	BA	3065	1/1	0.10	-4.76	7,7,7,7	0
55	MG	AA	1613	1/1	0.10	-4.82	20,20,20,20	0
55	MG	DA	3044	1/1	0.07	-4.82	61,61,61,61	0
55	MG	BA	3010	1/1	0.15	-4.84	3,3,3,3	0
55	MG	BA	3117	1/1	0.13	-4.84	4,4,4,4	0
55	MG	BA	3110	1/1	0.08	-4.86	23,23,23,23	0
55	MG	BA	3027	1/1	0.09	-4.88	22,22,22,22	0
55	MG	BA	3091	1/1	0.07	-4.88	28,28,28,28	0
55	MG	DA	3052	1/1	0.08	-4.90	35,35,35,35	0
55	MG	DA	3050	1/1	0.07	-4.91	29,29,29,29	0
55	MG	CA	1619	1/1	0.09	-5.01	26,26,26,26	0
55	MG	CA	1626	1/1	0.08	-5.04	42,42,42,42	0
55	MG	BA	3111	1/1	0.12	-5.19	23,23,23,23	0
55	MG	DA	3093	1/1	0.15	-5.32	65,65,65,65	0
55	MG	BA	3073	1/1	0.13	-5.35	13,13,13,13	0
55	MG	DA	3080	1/1	0.11	-5.37	39,39,39,39	0
55	MG	CA	1622	1/1	0.07	-5.38	40,40,40,40	0
55	MG	BA	3080	1/1	0.10	-5.42	18,18,18,18	0
55	MG	DA	3082	1/1	0.05	-5.43	50,50,50,50	0
55	MG	BA	3058	1/1	0.07	-5.46	13,13,13,13	0
55	MG	BA	3009	1/1	0.12	-5.72	6,6,6,6	0
55	MG	BA	3101	1/1	0.13	-5.87	2,2,2,2	0
55	MG	AA	1628	1/1	0.05	-5.89	37,37,37,37	0
55	MG	BA	3048	1/1	0.08	-5.96	16,16,16,16	0
55	MG	BA	3118	1/1	0.06	-5.97	11,11,11,11	0
55	MG	DA	3073	1/1	0.09	-5.97	37,37,37,37	0
55	MG	BA	3014	1/1	0.10	-5.98	6,6,6,6	0
55	MG	BA	3054	1/1	0.11	-5.98	5,5,5,5	0
55	MG	DA	3129	1/1	0.11	-5.99	38,38,38,38	0
55	MG	BA	3172	1/1	0.11	-6.00	23,23,23,23	0
55	MG	DA	3017	1/1	0.11	-6.09	40,40,40,40	0
55	MG	BA	3096	1/1	0.11	-6.11	5,5,5,5	0
55	MG	BA	3090	1/1	0.09	-6.20	17,17,17,17	0
55	MG	AA	1606	1/1	0.07	-6.26	31,31,31,31	0
55	MG	DA	3051	1/1	0.06	-6.31	35,35,35,35	0
55	MG	DA	3058	1/1	0.05	-6.32	37,37,37,37	0
55	MG	AA	1609	1/1	0.08	-6.41	20,20,20,20	0
55	MG	BA	3131	1/1	0.13	-6.42	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
55	MG	BA	3007	1/1	0.07	-6.44	25,25,25,25	0
55	MG	BA	3174	1/1	0.11	-6.50	20,20,20,20	0
55	MG	AA	1621	1/1	0.06	-6.51	33,33,33,33	0
55	MG	BA	3051	1/1	0.11	-6.59	6,6,6,6	0
55	MG	AA	1625	1/1	0.07	-6.76	31,31,31,31	0
55	MG	BA	3035	1/1	0.15	-7.17	2,2,2,2	0
55	MG	CA	1634	1/1	0.08	-7.34	49,49,49,49	0
55	MG	DA	3003	1/1	0.09	-7.40	52,52,52,52	0
55	MG	BA	3011	1/1	0.08	-7.40	13,13,13,13	0
55	MG	BA	3020	1/1	0.11	-7.41	7,7,7,7	0
55	MG	BA	3038	1/1	0.14	-7.47	8,8,8,8	0
55	MG	CA	1607	1/1	0.10	-7.55	42,42,42,42	0
55	MG	BA	3002	1/1	0.08	-7.84	15,15,15,15	0
55	MG	AA	1603	1/1	0.13	-7.88	34,34,34,34	0
55	MG	DA	3032	1/1	0.06	-7.92	49,49,49,49	0
55	MG	BA	3089	1/1	0.10	-8.24	12,12,12,12	0
55	MG	BA	3127	1/1	0.09	-8.39	1,1,1,1	0
55	MG	DA	3065	1/1	0.06	-8.80	33,33,33,33	0
55	MG	BA	3095	1/1	0.07	-8.81	8,8,8,8	0
55	MG	BA	3084	1/1	0.10	-9.16	12,12,12,12	0
55	MG	BA	3087	1/1	0.10	-9.23	18,18,18,18	0
55	MG	BB	202	1/1	0.08	-9.46	11,11,11,11	0
55	MG	DA	3144	1/1	0.04	-9.50	52,52,52,52	0
55	MG	AA	1611	1/1	0.07	-9.75	18,18,18,18	0
55	MG	BA	3005	1/1	0.05	-10.36	31,31,31,31	0
55	MG	BA	3094	1/1	0.05	-10.85	17,17,17,17	0
55	MG	BA	3135	1/1	0.09	-11.89	17,17,17,17	0
55	MG	AA	1602	1/1	0.09	-12.15	33,33,33,33	0
55	MG	BA	3026	1/1	0.06	-15.14	7,7,7,7	0
55	MG	BA	3043	1/1	0.08	-15.18	15,15,15,15	0
55	MG	CA	1652	1/1	0.17	-19.00	39,39,39,39	0
55	MG	BA	3029	1/1	0.12	-20.15	15,15,15,15	0
55	MG	BA	3028	1/1	0.11	-29.98	4,4,4,4	0
55	MG	BA	3173	1/1	0.19	-	20,20,20,20	0

6.5 Other polymers ⓘ

There are no such residues in this entry.