



wwPDB X-ray Structure Validation Summary Report

Jul 24, 2014 – 04:13 PM EDT

PDB ID : 4U1V
Title : Crystal structure of the E. coli ribosome bound to linopristin.
Authors : Noeske, J.; Huang, J.; Olivier, N.B.; Giacobbe, R.A.; Zambrowski, M.; Cate, J.H.D.
Deposited on : 2014-06-06
Resolution : 3.00 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>

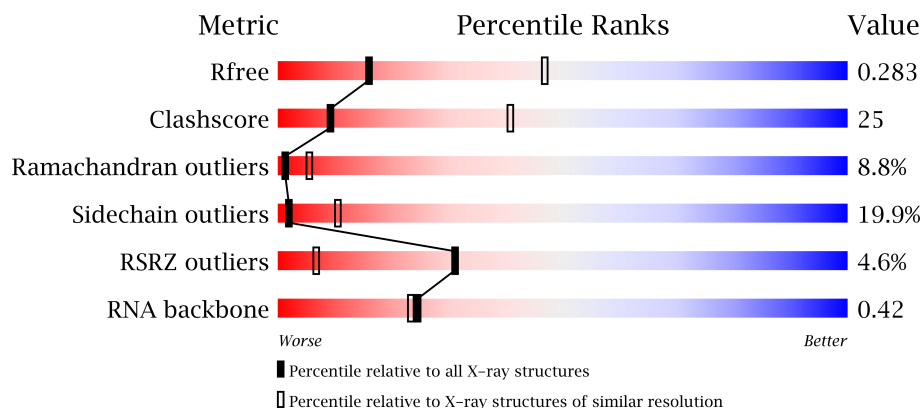
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)
RNA backbone	1838	1070 (3.50-2.50)

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	7	
54	D6	7	

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	1602	-	X
55	MG	AA	1603	-	X
55	MG	AA	1605	-	X
55	MG	AA	1610	-	X
55	MG	AA	1614	-	X
55	MG	AA	1622	-	X
55	MG	AA	1623	-	X
55	MG	AA	1626	-	X
55	MG	AA	1627	-	X
55	MG	AA	1635	-	X
55	MG	AA	1644	-	X
55	MG	AA	1646	-	X
55	MG	AA	1648	-	X
55	MG	AA	1650	-	X
55	MG	AA	1651	-	X
55	MG	AA	1653	-	X
55	MG	AA	1657	-	X
55	MG	AA	1658	-	X
55	MG	AA	1659	-	X
55	MG	AA	1661	-	X
55	MG	AA	1662	-	X
55	MG	AA	1665	-	X
55	MG	AA	1667	-	X
55	MG	AA	1668	-	X
55	MG	AA	1670	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
55	MG	AA	1671	-	X
55	MG	AM	201	-	X
55	MG	BA	3011	-	X
55	MG	BA	3014	-	X
55	MG	BA	3015	-	X
55	MG	BA	3016	-	X
55	MG	BA	3019	-	X
55	MG	BA	3025	-	X
55	MG	BA	3027	-	X
55	MG	BA	3033	-	X
55	MG	BA	3039	-	X
55	MG	BA	3040	-	X
55	MG	BA	3044	-	X
55	MG	BA	3053	-	X
55	MG	BA	3055	-	X
55	MG	BA	3056	-	X
55	MG	BA	3057	-	X
55	MG	BA	3061	-	X
55	MG	BA	3067	-	X
55	MG	BA	3072	-	X
55	MG	BA	3076	-	X
55	MG	BA	3083	-	X
55	MG	BA	3090	-	X
55	MG	BA	3092	-	X
55	MG	BA	3098	-	X
55	MG	BA	3104	-	X
55	MG	BA	3105	-	X
55	MG	BA	3106	-	X
55	MG	BA	3115	-	X
55	MG	BA	3119	-	X
55	MG	BA	3131	-	X
55	MG	BA	3133	-	X
55	MG	BA	3135	-	X
55	MG	BA	3136	-	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	3146	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
55	MG	BA	3150	-	X
55	MG	BA	3154	-	X
55	MG	BA	3157	-	X
55	MG	BA	3160	-	X
55	MG	BA	3164	-	X
55	MG	BA	3166	-	X
55	MG	BA	3168	-	X
55	MG	BA	3170	-	X
55	MG	BA	3171	-	X
55	MG	BA	3173	-	X
55	MG	BA	3176	-	X
55	MG	BA	3178	-	X
55	MG	BA	3179	-	X
55	MG	BA	3180	-	X
55	MG	BA	3183	-	X
55	MG	BA	3186	-	X
55	MG	BA	3190	-	X
55	MG	BA	3192	-	X
55	MG	BB	204	-	X
55	MG	CA	1605	-	X
55	MG	CA	1615	-	X
55	MG	CA	1618	-	X
55	MG	CA	1620	-	X
55	MG	CA	1625	-	X
55	MG	CA	1626	-	X
55	MG	CA	1627	-	X
55	MG	CA	1628	-	X
55	MG	CA	1630	-	X
55	MG	CA	1633	-	X
55	MG	CA	1637	-	X
55	MG	CA	1638	-	X
55	MG	CA	1642	-	X
55	MG	CA	1643	-	X
55	MG	CA	1644	-	X
55	MG	CA	1646	-	X
55	MG	CA	1647	-	X
55	MG	CA	1649	-	X
55	MG	CA	1650	-	X
55	MG	CA	1651	-	X
55	MG	CA	1653	-	X
55	MG	CA	1654	-	X
55	MG	CA	1655	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
55	MG	DA	3002	-	X
55	MG	DA	3004	-	X
55	MG	DA	3007	-	X
55	MG	DA	3014	-	X
55	MG	DA	3015	-	X
55	MG	DA	3016	-	X
55	MG	DA	3021	-	X
55	MG	DA	3026	-	X
55	MG	DA	3028	-	X
55	MG	DA	3029	-	X
55	MG	DA	3030	-	X
55	MG	DA	3032	-	X
55	MG	DA	3034	-	X
55	MG	DA	3041	-	X
55	MG	DA	3045	-	X
55	MG	DA	3056	-	X
55	MG	DA	3057	-	X
55	MG	DA	3061	-	X
55	MG	DA	3062	-	X
55	MG	DA	3064	-	X
55	MG	DA	3071	-	X
55	MG	DA	3072	-	X
55	MG	DA	3077	-	X
55	MG	DA	3089	-	X
55	MG	DA	3092	-	X
55	MG	DA	3093	-	X
55	MG	DA	3095	-	X
55	MG	DA	3099	-	X
55	MG	DA	3100	-	X
55	MG	DA	3102	-	X
55	MG	DA	3103	-	X
55	MG	DA	3104	-	X
55	MG	DA	3106	-	X
55	MG	DA	3110	-	X
55	MG	DA	3113	-	X
55	MG	DA	3116	-	X
55	MG	DA	3120	-	X
55	MG	DA	3132	-	X
55	MG	DA	3134	-	X
55	MG	DA	3136	-	X
55	MG	DA	3137	-	X
55	MG	DA	3138	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
55	MG	DA	3139	-	X
55	MG	DA	3141	-	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	3154	-	X
55	MG	DA	3155	-	X
55	MG	DA	3158	-	X
55	MG	DA	3159	-	X
55	MG	DA	3161	-	X
55	MG	DA	3164	-	X
55	MG	DA	3165	-	X
55	MG	DA	3166	-	X

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 288320 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			
			780	492	146	142	0	0	0

- 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		
			753	479	137	134	3	0	0
43	DV	94	Total	C	N	O	S		
			753	479	137	134	3	0	0

- 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		
			580	359	117	103	1	0	0
44	DW	75	Total	C	N	O	S		
			569	353	113	102	1	0	0

- 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		
			625	388	129	106	2	0	0
45	DX	77	Total	C	N	O	S		
			625	388	129	106	2	0	0

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
54	B6	7	Total	C	N	O	0	0	0
			69	50	9	10			
54	D6	7	Total	C	N	O	0	0	0
			69	50	9	10			

- 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	615	Total O 615 615	0	0
57	BB	14	Total O 14 14	0	0
57	BC	10	Total O 10 10	0	0
57	BD	4	Total O 4 4	0	0
57	BE	4	Total O 4 4	0	0
57	BF	1	Total O 1 1	0	0
57	BG	1	Total O 1 1	0	0
57	BJ	1	Total O 1 1	0	0
57	BL	6	Total O 6 6	0	0
57	BN	2	Total O 2 2	0	0
57	BS	1	Total O 1 1	0	0
57	BU	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

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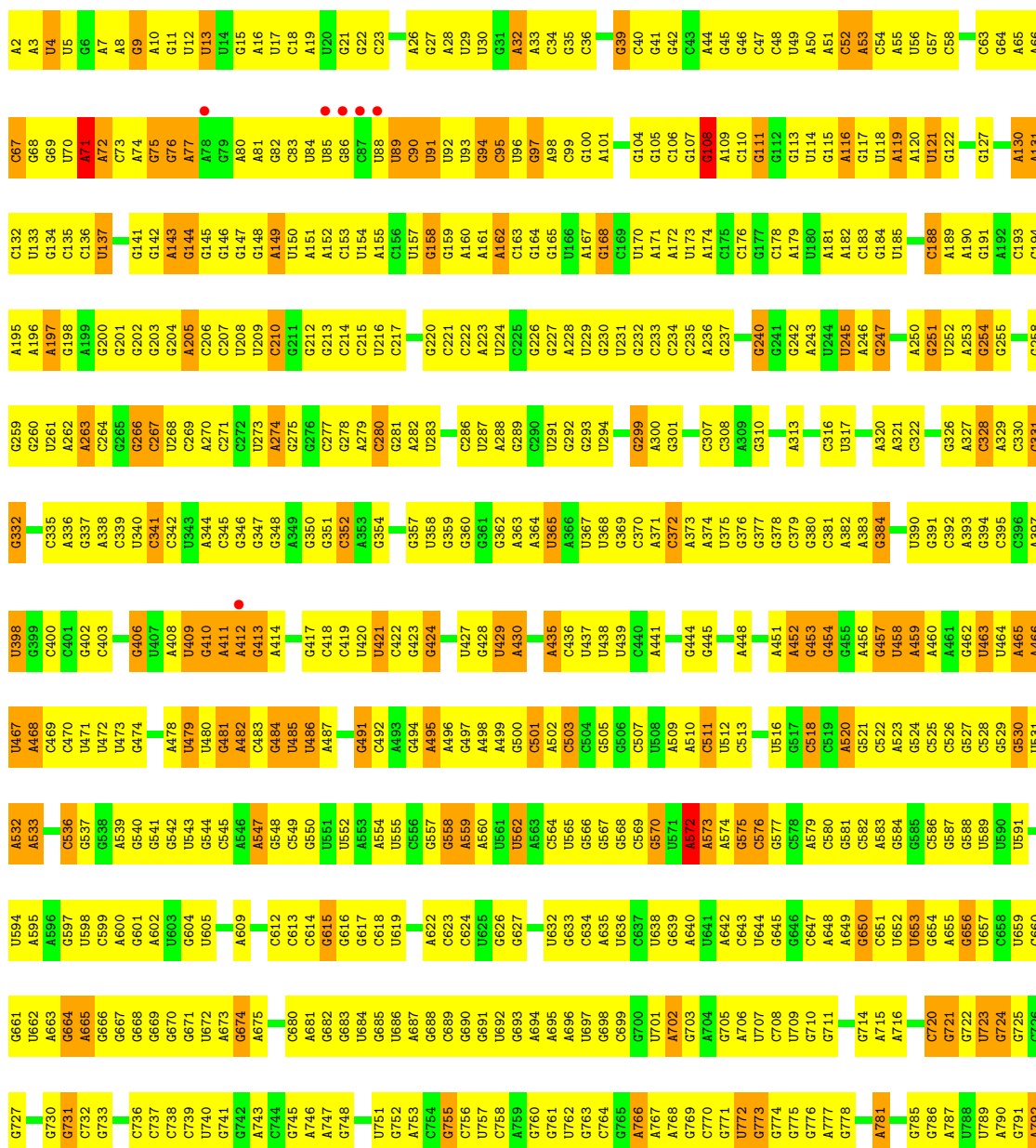
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57	CU	2	Total 2	O 2	0	0
57	DA	607	Total 607	O 607	0	0
57	DB	13	Total 13	O 13	0	0
57	DC	9	Total 9	O 9	0	0
57	DD	4	Total 4	O 4	0	0
57	DE	6	Total 6	O 6	0	0
57	DL	5	Total 5	O 5	0	0
57	DN	2	Total 2	O 2	0	0
57	DT	2	Total 2	O 2	0	0
57	DU	1	Total 1	O 1	0	0
57	DV	1	Total 1	O 1	0	0
57	D0	1	Total 1	O 1	0	0
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57	D3	2	Total 2	O 2	0	0
57	D4	1	Total 1	O 1	0	0

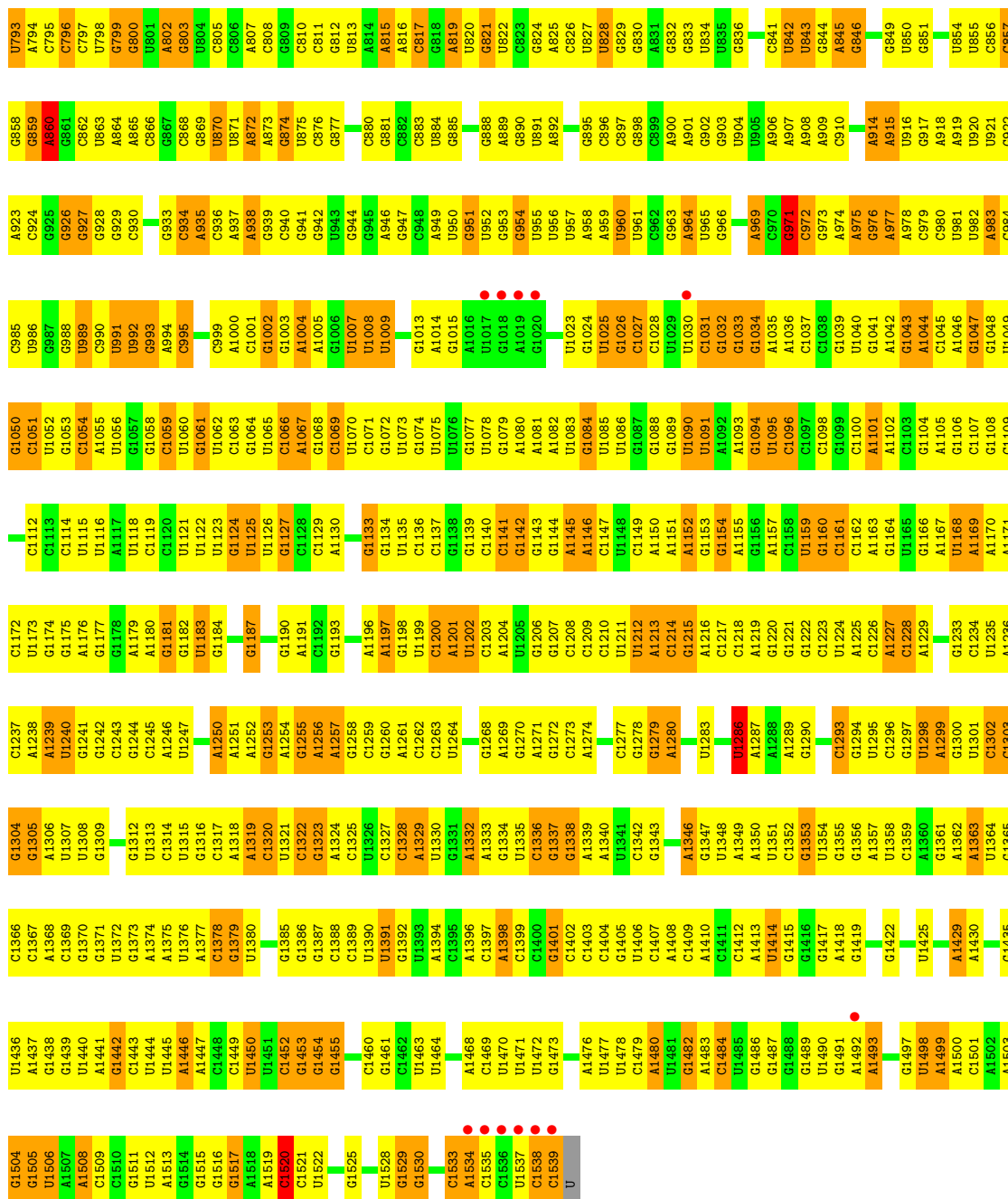
3 Residue-property plots

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

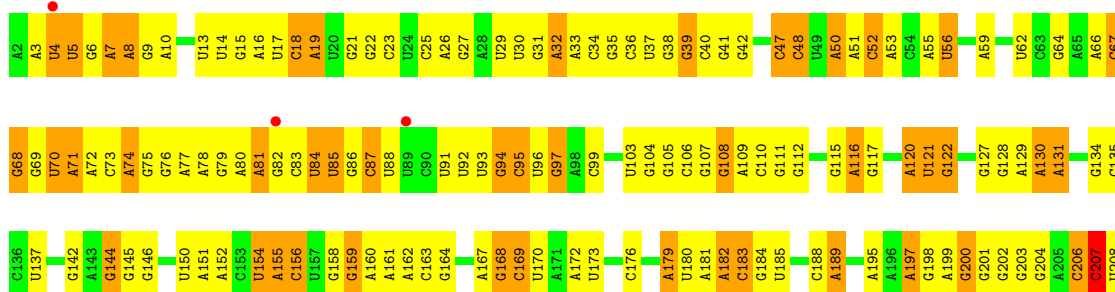
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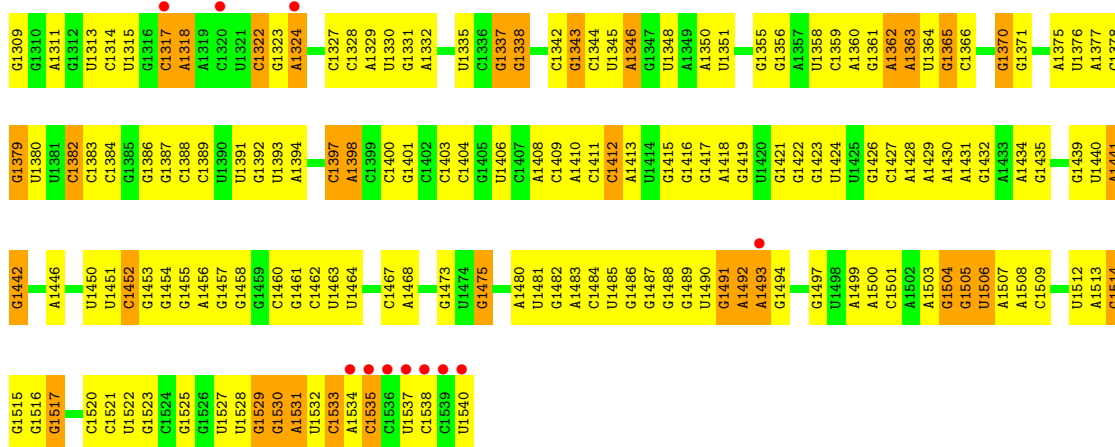


• Molecule 1: 16S rRNA

Chain CA:

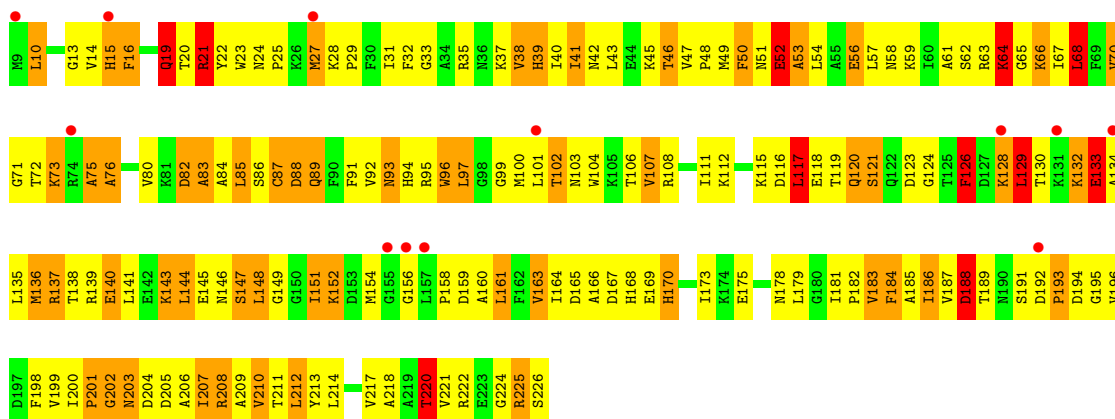


C1243	A1176	C1107	G976	C841	G773	U636	G558	U485	A415	C352	A279	U209
G1244	G1177	G1108	A977	U842	G774	C637	A559	U486	A418	A353	C280	C210
C1245	A1178	C1109	G978	U843	G775	G638	A560	U487	C418	A354	G281	G212
	G1179	G1110	A979	U844	G776	G639	A561	G494		C355	C285	C213
A1250	G1180	C1111	G980	A845	G777	G640	U562	A496	U421	A356	C286	C214
A1251	G1181	G1112	U981	G846	G778	U641	A563	A497	U422	G357	C289	C215
A1252	G1182	C1113	U982	G847	G779	A642	C564	G497	G423	U358	C290	C216
G1253	U1183	G1114	A983	C848	G780	C643	U565	A498	G424	G359	U217	U218
A1254	G1184	U1115	U984		A715	U644	G566	A499	G425	G360	C293	
G1255	G1185	U1116	U985	G851	A716	G645	A567	G500	U426	G361	U294	
A1256	G1186	U1117	G986	G852	G782	U646	U568	C501	U427	G362	C295	
A1257	G1187	U1118	U987	G853	A784	G649	C569	A502	G428	U365	C221	
G1258	U1188	G1119	G988	U854	G785	U650	G570	C503	U429	A366	C222	
	U1119	U1120	U989	U855	G786	C651	U571	C504	A430	U367	A223	
C1262	U1121	U1121	U990	G858	A787	U652	A572	G505	A431	U368	C224	
C1263	U1122	U1122	G991		A790	U653	A573	G506	A432	G369	G227	
U1264	G1123	G1123	G992	G859	G791	G724	A574			C370	A300	
C1265	U1124	U1124	U993	G860	G792		G575	A509	A435	C371	U304	
G1266	U1125	U1125	G994	G861	G793		G576	A510	A436	A371	C305	
	A1130	G1130	G995	G862	U794		G577	C511	U437	C372	C235	
A1196	G1131	G1131	A996	G863	G795		U578	C512	U438	A373	A236	
A1197	G1132	G1132	G997	G864	G796		G579	C513	U439	A374	G237	
G1198	U1133	U1133	C998	A865	C797		C580		U440	A375	C307	
G1199	C1134	C1134	C999	G866	U797		G581		A441	G376	C308	
U1200	U1135	U1135	A1000	C867	G798		C582		G442	G377	A309	
U1201	C1136	C1136	G1001	G868	G799		A583		C443	G378	G310	
U1202	U1137	U1137	G1002	G869	G800		G584		G444	C379	A313	
U1203	G1138	G1138	G1003	U870	G801		G585		G445	G380	C314	
A1204	U1139	U1139	U1004	U871	A802		C586		G446	A381	A315	
U1205	C1140	C1140	U1005	G872	G803					C382	U244	
U1206	U1141	U1141	G1006	G873	U804		A586		A451	A383	U245	
G1207	U1142	U1142	U1007	G874	C805		A587		A452	C384	A246	
U1208	G1143	G1143	U1008	G875	C806		A588		A453	G385	G247	
C1209	U1144	U1144	U1009	G876	G807		G589		A454	C386	C248	
A1280	A1145	A1145	G947	A878	G808		C590		A455	U387	U249	
C1281	C1146	C1146	C948		G809				A456	G388	A321	
C1282	U1147	U1147	A949	G881	C810		G604		A457	A389	G324	
U1283	C1148	C1148	U952	G882	G811		U605		U458	U390		
C1284	U1149	U1149	G953	G883	G812		G606		A459	G391	A327	
A1285	G1150	G1150	G954	G884	G813		A607		A460	C392	C328	
U1286	A1151	A1151	U955	G885	A814		A608		U463	A393	A329	
A1287	A1152	A1152	U956	G886	G815		A609		U464	C394	C330	
A1288	U1153	U1153	U957	G887	A816		G618		A465	A397	G331	
G1289	G1154	G1154	U958	G888	G817		U619		A466	U398	G332	
U1290	U1155	U1155	A958	G889	C817		C620		A467	G399	U333	
U1291	G1156	G1156	G959	G890			A621		A468	C395	A262	
G1292	U1157	U1157	U960	U891	G821		U625		C469	G402	C263	
C1293	C1158	C1158	U961	A892	U822		G626		G474	C403	G264	
G1294	U1159	U1159	C962	C893	G823		A627		C475	U405	G265	
C1295	G1160	G1160	G963	G894	G824		U628		U476	A398	G266	
C1296	C1161	C1161	A964	G895	G825		A629		U477	C399	C267	
G1297	U1162	U1162	U965	U896	U827		U630		G478	U406	U268	
U1298	C1163	C1163	G966	A900	G828		A631		C479	G407	C271	
A1299	U1164	U1164	C967	U901	G829		U632		C479	U408	A270	
G1300			A968	G902	G833		U633		G479	U409	G346	
U1301	C1165	C1165	G969	G903	U834		A695		G479	U410	G347	
C1302	G1166	G1166	C970	G904	U835		U692		G479	U411	C272	
G1303	U1167	U1167	G971	U906	G836		U693		G479	U412	U273	
A1288	A1170	A1170	G972	A907	U837		A694		G479	U413	A349	
A1239	A1171	A1171	C973	U908	G838		U695		G479	U414	A274	
U1240			G974	A909	U839		G696		G479	U415	G351	
G1304			A975	C910	G840		U697		G479	U416	G352	
G1305							U698		G479	U417	G353	
A1306							U699		G479	U418	G354	
U1307							U700		G479	U419	G355	
U1308							U701		G479	U420	G356	
							U702		G479	U421	G357	
							U703		G479	U422	G358	
							U704		G479	U423	G359	
							U705		G479	U424	G360	
							U706		G479	U425	G361	
							U707		G479	U426	G362	
							U708		G479	U427	G363	
							U709		G479	U428	G364	
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							U711		G479	U430	G366	
							U712		G479	U431	G367	
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							U720		G479	U439	G375	
							U721		G479	U440	G376	
							U722		G479	U441	G377	
							U723		G479	U442	G378	
							U724		G479	U443	G379	
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							U727		G479	U446	G382	
							U728		G479	U447	G383	
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							U730		G479	U449	G385	
							U731		G479	U450	G386	
							U732		G479	U451	G387	
							U733		G479	U452	G388	
							U734		G479	U453	G389	
							U735		G479	U454	G390	
							U736		G479	U455	G391	
							U737		G479	U456	G392	
							U738		G479	U457	G393	
							U739		G479	U458	G394	
							U740		G479	U459	G395	
							U741		G479	U460	G396	
							U742		G479	U461	G397	
							U743		G479	U462	G398	
							U744		G479	U463	G399	
							U745		G479	U464	G400	
							U746		G479	U465	G401	
							U747		G479	U466	G402	
							U748		G479	U467	G403	
							U749		G479	U468	G404	
							U750		G479	U469	G405	
							U751		G479	U470	G406	
							U752		G479	U471	G407	
							U753		G479	U472	G408	
							U754		G479	U473	G409	
							U755		G479	U474	G410	
							U756		G479	U475	G411	
							U757		G479	U476	G412	
							U758		G479	U477	G413	
							U759		G479	U478	G414	
							U760		G479	U479	G415	
							U761		G479	U480	G416	
							U762		G479	U481	G417	
							U763		G479	U482	G418	
							U764		G479	U483	G419	
							U765		G479	U484	G420	
							U766		G479	U485	G421	
							U767		G479	U486	G422	
							U768		G479	U487	G423	
							U769		G479	U488	G424	
							U770		G479	U489	G425	
							U771		G479	U490	G426	
							U772		G479	U491	G427	
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							U776					



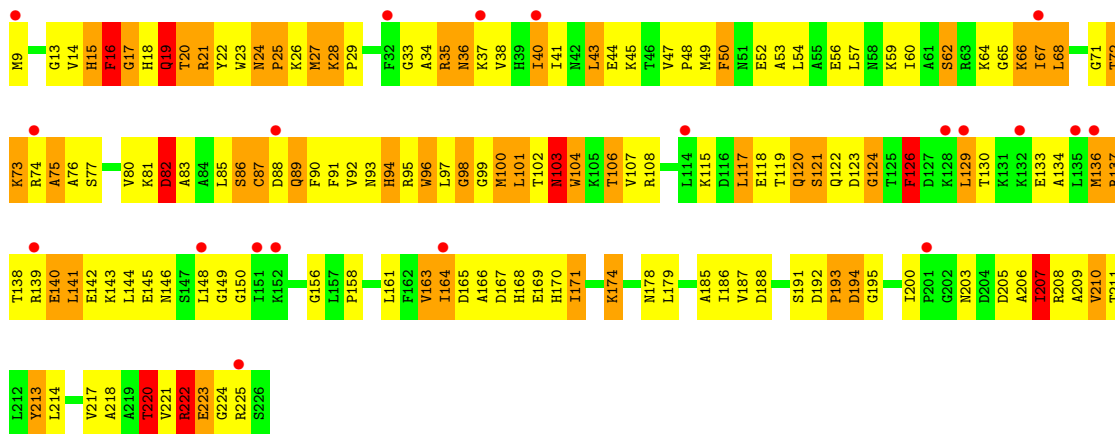
• Molecule 2: 30S ribosomal protein S2

Chain AB:



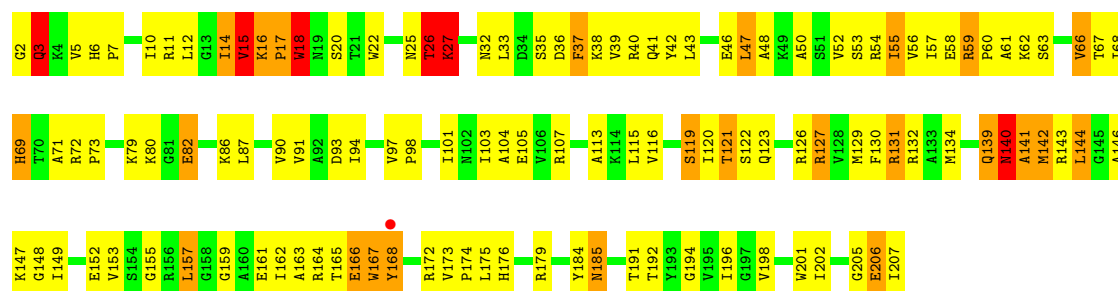
• Molecule 2: 30S ribosomal protein S2

Chain CB:



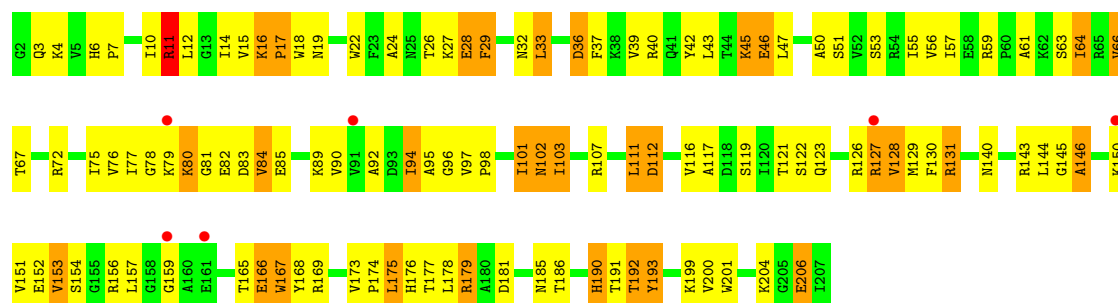
• Molecule 3: 30S ribosomal protein S3

Chain AC:



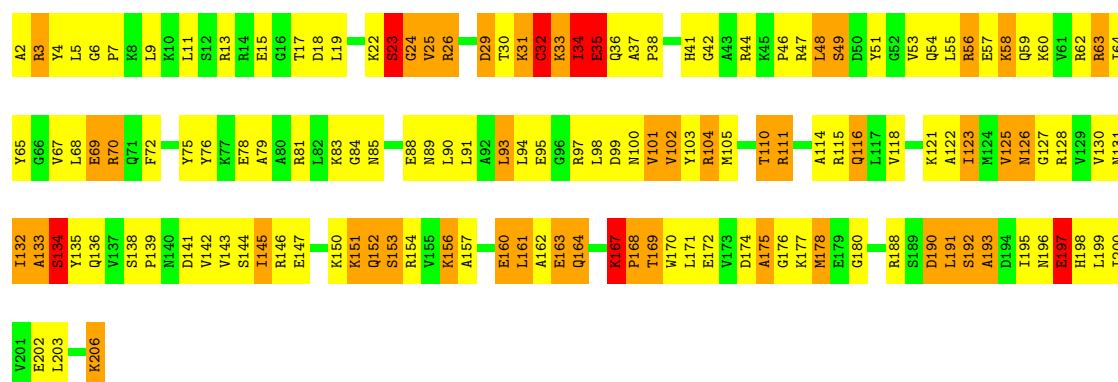
• Molecule 3: 30S ribosomal protein S3

Chain CC:



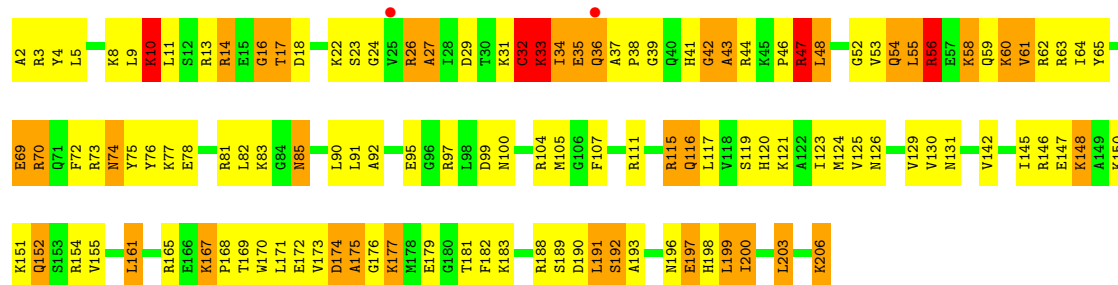
• Molecule 4: 30S ribosomal protein S4

Chain AD:

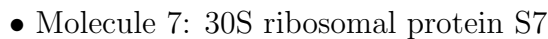
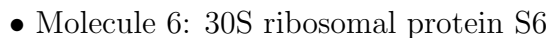
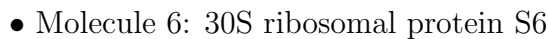
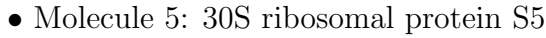


• Molecule 4: 30S ribosomal protein S4

Chain CD:



• Molecule 5: 30S ribosomal protein S5



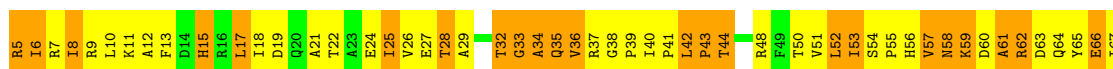
Response	Percentage
Yes	100%
No	0%





- Molecule 10: 30S ribosomal protein S10

Chain AJ:



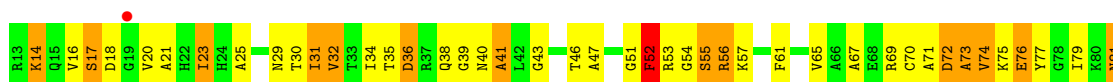
- Molecule 10: 30S ribosomal protein S10

Chain CJ:



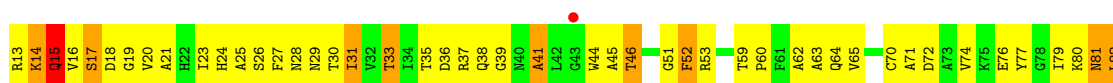
- Molecule 11: 30S ribosomal protein S11

Chain AK:



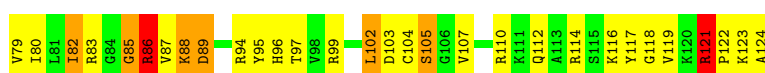
- Molecule 11: 30S ribosomal protein S11

Chain CK:



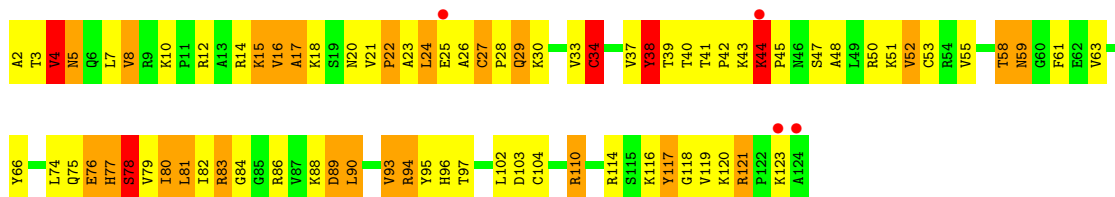
- Molecule 12: 30S ribosomal protein S12

Chain AL:



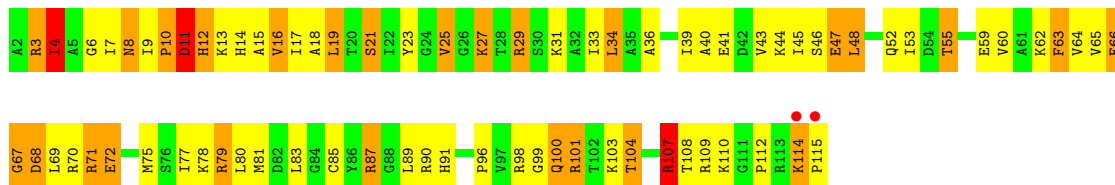
- Molecule 12: 30S ribosomal protein S12

Chain CL:



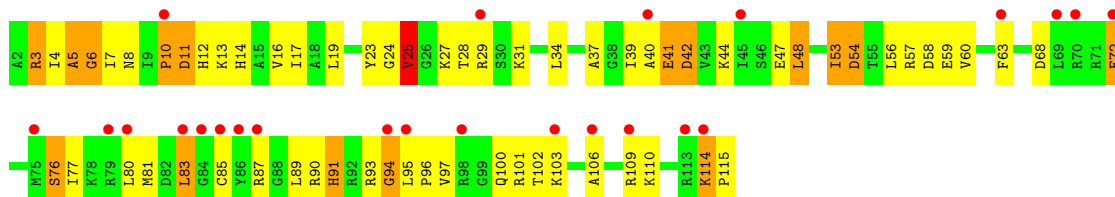
- Molecule 13: 30S ribosomal protein S13

Chain AM:



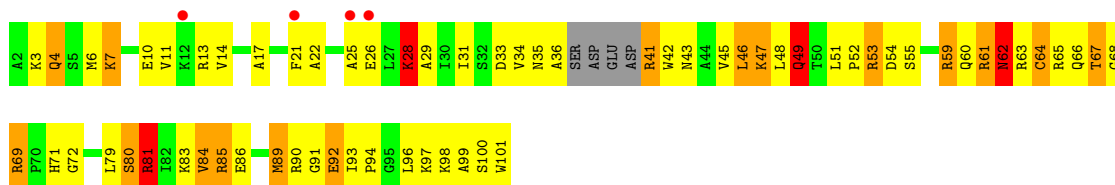
- Molecule 13: 30S ribosomal protein S13

Chain CM:



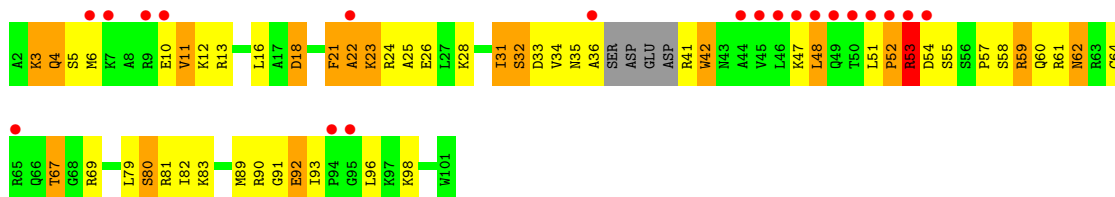
- Molecule 14: 30S ribosomal protein S14

Chain AN:



- Molecule 14: 30S ribosomal protein S14

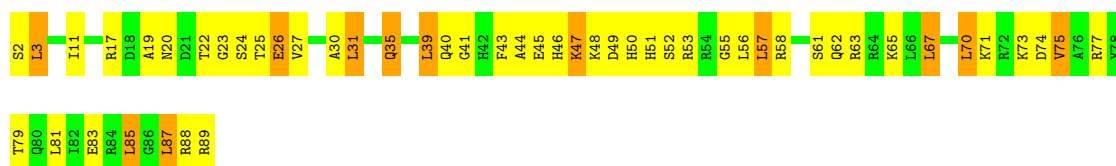
Chain CN:



- Molecule 15: 30S ribosomal protein S15

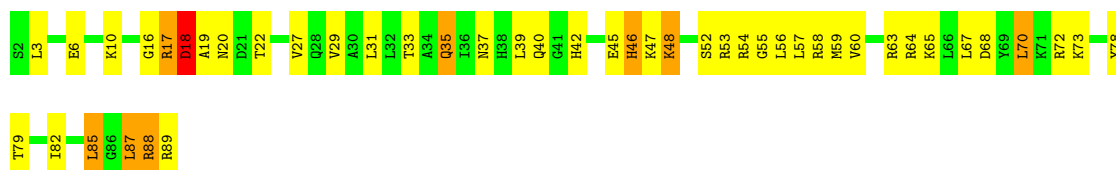
Chain AO:





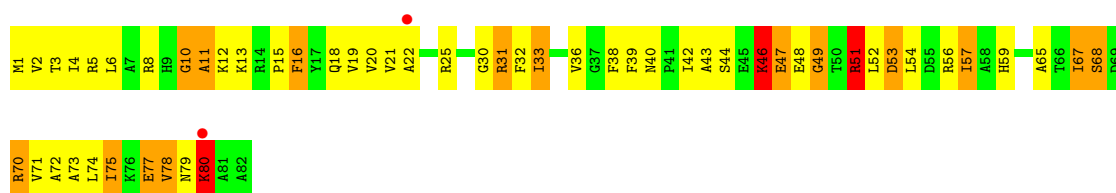
- Molecule 15: 30S ribosomal protein S15

Chain CO:



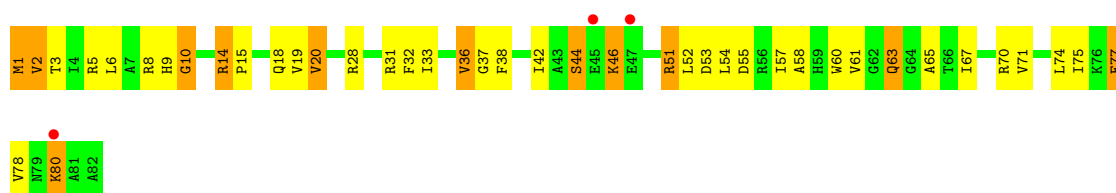
- Molecule 16: 30S ribosomal protein S16

Chain AP:



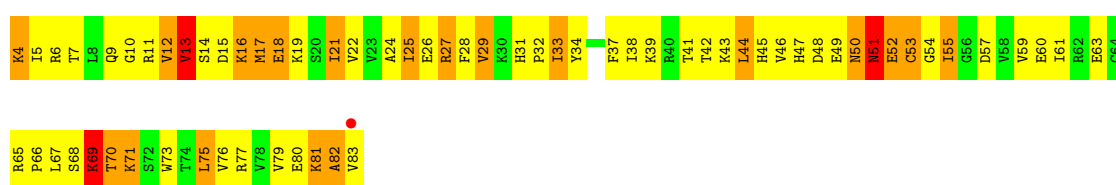
- Molecule 16: 30S ribosomal protein S16

Chain CP:



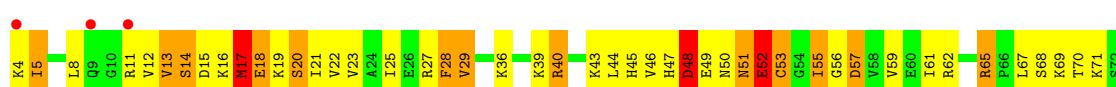
- Molecule 17: 30S ribosomal protein S17

Chain AQ:



- Molecule 17: 30S ribosomal protein S17

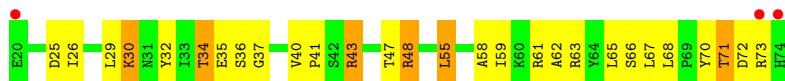
Chain CQ:





- Molecule 18: 30S ribosomal protein S18

Chain AR:



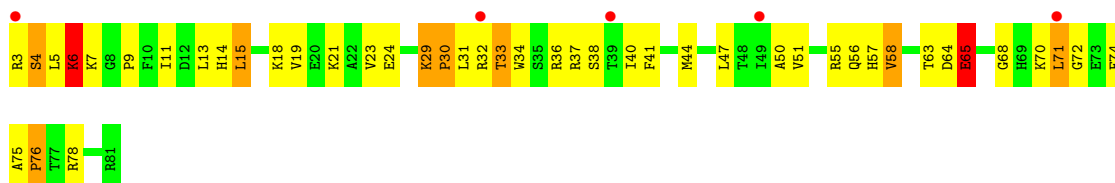
- Molecule 18: 30S ribosomal protein S18

Chain CR:



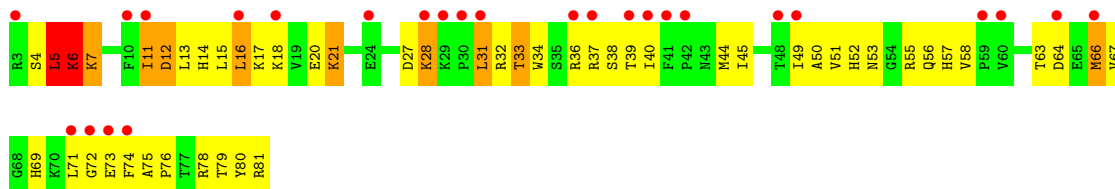
- Molecule 19: 30S ribosomal protein S19

Chain AS:



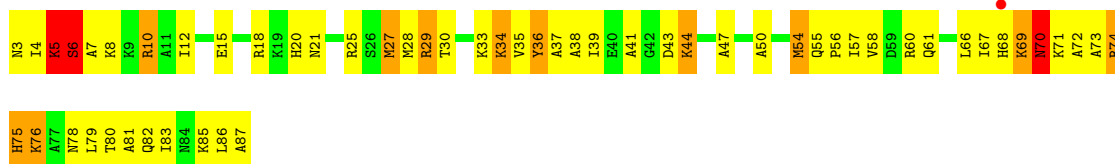
- Molecule 19: 30S ribosomal protein S19

Chain CS:



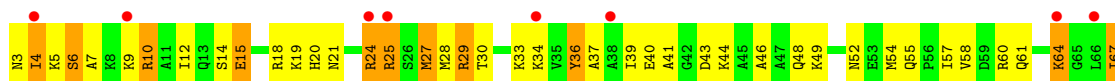
- Molecule 20: 30S ribosomal protein S20

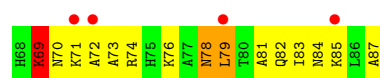
Chain AT:



- Molecule 20: 30S ribosomal protein S20

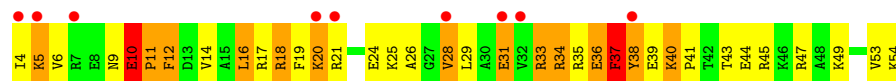
Chain CT:





- Molecule 21: 30S ribosomal protein S21

Chain AU:



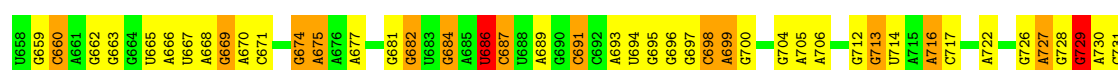
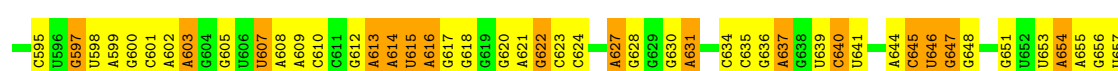
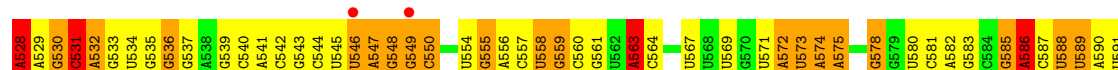
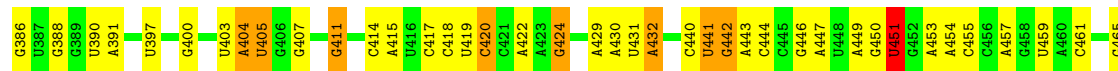
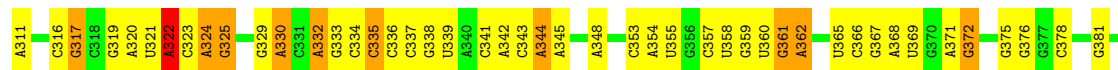
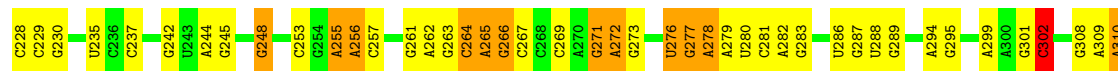
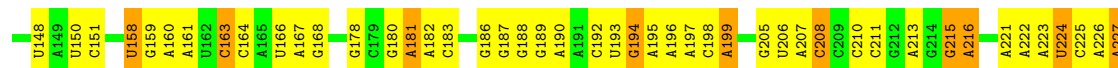
- Molecule 21: 30S ribosomal protein S21

Chain CU:



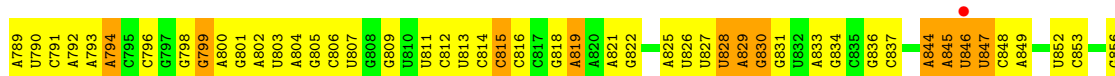
- Molecule 22: 23S rRNA

Chain BA:



G1731	A1655	A1586	G1514	G1448	G1382	A1321	A1260	C1196	U1132	G1071	G1002	A836	G859	A792	C732
C1732	C1656	G1587	A1515	G1449	A1383	A1322	C1261	G1197	A1133	C1072	G1003	C837	U860	A793	G733
G1733	G1657	A1588	G1516	G1450	A1384	G1323	A1262	U1198	A1134	A1073	U1004	G940	A861	A794	A734
A1735	C1658	U1589	C1451	C1451	A1385	G1324	U1263	U1199	C1135	G1074	C1005	C941	C864	C795	A735
A1736	G1659	A1590	U1520	G1452	A1386	U1325	A1264	C1200	G1136	C1075	C1006	G942	C865	C796	C737
G1737	G1660	A1591	U1523	A1453	A1387	U1326	A1265	A1204	G1137	C1076	C1007	A943	C866	G797	G738
G1738	G1661	C1592	G1524	C1454	G1388	A1327	G1266	A1205	G1138	A1077	A1008	A944	C867	A800	A739
A1739	U1662	A1593	G1525	G1455	A1392	A1328	U1267	A1206	C1139	U1078	A1009	A945	U868	G801	C740
G1740	C1663	A1594	A1525	G1456	A1393	U1329	A1268	C1207	C1140	C1079	A1010	A946	C868	A802	U741
C1741	A1664	C1595	G1527	U1457	A1394	G1330	A1269	C1208	U1141	A1080	G1011	A947	U870	U803	A742
U1742	C1667	C1599	U1542	G1458	A1395	G1332	A1271	U1209	A1143	U1082	C1013	C948	A877	A804	A743
G1743	A1668	U1600	A1532	U1460	U1396	G1333	A1272	A1144	A1144	U1083	A1014		A878	G805	U744
A1744	C1669	C1601	C1533	C1461	U1397	G1334	U1273	C1145	C1145	A1084	U1015		G879	C806	G745
A1746	U1670	A1603	U1534	U1467	C1398	C1335	A1274	A1151		A1085	G1016		U895	C807	G746
U1747	A1671	U1602	A1535	U1468	C1399	A1336	A1275	A1152	C1152	A1086	G1017		G808	G808	U747
C1748	A1672	C1536	G1537	A1469	G1400	G1337	A1276	G1215	C1153	G1087	U1018		U884	C885	G748
A1749	G1673	G1547	U1542	A1470	U1402	G1339	C1278	U1217	G1154	A1088	U1019		U885	C885	A749
C1675	A1608	A1608	U1542	G1471	A1403	U1340	G1279	G1218	A1155	A1089	A1020		A	C812	A750
	U1680	A1609	G1543	C1472	A1404	G1341	U1280	U1219	A1156	A1090	A1021		U	U811	A751
A1754	G1681	A1610	A1544	G1473	U1405	A1342	G1281	G1220	C1157	C1092	G1022		C	C814	A752
A1755	G1682	C1613	A1545	U1474	U1406	G1343	U1282	C1221	C1158	G1093	G1026		C	C815	A753
G1756	G1683	A1614	G1546	G1475	G1407	U1344	G1283	U1222	U1159	U1094	A1027		C	C816	U754
A1757	G1684	A1548	C1547	U1476	A1413	G1345	A1284	G1223	G1160	A1095	A1028		G	C817	U755
U1758	C1685	A1549	U1548	A1477	C1414	G1346	A1285	U1224	C1161	A1096			A892	C818	A756
A1759	G1686	A1618	A1549	G1478	C1414	A1347	A1286	U1225	G1162	U1097	U967		A896	A819	G757
G1760	G1687	G1619	A1551	G1479	U1415	A1348	A1287	A1226	G1163	A1098	G1031		C969	A820	G758
C1761	U1688	G1620	A1552	U1481	G1421	C1349	U1288	G1227	C1164	G1099	U1033		C	A821	G759
A1762	G1621	A1553	A1553	G1482	G1418	C1350	U1289		A1165	C1100			A899	G822	G760
G1763	G1622	U1554	U1562	G1483	A1419	U1352	C1290	U1231	G1166	U1101	G1036		A905	U824	U762
C1764	G1623	G1555	U1563	U1484	A1420	A1353	G1291	U1232	C1167	C1102	G1037		U906	A825	G763
U1765	U1624	C1556	C1564	U1487	G1422	A1354	U1292	G1233	C1168	A1103	G1038		C907	U826	G764
G1766	C1625	C1557	A1566	U1488	G1421	A1362	U1293	C1234	A1169	U1104			C908	U827	G765
G1767	A1626	C1558	C1568	C1488	G1422	G1355	U1294	G1235	C1170	U1105	C1043		A909	U828	U766
C1768	G1627	U1562	U1562	U1489	G1424	G1356	C1295	G1236	G1171	G1106	C1044		A910	G829	U767
U1769	G1628	U1563	U1564	A1490	G1425	G1357	C1296	G1237	C1172	G1107	C1045		A911	G830	G768
		U1564	C1564	G1491	G1426	G1358	C1297	A1237	U1173	U1108	A1046		C912	U831	U769
A1770	G1631	A1632	C1564	G1492	A1427	A1359	U1298	G1238	U1174	C1109	G1047		U913	U832	G770
A1773	G1633	G1633	C1565	C1428	C1428	G1360	U1299	G1239	A1175	G1110			C914	A833	G771
C1774	A1634	A1634	A1566	A1494	G1429	G1361	A1300	U1240	U1176	A1111	G1051		C915	G834	C772
U1775	G1635	A1635	G1567	A1495	G1430	C1362	A1301	A1241	G1177	G1112	C1052		G916		U773
G1776	U1636	A1636	C1568	A1496	A1431	G1363	A1302	U1242	C1178	U1113	C1053		A917	U839	G774
U1779	U1636	A1636	A1569	A1496	G1432	A1364	A1303	C1243	G1179	C1114	A1054		A918	C840	G775
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A1785	U1571	C1638	A1571	G1500	A1434	A1366	C1305	G1245	U1181	G1116	G1056		C987	U842	G777
A1786	G1573	A1640	G1573	G1436	G1435	A1367	A1307	A1247	G1183	C1117	A1057		C921	U843	G778
				A1503	C1437	G1368	U1307	U1249	U1184	U1119	U1058		C922	U844	U779
A1789	G1645	U1576	U1576	U1504	U1438	G1371	A1308	G1248	U1185	G1120	G1059		G923	A845	G780
C1790	C1646	C1577	C1577	A1504	U1438	U1372	U1312	G1250	G1186	C1121	U1061		C992	U847	A781
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C1793	G1649	A1580	A1580	C1507	G1441	U1375	C1314	A1253	A1189	G1124	C1064		U929	U852	G784
G1721	A1650	U1581	U1581	A1509	U1442	C1376	C1315	U1254	G1190	G1125	U1065		C995	C853	G785
A1722	C1651	C1582	C1582	G1510	U1443	G1377	U1316	U1255	G1191	A1126	A1066		A996	C854	G786
U1794	A1652	A1583	A1583	G1511	G1444	A1378	G1317	G1256	C1192	A1127	A1067		C998	C855	A788
C1795	G1653	C1512	C1512	C1511	G1445	U1379	U1318	U1257	G1193	G1128	G1068		A933	C856	A789
U1796	C1730	C1585	C1585	U1513	C1447	G1380	U1319	U1258	A1194	G1128	A1069		U999	G857	U790
G1797						G1381	C1320	G1259	G1195		A1070		C935		C791

A2726	A2727	U2728	A2729	A2730	A2731	A2732	A2733	A2734	A2735	A2736	A2737	A2738	A2739	A2740	A2741	A2742	A2743	A2744	A2745	A2746	A2747	A2748	A2749	A2750	A2751	A2752	A2753	A2754	A2755	A2756	A2757	A2758	A2759	A2760	A2761	A2762	A2763	A2764	A2765	A2766	A2767	A2768	A2769	A2770	A2771	A2772	A2773	A2774	A2775	A2776	A2777	A2778	A2779	A2780	A2781	A2782	A2783	A2784	A2785	A2786	A2787	A2788	A2789	A2790	A2791	A2792	A2793	A2794	A2795	A2796	A2797	A2798	A2799	A2800	A2801	A2802	A2803	A2804	A2805	A2806	A2807	A2808	A2809	A2810	A2811	A2812	A2813	A2814	A2815	A2816	A2817	A2818	A2819	A2820	A2821	A2822	A2823	A2824	A2825	A2826	A2827	A2828	A2829	A2830	A2831	A2832	A2833	A2834	A2835	A2836	A2837	A2838	A2839	A2840	A2841	A2842	A2843	A2844	A2845	A2846	A2847	A2848	A2849	A2850	A2851	A2852	A2853	A2854	A2855	A2856	A2857	A2858	A2859	A2860	A2861	A2862	A2863	A2864	A2865	A2866	A2867	A2868	A2869	A2870	A2871	A2872	A2873	A2874	A2875	A2876	A2877	A2878	A2879	A2880	A2881	A2882	A2883	A2884	A2885	A2886	A2887	A2888	A2889	A2890	A2891	A2892	A2893	A2894	A2895	A2896	A2897	A2898	A2899	A2900	A2901	A2902	A2903	A2904	A2905	A2906	A2907	A2908	A2909	A2910	A2911	A2912	A2913	A2914	A2915	A2916	A2917	A2918	A2919	A2920	A2921	A2922	A2923	A2924	A2925	A2926	A2927	A2928	A2929	A2930	A2931	A2932	A2933	A2934	A2935	A2936	A2937	A2938	A2939	A2940	A2941	A2942	A2943	A2944	A2945	A2946	A2947	A2948	A2949	A2950	A2951	A2952	A2953	A2954	A2955	A2956	A2957	A2958	A2959	A2960	A2961	A2962	A2963	A2964	A2965	A2966	A2967	A2968	A2969	A2970	A2971	A2972	A2973	A2974	A2975	A2976	A2977	A2978	A2979	A2980	A2981	A2982	A2983	A2984	A2985	A2986	A2987	A2988	A2989	A2990	A2991	A2992	A2993	A2994	A2995	A2996	A2997	A2998	A2999	A3000	A3001	A3002	A3003	A3004	A3005	A3006	A3007	A3008	A3009	A3010	A3011	A3012	A3013	A3014	A3015	A3016	A3017	A3018	A3019	A3020	A3021	A3022	A3023	A3024	A3025	A3026	A3027	A3028	A3029	A3030	A3031	A3032	A3033	A3034	A3035	A3036	A3037	A3038	A3039	A3040	A3041	A3042	A3043	A3044	A3045	A3046	A3047	A3048	A3049	A3050	A3051	A3052	A3053	A3054	A3055	A3056	A3057	A3058	A3059	A3060	A3061	A3062	A3063	A3064	A3065	A3066	A3067	A3068	A3069	A3070	A3071	A3072	A3073	A3074	A3075	A3076	A3077	A3078	A3079	A3080	A3081	A3082	A3083	A3084	A3085	A3086	A3087	A3088	A3089	A3090	A3091	A3092	A3093	A3094	A3095	A3096	A3097	A3098	A3099	A3100	A3101	A3102	A3103	A3104	A3105	A3106	A3107	A3108	A3109	A3110	A3111	A3112	A3113	A3114	A3115	A3116	A3117	A3118	A3119	A3120	A3121	A3122	A3123	A3124	A3125	A3126	A3127	A3128	A3129	A3130	A3131	A3132	A3133	A3134	A3135	A3136	A3137	A3138	A3139	A3140	A3141	A3142	A3143	A3144	A3145	A3146	A3147	A3148	A3149	A3150	A3151	A3152	A3153	A3154	A3155	A3156	A3157	A3158	A3159	A3160	A3161	A3162	A3163	A3164	A3165	A3166	A3167	A3168	A3169	A3170	A3171	A3172	A3173	A3174	A3175	A3176	A3177	A3178	A3179	A3180	A3181	A3182	A3183	A3184	A3185	A3186	A3187	A3188	A3189	A3190	A3191	A3192	A3193	A3194	A3195	A3196	A3197	A3198	A3199	A3200	A3201	A3202	A3203	A3204	A3205	A3206	A3207	A3208	A3209	A3210	A3211	A3212	A3213	A3214	A3215	A3216	A3217	A3218	A3219	A3220	A3221	A3222	A3223	A3224	A3225	A3226	A3227	A3228	A3229	A3230	A3231	A3232	A3233	A3234	A3235	A3236	A3237	A3238	A3239	A3240	A3241	A3242	A3243	A3244	A3245	A3246	A3247	A3248	A3249	A3250	A3251	A3252	A3253	A3254	A3255	A3256	A3257	A3258	A3259	A3260	A3261	A3262	A3263	A3264	A3265	A3266	A3267	A3268	A3269	A3270	A3271	A3272	A3273	A3274	A3275	A3276	A3277	A3278	A3279	A3280	A3281	A3282	A3283	A3284	A3285	A3286	A3287	A3288	A3289	A3290	A3291	A3292	A3293	A3294	A3295	A3296	A3297	A3298	A3299	A3300	A3301	A3302	A3303	A3304	A3305	A3306	A3307	A3308	A3309	A3310	A3311	A3312	A3313	A3314	A3315	A3316	A3317	A3318	A3319	A3320	A3321	A3322	A3323	A3324	A3325	A3326	A3327	A3328	A3329	A3330	A3331	A3332	A3333	A3334	A3335	A3336	A3337	A3338	A3339	A3340	A3341	A3342	A3343	A3344	A3345	A3346	A3347	A3348	A3349	A3350	A3351	A3352	A3353	A3354	A3355	A3356	A3357	A3358	A3359	A3360	A3361	A3362	A3363	A3364	A3365	A3366	A3367	A3368	A3369	A3370	A3371	A3372	A3373	A3374	A3375	A3376	A3377	A3378	A3379	A3380	A3381	A3382	A3383	A3384	A3385	A3386	A3387	A3388	A3389	A3390	A3391	A3392	A3393	A3394	A3395	A3396	A3397	A3398	A3399	A3400	A3401	A3402	A3403	A3404	A3405	A3406	A3407	A3408	A3409	A3410	A3411	A3412	A3413	A3414	A3415	A3416	A3417	A3418	A3419	A3420	A3421	A3422	A3423	A3424	A3425	A3426	A3427	A3428	A3429	A3430	A3431	A3432	A3433	A3434	A3435	A3436	A3437	A3438	A3439	A3440	A3441	A3442	A3443	A3444	A3445	A3446	A3447	A3448	A3449	A3450	A3451	A3452	A3453	A3454	A3455	A3456	A3457	A3458	A3459	A3460	A3461	A3462	A3463	A3464	A3465	A3466	A3467	A3468	A3469	A3470	A3471	A3472	A3473	A3474	A3475	A3476	A3477	A3478	A3479	A3480	A3481	A3482	A3483	A3484	A3485	A3486	A3487	A3488	A3489	A3490	A3491	A3492	A3493	A3494	A3495	A3496	A3497	A3498	A3499	A3500	A3501	A3502	A3503	A3504	A3505	A3506	A3507	A3508	A3509	A3510	A3511	A3512	A3513	A3514	A3515	A3516	A3517	A3518	A3519	A3520	A3521	A3522	A3523	A3524	A3525	A3526	A3527	A3528	A3529	A3530	A3531	A3532	A3533	A3534	A3535	A3536	A3537	A3538	A3539	A3540	A3541	A3542	A3543	A3544	A3545	A3546	A3547	A3548	A3549	A3550	A3551	A3552	A3553	A3554	A3555	A3556	A3557	A3558	A3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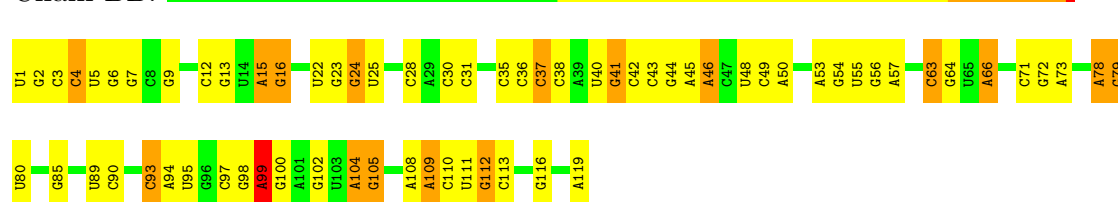




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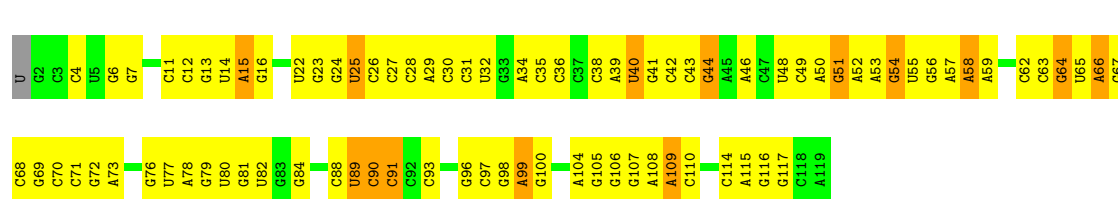
- Molecule 23: 5S rRNA

Chain BB:



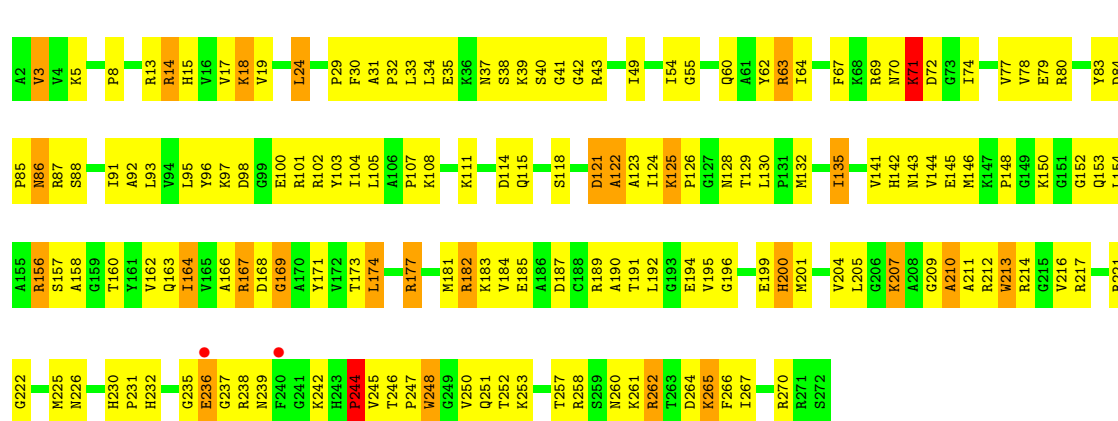
- Molecule 23: 5S rRNA

Chain DB:



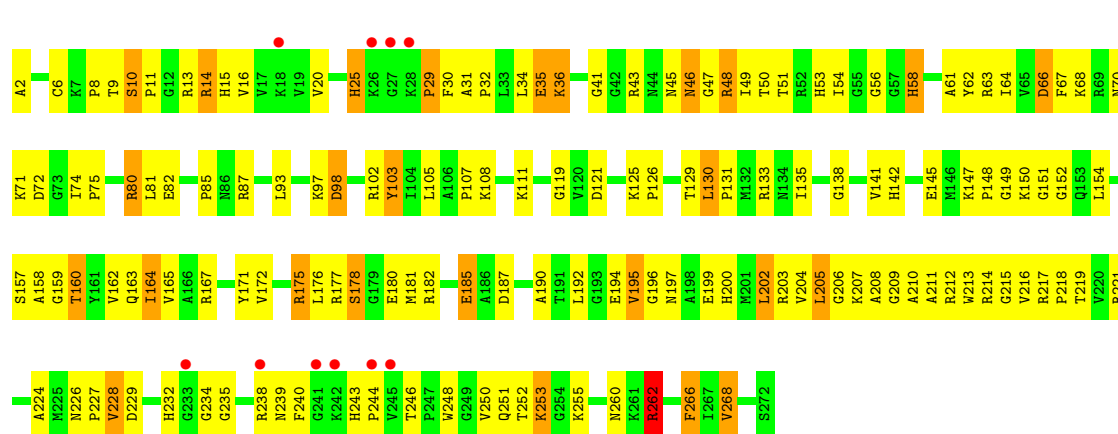
- Molecule 24: 50S ribosomal protein L2

Chain BC:

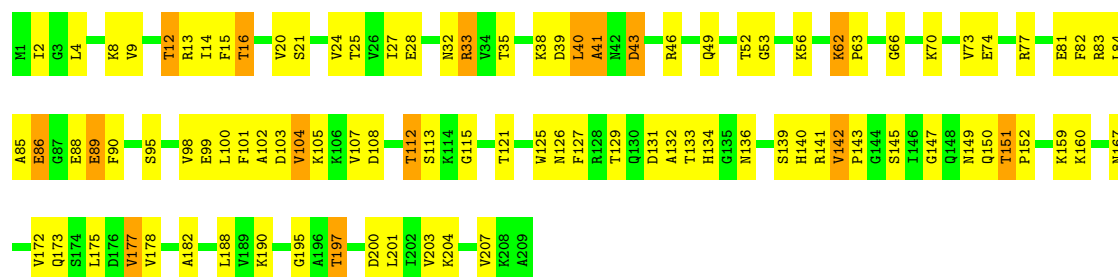


- Molecule 24: 50S ribosomal protein L2

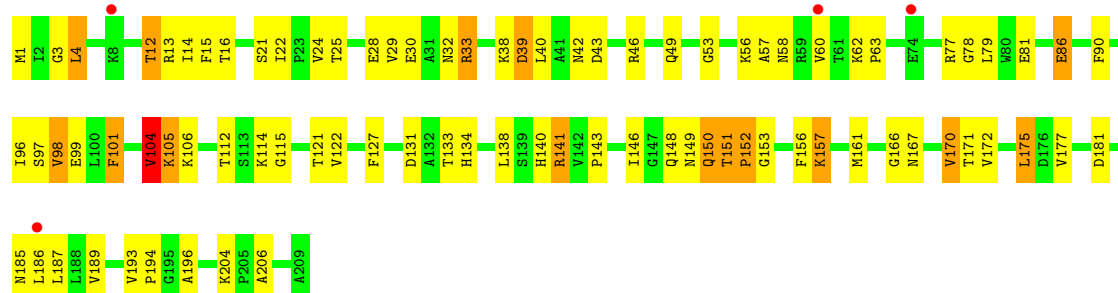
Chain DC:



- Molecule 25: 50S ribosomal protein L3

Chain BD: 

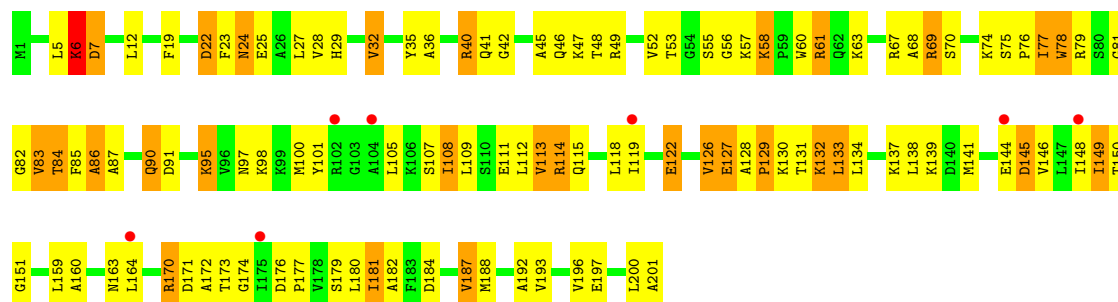
- Molecule 25: 50S ribosomal protein L3

Chain DD: 

- Molecule 26: 50S ribosomal protein L4

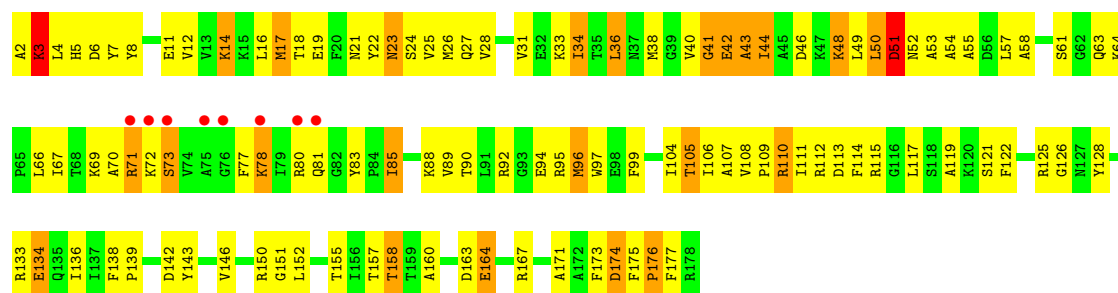
Chain BE: 

- Molecule 26: 50S ribosomal protein L4

Chain DE: 

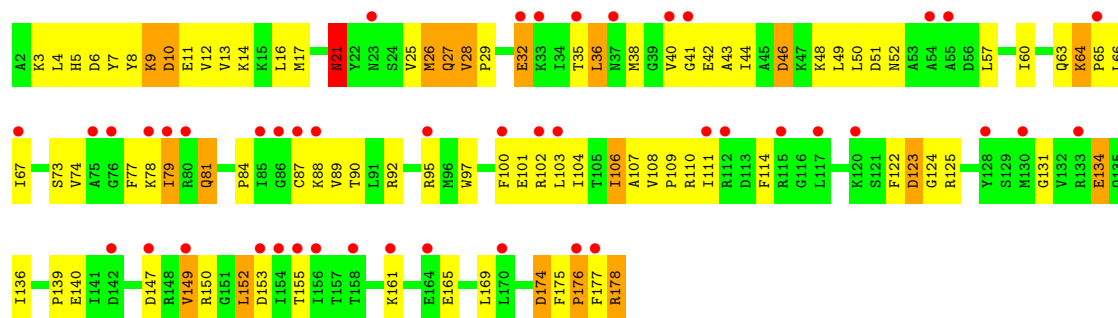
- Molecule 27: 50S ribosomal protein L5

Chain BF: 



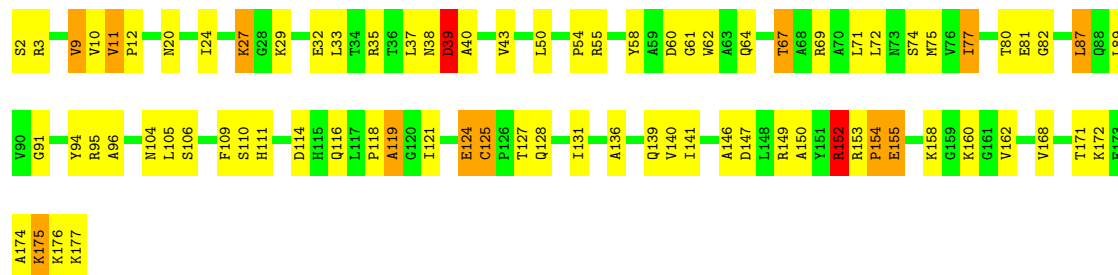
• Molecule 27: 50S ribosomal protein L5

Chain DF:



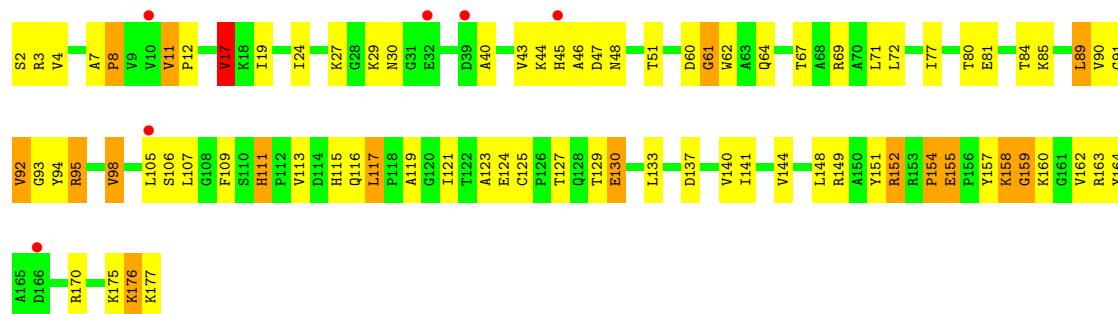
• Molecule 28: 50S ribosomal protein L6

Chain BG:



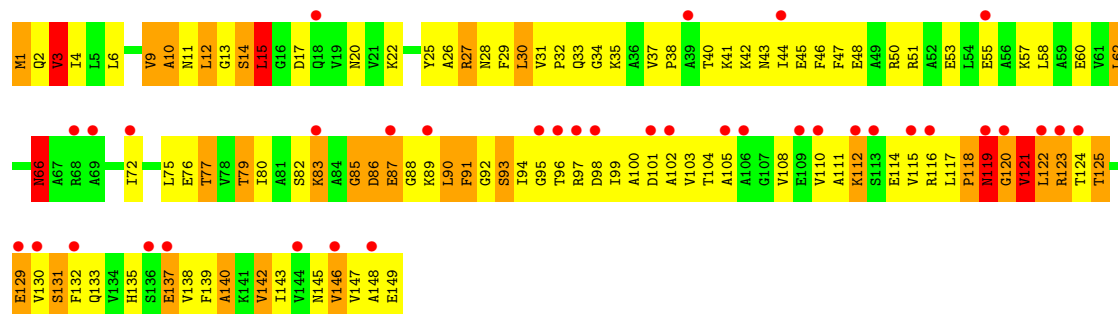
• Molecule 28: 50S ribosomal protein L6

Chain DG:



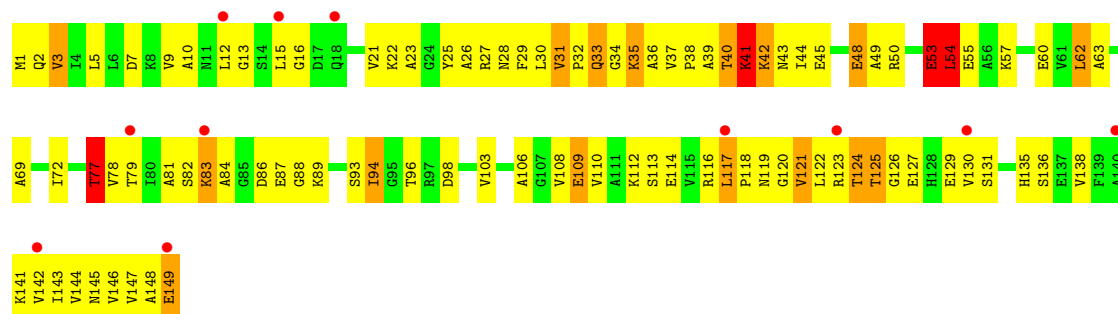
• Molecule 29: 50S ribosomal protein L9

Chain BH:



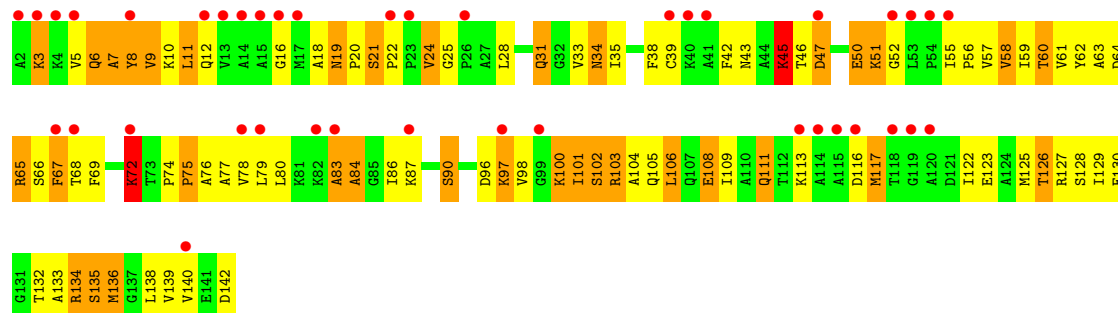
- Molecule 29: 50S ribosomal protein L9

Chain DH:



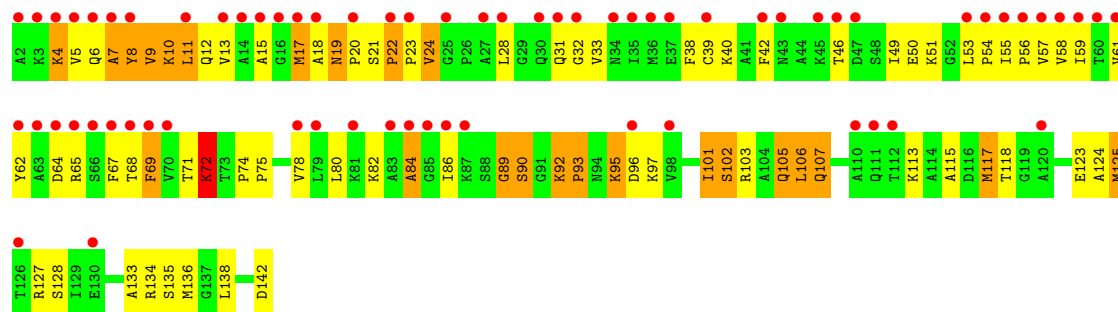
- Molecule 30: 50S ribosomal protein L11

Chain BI:

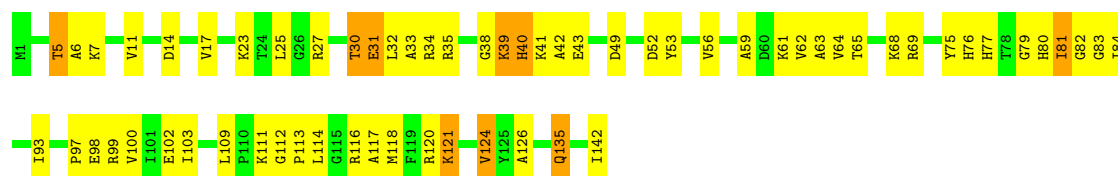


- Molecule 30: 50S ribosomal protein L11

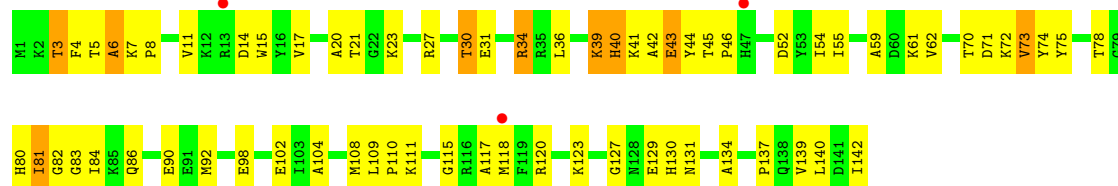
Chain DI:



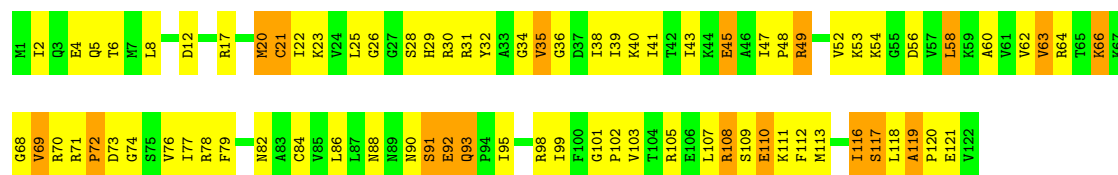
- Molecule 31: 50S ribosomal protein L13

Chain BJ: 

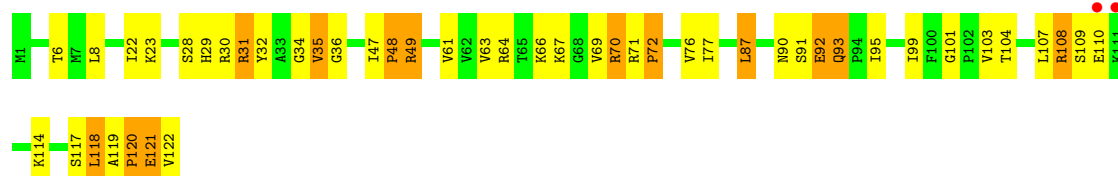
- Molecule 31: 50S ribosomal protein L13

Chain DJ: 

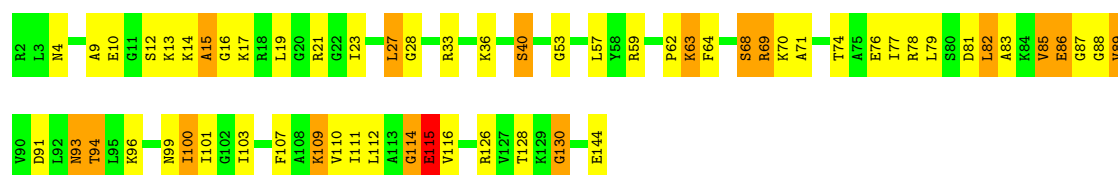
- Molecule 32: 50S ribosomal protein L14

Chain BK: 

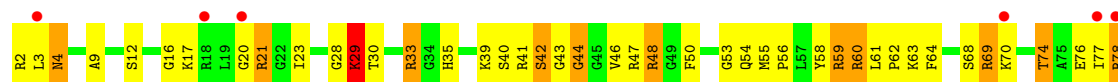
- Molecule 32: 50S ribosomal protein L14

Chain DK: 

- Molecule 33: 50S ribosomal protein L15

Chain BL: 

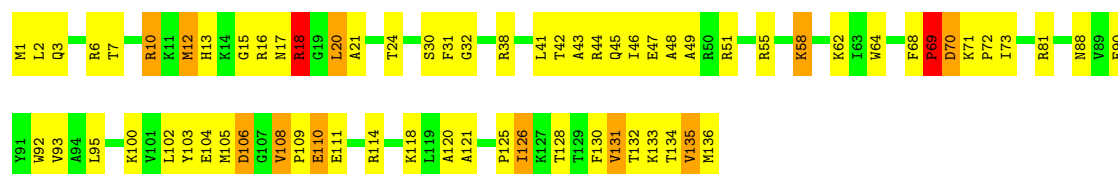
- Molecule 33: 50S ribosomal protein L15

Chain DL: 



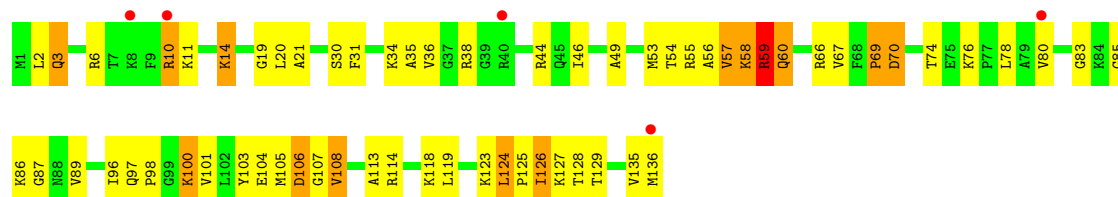
• Molecule 34: 50S ribosomal protein L16

Chain BM:



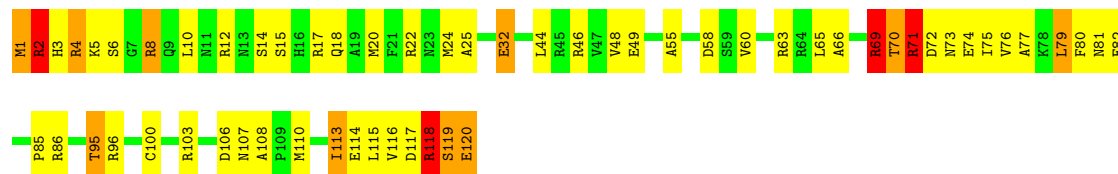
• Molecule 34: 50S ribosomal protein L16

Chain DM:



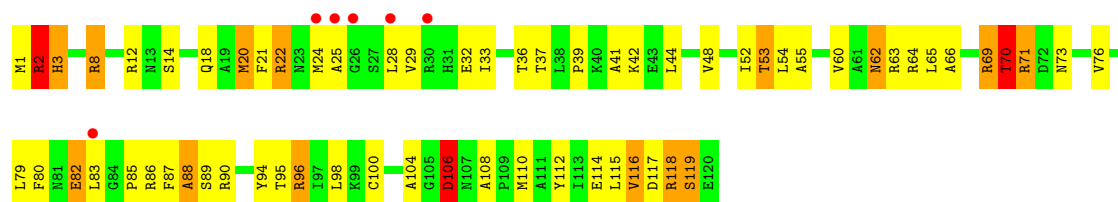
• Molecule 35: 50S ribosomal protein L17

Chain BN:



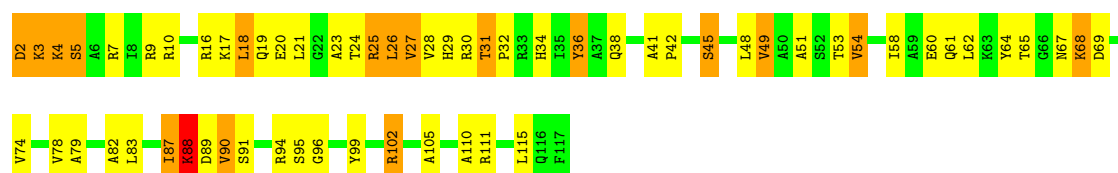
• Molecule 35: 50S ribosomal protein L17

Chain DN:



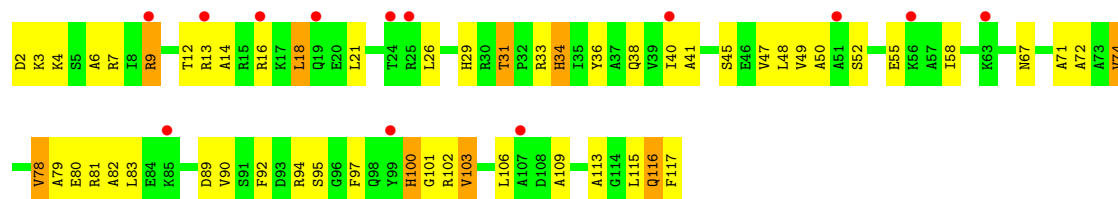
• Molecule 36: 50S ribosomal protein L18

Chain BO:



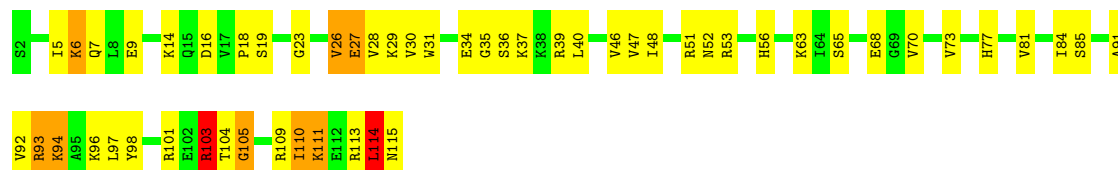
- Molecule 36: 50S ribosomal protein L18

Chain DO:



- Molecule 37: 50S ribosomal protein L19

Chain BP:



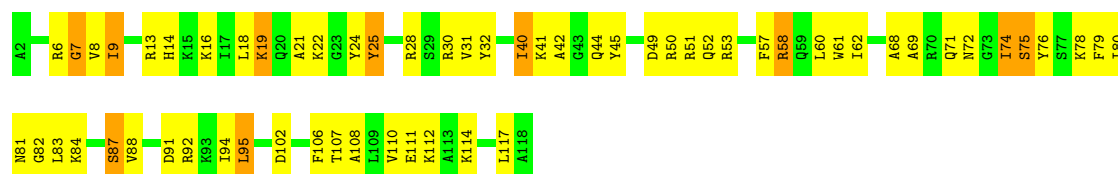
- Molecule 37: 50S ribosomal protein L19

Chain DP:



- Molecule 38: 50S ribosomal protein L20

Chain BQ:



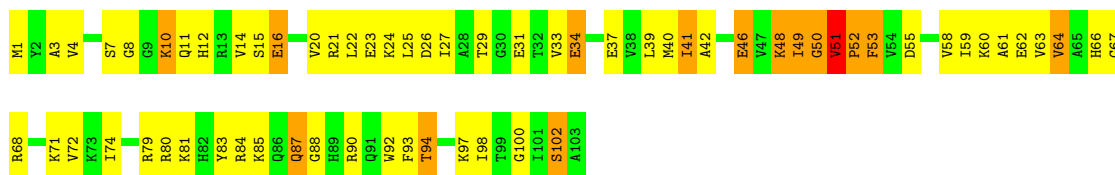
- Molecule 38: 50S ribosomal protein L20

Chain DQ:



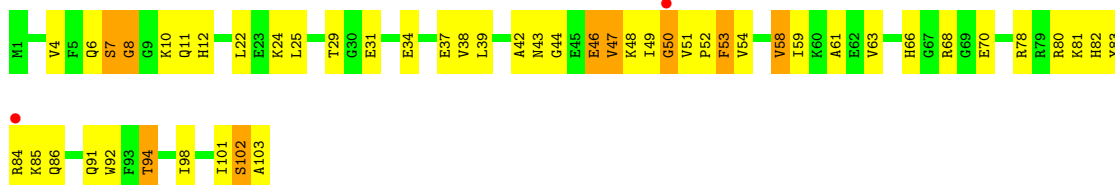
- Molecule 39: 50S ribosomal protein L21

Chain BR:



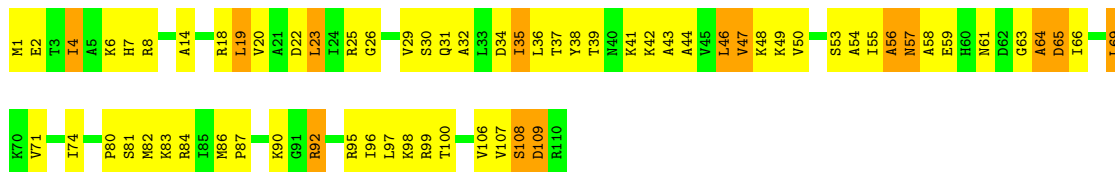
- Molecule 39: 50S ribosomal protein L21

Chain DR:



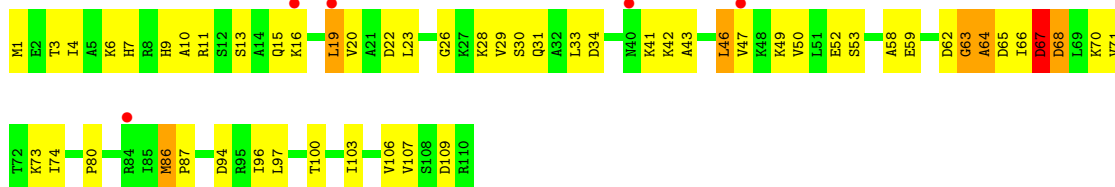
- Molecule 40: 50S ribosomal protein L22

Chain BS:



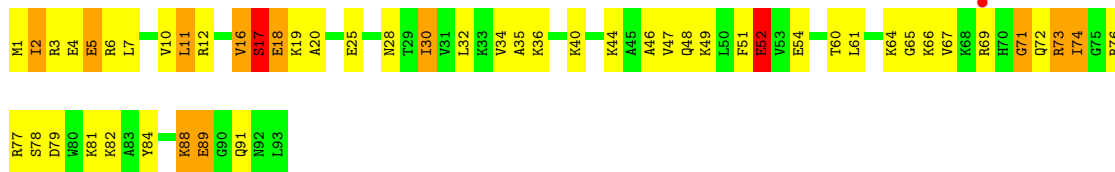
- Molecule 40: 50S ribosomal protein L22

Chain DS:



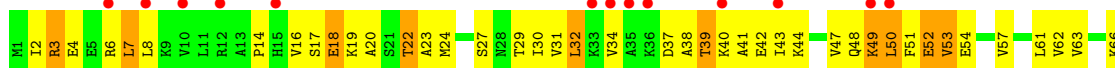
- Molecule 41: 50S ribosomal protein L23

Chain BT:



- Molecule 41: 50S ribosomal protein L23

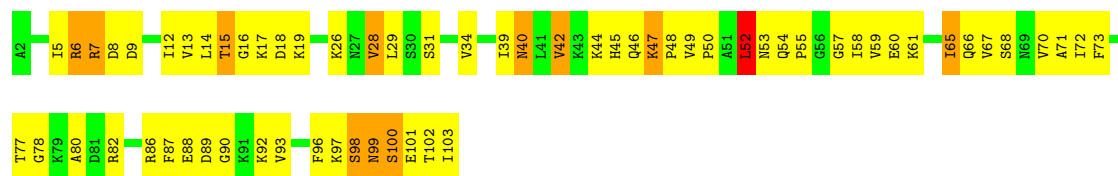
Chain DT:





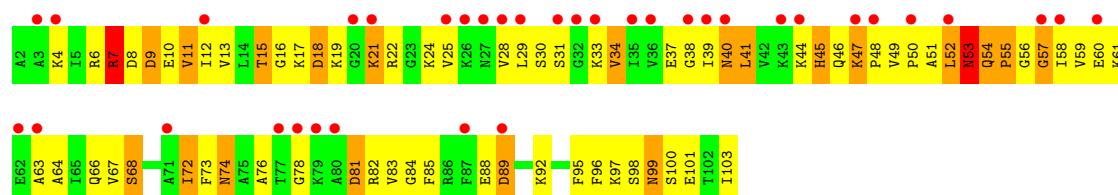
- Molecule 42: 50S ribosomal protein L24

Chain BU:



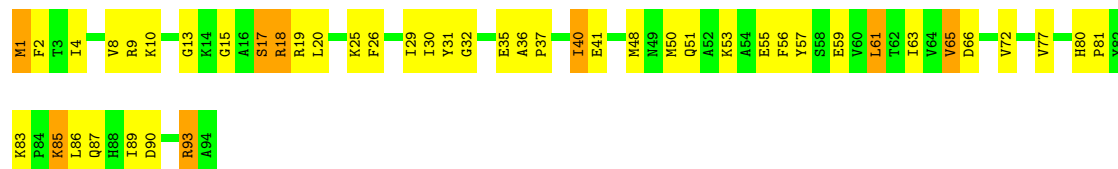
- Molecule 42: 50S ribosomal protein L24

Chain DU:



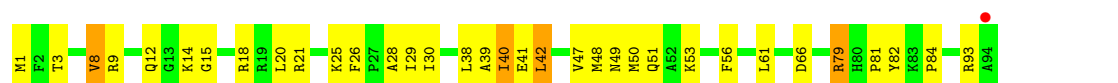
- Molecule 43: 50S ribosomal protein L25

Chain BV:



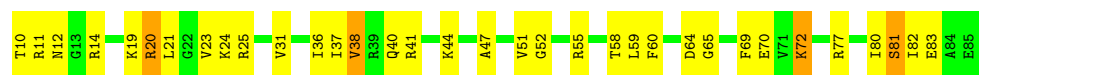
- Molecule 43: 50S ribosomal protein L25

Chain DV:



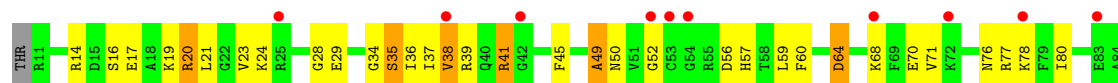
- Molecule 44: 50S ribosomal protein L27

Chain BW:



- Molecule 44: 50S ribosomal protein L27

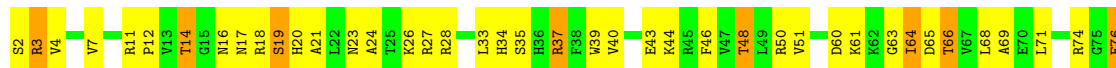
Chain DW:





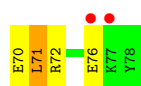
- Molecule 45: 50S ribosomal protein L28

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:



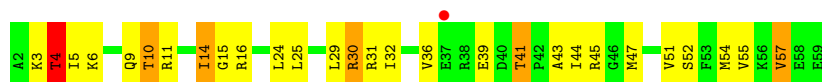
- Molecule 47: 50S ribosomal protein L30

Chain BZ:



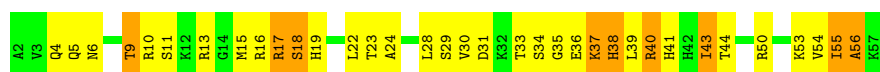
- Molecule 47: 50S ribosomal protein L30

Chain DZ:



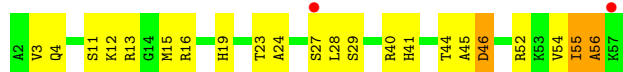
- Molecule 48: 50S ribosomal protein L32

Chain B0:



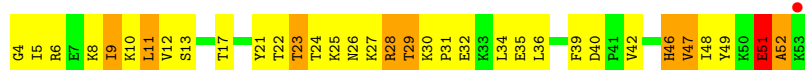
- Molecule 48: 50S ribosomal protein L32

Chain D0:



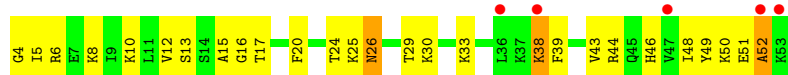
- Molecule 49: 50S ribosomal protein L33

Chain B1:



- Molecule 49: 50S ribosomal protein L33

Chain D1:



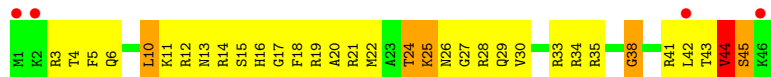
- Molecule 50: 50S ribosomal protein L34

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:



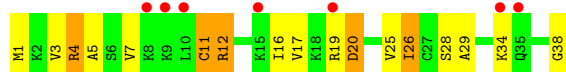
- Molecule 52: 50S ribosomal protein L36

Chain B4:



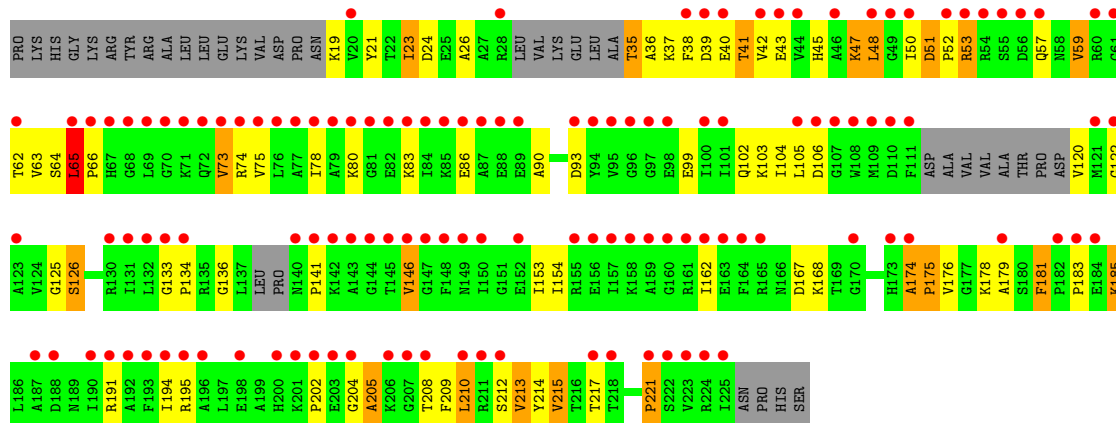
- Molecule 52: 50S ribosomal protein L36

Chain D4:



- Molecule 53: 50S ribosomal protein L1

Chain B5:



- Molecule 54: Linopristin

Chain B6:



- Molecule 54: Linopristin

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	211.49Å 433.90Å 621.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.15 – 3.00 69.15 – 3.00	Depositor EDS
% Data completeness (in resolution range)	90.2 (69.15-3.00) 90.2 (69.15-3.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.225 , 0.274 0.236 , 0.283	Depositor DCC
R_{free} test set	4092 reflections (0.40%)	DCC
Wilson B-factor (Å ²)	57.2	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 12.3	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 1017015 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	288320	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 2.64% 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, 04X, 004, MHW, 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	0.52	0/36944	1.02	48/57632 (0.1%)
1	CA	0.45	0/36966	0.96	27/57666 (0.0%)
2	AB	0.44	0/1736	0.65	0/2338
2	CB	0.38	0/1736	0.59	0/2338
3	AC	0.39	0/1652	0.61	0/2225
3	CC	0.37	0/1652	0.58	1/2225 (0.0%)
4	AD	0.39	0/1665	0.64	0/2227
4	CD	0.43	0/1665	0.65	0/2227
5	AE	0.41	0/1119	0.75	0/1504
5	CE	0.41	0/1119	0.73	0/1504
6	AF	0.41	0/836	0.77	2/1128 (0.2%)
6	CF	0.35	0/836	0.64	1/1128 (0.1%)
7	AG	0.37	0/1196	0.60	0/1602
7	CG	0.38	0/1196	0.54	0/1602
8	AH	0.40	0/989	0.63	0/1326
8	CH	0.34	0/989	0.57	0/1326
9	AI	0.39	0/1034	0.65	0/1375
9	CI	0.36	0/1034	0.59	0/1375
10	AJ	0.37	0/797	0.62	0/1077
10	CJ	0.36	0/797	0.61	0/1077
11	AK	0.38	0/893	0.63	0/1205
11	CK	0.37	0/893	0.61	0/1205
12	AL	0.41	0/969	0.71	0/1300
12	CL	0.41	0/969	0.73	0/1300
13	AM	0.38	0/893	0.70	1/1193 (0.1%)
13	CM	0.39	0/893	0.62	0/1193
14	AN	0.38	0/785	0.61	0/1043
14	CN	0.34	0/785	0.52	0/1043
15	AO	0.34	0/718	0.59	0/959
15	CO	0.32	0/718	0.57	0/959
16	AP	0.40	0/659	0.70	1/884 (0.1%)
16	CP	0.36	0/659	0.60	0/884

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.37	0/658	0.66	0/881
17	CQ	0.39	0/658	0.61	0/881
18	AR	0.37	0/463	0.61	0/621
18	CR	0.37	0/463	0.58	0/621
19	AS	0.43	0/653	0.66	0/877
19	CS	0.38	0/653	0.58	0/877
20	AT	0.43	0/671	0.63	0/888
20	CT	0.35	0/671	0.56	0/888
21	AU	0.50	0/431	0.71	0/570
21	CU	0.44	0/431	0.66	0/570
22	BA	0.90	44/69659 (0.1%)	1.39	725/108672 (0.7%)
22	DA	0.45	0/69659	0.95	28/108672 (0.0%)
23	BB	0.78	2/2850 (0.1%)	1.29	20/4444 (0.5%)
23	DB	0.39	0/2828	0.89	0/4410
24	BC	0.56	1/2122 (0.0%)	0.75	1/2852 (0.0%)
24	DC	0.37	0/2122	0.61	0/2852
25	BD	0.62	0/1586	0.80	1/2134 (0.0%)
25	DD	0.34	0/1586	0.55	0/2134
26	BE	0.54	0/1571	0.70	0/2113
26	DE	0.38	0/1571	0.60	0/2113
27	BF	0.41	0/1435	0.62	0/1926
27	DF	0.37	0/1435	0.53	0/1926
28	BG	0.45	0/1343	0.67	0/1816
28	DG	0.34	0/1343	0.52	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	0.44	0/1046	0.62	0/1410
30	DI	0.43	0/1046	0.59	0/1410
31	BJ	0.61	0/1152	0.75	1/1551 (0.1%)
31	DJ	0.35	0/1152	0.57	0/1551
32	BK	0.64	0/948	0.81	0/1268
32	DK	0.37	0/948	0.57	0/1268
33	BL	0.52	0/1054	0.75	0/1403
33	DL	0.38	0/1054	0.62	0/1403
34	BM	0.62	0/1093	0.80	1/1460 (0.1%)
34	DM	0.33	0/1093	0.56	0/1460
35	BN	0.61	0/974	0.88	3/1301 (0.2%)
35	DN	0.36	0/974	0.56	0/1301
36	BO	0.48	0/902	0.71	0/1209
36	DO	0.34	0/902	0.53	0/1209
37	BP	0.54	0/929	0.75	1/1242 (0.1%)
37	DP	0.37	0/929	0.58	0/1242
38	BQ	0.73	0/960	0.82	1/1278 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DQ	0.36	0/960	0.54	0/1278
39	BR	0.66	0/829	0.91	2/1107 (0.2%)
39	DR	0.36	0/829	0.59	0/1107
40	BS	0.72	0/864	0.81	0/1156
40	DS	0.36	0/864	0.63	0/1156
41	BT	0.49	0/745	0.68	0/994
41	DT	0.38	0/745	0.60	0/994
42	BU	0.48	0/788	0.72	0/1051
42	DU	0.43	0/788	0.61	0/1051
43	BV	0.52	0/766	0.70	0/1025
43	DV	0.32	0/766	0.48	0/1025
44	BW	0.64	0/587	0.79	0/776
44	DW	0.33	0/576	0.54	0/762
45	BX	0.45	0/635	0.73	0/848
45	DX	0.36	0/635	0.60	0/848
46	BY	0.46	0/510	0.71	0/677
46	DY	0.39	0/510	0.61	0/677
47	BZ	0.61	0/453	0.82	1/605 (0.2%)
47	DZ	0.32	0/453	0.58	0/605
48	B0	0.64	0/450	0.91	2/599 (0.3%)
48	D0	0.35	0/450	0.58	0/599
49	B1	0.46	0/417	0.67	0/554
49	D1	0.35	0/417	0.51	0/554
50	B2	0.55	0/380	0.83	0/498
50	D2	0.38	0/380	0.61	0/498
51	B3	0.58	0/513	0.75	0/676
51	D3	0.33	0/513	0.57	0/676
52	B4	0.60	0/303	0.71	0/397
52	D4	0.32	0/303	0.54	0/397
53	B5	0.39	0/1145	0.56	0/1556
54	B6	3.67	4/13 (30.8%)	4.12	3/15 (20.0%)
54	D6	3.86	3/13 (23.1%)	3.82	4/15 (26.7%)
All	All	0.59	54/310652 (0.0%)	1.02	876/464396 (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
5	CE	0	1
6	CF	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
11	AK	0	1
12	CL	0	2
21	AU	0	1
25	BD	0	1
25	DD	0	1
33	BL	0	1
48	B0	0	1
All	All	0	10

The worst 5 of 54 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1142	A	N9-C4	-12.83	1.30	1.37
22	BA	528	A	N9-C4	-10.27	1.31	1.37
22	BA	528	A	N3-C4	-8.70	1.29	1.34
22	BA	974	G	N9-C4	-8.12	1.31	1.38
22	BA	979	A	N9-C4	-7.80	1.33	1.37

The worst 5 of 876 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	974	G	C4-C5-N7	15.39	116.95	110.80
22	BA	974	G	C5-N7-C8	-15.02	96.79	104.30
22	BA	752	A	N1-C6-N6	14.90	127.54	118.60
22	BA	974	G	N1-C6-O6	14.51	128.61	119.90
22	BA	1779	U	N3-C4-O4	-13.09	110.24	119.40

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	AK	126	LYS	Peptide
21	AU	39	GLU	Peptide
48	B0	24	ALA	Peptide
25	BD	151	THR	Peptide
33	BL	28	GLY	Peptide

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32995	0	16607	1338	4
1	CA	33015	0	16617	1198	0
2	AB	1705	0	1732	164	0
2	CB	1705	0	1732	121	0
3	AC	1625	0	1696	89	0
3	CC	1625	0	1696	80	0
4	AD	1643	0	1707	133	0
4	CD	1643	0	1707	144	0
5	AE	1106	0	1148	83	0
5	CE	1106	0	1148	104	0
6	AF	818	0	808	62	0
6	CF	818	0	808	56	0
7	AG	1182	0	1238	65	0
7	CG	1182	0	1238	59	0
8	AH	979	0	1031	67	0
8	CH	979	0	1031	47	0
9	AI	1022	0	1070	77	0
9	CI	1022	0	1070	69	0
10	AJ	787	0	828	87	0
10	CJ	787	0	828	48	0
11	AK	877	0	887	79	0
11	CK	877	0	887	72	0
12	AL	955	0	1016	65	0
12	CL	955	0	1016	61	0
13	AM	884	0	941	80	0
13	CM	884	0	941	46	0
14	AN	774	0	824	66	0
14	CN	774	0	824	44	0
15	AO	710	0	728	35	0
15	CO	710	0	728	42	0
16	AP	649	0	666	53	0
16	CP	649	0	666	30	0
17	AQ	649	0	691	69	0
17	CQ	649	0	691	50	0
18	AR	456	0	478	22	0
18	CR	456	0	478	23	0
19	AS	638	0	665	48	0
19	CS	638	0	665	38	0
20	AT	665	0	714	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	CT	665	0	714	38	0
21	AU	426	0	449	61	0
21	CU	426	0	449	37	0
22	BA	62195	0	31280	2134	0
22	DA	62195	0	31280	2174	0
23	BB	2549	0	1291	56	0
23	DB	2529	0	1281	72	0
24	BC	2083	0	2154	157	0
24	DC	2083	0	2154	123	0
25	BD	1565	0	1616	92	0
25	DD	1565	0	1616	81	0
26	BE	1552	0	1619	75	0
26	DE	1552	0	1619	103	0
27	BF	1411	0	1444	105	0
27	DF	1411	0	1444	63	0
28	BG	1323	0	1371	61	0
28	DG	1323	0	1371	56	0
29	BH	1110	0	1147	154	0
29	DH	1110	0	1148	90	4
30	BI	1032	0	1085	82	0
30	DI	1032	0	1085	72	0
31	BJ	1129	0	1162	64	0
31	DJ	1129	0	1162	55	0
32	BK	939	0	1012	75	0
32	DK	939	0	1012	38	0
33	BL	1045	0	1117	51	0
33	DL	1045	0	1117	81	0
34	BM	1074	0	1157	47	0
34	DM	1074	0	1157	43	0
35	BN	961	0	1000	51	0
35	DN	961	0	1000	55	0
36	BO	892	0	923	57	0
36	DO	892	0	923	50	0
37	BP	917	0	962	48	0
37	DP	917	0	962	47	0
38	BQ	947	0	1019	61	0
38	DQ	947	0	1019	55	0
39	BR	816	0	839	84	0
39	DR	816	0	839	47	0
40	BS	857	0	922	64	0
40	DS	857	0	922	39	0
41	BT	739	0	807	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	DT	739	0	807	44	0
42	BU	780	0	831	50	0
42	DU	780	0	831	65	0
43	BV	753	0	780	31	0
43	DV	753	0	780	25	0
44	BW	580	0	594	23	0
44	DW	569	0	581	26	0
45	BX	625	0	652	35	0
45	DX	625	0	652	55	0
46	BY	509	0	543	29	0
46	DY	509	0	543	38	0
47	BZ	449	0	488	19	0
47	DZ	449	0	488	14	0
48	B0	444	0	458	33	0
48	D0	444	0	458	18	0
49	B1	410	0	440	32	0
49	D1	410	0	440	19	0
50	B2	377	0	418	19	0
50	D2	377	0	418	34	0
51	B3	504	0	572	22	0
51	D3	504	0	572	29	0
52	B4	302	0	340	12	0
52	D4	302	0	342	17	0
53	B5	1142	0	865	49	0
54	B6	69	0	44	5	0
54	D6	69	0	44	13	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	23	0
57	AL	1	0	0	0	0
57	AN	5	0	0	1	0
57	AT	2	0	0	1	0
57	AU	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	B2	1	0	0	0	0
57	B3	3	0	0	0	0
57	B4	2	0	0	0	0
57	BA	615	0	0	101	0
57	BB	14	0	0	0	0
57	BC	10	0	0	0	0
57	BD	4	0	0	2	0
57	BE	4	0	0	0	0
57	BF	1	0	0	1	0
57	BG	1	0	0	0	0
57	BJ	1	0	0	0	0
57	BL	6	0	0	0	0
57	BN	2	0	0	0	0
57	BS	1	0	0	0	0
57	BU	1	0	0	0	0
57	CA	189	0	0	20	0
57	CL	1	0	0	0	0
57	CN	3	0	0	2	0
57	CT	3	0	0	0	0
57	CU	2	0	0	0	0
57	D0	1	0	0	0	0
57	D2	2	0	0	0	0
57	D3	2	0	0	0	0
57	D4	1	0	0	0	0
57	DA	607	0	0	82	0
57	DB	13	0	0	3	0
57	DC	9	0	0	1	0
57	DD	4	0	0	2	0
57	DE	6	0	0	1	0
57	DL	5	0	0	1	0
57	DN	2	0	0	0	0
57	DT	2	0	0	0	0
57	DU	1	0	0	1	0
57	DV	1	0	0	0	0
All	All	288320	0	192877	11779	4

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 25.

The worst 5 of 11779 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
22:BA:1006:C:OP2	57:BA:3781:HOH:O	1.56	1.22

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
29:BH:117:LEU:O	29:BH:121:VAL:HG23	1.34	1.22
22:BA:2714:G:OP2	57:BA:3548:HOH:O	1.61	1.18
22:BA:1603:A:OP1	57:BA:3411:HOH:O	1.61	1.15
54:D6:4:PRO:HB2	54:D6:5:MHU:HM1	1.15	1.14

All (4) 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]	1.78	0.42
1:AA:368:U:OP1	29:DH:93:SER:OG[4_455]	1.93	0.27
1:AA:368:U:OP2	29:DH:123:ARG:NH2[4_455]	2.03	0.17
1:AA:368:U:OP2	29:DH:123:ARG:CZ[4_455]	2.07	0.13

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%)	135 (62%)	36 (17%)	45 (21%)	0	0
2	CB	216/218 (99%)	143 (66%)	36 (17%)	37 (17%)	0	1
3	AC	204/206 (99%)	142 (70%)	42 (21%)	20 (10%)	1	4
3	CC	204/206 (99%)	145 (71%)	41 (20%)	18 (9%)	1	5
4	AD	203/205 (99%)	133 (66%)	36 (18%)	34 (17%)	0	1
4	CD	203/205 (99%)	129 (64%)	48 (24%)	26 (13%)	0	2
5	AE	148/150 (99%)	98 (66%)	33 (22%)	17 (12%)	1	3
5	CE	148/150 (99%)	96 (65%)	29 (20%)	23 (16%)	0	1
6	AF	98/100 (98%)	61 (62%)	19 (19%)	18 (18%)	0	1
6	CF	98/100 (98%)	64 (65%)	18 (18%)	16 (16%)	0	1
7	AG	149/151 (99%)	110 (74%)	27 (18%)	12 (8%)	1	7
7	CG	149/151 (99%)	120 (80%)	21 (14%)	8 (5%)	3	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	AH	127/129 (98%)	80 (63%)	29 (23%)	18 (14%)	0	1
8	CH	127/129 (98%)	100 (79%)	19 (15%)	8 (6%)	2	12
9	AI	125/127 (98%)	90 (72%)	24 (19%)	11 (9%)	1	5
9	CI	125/127 (98%)	89 (71%)	27 (22%)	9 (7%)	2	8
10	AJ	96/98 (98%)	68 (71%)	7 (7%)	21 (22%)	0	0
10	CJ	96/98 (98%)	69 (72%)	18 (19%)	9 (9%)	1	5
11	AK	115/117 (98%)	83 (72%)	17 (15%)	15 (13%)	0	2
11	CK	115/117 (98%)	77 (67%)	28 (24%)	10 (9%)	1	5
12	AL	121/123 (98%)	92 (76%)	19 (16%)	10 (8%)	1	6
12	CL	121/123 (98%)	89 (74%)	17 (14%)	15 (12%)	1	2
13	AM	112/114 (98%)	79 (70%)	22 (20%)	11 (10%)	1	4
13	CM	112/114 (98%)	86 (77%)	15 (13%)	11 (10%)	1	4
14	AN	92/100 (92%)	57 (62%)	20 (22%)	15 (16%)	0	1
14	CN	92/100 (92%)	59 (64%)	20 (22%)	13 (14%)	0	2
15	AO	86/88 (98%)	60 (70%)	21 (24%)	5 (6%)	3	15
15	CO	86/88 (98%)	65 (76%)	18 (21%)	3 (4%)	6	30
16	AP	80/82 (98%)	52 (65%)	16 (20%)	12 (15%)	0	1
16	CP	80/82 (98%)	54 (68%)	20 (25%)	6 (8%)	2	8
17	AQ	78/80 (98%)	52 (67%)	16 (20%)	10 (13%)	0	2
17	CQ	78/80 (98%)	55 (70%)	13 (17%)	10 (13%)	0	2
18	AR	53/55 (96%)	40 (76%)	12 (23%)	1 (2%)	12	51
18	CR	53/55 (96%)	45 (85%)	4 (8%)	4 (8%)	2	8
19	AS	77/79 (98%)	52 (68%)	19 (25%)	6 (8%)	1	7
19	CS	77/79 (98%)	59 (77%)	14 (18%)	4 (5%)	3	18
20	AT	83/85 (98%)	51 (61%)	23 (28%)	9 (11%)	1	3
20	CT	83/85 (98%)	66 (80%)	11 (13%)	6 (7%)	2	8
21	AU	49/51 (96%)	23 (47%)	18 (37%)	8 (16%)	0	1
21	CU	49/51 (96%)	25 (51%)	10 (20%)	14 (29%)	0	0
24	BC	269/271 (99%)	208 (77%)	49 (18%)	12 (4%)	4	22
24	DC	269/271 (99%)	206 (77%)	42 (16%)	21 (8%)	1	7
25	BD	207/209 (99%)	176 (85%)	22 (11%)	9 (4%)	4	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	DD	207/209 (99%)	175 (84%)	24 (12%)	8 (4%)	5	26
26	BE	199/201 (99%)	164 (82%)	26 (13%)	9 (4%)	4	22
26	DE	199/201 (99%)	160 (80%)	27 (14%)	12 (6%)	2	14
27	BF	175/177 (99%)	136 (78%)	24 (14%)	15 (9%)	1	5
27	DF	175/177 (99%)	141 (81%)	23 (13%)	11 (6%)	2	12
28	BG	174/176 (99%)	146 (84%)	20 (12%)	8 (5%)	4	22
28	DG	174/176 (99%)	132 (76%)	33 (19%)	9 (5%)	3	18
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	4
30	BI	139/141 (99%)	79 (57%)	34 (24%)	26 (19%)	0	1
30	DI	139/141 (99%)	79 (57%)	42 (30%)	18 (13%)	0	2
31	BJ	140/142 (99%)	120 (86%)	17 (12%)	3 (2%)	11	47
31	DJ	140/142 (99%)	116 (83%)	18 (13%)	6 (4%)	4	23
32	BK	120/122 (98%)	94 (78%)	15 (12%)	11 (9%)	1	5
32	DK	120/122 (98%)	96 (80%)	14 (12%)	10 (8%)	1	6
33	BL	141/143 (99%)	108 (77%)	23 (16%)	10 (7%)	2	9
33	DL	141/143 (99%)	104 (74%)	28 (20%)	9 (6%)	2	11
34	BM	134/136 (98%)	114 (85%)	16 (12%)	4 (3%)	7	34
34	DM	134/136 (98%)	115 (86%)	13 (10%)	6 (4%)	4	22
35	BN	118/120 (98%)	97 (82%)	18 (15%)	3 (2%)	9	40
35	DN	118/120 (98%)	94 (80%)	16 (14%)	8 (7%)	2	10
36	BO	114/116 (98%)	87 (76%)	22 (19%)	5 (4%)	4	22
36	DO	114/116 (98%)	97 (85%)	15 (13%)	2 (2%)	13	53
37	BP	112/114 (98%)	97 (87%)	10 (9%)	5 (4%)	4	22
37	DP	112/114 (98%)	86 (77%)	19 (17%)	7 (6%)	2	12
38	BQ	115/117 (98%)	96 (84%)	15 (13%)	4 (4%)	6	30
38	DQ	115/117 (98%)	105 (91%)	9 (8%)	1 (1%)	25	73
39	BR	101/103 (98%)	89 (88%)	5 (5%)	7 (7%)	2	9
39	DR	101/103 (98%)	77 (76%)	17 (17%)	7 (7%)	2	9
40	BS	108/110 (98%)	91 (84%)	11 (10%)	6 (6%)	3	16
40	DS	108/110 (98%)	87 (81%)	14 (13%)	7 (6%)	2	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	BT	91/93 (98%)	69 (76%)	13 (14%)	9 (10%)	1	4
41	DT	91/93 (98%)	62 (68%)	19 (21%)	10 (11%)	1	3
42	BU	100/102 (98%)	75 (75%)	17 (17%)	8 (8%)	1	7
42	DU	100/102 (98%)	72 (72%)	15 (15%)	13 (13%)	0	2
43	BV	92/94 (98%)	83 (90%)	9 (10%)	0	100	100
43	DV	92/94 (98%)	76 (83%)	12 (13%)	4 (4%)	4	23
44	BW	74/76 (97%)	65 (88%)	9 (12%)	0	100	100
44	DW	73/76 (96%)	58 (80%)	10 (14%)	5 (7%)	2	10
45	BX	75/77 (97%)	64 (85%)	7 (9%)	4 (5%)	3	18
45	DX	75/77 (97%)	56 (75%)	15 (20%)	4 (5%)	3	18
46	BY	61/63 (97%)	38 (62%)	13 (21%)	10 (16%)	0	1
46	DY	61/63 (97%)	44 (72%)	11 (18%)	6 (10%)	1	4
47	BZ	56/58 (97%)	49 (88%)	4 (7%)	3 (5%)	3	17
47	DZ	56/58 (97%)	48 (86%)	5 (9%)	3 (5%)	3	17
48	B0	54/56 (96%)	42 (78%)	7 (13%)	5 (9%)	1	5
48	D0	54/56 (96%)	42 (78%)	8 (15%)	4 (7%)	2	8
49	B1	48/50 (96%)	39 (81%)	4 (8%)	5 (10%)	1	4
49	D1	48/50 (96%)	39 (81%)	6 (12%)	3 (6%)	2	12
50	B2	44/46 (96%)	36 (82%)	6 (14%)	2 (4%)	4	22
50	D2	44/46 (96%)	37 (84%)	4 (9%)	3 (7%)	2	10
51	B3	62/64 (97%)	51 (82%)	9 (14%)	2 (3%)	6	33
51	D3	62/64 (97%)	50 (81%)	9 (14%)	3 (5%)	4	20
52	B4	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
52	D4	36/38 (95%)	29 (81%)	6 (17%)	1 (3%)	8	37
53	B5	183/228 (80%)	100 (55%)	53 (29%)	30 (16%)	0	1
54	B6	2/7 (29%)	2 (100%)	0	0	100	100
54	D6	2/7 (29%)	1 (50%)	0	1 (50%)	0	0
All	All	11422/11686 (98%)	8514 (74%)	1907 (17%)	1001 (9%)	1	5

5 of 1001 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	22	TYR

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Mol	Chain	Res	Type
2	AB	64	LYS
2	AB	68	LEU
2	AB	73	LYS
2	AB	75	ALA

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%)	125 (69%)	55 (31%)	0	2
2	CB	180/180 (100%)	126 (70%)	54 (30%)	0	2
3	AC	170/170 (100%)	137 (81%)	33 (19%)	2	11
3	CC	170/170 (100%)	130 (76%)	40 (24%)	1	5
4	AD	172/172 (100%)	128 (74%)	44 (26%)	1	4
4	CD	172/172 (100%)	140 (81%)	32 (19%)	2	13
5	AE	113/113 (100%)	85 (75%)	28 (25%)	1	4
5	CE	113/113 (100%)	83 (74%)	30 (26%)	1	4
6	AF	87/87 (100%)	63 (72%)	24 (28%)	0	3
6	CF	87/87 (100%)	58 (67%)	29 (33%)	0	2
7	AG	124/124 (100%)	88 (71%)	36 (29%)	0	3
7	CG	124/124 (100%)	92 (74%)	32 (26%)	1	4
8	AH	104/104 (100%)	80 (77%)	24 (23%)	1	6
8	CH	104/104 (100%)	79 (76%)	25 (24%)	1	5
9	AI	105/105 (100%)	73 (70%)	32 (30%)	0	2
9	CI	105/105 (100%)	73 (70%)	32 (30%)	0	2
10	AJ	86/86 (100%)	61 (71%)	25 (29%)	0	2
10	CJ	86/86 (100%)	70 (81%)	16 (19%)	2	13
11	AK	90/90 (100%)	70 (78%)	20 (22%)	1	7
11	CK	90/90 (100%)	67 (74%)	23 (26%)	1	4
12	AL	103/103 (100%)	78 (76%)	25 (24%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	CL	103/103 (100%)	78 (76%)	25 (24%)	1	5
13	AM	92/92 (100%)	65 (71%)	27 (29%)	0	2
13	CM	92/92 (100%)	69 (75%)	23 (25%)	1	4
14	AN	79/83 (95%)	63 (80%)	16 (20%)	2	9
14	CN	79/83 (95%)	69 (87%)	10 (13%)	6	27
15	AO	75/76 (99%)	61 (81%)	14 (19%)	2	12
15	CO	75/76 (99%)	64 (85%)	11 (15%)	4	21
16	AP	65/65 (100%)	50 (77%)	15 (23%)	1	6
16	CP	65/65 (100%)	52 (80%)	13 (20%)	2	10
17	AQ	74/74 (100%)	50 (68%)	24 (32%)	0	2
17	CQ	74/74 (100%)	54 (73%)	20 (27%)	1	3
18	AR	48/48 (100%)	40 (83%)	8 (17%)	3	16
18	CR	48/48 (100%)	43 (90%)	5 (10%)	10	37
19	AS	70/70 (100%)	59 (84%)	11 (16%)	4	18
19	CS	70/70 (100%)	53 (76%)	17 (24%)	1	5
20	AT	65/65 (100%)	49 (75%)	16 (25%)	1	4
20	CT	65/65 (100%)	49 (75%)	16 (25%)	1	4
21	AU	44/44 (100%)	29 (66%)	15 (34%)	0	1
21	CU	44/44 (100%)	29 (66%)	15 (34%)	0	1
24	BC	216/216 (100%)	182 (84%)	34 (16%)	4	18
24	DC	216/216 (100%)	189 (88%)	27 (12%)	7	28
25	BD	164/164 (100%)	145 (88%)	19 (12%)	8	31
25	DD	164/164 (100%)	145 (88%)	19 (12%)	8	31
26	BE	165/165 (100%)	137 (83%)	28 (17%)	3	15
26	DE	165/165 (100%)	131 (79%)	34 (21%)	2	9
27	BF	148/148 (100%)	121 (82%)	27 (18%)	2	13
27	DF	148/148 (100%)	116 (78%)	32 (22%)	1	8
28	BG	137/137 (100%)	118 (86%)	19 (14%)	5	23
28	DG	137/137 (100%)	119 (87%)	18 (13%)	6	25
29	BH	114/114 (100%)	88 (77%)	26 (23%)	1	6
29	DH	114/114 (100%)	88 (77%)	26 (23%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	BI	109/109 (100%)	80 (73%)	29 (27%)	1	4
30	DI	109/109 (100%)	85 (78%)	24 (22%)	1	7
31	BJ	116/116 (100%)	106 (91%)	10 (9%)	15	50
31	DJ	116/116 (100%)	103 (89%)	13 (11%)	9	33
32	BK	103/103 (100%)	90 (87%)	13 (13%)	7	27
32	DK	103/103 (100%)	93 (90%)	10 (10%)	12	42
33	BL	102/102 (100%)	86 (84%)	16 (16%)	4	18
33	DL	102/102 (100%)	80 (78%)	22 (22%)	1	8
34	BM	109/109 (100%)	92 (84%)	17 (16%)	4	18
34	DM	109/109 (100%)	93 (85%)	16 (15%)	4	21
35	BN	100/100 (100%)	83 (83%)	17 (17%)	3	15
35	DN	100/100 (100%)	77 (77%)	23 (23%)	1	6
36	BO	86/86 (100%)	63 (73%)	23 (27%)	1	4
36	DO	86/86 (100%)	71 (83%)	15 (17%)	3	14
37	BP	99/99 (100%)	84 (85%)	15 (15%)	4	20
37	DP	99/99 (100%)	83 (84%)	16 (16%)	3	17
38	BQ	89/89 (100%)	75 (84%)	14 (16%)	4	18
38	DQ	89/89 (100%)	76 (85%)	13 (15%)	5	21
39	BR	84/84 (100%)	69 (82%)	15 (18%)	2	13
39	DR	84/84 (100%)	73 (87%)	11 (13%)	6	25
40	BS	93/93 (100%)	75 (81%)	18 (19%)	2	11
40	DS	93/93 (100%)	80 (86%)	13 (14%)	5	23
41	BT	80/80 (100%)	68 (85%)	12 (15%)	4	20
41	DT	80/80 (100%)	64 (80%)	16 (20%)	2	10
42	BU	83/83 (100%)	66 (80%)	17 (20%)	2	9
42	DU	83/83 (100%)	60 (72%)	23 (28%)	0	3
43	BV	78/78 (100%)	62 (80%)	16 (20%)	2	9
43	DV	78/78 (100%)	67 (86%)	11 (14%)	5	23
44	BW	57/58 (98%)	50 (88%)	7 (12%)	7	28
44	DW	56/58 (97%)	51 (91%)	5 (9%)	14	48
45	BX	67/67 (100%)	56 (84%)	11 (16%)	3	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	DX	67/67 (100%)	57 (85%)	10 (15%)	4	20
46	BY	55/55 (100%)	47 (86%)	8 (14%)	5	22
46	DY	55/55 (100%)	45 (82%)	10 (18%)	2	13
47	BZ	48/48 (100%)	42 (88%)	6 (12%)	7	28
47	DZ	48/48 (100%)	35 (73%)	13 (27%)	1	3
48	B0	47/47 (100%)	40 (85%)	7 (15%)	4	20
48	D0	47/47 (100%)	43 (92%)	4 (8%)	15	51
49	B1	45/45 (100%)	37 (82%)	8 (18%)	2	14
49	D1	45/45 (100%)	39 (87%)	6 (13%)	6	25
50	B2	38/38 (100%)	33 (87%)	5 (13%)	6	25
50	D2	38/38 (100%)	32 (84%)	6 (16%)	4	18
51	B3	51/51 (100%)	40 (78%)	11 (22%)	1	8
51	D3	51/51 (100%)	47 (92%)	4 (8%)	18	55
52	B4	34/34 (100%)	29 (85%)	5 (15%)	4	21
52	D4	34/34 (100%)	29 (85%)	5 (15%)	4	21
53	B5	61/180 (34%)	47 (77%)	14 (23%)	1	6
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%)	7518 (80%)	1872 (20%)	2	10

5 of 1872 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
42	BU	15	THR
3	CC	185	ASN
38	DQ	51	ARG
43	BV	65	VAL
53	B5	39	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
37	BP	56	HIS
51	B3	31	HIS
37	DP	41	GLN

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Mol	Chain	Res	Type
48	B0	42	HIS
51	B3	43	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1537/1539 (99%)	361 (23%)	0
1	CA	1538/1539 (99%)	335 (21%)	0
22	BA	2895/2903 (99%)	672 (23%)	0
22	DA	2895/2903 (99%)	609 (21%)	0
23	BB	118/119 (99%)	27 (22%)	0
23	DB	117/119 (98%)	25 (21%)	0
All	All	9100/9122 (99%)	2029 (22%)	0

5 of 2029 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	5	U
1	AA	9	G
1	AA	13	U
1	AA	32	A

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	2.70	4 (44%)	8,11,13	3.13	6 (75%)
54	DBB	B6	3	54	5,5,6	6.75	1 (20%)	3,5,7	4.31	1 (33%)

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	4.68	7 (46%)	16,19,21	2.07	3 (18%)
54	04X	B6	6	54	16,16,17	2.88	5 (31%)	18,20,22	5.07	11 (61%)
54	004	B6	7	54	10,10,11	4.73	7 (70%)	10,12,14	11.23	2 (20%)
54	MHW	D6	1	54	9,9,10	2.55	3 (33%)	8,11,13	2.25	7 (87%)
54	DBB	D6	3	54	5,5,6	6.42	1 (20%)	3,5,7	1.74	2 (66%)
54	MHU	D6	5	54	15,15,16	4.94	7 (46%)	16,19,21	2.08	3 (18%)
54	04X	D6	6	54	16,16,17	2.94	4 (25%)	18,20,22	6.16	12 (66%)
54	004	D6	7	54	10,10,11	5.46	7 (70%)	10,12,14	10.33	3 (30%)

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	04X	B6	6	54	-	0/4/24/26	0/2/2/2
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	-	1/10/12/14	0/1/1/1
54	04X	D6	6	54	-	0/4/24/26	0/2/2/2
54	004	D6	7	54	-	0/4/6/8	0/1/1/1

The worst 5 of 46 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	D6	5	MHU	O-C	15.89	1.22	1.11
54	B6	3	DBB	O-C	14.95	1.21	1.11
54	B6	5	MHU	O-C	14.88	1.21	1.11
54	D6	3	DBB	O-C	14.12	1.21	1.11
54	B6	7	004	CB-CA	-11.32	1.45	1.52

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	B6	7	004	C-CA-N	35.25	117.26	113.27
54	D6	7	004	C-CA-N	-32.06	109.64	113.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	D6	6	04X	C0-N1-C1	17.27	135.46	110.98
54	B6	6	04X	C0-N1-C1	14.39	131.37	110.98
54	D6	6	04X	CE-N-CA	12.44	121.04	110.86

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	D6	5	MHU	C-CA-N-CM

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
54	B6	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B6	2:THR	C	3:DBB	N	1.61

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%)	-0.47	18 (1%) 75 20	14, 54, 137, 179	0
1	CA	1539/1539 (100%)	-0.29	27 (1%) 65 14	27, 72, 145, 177	0
2	AB	218/218 (100%)	0.64	12 (5%) 24 5	43, 76, 100, 125	0
2	CB	218/218 (100%)	0.80	20 (9%) 9 2	63, 86, 106, 126	0
3	AC	206/206 (100%)	0.01	1 (0%) 88 36	39, 61, 83, 96	0
3	CC	206/206 (100%)	0.61	6 (2%) 49 9	57, 79, 97, 109	0
4	AD	205/205 (100%)	-0.04	0 100 100	35, 58, 79, 106	0
4	CD	205/205 (100%)	-0.16	2 (0%) 79 22	21, 40, 71, 90	0
5	AE	150/150 (100%)	-0.02	0 100 100	27, 51, 82, 106	0
5	CE	150/150 (100%)	-0.04	0 100 100	34, 59, 87, 104	0
6	AF	100/100 (100%)	-0.22	0 100 100	38, 59, 76, 84	0
6	CF	100/100 (100%)	-0.14	0 100 100	46, 74, 96, 104	0
7	AG	151/151 (100%)	0.44	5 (3%) 44 8	54, 78, 98, 108	0
7	CG	151/151 (100%)	0.95	15 (9%) 8 2	77, 97, 107, 113	0
8	AH	129/129 (100%)	-0.13	0 100 100	30, 50, 73, 81	0
8	CH	129/129 (100%)	0.03	0 100 100	45, 65, 81, 90	0
9	AI	127/127 (100%)	0.65	7 (5%) 24 5	51, 73, 97, 113	0
9	CI	127/127 (100%)	0.89	13 (10%) 7 2	71, 91, 109, 126	0
10	AJ	98/98 (100%)	0.23	3 (3%) 47 9	46, 68, 92, 122	0
10	CJ	98/98 (100%)	1.12	16 (16%) 2 1	71, 93, 110, 124	0
11	AK	117/117 (100%)	0.28	2 (1%) 67 15	32, 64, 91, 110	0
11	CK	117/117 (100%)	-0.01	1 (0%) 81 24	44, 68, 82, 91	0
12	AL	123/123 (100%)	0.05	1 (0%) 83 26	23, 39, 68, 94	0
12	CL	123/123 (100%)	0.03	4 (3%) 44 8	39, 52, 79, 99	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	114/114 (100%)	0.19	2 (1%) 65 14	49, 71, 92, 105	0
13	CM	114/114 (100%)	1.26	24 (21%) 1 1	90, 103, 116, 120	0
14	AN	96/100 (96%)	0.47	4 (4%) 35 7	43, 63, 94, 106	0
14	CN	96/100 (96%)	1.10	20 (20%) 1 1	69, 91, 110, 118	0
15	AO	88/88 (100%)	-0.02	0 100 100	31, 51, 68, 98	0
15	CO	88/88 (100%)	-0.02	0 100 100	43, 63, 81, 105	0
16	AP	82/82 (100%)	0.28	2 (2%) 56 11	35, 49, 84, 100	0
16	CP	82/82 (100%)	0.40	3 (3%) 39 8	45, 62, 88, 106	0
17	AQ	80/80 (100%)	-0.02	1 (1%) 74 19	27, 54, 81, 124	0
17	CQ	80/80 (100%)	0.33	3 (3%) 38 7	44, 72, 96, 105	0
18	AR	55/55 (100%)	-0.07	3 (5%) 24 5	39, 53, 81, 112	0
18	CR	55/55 (100%)	0.04	1 (1%) 65 14	46, 56, 82, 111	0
19	AS	79/79 (100%)	0.55	5 (6%) 19 5	55, 72, 92, 101	0
19	CS	79/79 (100%)	1.71	26 (32%) 1 0	87, 103, 114, 123	0
20	AT	85/85 (100%)	0.05	1 (1%) 75 20	35, 51, 74, 111	0
20	CT	85/85 (100%)	0.88	12 (14%) 3 1	53, 72, 93, 96	0
21	AU	51/51 (100%)	1.14	9 (17%) 2 1	56, 76, 95, 108	0
21	CU	51/51 (100%)	0.38	3 (5%) 22 5	48, 72, 94, 108	0
22	BA	2897/2903 (99%)	-0.26	98 (3%) 43 8	0, 14, 130, 195	0
22	DA	2897/2903 (99%)	-0.18	53 (1%) 65 14	42, 83, 144, 183	0
23	BB	119/119 (100%)	-0.61	0 100 100	1, 24, 54, 90	0
23	DB	118/119 (99%)	-0.42	0 100 100	66, 111, 133, 141	0
24	BC	271/271 (100%)	-0.20	2 (0%) 84 28	3, 21, 43, 55	0
24	DC	271/271 (100%)	0.26	10 (3%) 39 8	42, 62, 76, 91	0
25	BD	209/209 (100%)	-0.33	0 100 100	0, 9, 38, 71	0
25	DD	209/209 (100%)	0.27	4 (1%) 64 13	46, 66, 81, 99	0
26	BE	201/201 (100%)	-0.30	0 100 100	0, 24, 56, 91	0
26	DE	201/201 (100%)	0.54	7 (3%) 42 8	45, 81, 98, 106	0
27	BF	177/177 (100%)	0.10	8 (4%) 32 7	15, 46, 88, 97	0
27	DF	177/177 (100%)	1.35	45 (25%) 1 1	85, 102, 117, 125	0
28	BG	176/176 (100%)	-0.16	0 100 100	15, 38, 64, 88	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DG	176/176 (100%)	0.67	6 (3%) 43 8	71, 90, 104, 117	0
29	BH	149/149 (100%)	1.29	37 (24%) 1 1	25, 102, 121, 129	0
29	DH	149/149 (100%)	0.60	11 (7%) 14 3	25, 92, 107, 115	0
30	BI	141/141 (100%)	1.56	40 (28%) 1 0	84, 108, 121, 136	0
30	DI	141/141 (100%)	2.11	67 (47%) 1 0	96, 114, 123, 127	0
31	BJ	142/142 (100%)	-0.34	0 100 100	1, 5, 23, 43	0
31	DJ	142/142 (100%)	0.22	3 (2%) 60 12	48, 64, 79, 96	0
32	BK	122/122 (100%)	-0.38	0 100 100	2, 11, 37, 67	0
32	DK	122/122 (100%)	0.29	2 (1%) 68 16	48, 61, 81, 96	0
33	BL	143/143 (100%)	-0.27	0 100 100	0, 21, 48, 76	0
33	DL	143/143 (100%)	0.80	13 (9%) 9 2	42, 77, 91, 113	0
34	BM	136/136 (100%)	-0.34	0 100 100	1, 9, 30, 87	0
34	DM	136/136 (100%)	0.42	5 (3%) 39 8	42, 67, 82, 108	0
35	BN	120/120 (100%)	-0.33	0 100 100	1, 6, 17, 62	0
35	DN	120/120 (100%)	0.37	6 (5%) 28 6	54, 74, 88, 110	0
36	BO	116/116 (100%)	-0.20	0 100 100	14, 27, 46, 52	0
36	DO	116/116 (100%)	0.93	13 (11%) 6 2	74, 91, 102, 114	0
37	BP	114/114 (100%)	-0.24	0 100 100	5, 19, 48, 70	0
37	DP	114/114 (100%)	0.28	0 100 100	56, 68, 84, 93	0
38	BQ	117/117 (100%)	-0.34	0 100 100	0, 3, 11, 42	0
38	DQ	117/117 (100%)	0.21	2 (1%) 67 15	52, 66, 77, 84	0
39	BR	103/103 (100%)	-0.35	0 100 100	1, 9, 31, 63	0
39	DR	103/103 (100%)	0.47	2 (1%) 64 13	50, 75, 87, 97	0
40	BS	110/110 (100%)	-0.28	0 100 100	1, 3, 23, 84	0
40	DS	110/110 (100%)	0.70	5 (4%) 32 7	56, 73, 89, 96	0
41	BT	93/93 (100%)	0.05	1 (1%) 77 21	10, 27, 80, 101	0
41	DT	93/93 (100%)	1.13	17 (18%) 2 1	63, 83, 103, 110	0
42	BU	102/102 (100%)	-0.08	0 100 100	10, 30, 61, 92	0
42	DU	102/102 (100%)	1.54	36 (35%) 1 0	70, 88, 106, 112	0
43	BV	94/94 (100%)	-0.29	0 100 100	4, 22, 43, 54	0
43	DV	94/94 (100%)	0.23	1 (1%) 77 21	65, 82, 94, 99	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BW	76/76 (100%)	-0.27	0 100 100	3, 10, 27, 48	0
44	DW	75/76 (98%)	0.95	11 (14%) 3 1	54, 79, 88, 108	0
45	BX	77/77 (100%)	-0.23	0 100 100	6, 24, 52, 77	0
45	DX	77/77 (100%)	0.47	4 (5%) 26 6	49, 69, 86, 89	0
46	BY	63/63 (100%)	0.00	1 (1%) 68 16	22, 44, 74, 96	0
46	DY	63/63 (100%)	0.61	5 (7%) 13 3	71, 90, 99, 103	0
47	BZ	58/58 (100%)	-0.28	0 100 100	2, 7, 29, 41	0
47	DZ	58/58 (100%)	0.21	1 (1%) 67 15	52, 70, 84, 89	0
48	B0	56/56 (100%)	-0.38	0 100 100	0, 8, 35, 70	0
48	D0	56/56 (100%)	0.43	2 (3%) 41 8	53, 74, 91, 104	0
49	B1	50/50 (100%)	-0.19	1 (2%) 62 12	13, 31, 54, 87	0
49	D1	50/50 (100%)	0.65	5 (10%) 8 2	68, 84, 93, 105	0
50	B2	46/46 (100%)	-0.26	1 (2%) 59 12	3, 9, 17, 90	0
50	D2	46/46 (100%)	0.73	4 (8%) 10 3	53, 66, 79, 100	0
51	B3	64/64 (100%)	-0.27	0 100 100	4, 9, 18, 31	0
51	D3	64/64 (100%)	0.69	6 (9%) 9 2	58, 71, 79, 85	0
52	B4	38/38 (100%)	-0.07	0 100 100	11, 20, 35, 52	0
52	D4	38/38 (100%)	1.09	7 (18%) 2 1	63, 74, 85, 99	0
53	B5	191/228 (83%)	2.68	127 (66%) 0 0	85, 111, 123, 134	0
54	B6	6/7 (85%)	1.02	1 (16%) 2 1	5, 9, 17, 17	0
54	D6	6/7 (85%)	1.99	2 (33%) 1 0	53, 58, 61, 62	0
All	All	20746/20808 (99%)	0.07	944 (4%) 31 7	0, 64, 119, 195	0

The worst 5 of 944 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	BA	2104	C	13.3
22	BA	2185	U	13.0
22	BA	2100	G	12.3
22	BA	2184	A	11.9
30	BI	53	LEU	11.5

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	MHU	D6	5	15/16	0.37	1.99	45,58,69,72	0
54	004	B6	7	10/11	0.28	1.85	2,4,6,6	0
54	MHW	B6	1	9/10	0.21	1.35	8,13,21,30	0
54	DBB	B6	3	6/7	0.29	1.33	8,14,20,33	0
54	MHW	D6	1	9/10	0.22	1.20	55,59,63,66	0
54	DBB	D6	3	6/7	0.56	1.08	45,50,65,70	0
54	MHU	B6	5	15/16	0.24	0.74	3,7,15,15	0
54	004	D6	7	10/11	0.22	0.09	47,52,61,64	0
54	04X	D6	6	15/16	0.26	-0.14	47,59,67,73	0
54	04X	B6	6	15/16	0.19	-0.74	6,11,15,20	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	AA	1614	1/1	0.25	175.36	66,66,66,66	0
55	MG	CA	1654	1/1	0.25	129.00	26,26,26,26	0
55	MG	AA	1661	1/1	0.44	123.80	23,23,23,23	0
55	MG	CA	1647	1/1	0.34	93.97	35,35,35,35	0
55	MG	DA	3139	1/1	0.65	73.50	47,47,47,47	0
55	MG	CA	1650	1/1	0.67	70.09	50,50,50,50	0
55	MG	AA	1659	1/1	0.49	70.09	32,32,32,32	0
55	MG	AA	1644	1/1	0.65	69.43	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	AA	1665	1/1	0.68	67.85	53,53,53,53	0
55	MG	DA	3061	1/1	1.67	64.18	97,97,97,97	0
55	MG	BA	3061	1/1	0.68	55.41	66,66,66,66	0
55	MG	BB	204	1/1	0.35	48.36	0,0,0,0	0
55	MG	AA	1667	1/1	0.72	44.48	54,54,54,54	0
55	MG	DA	3132	1/1	0.78	43.58	85,85,85,85	0
55	MG	BA	3098	1/1	0.61	36.84	73,73,73,73	0
55	MG	CA	1655	1/1	0.79	35.02	67,67,67,67	0
55	MG	DA	3062	1/1	0.77	34.00	70,70,70,70	0
55	MG	CA	1637	1/1	0.41	33.93	80,80,80,80	0
55	MG	AA	1627	1/1	0.51	33.63	76,76,76,76	0
55	MG	AA	1668	1/1	0.34	33.07	33,33,33,33	0
55	MG	BA	3180	1/1	0.57	33.06	25,25,25,25	0
55	MG	BA	3176	1/1	0.27	32.59	24,24,24,24	0
55	MG	DA	3120	1/1	0.52	31.35	95,95,95,95	0
55	MG	AA	1651	1/1	0.35	31.29	55,55,55,55	0
55	MG	DA	3015	1/1	0.57	30.40	77,77,77,77	0
55	MG	DA	3077	1/1	0.27	29.91	76,76,76,76	0
55	MG	BA	3190	1/1	0.38	28.88	42,42,42,42	0
55	MG	BA	3186	1/1	0.26	28.48	12,12,12,12	0
55	MG	DA	3099	1/1	0.50	27.83	82,82,82,82	0
55	MG	AA	1657	1/1	0.42	27.29	37,37,37,37	0
55	MG	DA	3026	1/1	0.81	27.22	75,75,75,75	0
55	MG	DA	3089	1/1	0.57	26.13	91,91,91,91	0
55	MG	CA	1633	1/1	0.77	25.54	82,82,82,82	0
55	MG	BA	3015	1/1	0.41	24.15	61,61,61,61	0
55	MG	DA	3016	1/1	0.53	23.88	84,84,84,84	0
55	MG	DA	3136	1/1	0.44	23.33	81,81,81,81	0
55	MG	BA	3179	1/1	0.36	22.89	30,30,30,30	0
55	MG	BA	3025	1/1	0.21	22.27	40,40,40,40	0
55	MG	DA	3014	1/1	0.36	21.70	73,73,73,73	0
55	MG	BA	3119	1/1	0.38	21.60	49,49,49,49	0
55	MG	CA	1644	1/1	0.43	21.07	36,36,36,36	0
55	MG	AA	1671	1/1	0.45	21.07	54,54,54,54	0
55	MG	BA	3178	1/1	0.36	20.93	12,12,12,12	0
55	MG	DA	3164	1/1	0.74	19.34	56,56,56,56	0
55	MG	BA	3044	1/1	0.21	16.59	8,8,8,8	0
55	MG	DA	3155	1/1	0.31	16.35	37,37,37,37	0
55	MG	BA	3040	1/1	0.37	16.19	2,2,2,2	0
55	MG	CA	1653	1/1	0.38	15.56	48,48,48,48	0
55	MG	DA	3007	1/1	0.33	15.09	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CA	1615	1/1	0.26	15.08	56,56,56,56	0
55	MG	CA	1618	1/1	0.21	14.88	35,35,35,35	0
55	MG	BA	3027	1/1	0.37	14.67	36,36,36,36	0
55	MG	BA	3056	1/1	0.21	14.55	22,22,22,22	0
55	MG	AA	1646	1/1	0.23	14.19	50,50,50,50	0
55	MG	DA	3113	1/1	0.45	13.85	75,75,75,75	0
55	MG	DA	3002	1/1	0.46	13.64	81,81,81,81	0
55	MG	DA	3151	1/1	0.47	13.62	40,40,40,40	0
55	MG	BA	3141	1/1	0.39	13.42	0,0,0,0	0
55	MG	DA	3141	1/1	0.43	13.37	45,45,45,45	0
55	MG	DA	3057	1/1	0.30	13.07	82,82,82,82	0
55	MG	AA	1602	1/1	0.34	12.92	53,53,53,53	0
55	MG	DA	3100	1/1	0.34	12.90	73,73,73,73	0
55	MG	BA	3131	1/1	0.38	12.62	37,37,37,37	0
55	MG	DA	3071	1/1	0.56	12.28	93,93,93,93	0
55	MG	DA	3072	1/1	0.46	11.45	89,89,89,89	0
55	MG	BA	3154	1/1	0.29	11.32	21,21,21,21	0
55	MG	BA	3136	1/1	0.55	11.31	43,43,43,43	0
55	MG	BA	3150	1/1	0.19	11.17	37,37,37,37	0
55	MG	AA	1670	1/1	0.35	11.16	45,45,45,45	0
55	MG	CA	1605	1/1	0.24	10.49	78,78,78,78	0
55	MG	BA	3138	1/1	0.28	10.37	0,0,0,0	0
55	MG	DA	3041	1/1	0.40	10.13	66,66,66,66	0
55	MG	DA	3161	1/1	0.28	9.75	48,48,48,48	0
55	MG	DA	3030	1/1	0.31	9.55	61,61,61,61	0
55	MG	BA	3170	1/1	0.18	8.82	22,22,22,22	0
55	MG	DA	3150	1/1	0.20	8.81	50,50,50,50	0
55	MG	BA	3142	1/1	0.21	8.66	0,0,0,0	0
55	MG	DA	3056	1/1	0.30	8.63	80,80,80,80	0
55	MG	DA	3142	1/1	0.39	8.58	39,39,39,39	0
55	MG	DA	3093	1/1	0.38	8.56	99,99,99,99	0
55	MG	BA	3157	1/1	0.30	8.34	34,34,34,34	0
55	MG	DA	3159	1/1	0.30	8.27	57,57,57,57	0
55	MG	DA	3138	1/1	0.34	7.92	37,37,37,37	0
55	MG	DA	3158	1/1	0.41	7.88	58,58,58,58	0
55	MG	AA	1635	1/1	0.24	7.80	76,76,76,76	0
55	MG	AM	201	1/1	0.59	7.69	50,50,50,50	0
55	MG	DA	3102	1/1	0.40	7.57	72,72,72,72	0
55	MG	DA	3154	1/1	0.28	7.39	40,40,40,40	0
55	MG	CA	1625	1/1	0.17	7.08	18,18,18,18	0
55	MG	DA	3165	1/1	0.35	7.05	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3103	1/1	0.30	6.97	67,67,67,67	0
55	MG	CA	1649	1/1	0.19	6.94	24,24,24,24	0
55	MG	DA	3092	1/1	0.37	6.83	94,94,94,94	0
55	MG	BA	3055	1/1	0.31	6.79	50,50,50,50	0
55	MG	DA	3032	1/1	0.25	6.73	78,78,78,78	0
55	MG	BA	3115	1/1	0.42	6.69	76,76,76,76	0
55	MG	BA	3143	1/1	0.31	6.51	3,3,3,3	0
55	MG	CA	1628	1/1	0.26	6.40	100,100,100,100	0
55	MG	CA	1643	1/1	0.36	6.28	41,41,41,41	0
55	MG	BA	3135	1/1	0.26	6.25	48,48,48,48	0
55	MG	BA	3173	1/1	0.23	6.19	30,30,30,30	0
55	MG	DA	3029	1/1	0.33	6.07	66,66,66,66	0
55	MG	AA	1603	1/1	0.19	6.05	57,57,57,57	0
55	MG	CA	1642	1/1	0.23	5.95	25,25,25,25	0
55	MG	BA	3076	1/1	0.29	5.91	56,56,56,56	0
55	MG	BA	3192	1/1	0.24	5.69	11,11,11,11	0
55	MG	BA	3057	1/1	0.26	5.66	20,20,20,20	0
55	MG	BA	3019	1/1	0.25	5.64	1,1,1,1	0
55	MG	CA	1626	1/1	0.27	5.51	66,66,66,66	0
55	MG	BA	3146	1/1	0.21	5.48	22,22,22,22	0
55	MG	DA	3148	1/1	0.27	5.40	51,51,51,51	0
55	MG	DA	3021	1/1	0.38	5.37	62,62,62,62	0
55	MG	BA	3171	1/1	0.22	5.31	20,20,20,20	0
55	MG	CA	1627	1/1	0.31	5.30	88,88,88,88	0
55	MG	BA	3168	1/1	0.22	5.21	21,21,21,21	0
55	MG	BA	3133	1/1	0.38	5.19	57,57,57,57	0
55	MG	BA	3183	1/1	0.22	5.05	22,22,22,22	0
55	MG	BA	3160	1/1	0.22	4.99	5,5,5,5	0
55	MG	BA	3166	1/1	0.21	4.97	37,37,37,37	0
55	MG	BA	3104	1/1	0.26	4.94	0,0,0,0	0
55	MG	BA	3137	1/1	0.27	4.89	2,2,2,2	0
55	MG	AA	1648	1/1	0.26	4.85	39,39,39,39	0
55	MG	BA	3090	1/1	0.19	4.73	33,33,33,33	0
55	MG	DA	3028	1/1	0.59	4.51	86,86,86,86	0
55	MG	DA	3106	1/1	0.30	4.36	70,70,70,70	0
55	MG	CA	1630	1/1	0.66	4.28	102,102,102,102	0
55	MG	BA	3140	1/1	0.15	4.21	7,7,7,7	0
55	MG	DA	3104	1/1	0.17	4.14	76,76,76,76	0
55	MG	AA	1650	1/1	0.22	3.91	20,20,20,20	0
55	MG	BA	3083	1/1	0.20	3.76	34,34,34,34	0
55	MG	BA	3014	1/1	0.23	3.76	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	1622	1/1	0.21	3.72	21,21,21,21	0
55	MG	BA	3106	1/1	0.24	3.50	0,0,0,0	0
55	MG	DA	3166	1/1	0.17	3.49	44,44,44,44	0
55	MG	DA	3110	1/1	0.24	3.35	45,45,45,45	0
55	MG	CA	1638	1/1	0.17	3.30	74,74,74,74	0
55	MG	CA	1620	1/1	0.14	3.15	81,81,81,81	0
55	MG	AA	1658	1/1	0.19	3.11	35,35,35,35	0
55	MG	DA	3064	1/1	0.22	3.09	48,48,48,48	0
55	MG	BA	3033	1/1	0.21	2.97	0,0,0,0	0
55	MG	DA	3116	1/1	0.35	2.96	92,92,92,92	0
55	MG	DA	3134	1/1	0.52	2.86	87,87,87,87	0
55	MG	BA	3067	1/1	0.20	2.86	0,0,0,0	0
55	MG	CA	1646	1/1	0.19	2.77	36,36,36,36	0
55	MG	DA	3004	1/1	0.37	2.72	87,87,87,87	0
55	MG	DA	3137	1/1	0.31	2.71	84,84,84,84	0
55	MG	BA	3016	1/1	0.22	2.70	31,31,31,31	0
55	MG	BA	3139	1/1	0.23	2.69	0,0,0,0	0
55	MG	DA	3045	1/1	0.22	2.67	61,61,61,61	0
55	MG	AA	1610	1/1	0.14	2.64	51,51,51,51	0
55	MG	BA	3105	1/1	0.22	2.52	0,0,0,0	0
55	MG	AA	1605	1/1	0.20	2.49	29,29,29,29	0
55	MG	AA	1626	1/1	0.22	2.42	26,26,26,26	0
55	MG	BA	3072	1/1	0.19	2.39	2,2,2,2	0
55	MG	BA	3092	1/1	0.16	2.39	42,42,42,42	0
55	MG	DA	3034	1/1	0.22	2.33	58,58,58,58	0
55	MG	AA	1662	1/1	0.32	2.32	49,49,49,49	0
55	MG	AA	1623	1/1	0.14	2.31	49,49,49,49	0
55	MG	DA	3149	1/1	0.15	2.28	49,49,49,49	0
55	MG	CA	1651	1/1	0.25	2.28	72,72,72,72	0
55	MG	BA	3164	1/1	0.29	2.26	6,6,6,6	0
55	MG	DA	3095	1/1	0.23	2.25	69,69,69,69	0
55	MG	BA	3053	1/1	0.18	2.24	0,0,0,0	0
55	MG	BA	3039	1/1	0.21	2.22	1,1,1,1	0
55	MG	BA	3011	1/1	0.21	2.17	30,30,30,30	0
55	MG	AA	1653	1/1	0.16	2.11	34,34,34,34	0
55	MG	BA	3128	1/1	0.19	1.95	3,3,3,3	0
55	MG	BA	3125	1/1	0.19	1.89	2,2,2,2	0
55	MG	DA	3020	1/1	0.20	1.87	44,44,44,44	0
55	MG	BA	3189	1/1	0.19	1.84	0,0,0,0	0
55	MG	BA	3144	1/1	0.27	1.80	24,24,24,24	0
55	MG	BA	3152	1/1	0.26	1.76	8,8,8,8	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	3109	1/1	0.19	1.75	1,1,1,1	0
55	MG	BA	3194	1/1	0.18	1.74	22,22,22,22	0
55	MG	BA	3149	1/1	0.21	1.70	0,0,0,0	0
55	MG	DA	3060	1/1	0.24	1.62	72,72,72,72	0
55	MG	BA	3167	1/1	0.16	1.52	22,22,22,22	0
55	MG	CA	1636	1/1	0.31	1.43	97,97,97,97	0
55	MG	AA	1631	1/1	0.17	1.41	52,52,52,52	0
55	MG	AA	1663	1/1	0.18	1.40	49,49,49,49	0
55	MG	CA	1623	1/1	0.21	1.35	66,66,66,66	0
55	MG	CA	1606	1/1	0.28	1.33	76,76,76,76	0
55	MG	AA	1669	1/1	0.24	1.28	34,34,34,34	0
55	MG	DA	3011	1/1	0.33	1.25	74,74,74,74	0
55	MG	BA	3116	1/1	0.20	1.24	30,30,30,30	0
55	MG	AA	1629	1/1	0.17	1.23	54,54,54,54	0
55	MG	DA	3044	1/1	0.19	1.17	83,83,83,83	0
55	MG	BA	3005	1/1	0.15	1.08	43,43,43,43	0
55	MG	DA	3152	1/1	0.33	1.02	55,55,55,55	0
55	MG	BA	3086	1/1	0.20	1.01	0,0,0,0	0
55	MG	DA	3040	1/1	0.17	1.00	66,66,66,66	0
55	MG	CA	1603	1/1	0.15	0.90	45,45,45,45	0
55	MG	DA	3085	1/1	0.19	0.87	78,78,78,78	0
55	MG	DA	3075	1/1	0.25	0.79	61,61,61,61	0
55	MG	AA	1655	1/1	0.15	0.76	20,20,20,20	0
55	MG	DA	3067	1/1	0.17	0.72	43,43,43,43	0
55	MG	DA	3006	1/1	0.21	0.69	98,98,98,98	0
55	MG	CA	1645	1/1	0.12	0.66	32,32,32,32	0
55	MG	CA	1640	1/1	0.16	0.59	36,36,36,36	0
55	MG	AA	1643	1/1	0.13	0.54	23,23,23,23	0
55	MG	DA	3163	1/1	0.20	0.47	47,47,47,47	0
55	MG	CA	1641	1/1	0.42	0.45	58,58,58,58	0
55	MG	BA	3096	1/1	0.17	0.42	2,2,2,2	0
55	MG	DA	3083	1/1	0.17	0.40	65,65,65,65	0
55	MG	DA	3130	1/1	0.17	0.38	43,43,43,43	0
55	MG	AA	1666	1/1	0.17	0.35	32,32,32,32	0
55	MG	DA	3126	1/1	0.18	0.35	61,61,61,61	0
55	MG	CA	1648	1/1	0.15	0.32	51,51,51,51	0
55	MG	BA	3187	1/1	0.19	0.28	3,3,3,3	0
55	MG	AA	1632	1/1	0.13	0.26	40,40,40,40	0
55	MG	BA	3046	1/1	0.16	0.24	3,3,3,3	0
55	MG	DA	3069	1/1	0.17	0.16	77,77,77,77	0
55	MG	DA	3107	1/1	0.17	0.15	56,56,56,56	0
55	MG	DA	3109	1/1	0.18	0.10	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DB	202	1/1	0.13	0.03	57,57,57,57	0
55	MG	DA	3144	1/1	0.30	0.02	58,58,58,58	0
55	MG	AA	1615	1/1	0.14	0.00	63,63,63,63	0
55	MG	CA	1631	1/1	0.25	-0.07	98,98,98,98	0
55	MG	DA	3048	1/1	0.16	-0.08	93,93,93,93	0
55	MG	DA	3131	1/1	0.17	-0.10	50,50,50,50	0
55	MG	CM	201	1/1	0.41	-0.14	50,50,50,50	0
55	MG	BA	3099	1/1	0.18	-0.15	21,21,21,21	0
55	MG	BA	3118	1/1	0.16	-0.16	34,34,34,34	0
55	MG	DA	3108	1/1	0.14	-0.22	55,55,55,55	0
55	MG	DA	3084	1/1	0.15	-0.23	75,75,75,75	0
55	MG	CA	1611	1/1	0.12	-0.27	69,69,69,69	0
55	MG	BA	3074	1/1	0.25	-0.28	32,32,32,32	0
55	MG	DA	3078	1/1	0.20	-0.28	95,95,95,95	0
55	MG	BA	3102	1/1	0.19	-0.29	17,17,17,17	0
55	MG	BA	3185	1/1	0.14	-0.30	5,5,5,5	0
55	MG	DA	3133	1/1	0.23	-0.31	55,55,55,55	0
55	MG	BA	3037	1/1	0.18	-0.36	0,0,0,0	0
55	MG	BA	3069	1/1	0.14	-0.43	64,64,64,64	0
55	MG	BA	3023	1/1	0.17	-0.45	0,0,0,0	0
55	MG	AA	1636	1/1	0.19	-0.48	42,42,42,42	0
55	MG	DA	3058	1/1	0.15	-0.51	70,70,70,70	0
55	MG	BA	3132	1/1	0.22	-0.56	32,32,32,32	0
55	MG	DA	3094	1/1	0.15	-0.60	83,83,83,83	0
55	MG	AA	1647	1/1	0.15	-0.66	44,44,44,44	0
55	MG	DA	3042	1/1	0.14	-0.70	69,69,69,69	0
55	MG	DA	3147	1/1	0.11	-0.72	35,35,35,35	0
55	MG	BA	3151	1/1	0.13	-0.80	23,23,23,23	0
55	MG	DA	3024	1/1	0.16	-0.81	45,45,45,45	0
55	MG	AA	1639	1/1	0.09	-0.83	67,67,67,67	0
55	MG	BA	3145	1/1	0.15	-0.83	26,26,26,26	0
55	MG	AA	1637	1/1	0.14	-0.84	16,16,16,16	0
55	MG	BA	3195	1/1	0.13	-0.84	36,36,36,36	0
55	MG	DA	3019	1/1	0.15	-0.86	84,84,84,84	0
55	MG	DA	3140	1/1	0.16	-0.88	42,42,42,42	0
55	MG	DA	3036	1/1	0.13	-0.89	57,57,57,57	0
55	MG	AA	1607	1/1	0.14	-0.89	48,48,48,48	0
55	MG	BA	3064	1/1	0.15	-0.96	0,0,0,0	0
55	MG	CA	1639	1/1	0.13	-0.96	43,43,43,43	0
55	MG	BA	3036	1/1	0.15	-0.97	23,23,23,23	0
55	MG	DA	3050	1/1	0.14	-0.98	52,52,52,52	0
55	MG	AA	1664	1/1	0.13	-1.00	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CA	1652	1/1	0.10	-1.00	62,62,62,62	0
55	MG	BA	3094	1/1	0.11	-1.00	20,20,20,20	0
55	MG	BA	3004	1/1	0.14	-1.01	52,52,52,52	0
55	MG	DA	3047	1/1	0.14	-1.01	71,71,71,71	0
55	MG	BA	3022	1/1	0.15	-1.03	0,0,0,0	0
55	MG	BA	3155	1/1	0.17	-1.06	2,2,2,2	0
55	MG	AA	1652	1/1	0.12	-1.06	40,40,40,40	0
55	MG	DA	3070	1/1	0.11	-1.08	93,93,93,93	0
55	MG	CA	1613	1/1	0.14	-1.09	17,17,17,17	0
55	MG	DA	3046	1/1	0.12	-1.09	62,62,62,62	0
55	MG	DA	3118	1/1	0.11	-1.10	73,73,73,73	0
55	MG	AA	1617	1/1	0.10	-1.10	62,62,62,62	0
55	MG	DA	3017	1/1	0.18	-1.12	39,39,39,39	0
55	MG	DQ	201	1/1	0.23	-1.13	40,40,40,40	0
55	MG	DA	3088	1/1	0.10	-1.14	69,69,69,69	0
55	MG	CA	1622	1/1	0.14	-1.14	57,57,57,57	0
55	MG	AA	1638	1/1	0.11	-1.16	63,63,63,63	0
55	MG	BA	3163	1/1	0.13	-1.16	27,27,27,27	0
55	MG	DA	3018	1/1	0.09	-1.20	68,68,68,68	0
55	MG	DA	3010	1/1	0.12	-1.23	64,64,64,64	0
55	MG	BA	3126	1/1	0.14	-1.23	3,3,3,3	0
55	MG	DA	3129	1/1	0.11	-1.24	70,70,70,70	0
55	MG	BA	3047	1/1	0.11	-1.26	40,40,40,40	0
55	MG	DA	3121	1/1	0.15	-1.28	60,60,60,60	0
55	MG	BA	3030	1/1	0.15	-1.30	3,3,3,3	0
55	MG	AA	1654	1/1	0.11	-1.34	41,41,41,41	0
55	MG	DA	3115	1/1	0.09	-1.34	79,79,79,79	0
55	MG	DA	3101	1/1	0.07	-1.35	63,63,63,63	0
55	MG	CA	1629	1/1	0.10	-1.38	84,84,84,84	0
55	MG	BA	3049	1/1	0.15	-1.40	3,3,3,3	0
56	ZN	B4	101	1/1	0.07	-1.46	76,76,76,76	0
56	ZN	D4	101	1/1	0.06	-1.46	74,74,74,74	0
55	MG	CA	1609	1/1	0.12	-1.47	78,78,78,78	0
55	MG	BA	3121	1/1	0.06	-1.47	14,14,14,14	0
55	MG	DA	3008	1/1	0.14	-1.48	80,80,80,80	0
55	MG	AA	1608	1/1	0.15	-1.49	20,20,20,20	0
55	MG	CA	1608	1/1	0.13	-1.49	65,65,65,65	0
55	MG	BA	3162	1/1	0.13	-1.51	23,23,23,23	0
55	MG	BA	3013	1/1	0.17	-1.54	0,0,0,0	0
55	MG	DA	3031	1/1	0.14	-1.56	59,59,59,59	0
55	MG	DA	3098	1/1	0.09	-1.56	50,50,50,50	0
55	MG	BA	3042	1/1	0.13	-1.58	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	3097	1/1	0.13	-1.58	67,67,67,67	0
55	MG	BA	3107	1/1	0.13	-1.59	3,3,3,3	0
55	MG	DA	3125	1/1	0.13	-1.60	86,86,86,86	0
55	MG	CA	1614	1/1	0.04	-1.62	52,52,52,52	0
55	MG	BA	3017	1/1	0.15	-1.65	0,0,0,0	0
55	MG	BA	3153	1/1	0.17	-1.65	2,2,2,2	0
55	MG	DA	3037	1/1	0.08	-1.65	76,76,76,76	0
55	MG	BA	3188	1/1	0.11	-1.69	35,35,35,35	0
55	MG	DA	3145	1/1	0.10	-1.70	68,68,68,68	0
55	MG	DA	3157	1/1	0.14	-1.70	29,29,29,29	0
55	MG	CA	1601	1/1	0.15	-1.75	52,52,52,52	0
55	MG	BA	3161	1/1	0.16	-1.76	15,15,15,15	0
55	MG	BA	3068	1/1	0.17	-1.76	1,1,1,1	0
55	MG	BA	3100	1/1	0.08	-1.76	9,9,9,9	0
55	MG	BA	3108	1/1	0.16	-1.77	5,5,5,5	0
55	MG	CA	1602	1/1	0.12	-1.79	69,69,69,69	0
55	MG	BB	201	1/1	0.10	-1.79	28,28,28,28	0
55	MG	DA	3023	1/1	0.11	-1.82	60,60,60,60	0
55	MG	AA	1630	1/1	0.12	-1.83	67,67,67,67	0
55	MG	BA	3077	1/1	0.07	-1.84	38,38,38,38	0
55	MG	DA	3012	1/1	0.13	-1.86	39,39,39,39	0
55	MG	BA	3191	1/1	0.14	-1.86	26,26,26,26	0
55	MG	DA	3038	1/1	0.11	-1.86	63,63,63,63	0
55	MG	DA	3135	1/1	0.07	-1.87	46,46,46,46	0
55	MG	DA	3080	1/1	0.11	-1.88	91,91,91,91	0
55	MG	AA	1618	1/1	0.10	-1.95	34,34,34,34	0
55	MG	CA	1635	1/1	0.10	-1.97	94,94,94,94	0
55	MG	BA	3066	1/1	0.14	-1.98	2,2,2,2	0
55	MG	DA	3127	1/1	0.14	-1.98	88,88,88,88	0
55	MG	DA	3063	1/1	0.11	-2.01	53,53,53,53	0
55	MG	DA	3146	1/1	0.07	-2.02	41,41,41,41	0
55	MG	DA	3112	1/1	0.11	-2.05	64,64,64,64	0
55	MG	BA	3007	1/1	0.09	-2.11	32,32,32,32	0
55	MG	DA	3079	1/1	0.07	-2.18	94,94,94,94	0
55	MG	AA	1640	1/1	0.10	-2.19	57,57,57,57	0
55	MG	BA	3177	1/1	0.10	-2.22	9,9,9,9	0
55	MG	BA	3045	1/1	0.11	-2.22	4,4,4,4	0
55	MG	DA	3035	1/1	0.10	-2.25	71,71,71,71	0
55	MG	DA	3162	1/1	0.10	-2.26	48,48,48,48	0
55	MG	DA	3122	1/1	0.07	-2.32	64,64,64,64	0
55	MG	DA	3156	1/1	0.15	-2.36	58,58,58,58	0
55	MG	DA	3003	1/1	0.12	-2.38	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3111	1/1	0.11	-2.39	81,81,81,81	0
55	MG	DA	3117	1/1	0.10	-2.40	55,55,55,55	0
55	MG	DA	3027	1/1	0.12	-2.41	82,82,82,82	0
55	MG	BA	3089	1/1	0.14	-2.42	1,1,1,1	0
55	MG	DA	3013	1/1	0.14	-2.42	64,64,64,64	0
55	MG	BA	3063	1/1	0.13	-2.42	2,2,2,2	0
55	MG	DA	3114	1/1	0.10	-2.43	52,52,52,52	0
55	MG	DA	3105	1/1	0.12	-2.50	52,52,52,52	0
55	MG	BA	3085	1/1	0.16	-2.54	11,11,11,11	0
55	MG	BA	3021	1/1	0.15	-2.57	2,2,2,2	0
55	MG	DB	203	1/1	0.07	-2.59	90,90,90,90	0
55	MG	DA	3066	1/1	0.13	-2.59	45,45,45,45	0
55	MG	DA	3025	1/1	0.10	-2.60	65,65,65,65	0
55	MG	BA	3113	1/1	0.12	-2.73	2,2,2,2	0
55	MG	AA	1624	1/1	0.09	-2.75	50,50,50,50	0
55	MG	DA	3001	1/1	0.07	-2.78	37,37,37,37	0
55	MG	BA	3165	1/1	0.12	-2.79	3,3,3,3	0
55	MG	BA	3169	1/1	0.10	-2.81	4,4,4,4	0
55	MG	BA	3093	1/1	0.10	-2.83	26,26,26,26	0
55	MG	CA	1612	1/1	0.05	-2.86	43,43,43,43	0
55	MG	BA	3018	1/1	0.08	-2.87	10,10,10,10	0
55	MG	BA	3073	1/1	0.14	-2.88	9,9,9,9	0
55	MG	BA	3123	1/1	0.12	-2.91	11,11,11,11	0
55	MG	DA	3123	1/1	0.14	-2.92	44,44,44,44	0
55	MG	BA	3002	1/1	0.12	-2.97	18,18,18,18	0
55	MG	DA	3153	1/1	0.12	-3.00	68,68,68,68	0
55	MG	CA	1610	1/1	0.07	-3.00	58,58,58,58	0
55	MG	DB	201	1/1	0.05	-3.01	96,96,96,96	0
55	MG	CA	1621	1/1	0.08	-3.01	67,67,67,67	0
55	MG	DA	3096	1/1	0.08	-3.02	54,54,54,54	0
55	MG	DA	3081	1/1	0.14	-3.07	62,62,62,62	0
55	MG	CA	1607	1/1	0.12	-3.10	55,55,55,55	0
55	MG	BA	3147	1/1	0.14	-3.10	11,11,11,11	0
55	MG	CA	1604	1/1	0.07	-3.12	78,78,78,78	0
55	MG	CA	1632	1/1	0.06	-3.12	75,75,75,75	0
55	MG	BA	3193	1/1	0.15	-3.14	12,12,12,12	0
55	MG	DA	3022	1/1	0.12	-3.16	43,43,43,43	0
55	MG	DA	3049	1/1	0.11	-3.17	69,69,69,69	0
55	MG	DA	3068	1/1	0.07	-3.19	60,60,60,60	0
55	MG	BA	3079	1/1	0.09	-3.19	21,21,21,21	0
55	MG	AA	1656	1/1	0.07	-3.21	32,32,32,32	0
55	MG	BA	3112	1/1	0.09	-3.24	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3076	1/1	0.12	-3.24	59,59,59,59	0
55	MG	BA	3051	1/1	0.13	-3.26	4,4,4,4	0
55	MG	BA	3159	1/1	0.13	-3.28	24,24,24,24	0
55	MG	BA	3008	1/1	0.11	-3.29	0,0,0,0	0
55	MG	DA	3053	1/1	0.10	-3.29	39,39,39,39	0
55	MG	BA	3117	1/1	0.15	-3.31	1,1,1,1	0
55	MG	DA	3082	1/1	0.10	-3.31	65,65,65,65	0
55	MG	BB	202	1/1	0.10	-3.37	4,4,4,4	0
55	MG	BA	3175	1/1	0.09	-3.39	9,9,9,9	0
55	MG	AA	1628	1/1	0.04	-3.44	39,39,39,39	0
55	MG	BA	3110	1/1	0.11	-3.50	26,26,26,26	0
55	MG	AA	1604	1/1	0.07	-3.50	48,48,48,48	0
55	MG	AA	1616	1/1	0.08	-3.59	62,62,62,62	0
55	MG	AA	1620	1/1	0.06	-3.63	55,55,55,55	0
55	MG	AA	1645	1/1	0.09	-3.65	42,42,42,42	0
55	MG	DA	3009	1/1	0.09	-3.70	69,69,69,69	0
55	MG	BA	3078	1/1	0.03	-3.71	38,38,38,38	0
55	MG	BA	3029	1/1	0.14	-3.72	35,35,35,35	0
55	MG	CA	1617	1/1	0.11	-3.77	41,41,41,41	0
55	MG	BA	3032	1/1	0.12	-3.77	2,2,2,2	0
55	MG	AA	1612	1/1	0.12	-3.82	38,38,38,38	0
55	MG	AA	1634	1/1	0.09	-3.85	49,49,49,49	0
55	MG	DA	3005	1/1	0.09	-3.86	90,90,90,90	0
55	MG	DA	3086	1/1	0.12	-3.92	61,61,61,61	0
55	MG	BA	3184	1/1	0.11	-3.96	8,8,8,8	0
55	MG	BA	3020	1/1	0.12	-3.98	5,5,5,5	0
55	MG	BA	3075	1/1	0.12	-3.99	6,6,6,6	0
55	MG	AA	1625	1/1	0.08	-4.05	51,51,51,51	0
55	MG	BA	3052	1/1	0.09	-4.11	21,21,21,21	0
55	MG	BA	3097	1/1	0.11	-4.12	0,0,0,0	0
55	MG	BA	3124	1/1	0.09	-4.13	9,9,9,9	0
55	MG	BA	3065	1/1	0.12	-4.18	1,1,1,1	0
55	MG	BA	3082	1/1	0.07	-4.28	6,6,6,6	0
55	MG	DA	3054	1/1	0.09	-4.29	62,62,62,62	0
55	MG	BA	3003	1/1	0.11	-4.32	29,29,29,29	0
55	MG	BA	3012	1/1	0.15	-4.32	0,0,0,0	0
55	MG	CA	1619	1/1	0.10	-4.39	27,27,27,27	0
55	MG	DA	3091	1/1	0.14	-4.42	79,79,79,79	0
55	MG	AA	1641	1/1	0.12	-4.43	7,7,7,7	0
55	MG	BA	3148	1/1	0.12	-4.47	13,13,13,13	0
55	MG	BA	3101	1/1	0.08	-4.51	11,11,11,11	0
55	MG	BB	203	1/1	0.09	-4.57	7,7,7,7	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	3006	1/1	0.06	-4.63	13,13,13,13	0
55	MG	AA	1609	1/1	0.08	-4.71	33,33,33,33	0
55	MG	DA	3059	1/1	0.07	-4.85	42,42,42,42	0
55	MG	BA	3095	1/1	0.07	-4.86	14,14,14,14	0
55	MG	AA	1601	1/1	0.09	-4.86	61,61,61,61	0
55	MG	AA	1642	1/1	0.07	-4.88	25,25,25,25	0
55	MG	BA	3070	1/1	0.11	-4.95	37,37,37,37	0
55	MG	AA	1660	1/1	0.09	-5.05	41,41,41,41	0
55	MG	DA	3087	1/1	0.05	-5.12	58,58,58,58	0
55	MG	BA	3028	1/1	0.10	-5.13	3,3,3,3	0
55	MG	AA	1621	1/1	0.10	-5.15	37,37,37,37	0
55	MG	BA	3091	1/1	0.06	-5.19	48,48,48,48	0
55	MG	BA	3059	1/1	0.13	-5.22	5,5,5,5	0
55	MG	DA	3043	1/1	0.08	-5.23	67,67,67,67	0
55	MG	BA	3130	1/1	0.16	-5.27	2,2,2,2	0
55	MG	BA	3088	1/1	0.08	-5.33	29,29,29,29	0
55	MG	AA	1633	1/1	0.08	-5.42	35,35,35,35	0
55	MG	AA	1619	1/1	0.14	-5.55	65,65,65,65	0
55	MG	BA	3122	1/1	0.16	-5.57	0,0,0,0	0
55	MG	DA	3090	1/1	0.06	-5.74	59,59,59,59	0
55	MG	BA	3048	1/1	0.08	-5.76	26,26,26,26	0
55	MG	CA	1616	1/1	0.09	-5.79	38,38,38,38	0
55	MG	DA	3124	1/1	0.16	-5.93	41,41,41,41	0
55	MG	AA	1649	1/1	0.11	-6.03	28,28,28,28	0
55	MG	DA	3051	1/1	0.05	-6.11	33,33,33,33	0
55	MG	BA	3001	1/1	0.05	-6.12	21,21,21,21	0
55	MG	BA	3111	1/1	0.07	-6.22	27,27,27,27	0
55	MG	DA	3073	1/1	0.10	-6.30	35,35,35,35	0
55	MG	BA	3129	1/1	0.13	-6.33	0,0,0,0	0
55	MG	BA	3038	1/1	0.13	-6.39	1,1,1,1	0
55	MG	BA	3050	1/1	0.06	-6.41	7,7,7,7	0
55	MG	DA	3074	1/1	0.08	-6.57	47,47,47,47	0
55	MG	BA	3120	1/1	0.11	-6.59	11,11,11,11	0
55	MG	DA	3119	1/1	0.08	-6.79	58,58,58,58	0
55	MG	BA	3127	1/1	0.10	-6.96	2,2,2,2	0
55	MG	BA	3058	1/1	0.07	-6.96	15,15,15,15	0
55	MG	BA	3054	1/1	0.08	-7.03	7,7,7,7	0
55	MG	BA	3026	1/1	0.09	-7.07	6,6,6,6	0
55	MG	DA	3128	1/1	0.08	-7.12	74,74,74,74	0
55	MG	BA	3134	1/1	0.08	-7.13	3,3,3,3	0
55	MG	BA	3071	1/1	0.14	-7.58	17,17,17,17	0
55	MG	BA	3043	1/1	0.07	-7.67	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
55	MG	DA	3052	1/1	0.06	-7.69	47,47,47,47	0
55	MG	BA	3031	1/1	0.10	-7.72	7,7,7,7	0
55	MG	BA	3172	1/1	0.12	-7.84	16,16,16,16	0
55	MG	DA	3039	1/1	0.08	-7.99	53,53,53,53	0
55	MG	AA	1606	1/1	0.06	-8.07	58,58,58,58	0
55	MG	BA	3009	1/1	0.07	-8.10	2,2,2,2	0
55	MG	DA	3143	1/1	0.13	-8.35	35,35,35,35	0
55	MG	BA	3080	1/1	0.10	-8.39	24,24,24,24	0
55	MG	DA	3055	1/1	0.07	-8.88	57,57,57,57	0
55	MG	BA	3024	1/1	0.06	-8.90	3,3,3,3	0
55	MG	BA	3062	1/1	0.11	-8.97	4,4,4,4	0
55	MG	DA	3065	1/1	0.08	-9.15	41,41,41,41	0
55	MG	AA	1613	1/1	0.07	-9.15	23,23,23,23	0
55	MG	BA	3060	1/1	0.12	-9.77	29,29,29,29	0
55	MG	BA	3035	1/1	0.06	-9.84	0,0,0,0	0
55	MG	BA	3103	1/1	0.06	-10.00	7,7,7,7	0
55	MG	BA	3087	1/1	0.09	-10.67	27,27,27,27	0
55	MG	BA	3084	1/1	0.10	-10.71	7,7,7,7	0
55	MG	AA	1611	1/1	0.07	-10.94	21,21,21,21	0
55	MG	BA	3041	1/1	0.09	-11.08	11,11,11,11	0
55	MG	BA	3158	1/1	0.11	-11.25	15,15,15,15	0
55	MG	BA	3034	1/1	0.10	-11.92	5,5,5,5	0
55	MG	BA	3156	1/1	0.13	-12.08	9,9,9,9	0
55	MG	BA	3114	1/1	0.09	-12.49	28,28,28,28	0
55	MG	CA	1624	1/1	0.07	-12.86	52,52,52,52	0
55	MG	BA	3010	1/1	0.09	-15.36	1,1,1,1	0
55	MG	BA	3081	1/1	0.08	-18.57	0,0,0,0	0
55	MG	DA	3033	1/1	0.08	-18.59	54,54,54,54	0
55	MG	CA	1634	1/1	0.05	-25.48	58,58,58,58	0
55	MG	DA	3167	1/1	0.16	-	30,30,30,30	0
55	MG	BA	3174	1/1	0.16	-	5,5,5,5	0
55	MG	BA	3182	1/1	0.22	-	14,14,14,14	0
55	MG	BA	3181	1/1	0.12	-	26,26,26,26	0
55	MG	DA	3160	1/1	0.17	-	47,47,47,47	0

6.5 Other polymers ⓘ

There are no such residues in this entry.