



wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 07:14 PM BST

PDB ID : 4V6C
Title : Crystal structure of the E. coli 70S ribosome in an intermediate state of ratcheting
Authors : Zhang, W.; Dunkle, J.A.; Cate, J.H.D.
Deposited on : 2009-06-27
Resolution : 3.19 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

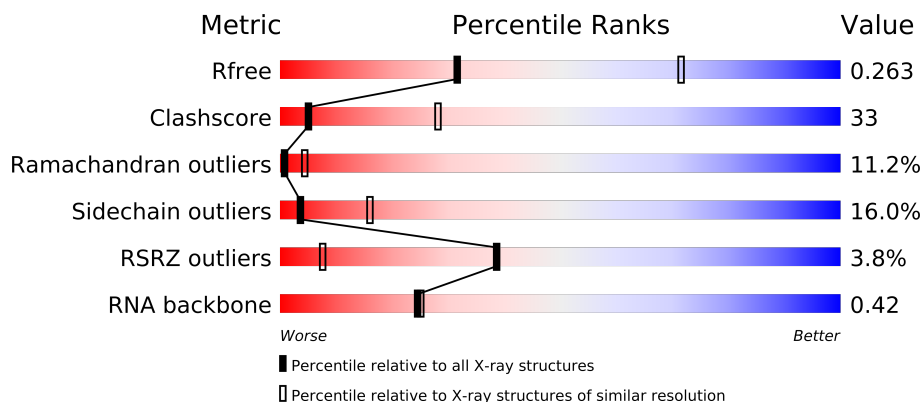
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 3.19 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	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)
RNA backbone	1838	1002 (3.72-2.68)

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	AB	241	
1	CB	241	
2	AC	233	
2	CC	233	
3	AD	206	
3	CD	206	
4	AE	167	
4	CE	167	
5	AF	135	
5	CF	135	
6	AG	179	
6	CG	179	

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Mol	Chain	Length	Quality of chain
7	AH	130	
7	CH	130	
8	AI	130	
8	CI	130	
9	AJ	103	
9	CJ	103	
10	AK	129	
10	CK	129	
11	AL	124	
11	CL	124	
12	AM	118	
12	CM	118	
13	AN	101	
13	CN	101	
14	AO	89	
14	CO	89	
15	AP	82	
15	CP	82	
16	AQ	84	
16	CQ	84	
17	AR	75	
17	CR	75	
18	AS	92	
18	CS	92	
19	AT	87	
19	CT	87	
20	AU	71	
20	CU	71	
21	AA	1533	
22	BA	2903	
22	DA	2903	
23	BB	118	
24	BC	273	
24	DC	273	
25	BD	209	
25	DD	209	
26	BE	201	
26	DE	201	
27	BF	179	
27	DF	179	
28	BG	177	
28	DG	177	

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Mol	Chain	Length	Quality of chain
29	BH	149	
29	DH	149	
30	BI	142	
30	DI	142	
31	BJ	142	
31	DJ	142	
32	BK	123	
32	DK	123	
33	BL	144	
33	DL	144	
34	BM	136	
34	DM	136	
35	BN	127	
35	DN	127	
36	BO	117	
36	DO	117	
37	BP	115	
37	DP	115	
38	BQ	118	
38	DQ	118	
39	BR	103	
39	DR	103	
40	BS	110	
40	DS	110	
41	BT	100	
41	DT	100	
42	BU	104	
42	DU	104	
43	BV	94	
43	DV	94	
44	BW	85	
44	DW	85	
45	BX	78	
45	DX	78	
46	BY	63	
46	DY	63	
47	BZ	59	
47	DZ	59	
48	B0	57	
48	D0	57	
49	B1	55	
49	D1	55	

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Mol	Chain	Length	Quality of chain
50	B2	46	
50	D2	46	
51	B3	65	
51	D3	65	
52	B4	38	
52	D4	38	
53	CA	1530	
54	DB	117	

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	1609	-	X
55	MG	AA	1611	-	X
55	MG	AA	1615	-	X
55	MG	AA	1619	-	X
55	MG	AA	1622	-	X
55	MG	AA	1626	-	X
55	MG	AA	1627	-	X
55	MG	AA	1628	-	X
55	MG	AA	1636	-	X
55	MG	AA	1641	-	X
55	MG	BA	3011	-	X
55	MG	BA	3014	-	X
55	MG	BA	3015	-	X
55	MG	BA	3020	-	X
55	MG	BA	3026	-	X
55	MG	BA	3028	-	X
55	MG	BA	3035	-	X
55	MG	BA	3037	-	X
55	MG	BA	3038	-	X
55	MG	BA	3040	-	X
55	MG	BA	3045	-	X
55	MG	BA	3049	-	X
55	MG	BA	3056	-	X
55	MG	BA	3057	-	X
55	MG	BA	3058	-	X
55	MG	BA	3060	-	X
55	MG	BA	3061	-	X
55	MG	BA	3062	-	X
55	MG	BA	3071	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
55	MG	BA	3072	-	X
55	MG	BA	3077	-	X
55	MG	BA	3084	-	X
55	MG	BA	3088	-	X
55	MG	BA	3092	-	X
55	MG	BA	3103	-	X
55	MG	BA	3105	-	X
55	MG	BA	3109	-	X
55	MG	BA	3110	-	X
55	MG	BA	3117	-	X
55	MG	BA	3120	-	X
55	MG	BA	3125	-	X
55	MG	BA	3127	-	X
55	MG	BA	3132	-	X
55	MG	BA	3134	-	X
55	MG	BA	3136	-	X
55	MG	BA	3137	-	X
55	MG	BB	201	-	X
55	MG	CA	1603	-	X
55	MG	CA	1610	-	X
55	MG	CA	1612	-	X
55	MG	CA	1614	-	X
55	MG	CA	1615	-	X
55	MG	CA	1619	-	X
55	MG	CA	1620	-	X
55	MG	CA	1624	-	X
55	MG	CA	1625	-	X
55	MG	CA	1626	-	X
55	MG	CA	1627	-	X
55	MG	CA	1628	-	X
55	MG	DA	3002	-	X
55	MG	DA	3005	-	X
55	MG	DA	3007	-	X
55	MG	DA	3013	-	X
55	MG	DA	3015	-	X
55	MG	DA	3020	-	X
55	MG	DA	3021	-	X
55	MG	DA	3022	-	X
55	MG	DA	3027	-	X
55	MG	DA	3029	-	X
55	MG	DA	3039	-	X
55	MG	DA	3042	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
55	MG	DA	3058	-	X
55	MG	DA	3059	-	X
55	MG	DA	3060	-	X
55	MG	DA	3061	-	X
55	MG	DA	3063	-	X
55	MG	DA	3064	-	X
55	MG	DA	3065	-	X
55	MG	DA	3070	-	X
55	MG	DA	3075	-	X
55	MG	DA	3079	-	X
55	MG	DA	3098	-	X
55	MG	DA	3101	-	X
55	MG	DA	3109	-	X
55	MG	DA	3110	-	X
55	MG	DA	3115	-	X
55	MG	DA	3116	-	X
55	MG	DA	3127	-	X
55	MG	DA	3129	-	X
55	MG	DA	3131	-	X
55	MG	DA	3132	-	X
55	MG	DA	3134	-	X
55	MG	DJ	201	-	X

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 284450 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 protein called 30S ribosomal protein S2.

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AG	151	Total	C	N	O	S	0	0	0
			1181	735	227	215	4			
6	CG	150	Total	C	N	O	S	0	0	0
			1174	730	226	214	4			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 15 is a protein called 30S ribosomal protein S16.

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

- Molecule 16 is a protein called 30S ribosomal protein S17.

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

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

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

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

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

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

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

- Molecule 20 is a protein called 30S ribosomal protein S21.

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

- Molecule 21 is a RNA chain called 16S rRNA.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	BA	2854	Total	C	N	O	P	0	0	0
			61274	27334	11279	19807	2854			
22	DA	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BF	177	Total	C	N	O	S	0	0	0
			1410	899	249	256	6			
27	DF	178	Total	C	N	O	S	0	0	0
			1420	905	251	258	6			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BK	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	DK	122	Total	C	N	O	S	0	0	0
			938	587	180	165	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
			960	593	196	166	5			
35	DN	120	Total	C	N	O	S	0	0	0
			960	593	196	166	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	0	0	0
			947	604	192	151			
38	DQ	117	Total	C	N	O	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
			738	466	139	131	2			
41	DT	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 54 is a RNA chain called 5S rRNA.

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

- 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	137	Total	Mg	0	0
			137	137		
55	CA	42	Total	Mg	0	0
			42	42		
55	DJ	1	Total	Mg	0	0
			1	1		
55	AA	43	Total	Mg	0	0
			43	43		
55	DA	135	Total	Mg	0	0
			135	135		
55	DB	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	AE	1	Total	O	0	0
			1	1		
57	AL	3	Total	O	0	0
			3	3		
57	AN	6	Total	O	0	0
			6	6		
57	AT	2	Total	O	0	0
			2	2		
57	AU	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	AA	195	Total 195	O 195	0	0
57	BA	610	Total 610	O 610	0	0
57	BB	20	Total 20	O 20	0	0
57	BC	10	Total 10	O 10	0	0
57	BD	2	Total 2	O 2	0	0
57	BL	4	Total 4	O 4	0	0
57	BN	3	Total 3	O 3	0	0
57	BQ	1	Total 1	O 1	0	0
57	BT	2	Total 2	O 2	0	0
57	B0	1	Total 1	O 1	0	0
57	B2	1	Total 1	O 1	0	0
57	B3	3	Total 3	O 3	0	0
57	B4	3	Total 3	O 3	0	0
57	CE	5	Total 5	O 5	0	0
57	CI	1	Total 1	O 1	0	0
57	CL	1	Total 1	O 1	0	0
57	CN	3	Total 3	O 3	0	0
57	CT	3	Total 3	O 3	0	0
57	CU	2	Total 2	O 2	0	0
57	CA	192	Total 192	O 192	0	0
57	DA	599	Total 599	O 599	0	0

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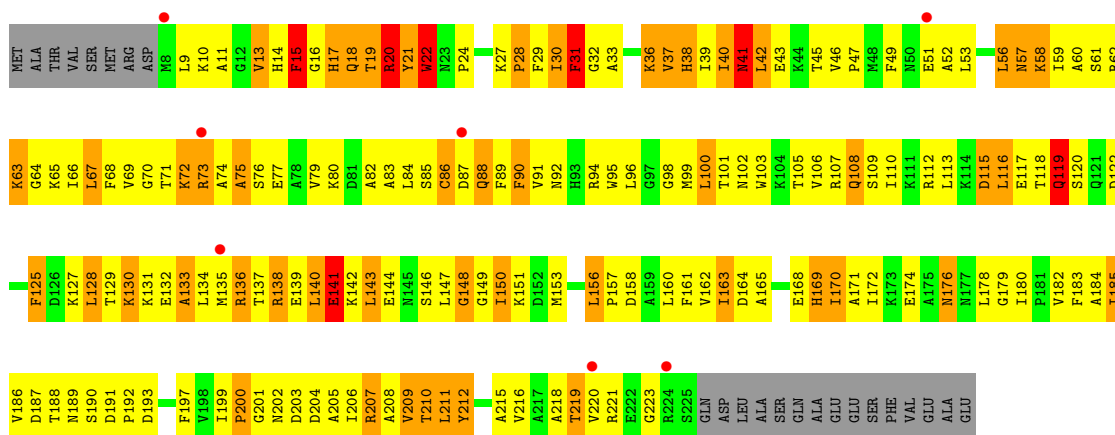
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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57	DC	13	Total 13	O 13	0	0
57	DD	4	Total 4	O 4	0	0
57	DE	3	Total 3	O 3	0	0
57	DJ	3	Total 3	O 3	0	0
57	DL	5	Total 5	O 5	0	0
57	DN	2	Total 2	O 2	0	0
57	DT	2	Total 2	O 2	0	0
57	DU	1	Total 1	O 1	0	0
57	DV	1	Total 1	O 1	0	0
57	D2	1	Total 1	O 1	0	0
57	D3	1	Total 1	O 1	0	0
57	D4	4	Total 4	O 4	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

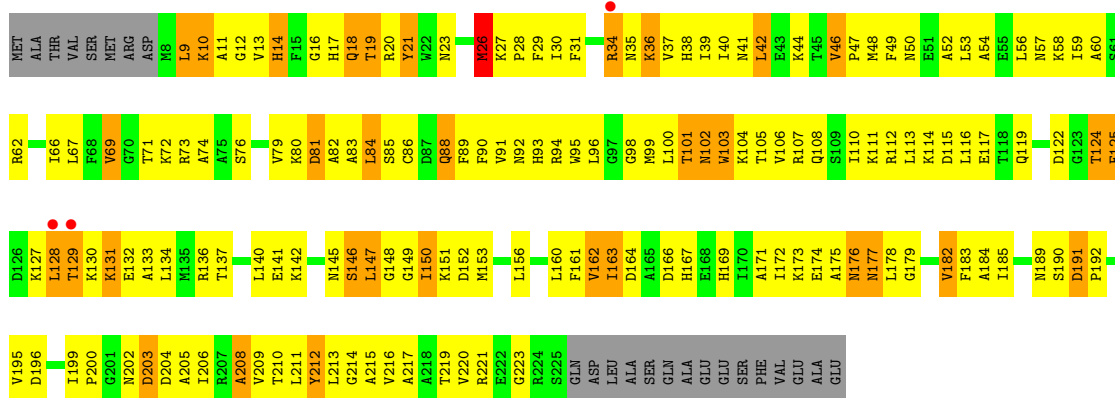
• Molecule 1: 30S ribosomal protein S2

Chain AB: 



• Molecule 1: 30S ribosomal protein S2

Chain CB: 

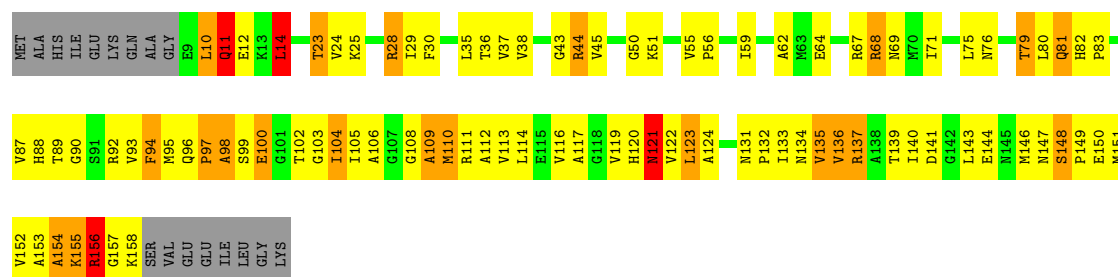


• Molecule 2: 30S ribosomal protein S3

Chain AC: 

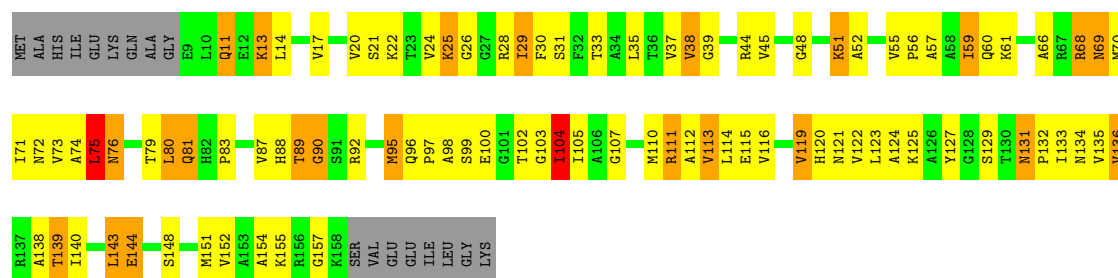


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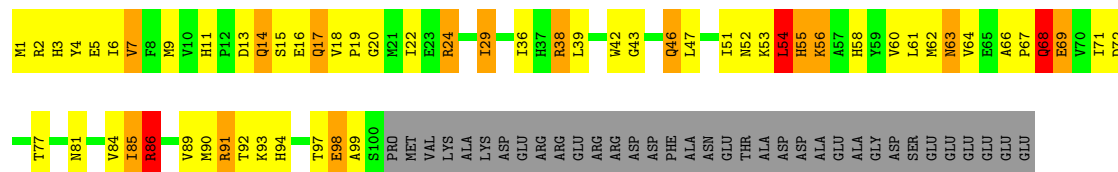
- Molecule 4: 30S ribosomal protein S5

Chain CE:



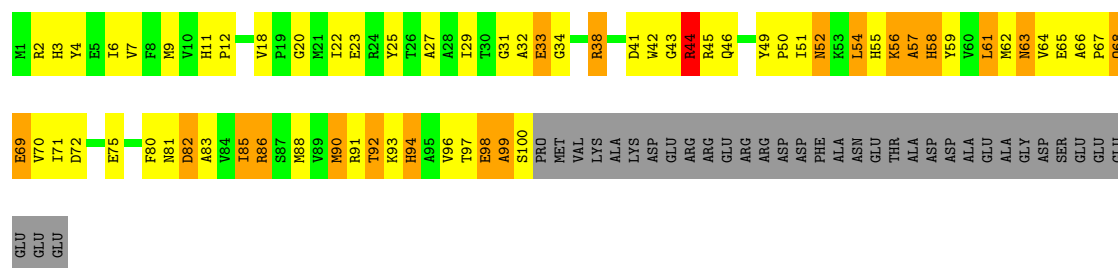
- Molecule 5: 30S ribosomal protein S6

Chain AF:



- Molecule 5: 30S ribosomal protein S6

Chain CF:

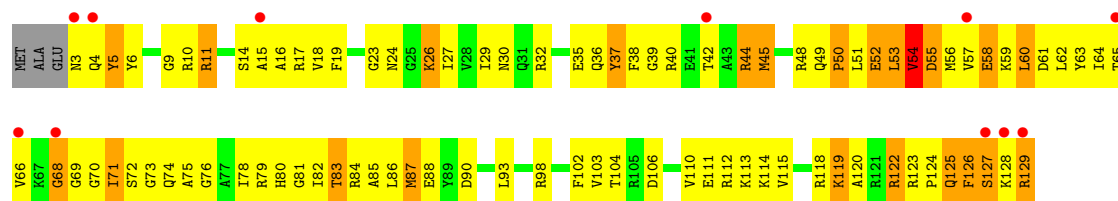


- Molecule 6: 30S ribosomal protein S7

Chain AG:

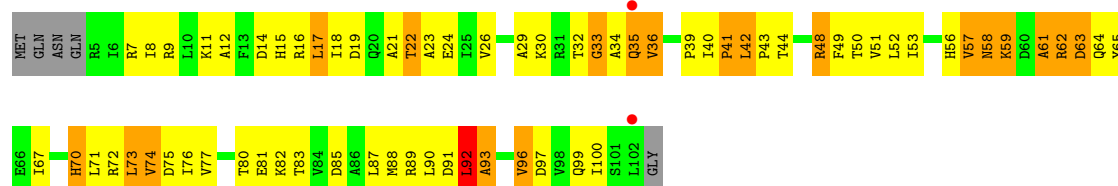






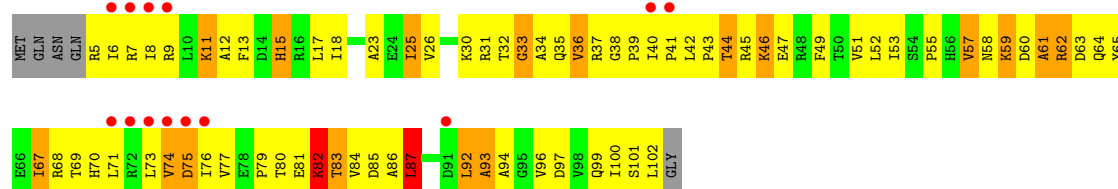
• Molecule 9: 30S ribosomal protein S10

Chain AJ:



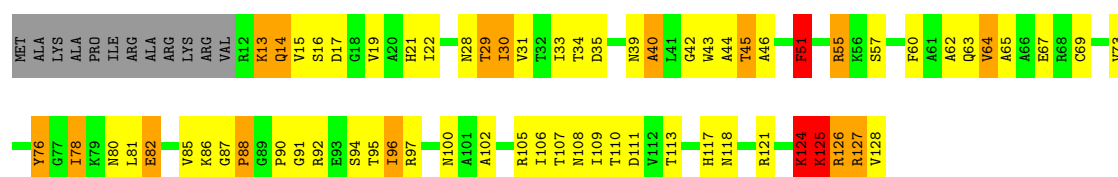
• Molecule 9: 30S ribosomal protein S10

Chain CJ:



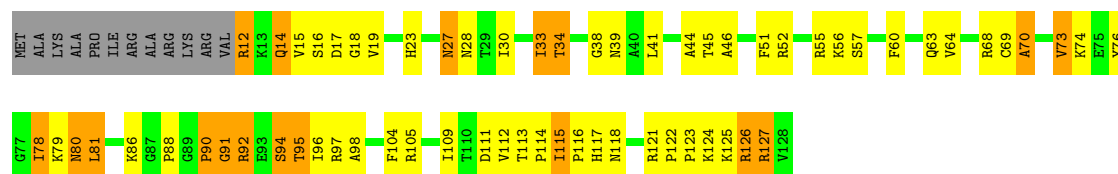
• Molecule 10: 30S ribosomal protein S11

Chain AK:



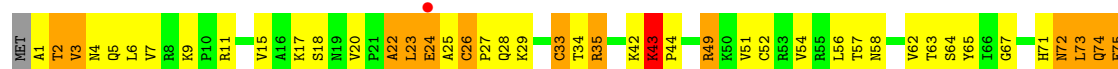
• Molecule 10: 30S ribosomal protein S11

Chain CK:



• Molecule 11: 30S ribosomal protein S12

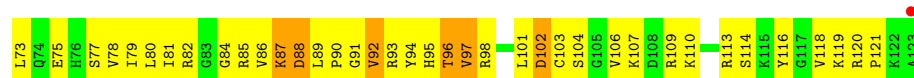
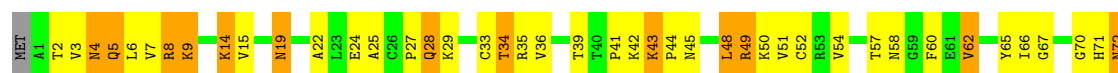
Chain AL:





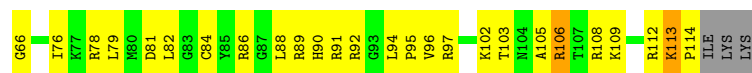
- Molecule 11: 30S ribosomal protein S12

Chain CL:



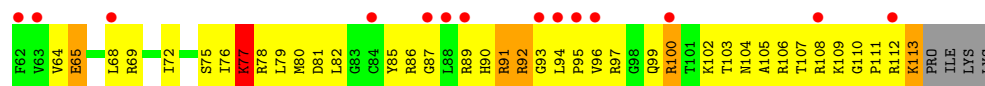
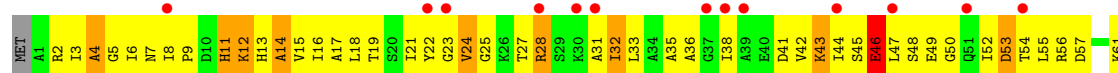
- Molecule 12: 30S ribosomal protein S13

Chain AM:



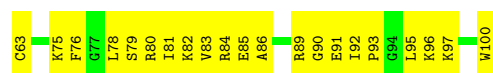
- Molecule 12: 30S ribosomal protein S13

Chain CM:



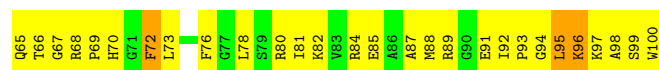
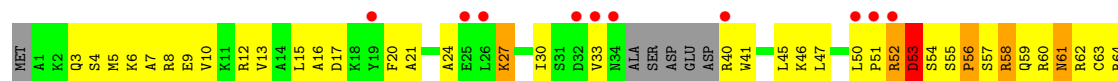
- Molecule 13: 30S ribosomal protein S14

Chain AN:



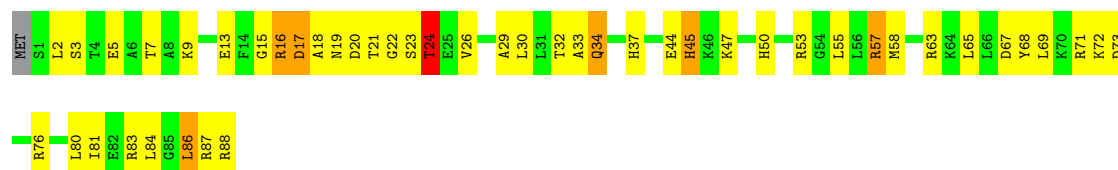
- Molecule 13: 30S ribosomal protein S14

Chain CN:



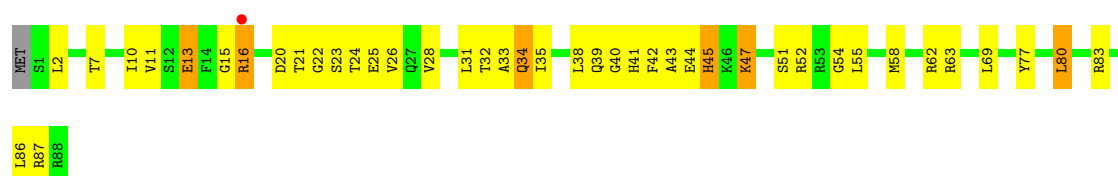
- Molecule 14: 30S ribosomal protein S15

Chain AO:



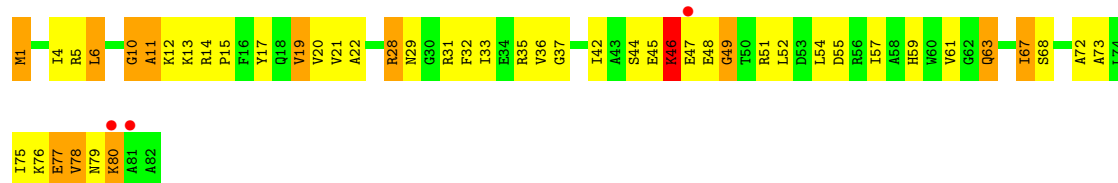
- Molecule 14: 30S ribosomal protein S15

Chain CO:



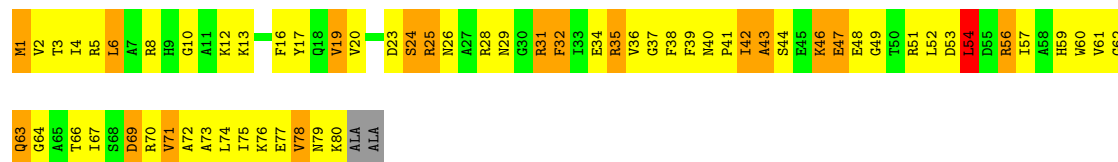
- Molecule 15: 30S ribosomal protein S16

Chain AP:



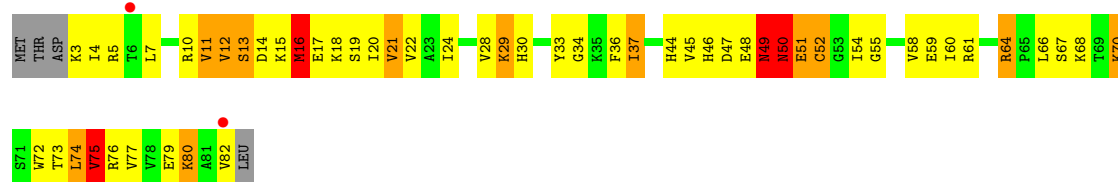
- Molecule 15: 30S ribosomal protein S16

Chain CP:



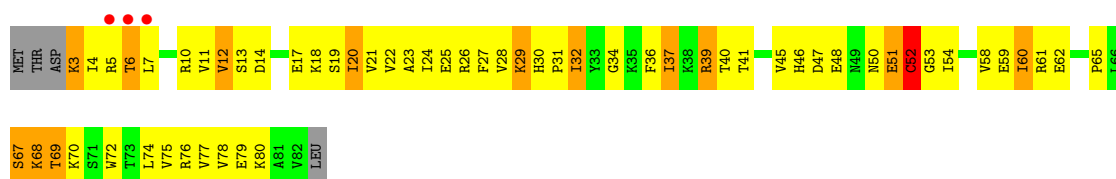
- Molecule 16: 30S ribosomal protein S17

Chain AQ:



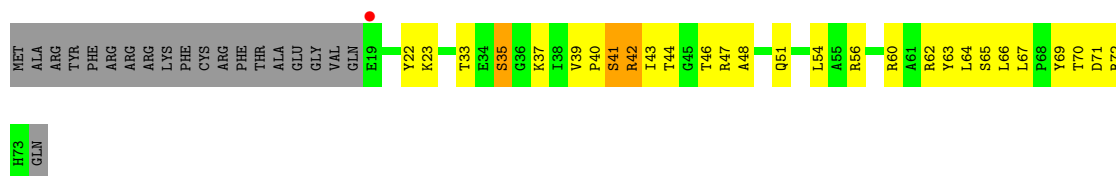
- Molecule 16: 30S ribosomal protein S17

Chain CQ:



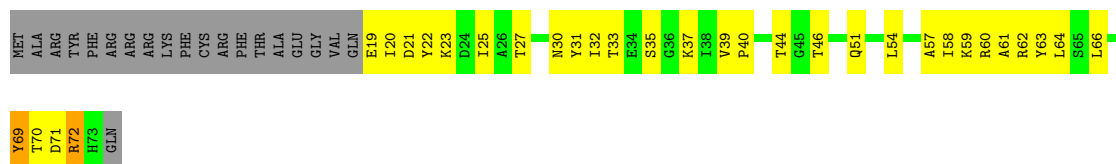
- Molecule 17: 30S ribosomal protein S18

Chain AR:



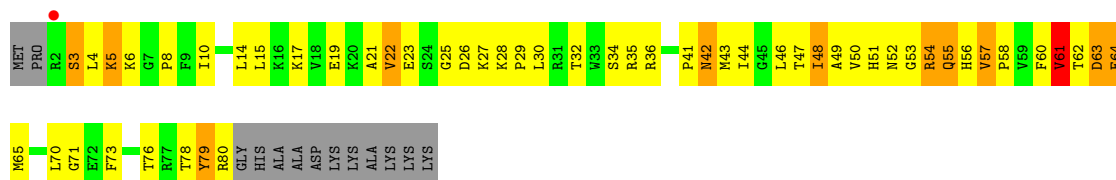
- Molecule 17: 30S ribosomal protein S18

Chain CR:



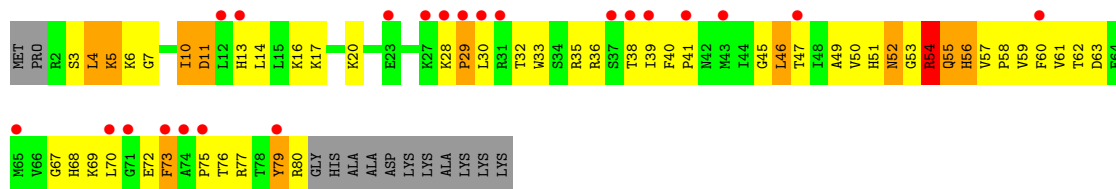
- Molecule 18: 30S ribosomal protein S19

Chain AS:



- Molecule 18: 30S ribosomal protein S19

Chain CS:



- Molecule 19: 30S ribosomal protein S20

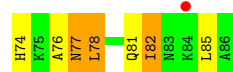
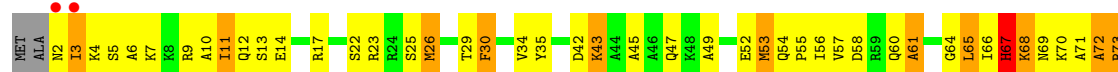
Chain AT:





- Molecule 19: 30S ribosomal protein S20

Chain CT:



- Molecule 20: 30S ribosomal protein S21

Chain AU:



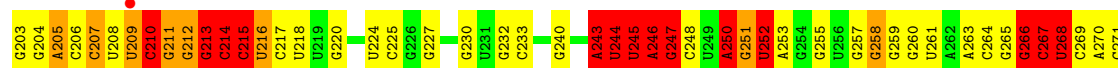
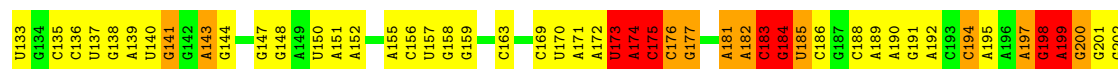
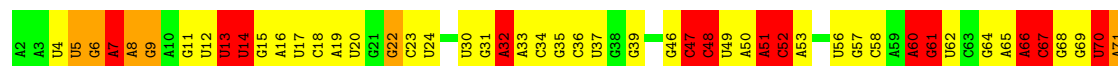
- Molecule 20: 30S ribosomal protein S21

Chain CU:



- Molecule 21: 16S rRNA

Chain AA:

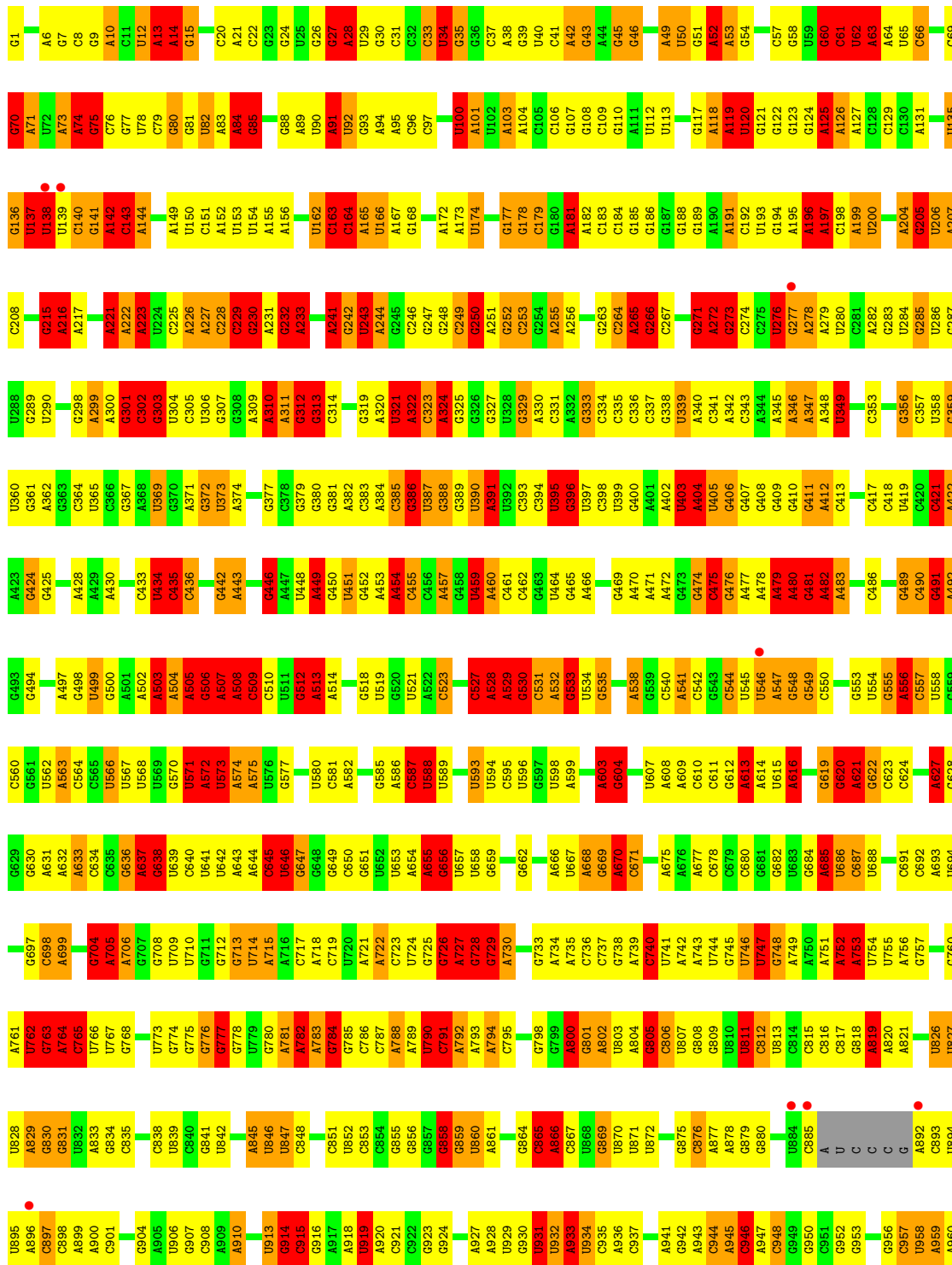


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A1413	A1339	G1277	U1211	G1138	G1064	A996	G929	U856	A776	U707	C623	A559	C422	C352
U1414	G1278	G1279	U1212	G1139	U1065	U987	C930	C856		C708	C624	A560	G423	A353
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G1417	C1344	C1281	C1214	G1142	G1068	A1000	C933	G859	C783	A715	A635	A563	U426	A356
A1418	U1345	C1282	G1215	G1143	C1069	G1001	C934	A860		A716		C564	U427	G357
G1423	G1347	U1283	C1216	A1144	U1070	G1002	A935	G861			U641	U565	U428	U358
U1424	C1348	C1284	C1217	A1145	C1071	A1003	C936	U870	U788	U717	A642	U566	G429	U359
U1425	A1349	A1285	C1218	A1146	G1072	A1004	A937	U871	A790	A718	A643	U567	U430	
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A1429	G1353	U1290	C1223		U1080	U1008		U875	U794	U723	U652	U571	U434	A366
A1430	U1354	U1291	U1224	A1157	A1082	A1012	G945	C876	C795	G724	G653	A572	A435	U367
A1431	G1355	G1292	A1225	C1158	U1083	G1013	A946	G877	C796	G725	G654	A573	C436	U368
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A1433	A1357	G1294	A1227	U1160	U1085	G1015	C948	C879	U798	G727	U656	C507	U438	
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A1441	C1366	C1302	U1235	U1168	G1094	G1024	A958	G890	C810	C736	A665	U584	A452	A383
G1442	G1367	C1303	A1236	A1169	U1095	U1025	A959	U891	C811	C737	G666	G585	A453	G384
C1443	U1370	G1304	C1237	A1170	C1096	G1026	U960	A892	G812	C738	G667	C586	G454	C385
A1446	G1371	G1305	A1238	A1171	C1097	U1029	U961	C893	U813	C739		C587		C386
A1447	U1372	A1306	A1239	C1172	C1098	U1030	U965	G894	A814	U740	U672	C588	U458	U387
A1448	G1373	U1307	U1240	U1173	A1101	G1031	G966	G895	A815	G741	A673	U589	A459	G388
C1449	U1379	U1308	G1242	G1174	A1102	G1032	C967	A896	A816		G674	U590	A460	A389
U1450	G1312	G1243	G1243	A1180	C1103	G1033	U968	A900	C817	A747	A675	U591	A461	U390
U1451	U1381	G1244	C1245	G1181	G1034	G1034	A968	A901	G818	G748	A676	G592	G462	G391
C1452	C1314	C1245	C1245	G1182	A1035	A1035	A969	A901	A819	A749	U677	U593	U463	C392
G1453	U1315	U1246	A1246	U1183	A1036	A1036	C970	G902	U820	C750	G683	U594	U464	A393
A1454	G1316	U1247	U1247	G1184	C1112	C1037	G971	G903	G821	G751	U684	A595	A465	G394
G1455	C1317	A1248	C1248	G1187	C1113	C1038	C972	U904	U822	G752	G685	A596	A466	C395
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G1457	A1319	A1250	A1250	G1190	U1115	U1040	A974	A908	C826	C754	U686	U534	A468	A397
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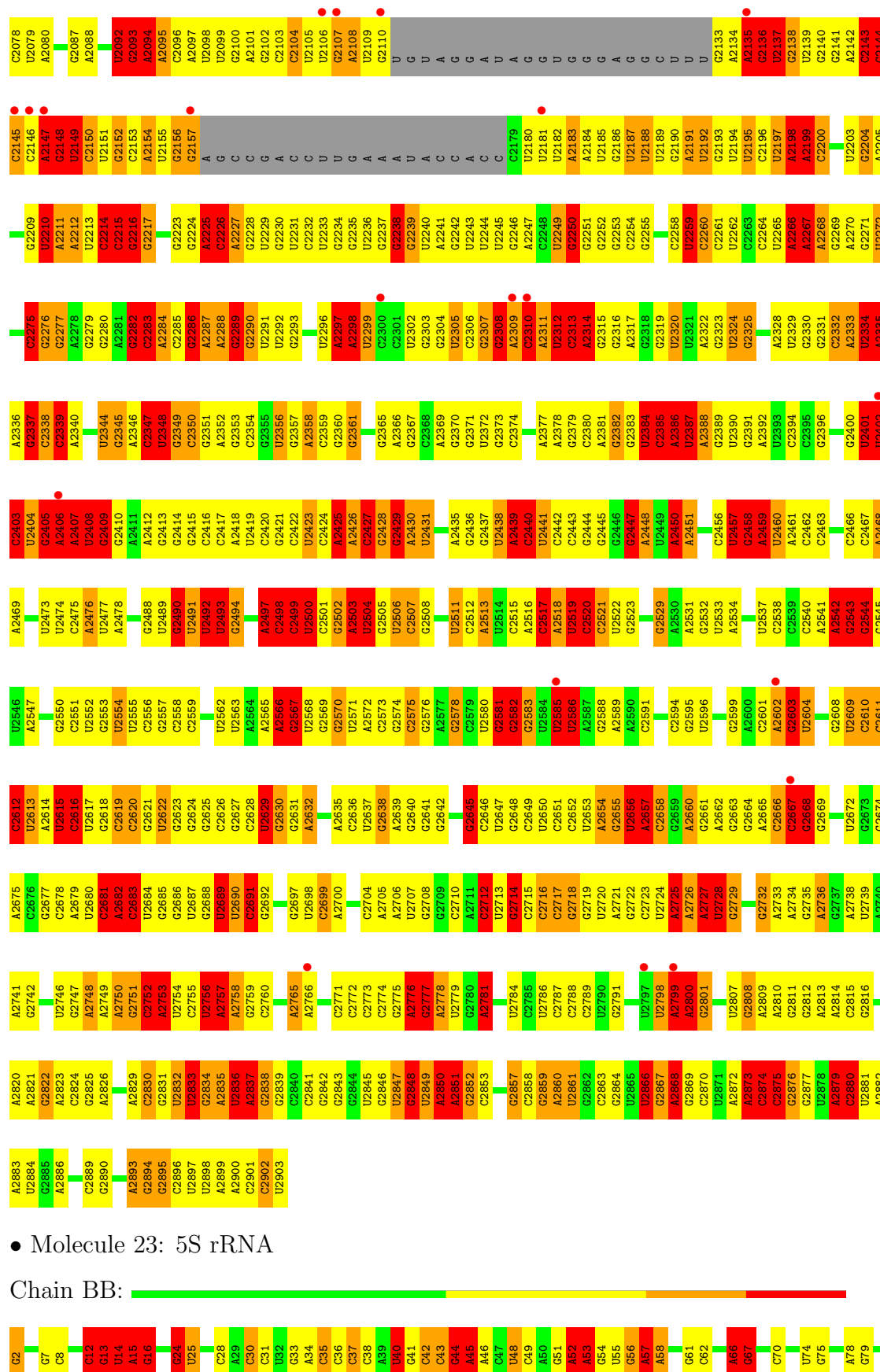


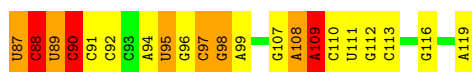




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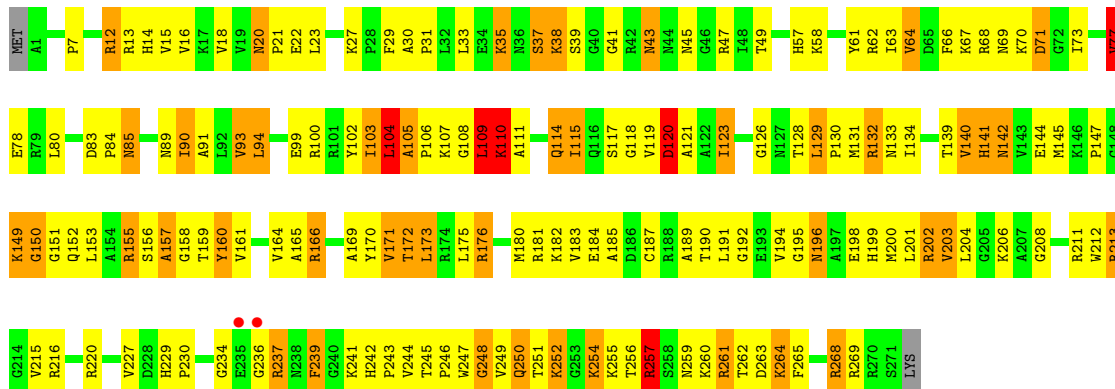
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C2055	C1989		G1946	A1783	A1717	A1650	A1587	A1526	U1458	C1330	A1265	G1198	U1131
G2056	U1990	C1925	A1847	A1784	G1718	G1651	G1588	C1527	G1459	G1331	G1266		U1132
U2057	C1991	U1926	U1848	U1785		A1652	G1589	A1528	U1460	G1332	U1267		A1133
A2058	U1992	A1927	A1849	A1786	G1721	G1653	U1590	G1529	C1462	G1333	A1268	U1201	A1134
G2059	C1993	C1927	C1854	U1787	U1722	A1654	A1591	U1530	U1461	U1334	A1269	G1202	G1135
A2060	U1994	A1928	U1854	C1788	G1723	A1655	C1592	A1531	G1465	C1335	C1270	U1203	G1136
C2061	G1995	G1928	U1855	U1789	G1724	C1656	C1593	A1532	U1466	G1336	A1271	A1204	G1137
A2062	C1996	U1930	G1865	C1790	U1725		A1593	G1527		G1337	U1272	A1205	G1138
C2063	C1997	A1932	U1866	U1796		G1661	U1594	A1529	C1463	G1338	U1273	G1206	G1139
A2064	C1998		A1867	U1797	C1732	U1662	C1595	U1533	U1468	G1339	A1274	C1207	G1140
C2065	C1999	G1935	G1868	C1798	G1730	A1664	A1596	A1534	G1469	U1401	A1275	C1208	U1141
G2066	C2000	A1936	U1869	U1799	U1731	A1665	U1597	A1535	G1601	U1402	A1276	G1210	A1142
C2067	C2001	A1937	G1870	U1796	C1733	G1666	U1598	A1536	A1470	A1403	G1277	G1211	A1143
U2068	U2007	A1938	C1871	U1797	G1734	A1668	A1599	C1537	A1471	U1404	A1278	G1212	A1144
G2069	C2008	U1939	U1872	U1798	A1735	A1689	U1602	C1538	A1472	U1405	G1279	A1213	A1145
A2070	A2009	G1940	C1873	C1799	U1736	A1690	A1603	U1539	U1473	U1406	G1280	G1214	C1146
C2071	C2010	C1941	C1874	C1800	U1737	U1670	C1604	U1540	U1474	U1407	G1281	G1215	
G2072	U2011	C1942	A1871	A1801	G1737	U1671	C1605	U1541		U1411			
C2073	C2012	U1943	A1872	A1802	G1738	A1672	C1606	U1542	G1475	U1412			
U2074	U2013	U1944	G1873	A1803	A1739	G1673	C1607	U1543	U1476				
A2075	A2014	G1945	C1874	C1804	G1740	G1674	C1608	C1544	A1477				
U2076							A1608		G1478				
A2077													





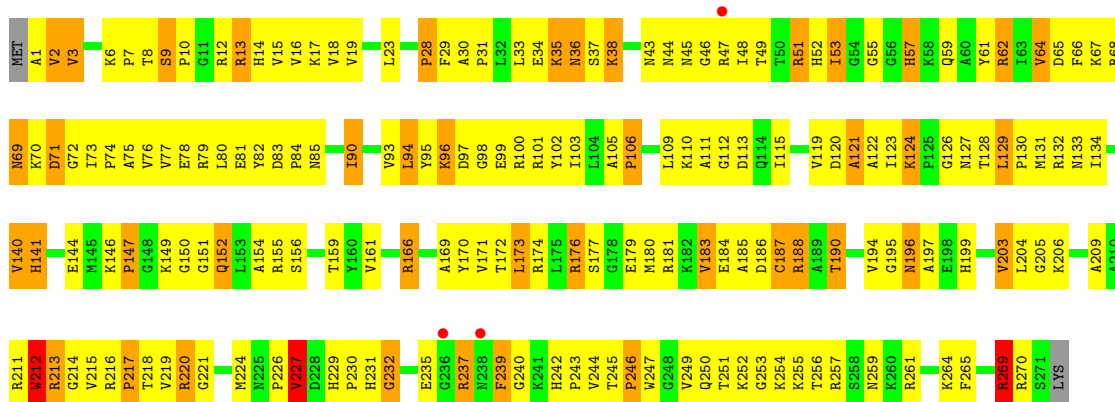
• Molecule 24: 50S ribosomal protein L2

Chain BC:



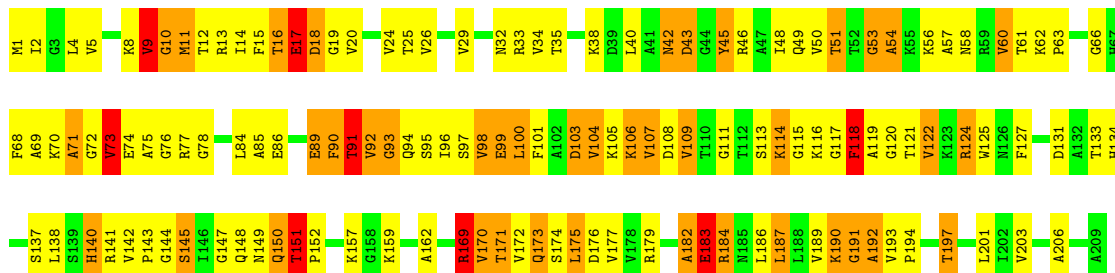
• Molecule 24: 50S ribosomal protein L2

Chain DC:



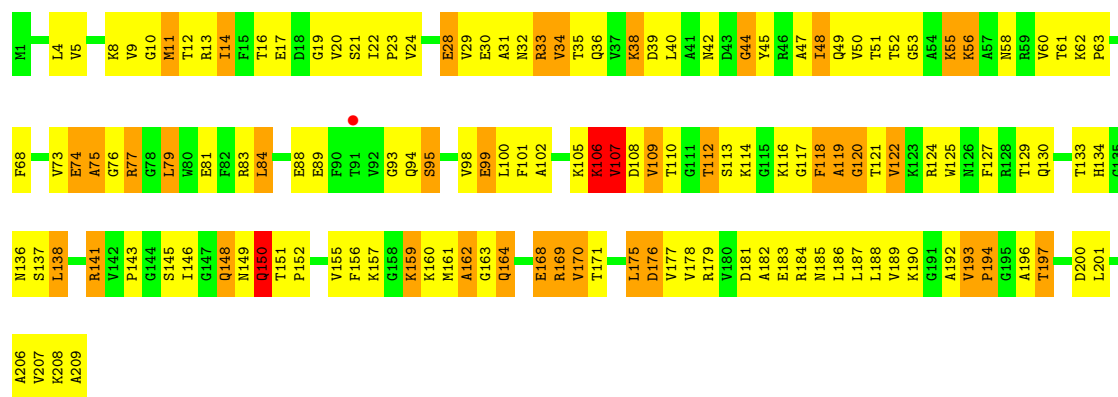
• Molecule 25: 50S ribosomal protein L3

Chain BD:



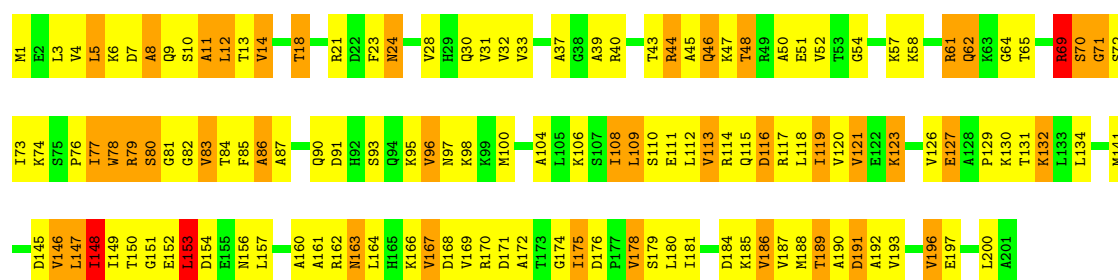
• Molecule 25: 50S ribosomal protein L3

Chain DD:



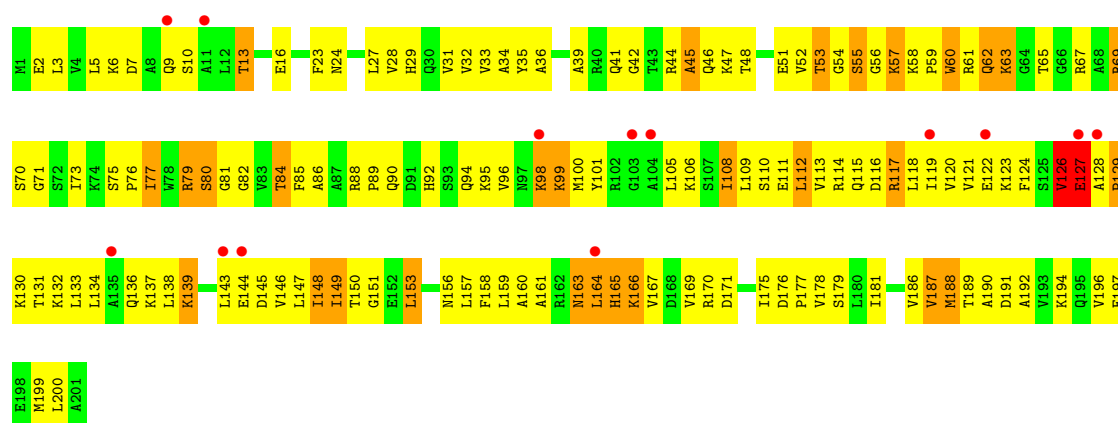
• Molecule 26: 50S ribosomal protein L4

Chain BE:



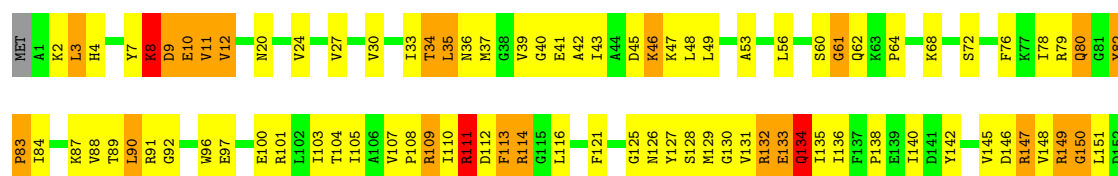
• Molecule 26: 50S ribosomal protein L4

Chain DE:



• Molecule 27: 50S ribosomal protein L5

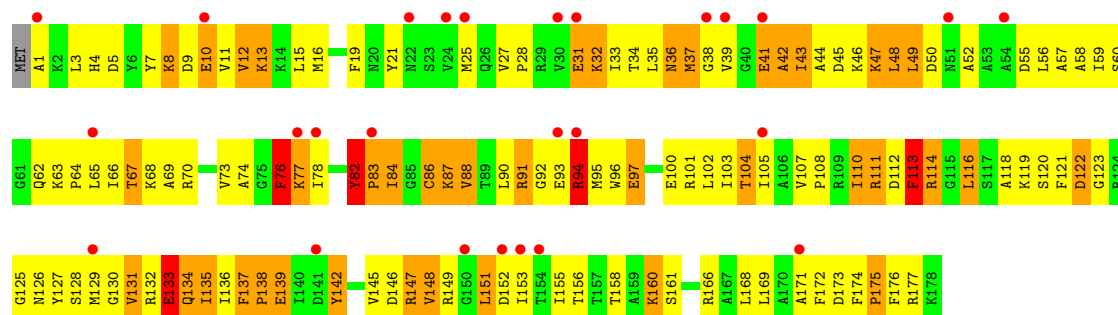
Chain BF:





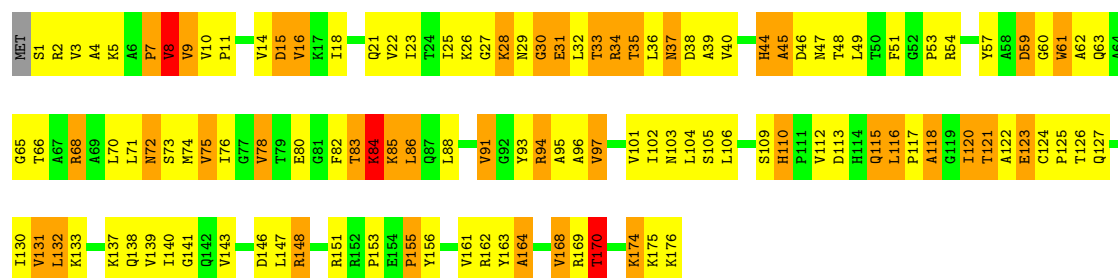
• Molecule 27: 50S ribosomal protein L5

Chain DF:



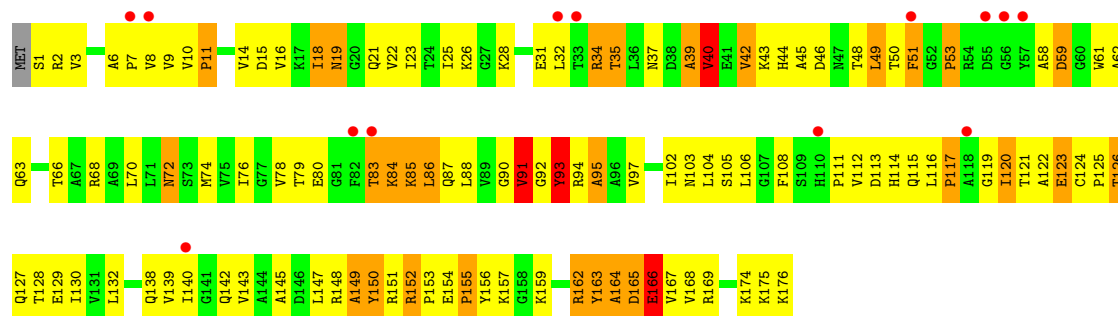
• Molecule 28: 50S ribosomal protein L6

Chain BG:



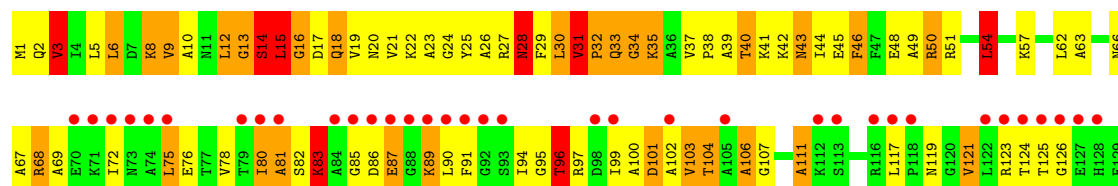
• Molecule 28: 50S ribosomal protein L6

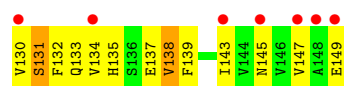
Chain DG:



• Molecule 29: 50S ribosomal protein L9

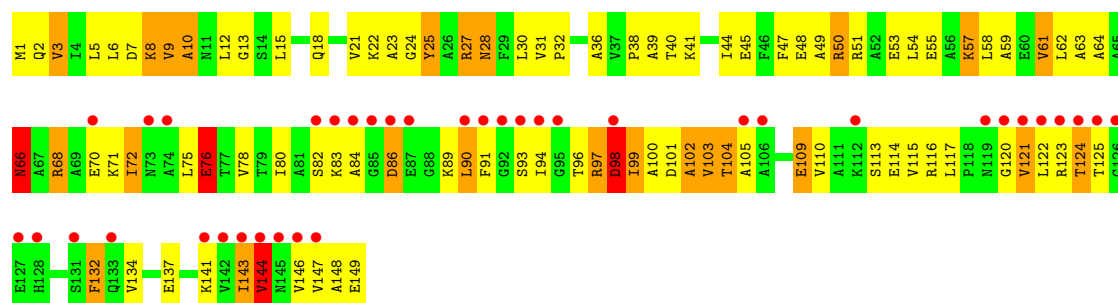
Chain BH:





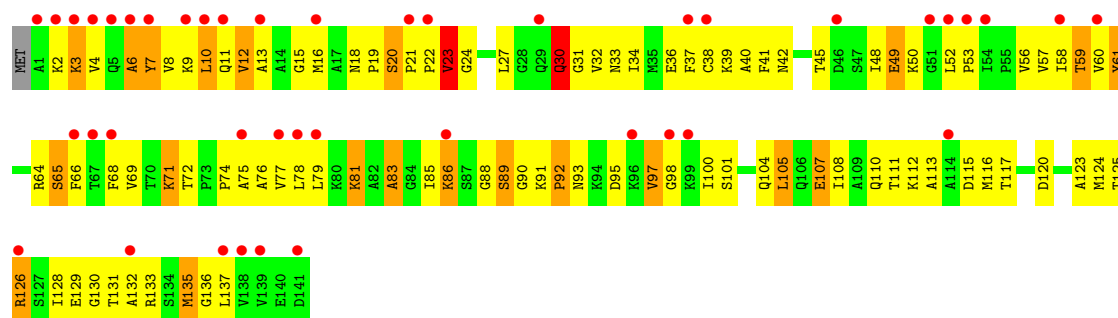
- Molecule 29: 50S ribosomal protein L9

Chain DH:



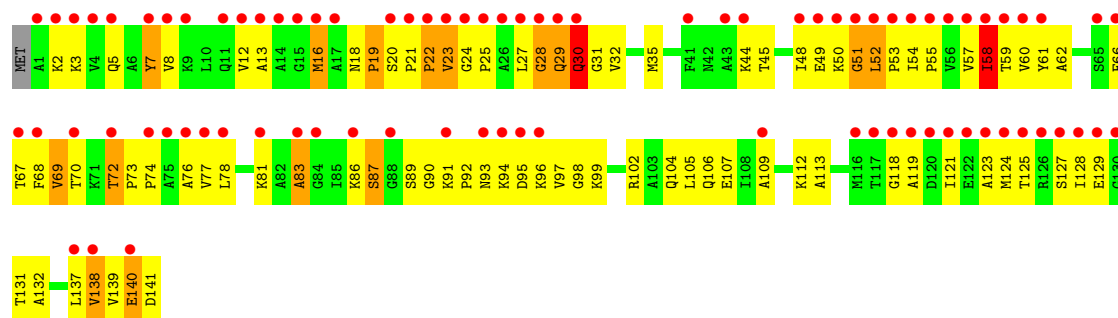
- Molecule 30: 50S ribosomal protein L11

Chain BI:



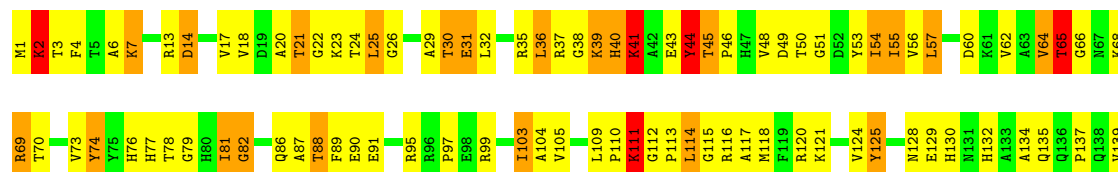
- Molecule 30: 50S ribosomal protein L11

Chain DI:



- Molecule 31: 50S ribosomal protein L13

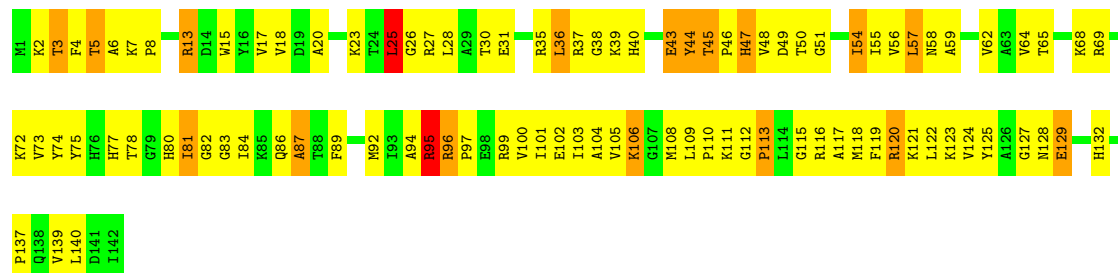
Chain BJ:





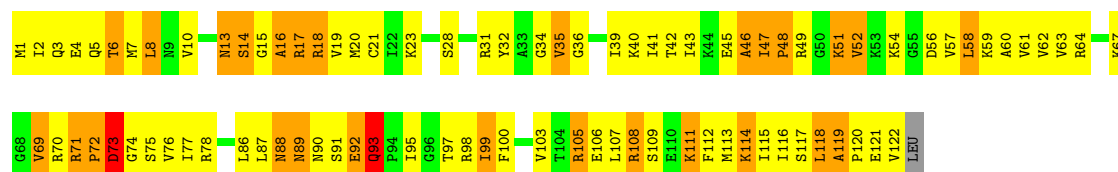
- Molecule 31: 50S ribosomal protein L13

Chain DJ:



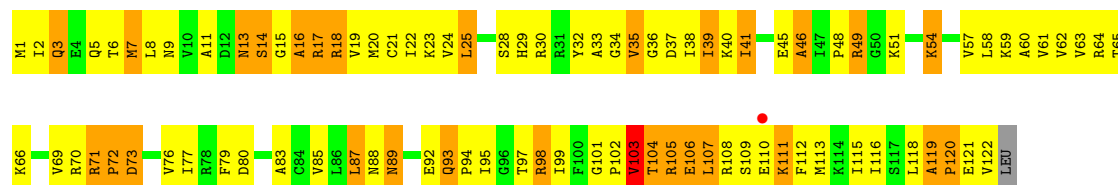
- Molecule 32: 50S ribosomal protein L14

Chain BK:



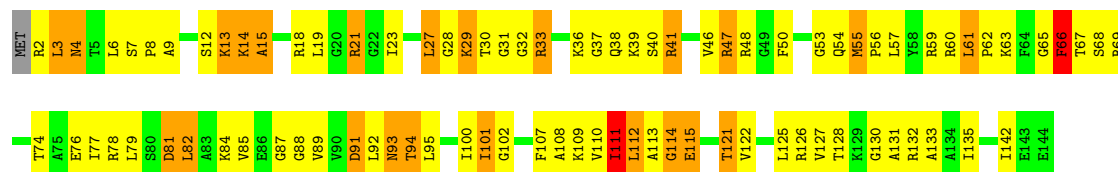
- Molecule 32: 50S ribosomal protein L14

Chain DK:



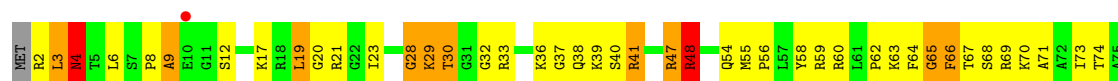
- Molecule 33: 50S ribosomal protein L15

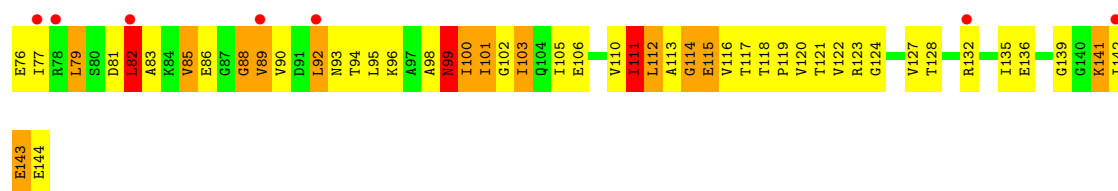
Chain BL:



- Molecule 33: 50S ribosomal protein L15

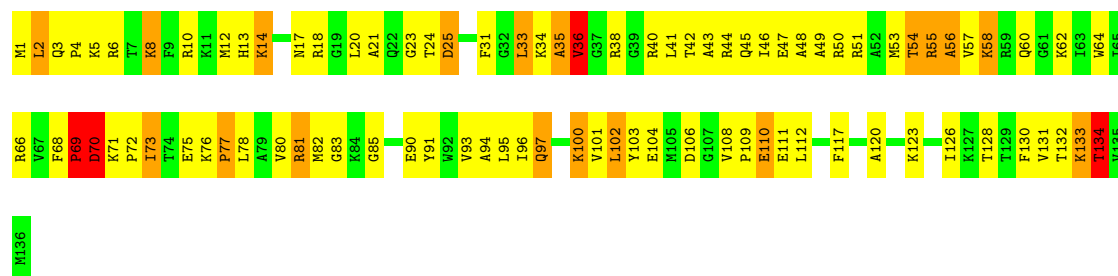
Chain DL:





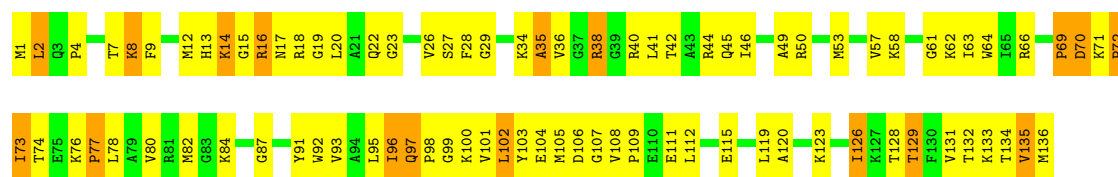
- Molecule 34: 50S ribosomal protein L16

Chain BM:



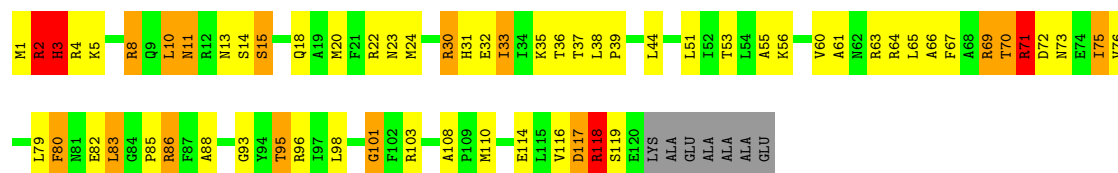
- Molecule 34: 50S ribosomal protein L16

Chain DM:



- Molecule 35: 50S ribosomal protein L17

Chain BN:



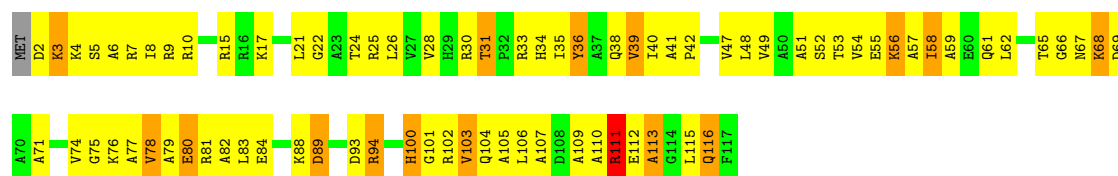
- Molecule 35: 50S ribosomal protein L17

Chain DN:



- Molecule 36: 50S ribosomal protein L18

Chain BO: 



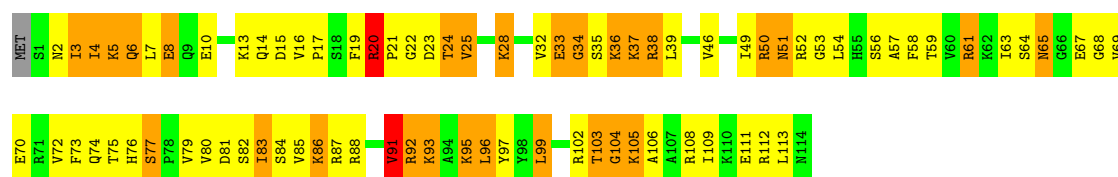
- Molecule 36: 50S ribosomal protein L18

Chain DO: 



- Molecule 37: 50S ribosomal protein L19

Chain BP: 



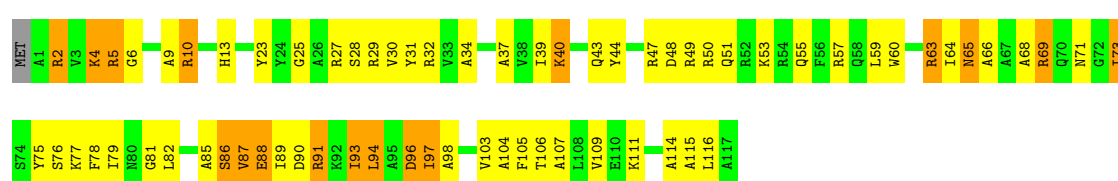
- Molecule 37: 50S ribosomal protein L19

Chain DP: 



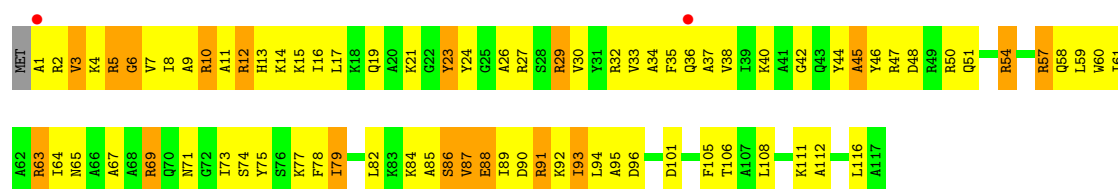
- Molecule 38: 50S ribosomal protein L20

Chain BQ: 



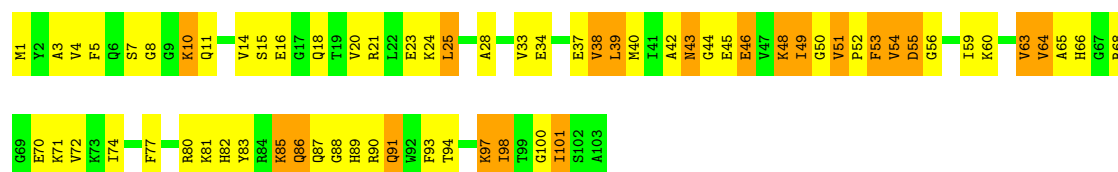
- Molecule 38: 50S ribosomal protein L20

Chain DQ: 



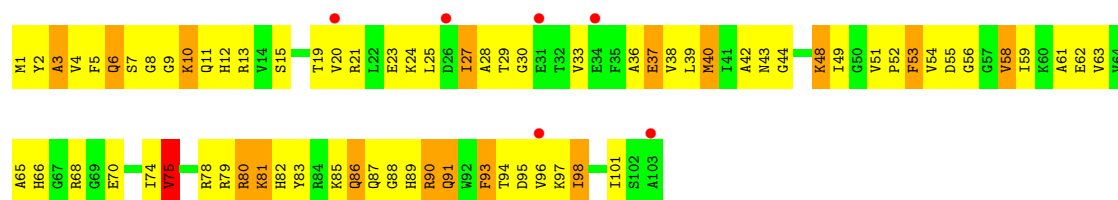
• Molecule 39: 50S ribosomal protein L21

Chain BR:



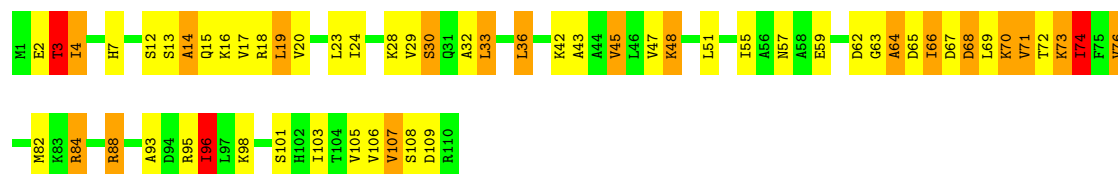
• Molecule 39: 50S ribosomal protein L21

Chain DR:



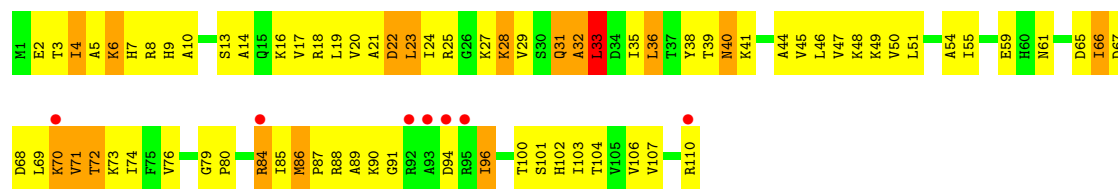
• Molecule 40: 50S ribosomal protein L22

Chain BS:



• Molecule 40: 50S ribosomal protein L22

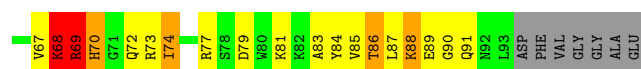
Chain DS:



• Molecule 41: 50S ribosomal protein L23

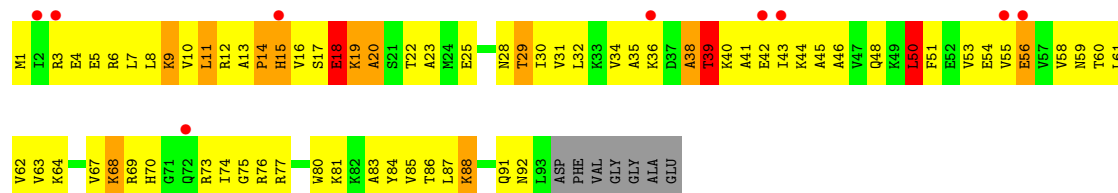
Chain BT:





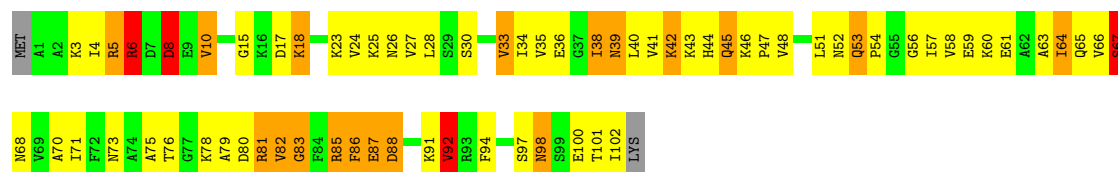
• Molecule 41: 50S ribosomal protein L23

Chain DT:



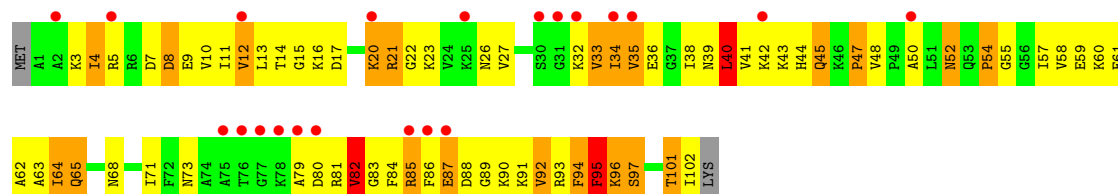
• Molecule 42: 50S ribosomal protein L24

Chain BU:



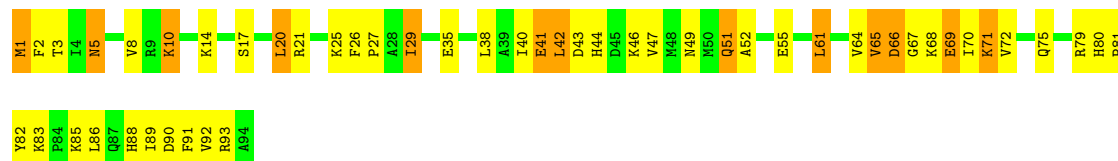
• Molecule 42: 50S ribosomal protein L24

Chain DU:



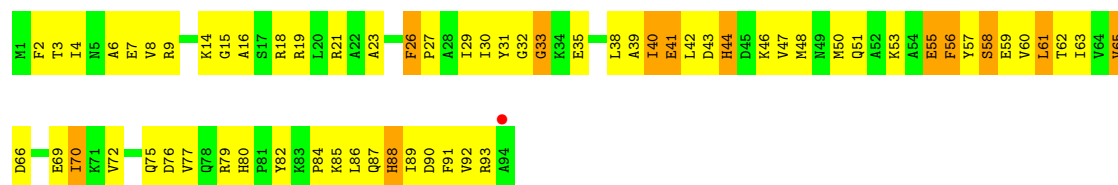
• Molecule 43: 50S ribosomal protein L25

Chain BV:



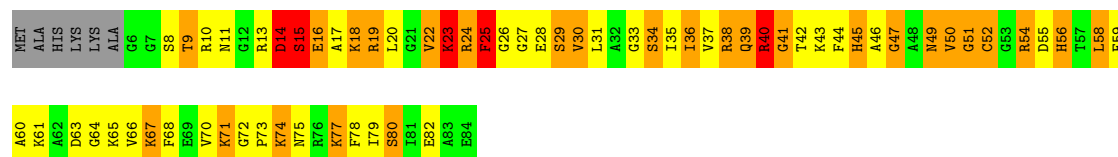
• Molecule 43: 50S ribosomal protein L25

Chain DV:



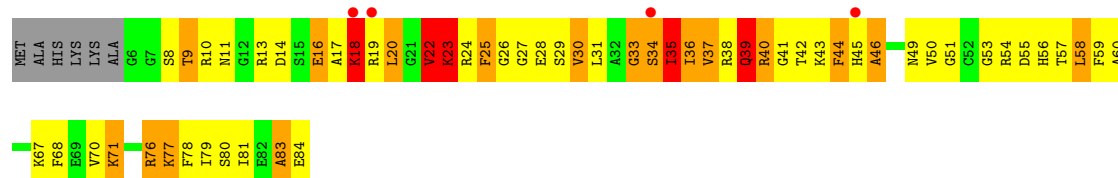
• Molecule 44: 50S ribosomal protein L27

Chain BW:



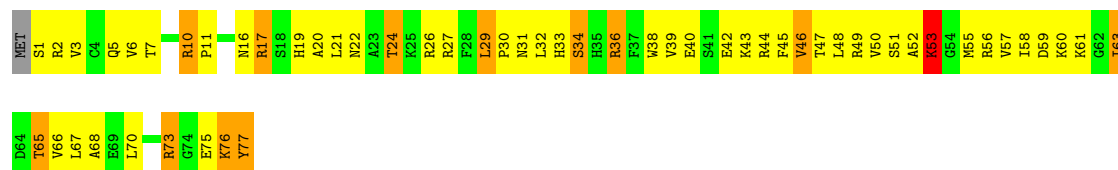
- Molecule 44: 50S ribosomal protein L27

Chain DW:



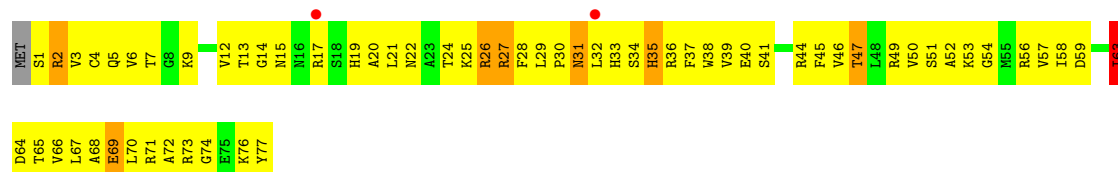
- Molecule 45: 50S ribosomal protein L28

Chain BX:



- Molecule 45: 50S ribosomal protein L28

Chain DX:



- Molecule 46: 50S ribosomal protein L29

Chain BY:



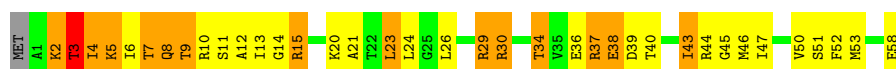
- Molecule 46: 50S ribosomal protein L29

Chain DY:



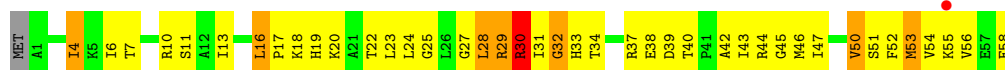
- Molecule 47: 50S ribosomal protein L30

Chain BZ:



- Molecule 47: 50S ribosomal protein L30

Chain DZ:



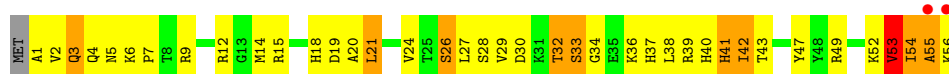
- Molecule 48: 50S ribosomal protein L32

Chain B0:



- Molecule 48: 50S ribosomal protein L32

Chain D0:



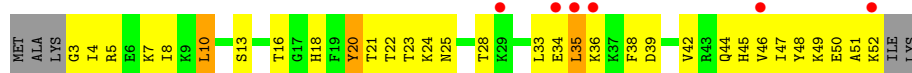
- Molecule 49: 50S ribosomal protein L33

Chain B1:



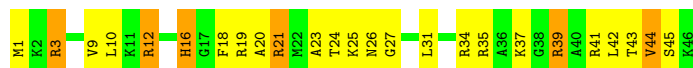
- Molecule 49: 50S ribosomal protein L33

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:



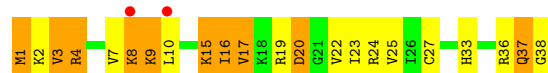
- Molecule 52: 50S ribosomal protein L36

Chain B4:



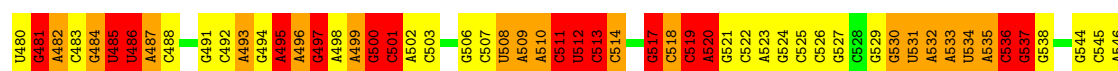
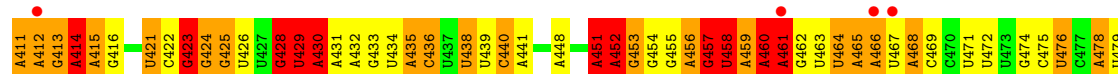
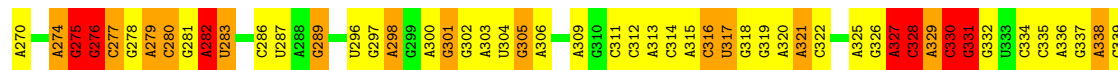
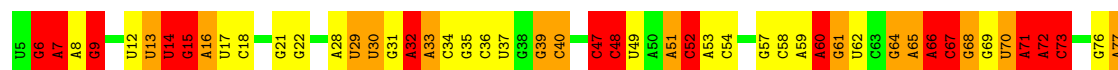
- Molecule 52: 50S ribosomal protein L36

Chain D4:



- Molecule 53: 16S rRNA

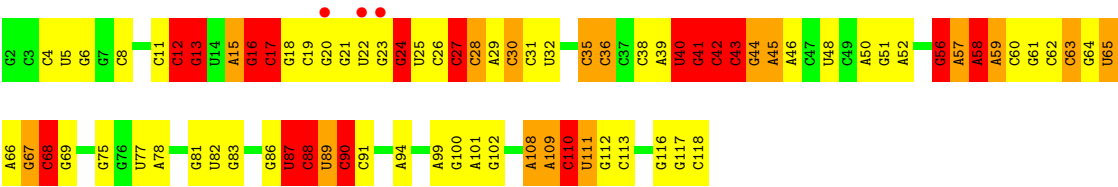
Chain CA:



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U1436	G1439	U1440	A1441	G1442	C1443	U1444	A1445	A1446	A1447	C1448	C1449	A1450	A1451	C1452	G1453	G1454	G1455	A1456	G1457	G1458	G1461	C1462	U1463	U1464	A1465	G1466	A1467	A1468	U1471	U1472	G1473	A1476	U1477	U1478	U1479	A1480	U1481	G1482	A1483	C1484	U1485	G1486	G1487	G1488	G1489	U1490	A1491	A1492	A1493	G1494	U1495	C1496	G1497	U1498	A1499										
C1366	C1367	A1368	C1369	G1370	G1371	U1372	U1373	A1374	A1375	U1376	A1377	C1378	C1379	U1380	U1381	C1382	C1383	C1384	G1385	G1386	G1387	C1388	U1391	G1392	U1393	A1394	C1395	A1396	C1397	A1398	C1399	C1400	G1401	G1402	C1403	U1341	G1404	U1478	U1479	A1480	U1481	G1482	A1483	C1484	U1485	G1486	G1487	G1488	G1489	U1490	A1491	A1492	A1493	G1494	U1495	C1496	G1497	U1498	A1499						
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A1239	U1240	G1241	C1242	G1243	G1244	C1245	U1247	A1248	C1249	A1250	A1251	A1252	U1253	A1254	G1255	A1256	U1257	G1258	C1259	G1260	A1261	C1262	C1263	U1264	C1265	A1266	C1267	G1268	A1269	G1270	C1271	G1272	C1273	A1274	G1278	G1279	A1280	C1281	C1282	U1283	G1284	U1341	G1404	U1478	U1479	A1480	U1481	G1482	A1483	C1484	U1485	G1486	G1487	G1488	G1489	U1490	A1491	A1492	A1493	G1494	U1495	C1496	G1497	U1498	A1499
C1303	G1304	G1305	U1308	G1309	G1310	G1311	G1312	U1313	C1314	U1315	U1316	U1317	U1318	C1319	C1320	U1321	C1322	G1323	A1324	G1325	U1326	C1327	C1328	A1329	U1330	G1331	A1332	A1333	G1334	U1335	C1336	G1337	G1338	A1339	C1403	U1341	G1404	U1478	U1479	A1480	U1481	G1482	A1483	C1484	U1485	G1486	G1487	G1488	G1489	U1490	A1491	A1492	A1493	G1494	U1495	C1496	G1497	U1498	A1499						
A1239	U1240	G1241	C1242	G1243	G1244	C1245	U1247	A1248	C1249	A1250	A1251	A1252	U1253	A1254	G1255	A1256	U1257	G1258	C1259	G1260	A1261	C1262	C1263	U1264	C1265	A1266	C1267	G1268	A1269	G1270	C1271	G1272	C1273	A1274	G1278	G1279	A1280	C1281	C1282	U1283	G1284	U1341	G1404	U1478	U1479	A1480	U1481	G1482	A1483	C1484	U1485	G1486	G1487	G1488	G1489	U1490	A1491	A1492	A1493	G1494	U1495	C1496	G1497	U1498	A1499
C1303	G1304	G1305	U1308	G1309	G1310	G1311	G1312	U1313	C1314	U1315	U1316	U1317	U1318	C1319	C1320	U1321	C1322	G1323	A1324	G1325	U1326	C1327	C1328	A1329	U1330	G1331	A1332	A1333	G1334	U1335	C1336	G1337	G1338	A1339	C1403	U1341	G1404	U1478	U1479	A1480	U1481	G1482	A1483	C1484	U1485	G1486	G1487	G1488	G1489	U1490	A1491	A1492	A1493	G1494	U1495	C1496	G1497	U1498	A1499						
A1239	U1240	G1241	C1242	G1243	G1244	C1245	U1247	A1248	C1249	A1250	A1251	A1252	U1253	A1254	G1255	A1256	U1257	G1258	C1259	G1260	A1261	C1262	C1263	U1264	C1265	A1266	C1267	G1268	A1269	G1270	C1271	G1272	C1273	A1274	G1278	G1279	A1280	C1281	C1282	U1283	G1284	U1341	G1404	U1478	U1479	A1480	U1481	G1482	A1483	C1484	U1485	G1486	G1487	G1488	G1489	U1490	A1491	A1492	A1493	G1494	U1495	C1496	G1497	U1498	A1499
C1303	G1304	G1305	U1308	G1309	G1310	G1311	G1312	U1313	C1314	U1315	U1316	U1317	U1318	C1319	C1320	U1321	C1322	G1323	A1324	G1325	U1326	C1327	C1328	A1329	U1330	G1331	A1332	A1333	G1334	U1335	C1336	G1337	G1338	A1339	C1403	U1341	G1404	U1478	U1479	A1480	U1481	G1482	A1483	C1484	U1485	G1486	G1487	G1488	G1489	U1490	A1491	A1492	A1493	G1494	U1495	C1496	G1497	U1498	A1499						
A1239	U1240	G1241	C1242	G1243	G1244	C1245	U1247	A1248	C1249	A1250	A1251	A1252	U1253	A1254	G1255	A1256	U1257	G1258	C1259	G1260	A1261	C1262	C1263	U1264	C1265	A1266	C1267	G1268	A1269	G1270	C1271	G1272	C1273	A1274	G1278	G1279	A1280	C1281	C1282	U1283	G1284	U1341	G1404	U1478	U1479	A1480	U1481	G1482	A1483	C1484	U1485	G1486	G1487	G1488	G1489	U1490	A1491	A1492	A1493	G1494	U1495	C1496	G1497	U1498	A1499
C1303	G1304	G1305	U1308	G1309	G1310	G1311	G1312	U1313	C1314	U1315	U1316	U1317	U1318	C1319	C1320	U1321	C1322	G1323	A1324	G1325	U1326	C1327	C1328	A1329	U1330	G1331	A1332	A1333	G1334	U1335	C1336	G1337	G1338	A1339	C1403	U1341	G1404	U1478	U1479	A1480	U1481	G1482	A1483	C1484	U1485	G1486	G1487	G1488	G1489	U1490	A1491	A1492	A1493	G1494	U1495	C1496	G1497	U1498	A1499						
A1239	U1240	G1241	C1242	G1243	G1244	C1245	U1247	A1248	C1249	A1250	A1251	A1252	U1253	A1254	G1255	A1256	U1257	G1258	C1259	G1260	A1261	C1262	C1263	U1264	C1265	A1266	C1267	G1268	A1269	G1270	C1271	G1272	C1273	A1274	G1278	G1279	A1280	C1281	C1282	U1283	G1284	U1341	G1404	U1478	U1479	A1480	U1481	G1482	A1483	C1484	U1485	G1486	G1487	G1488	G1489	U1490	A1491	A1492	A1493	G1494	U1495	C1496	G1497	U1498	A1499
C1303	G1304	G1305	U1308	G1309	G1310	G1311	G1312	U1313	C1314	U1315	U1316	U1317	U1318	C1319	C1320	U1321	C1322	G1323	A1324	G1325	U1326	C1327	C1328	A1329	U1330	G1331	A1332	A1333	G1334	U1335	C1336	G1337	G1338	A1339	C1403	U1341	G1404	U1478	U1479	A1480	U1481	G1482	A1483	C1484	U1485	G1486	G1487	G1488	G1489	U1490	A1491	A1492	A1493	G1494	U1495	C1496	G1497	U1498	A1499						
A1239	U1240	G1241	C1242	G1243	G1244	C1245	U1247	A1248	C1249	A1250	A1251	A1252	U1253	A1254	G1255	A1256	U1257	G1258	C1259	G1260	A1261	C1262	C1263	U1264	C1265	A1266	C1267	G1268	A1269	G1270	C1271	G1272	C1273	A1274	G1278	G1279	A1280	C1281	C1282	U1283	G1284	U1341	G1404	U1478	U1479	A1480	U1481	G1482	A1483	C1484	U1485	G1486	G1487	G1488	G1489	U1490	A1491	A1492	A1493	G1494	U1495	C1496	G1497	U1498	A1499
C1303	G1304	G1305	U1308	G1309	G1310	G1311	G1312	U1313	C1314	U1315	U1316	U1317	U1318	C1319	C1320	U1321	C1322	G1323	A1324	G1325	U1326	C1327	C1328	A1329	U1330	G1331	A1332	A1333	G1334	U1335	C1336	G1337	G1338	A1339	C1403	U1341	G1404	U1478	U1479	A1480	U1481	G1482	A1483	C1484	U1485	G1486	G1487	G1488	G1489	U1490	A1491	A1492	A1493	G1494	U1495	C1496	G1497	U1498	A1499						
A1239	U1240	G1241	C1242	G1243	G1244	C1245	U1247	A1248	C1249	A1250	A1251	A1252	U1253	A1254	G1255	A1256	U1257	G1258	C1259	G1260	A1261	C1262	C1263	U1264	C1265	A1266	C1267	G1268	A1269	G1270	C1271	G1272	C1273	A1274	G1278	G1279	A1280	C1281	C1282	U1283	G1284	U1341	G1404	U1478	U1479	A1480	U1481	G1482	A1483	C1484	U1485	G1486	G1487	G1488	G1489	U1490	A1491	A1492	A1493	G1494	U1495	C1496	G1497	U1498	A1499
C1303	G1304	G1305	U1308	G1309	G1310	G1311	G1312	U1313	C1314	U1315	U1316	U1317	U1318	C1319	C1320	U1321	C1322	G1323	A1324	G1325	U1326	C1327	C1328	A1329	U1330	G1331	A1332	A1333	G1334	U1335	C1336	G1337	G1338	A1339	C1403	U1341	G1404	U1478	U1479	A1480	U1481	G1482	A1483	C1484	U1485	G1486	G1487	G1488	G1489	U1490	A1491	A1492	A1493	G1494	U1495	C1496	G1497	U1498	A1499						
A1239	U1240	G1241	C1242	G1243	G1244	C1245	U1247	A1248	C1249	A1250	A1251	A1252	U1253	A1254	G1255	A1256	U1257	G1258	C1259	G1260	A1261	C1262	C1263	U1264	C1265	A1266	C1267	G1268	A1269	G1270	C1271	G1272	C1273	A1274	G1278	G1279	A1280	C1281	C1282	U1283	G1284	U1341	G1404	U1478	U1479	A1480	U1481	G1482	A1483	C1484	U1485	G1486	G1487	G1488	G1489	U1490	A1491	A1492	A1493	G1494	U1495	C1496	G1497	U1498	A1499
C1303	G1304	G1305	U1308	G1309	G1310	G1311	G1312	U1313	C1314	U1315	U1316	U1317	U1318	C1319	C1320	U1321	C1322	G1323	A1324	G1325	U1326	C1327	C1328	A1329	U1330	G1331	A1332	A1333	G1334	U1335	C1336	G1337	G1338	A1339	C1403	U1341	G1404	U1478	U1479	A1480	U1481	G1482	A1483	C1484	U1485	G1486	G1487	G1488	G1489	U1490	A1491	A1492	A1493	G1494	U1495	C1496	G1497	U1498	A1499						
A1239	U1240	G1241	C1242	G1243	G1244	C1245	U1247	A1248	C1249	A1250	A1251	A1252	U1253	A1254	G1255	A1256	U1257	G1258	C1259	G1260	A1261	C1262	C1263	U1264	C1265	A1266	C1267	G1268	A1269	G1270	C1271	G1272	C1273	A1274	G1278	G1279	A1280	C1281	C1282	U1283	G1284	U1341	G1404	U1478	U1479	A1480	U1481	G1482	A1483	C1484	U1485	G1486	G1487	G1488	G1489	U1490	A1491	A1492	A1493	G1494	U1495	C1496	G1497	U1498	A1499
C1303	G1304	G1305	U1308	G1309	G1310	G1311	G1312	U1313	C1314	U1315	U1316	U1317	U1318	C1319	C1320	U1321	C1322	G1323	A1324	G1325	U1326	C1327	C1328	A1329	U1330	G1331	A1332	A1333	G1334	U1335	C1336	G1337	G1338	A1339	C1403	U1341	G1404	U1478	U1479	A1480	U1481	G1482																							

● Molecule 54: 5S rRNA

Chain DB: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.89Å 434.93Å 622.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.88 – 3.19 39.88 – 3.19	Depositor EDS
% Data completeness (in resolution range)	95.8 (39.88-3.19) 95.8 (39.88-3.19)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 3.18Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.195 , 0.252 0.211 , 0.263	Depositor DCC
R_{free} test set	18197 reflections (2.05%)	DCC
Wilson B-factor (Å ²)	63.6	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 40.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 904292 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	284450	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.53% 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, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AB	0.30	0/1735	0.52	0/2338
1	CB	0.27	0/1735	0.49	0/2338
2	AC	0.30	0/1651	0.53	1/2225 (0.0%)
2	CC	0.25	0/1651	0.45	0/2225
3	AD	0.31	0/1665	0.52	0/2227
3	CD	0.39	0/1665	0.60	0/2227
4	AE	0.36	0/1118	0.63	1/1504 (0.1%)
4	CE	0.34	0/1118	0.54	0/1504
5	AF	0.32	0/835	0.49	0/1128
5	CF	0.28	0/835	0.50	0/1128
6	AG	0.27	0/1195	0.48	0/1602
6	CG	0.25	0/1187	0.46	0/1591
7	AH	0.33	0/989	0.55	0/1326
7	CH	0.28	0/989	0.50	0/1326
8	AI	0.27	0/1034	0.49	0/1375
8	CI	0.24	0/1034	0.43	0/1375
9	AJ	0.29	0/796	0.53	0/1077
9	CJ	0.24	0/796	0.48	0/1077
10	AK	0.31	0/893	0.56	0/1205
10	CK	0.29	0/893	0.50	0/1205
11	AL	0.39	0/969	0.69	0/1300
11	CL	0.32	0/969	0.57	0/1300
12	AM	0.26	0/892	0.49	0/1193
12	CM	0.20	0/884	0.41	0/1181
13	AN	0.30	0/785	0.54	0/1043
13	CN	0.22	0/780	0.39	0/1036
14	AO	0.30	0/722	0.49	0/964
14	CO	0.26	0/722	0.45	0/964
15	AP	0.30	0/659	0.50	0/884
15	CP	0.30	0/648	0.51	0/870
16	AQ	0.39	0/657	0.59	0/881
16	CQ	0.31	0/657	0.51	0/881

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AR	0.30	0/462	0.50	0/621
17	CR	0.30	0/462	0.47	0/621
18	AS	0.28	0/652	0.49	0/877
18	CS	0.21	0/652	0.43	0/877
19	AT	0.35	0/671	0.56	0/888
19	CT	0.27	0/671	0.50	0/888
20	AU	0.39	0/430	0.54	0/570
20	CU	0.39	0/430	0.63	0/570
21	AA	0.55	1/36834 (0.0%)	1.38	581/57462 (1.0%)
22	BA	0.78	12/68626 (0.0%)	1.59	1420/107056 (1.3%)
22	DA	0.50	0/68314	1.35	1136/106569 (1.1%)
23	BB	0.71	0/2828	1.50	45/4410 (1.0%)
24	BC	0.44	0/2121	0.70	1/2852 (0.0%)
24	DC	0.31	0/2121	0.53	0/2852
25	BD	0.53	0/1586	0.76	1/2134 (0.0%)
25	DD	0.30	0/1586	0.56	0/2134
26	BE	0.43	0/1571	0.64	0/2113
26	DE	0.26	0/1571	0.47	0/2113
27	BF	0.33	0/1434	0.54	0/1926
27	DF	0.23	0/1444	0.47	0/1937
28	BG	0.40	0/1343	0.64	0/1816
28	DG	0.24	0/1343	0.48	0/1816
29	BH	0.31	0/1122	0.50	0/1515
29	DH	0.28	0/1122	0.50	0/1515
30	BI	0.23	0/1046	0.47	0/1410
30	DI	0.21	0/1046	0.43	0/1410
31	BJ	0.57	0/1152	0.80	1/1551 (0.1%)
31	DJ	0.28	0/1152	0.55	1/1551 (0.1%)
32	BK	0.51	0/947	0.77	0/1268
32	DK	0.33	0/947	0.56	0/1268
33	BL	0.43	0/1054	0.75	0/1403
33	DL	0.27	0/1054	0.52	0/1403
34	BM	0.50	0/1093	0.70	0/1460
34	DM	0.27	0/1093	0.46	0/1460
35	BN	0.47	0/973	0.70	0/1301
35	DN	0.28	0/973	0.50	0/1301
36	BO	0.42	0/902	0.63	0/1209
36	DO	0.22	0/902	0.42	0/1209
37	BP	0.50	0/929	0.73	0/1242
37	DP	0.30	0/929	0.50	0/1242
38	BQ	0.57	0/960	0.73	0/1278
38	DQ	0.29	0/960	0.46	0/1278
39	BR	0.60	1/829 (0.1%)	0.75	0/1107

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	DR	0.28	0/829	0.49	0/1107
40	BS	0.53	0/864	0.72	0/1156
40	DS	0.29	0/864	0.52	0/1156
41	BT	0.46	0/744	0.74	0/994
41	DT	0.24	0/744	0.48	0/994
42	BU	0.44	0/787	0.70	0/1051
42	DU	0.25	0/787	0.47	0/1051
43	BV	0.42	0/766	0.58	0/1025
43	DV	0.25	0/766	0.43	0/1025
44	BW	0.56	0/603	0.87	0/797
44	DW	0.26	0/603	0.48	0/797
45	BX	0.42	0/635	0.70	1/848 (0.1%)
45	DX	0.27	0/635	0.55	0/848
46	BY	0.35	0/510	0.65	0/677
46	DY	0.22	0/510	0.45	0/677
47	BZ	0.51	0/453	0.77	0/605
47	DZ	0.26	0/453	0.49	0/605
48	B0	0.45	0/450	0.71	0/599
48	D0	0.28	0/450	0.51	0/599
49	B1	0.40	0/416	0.63	0/554
49	D1	0.27	0/416	0.46	0/554
50	B2	0.46	0/380	0.73	0/498
50	D2	0.28	0/380	0.50	0/498
51	B3	0.45	0/513	0.69	0/676
51	D3	0.27	0/513	0.51	0/676
52	B4	0.55	0/303	0.78	0/397
52	D4	0.27	0/303	0.49	0/397
53	CA	0.50	0/36762	1.32	542/57350 (0.9%)
54	DB	0.44	0/2803	1.26	34/4371 (0.8%)
All	All	0.55	14/306737 (0.0%)	1.26	3765/458565 (0.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
25	BD	0	1
32	BK	0	1
35	BN	0	1
51	B3	0	1
All	All	0	4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1142	A	N9-C4	-10.15	1.31	1.37
22	BA	2451	A	C8-N7	8.00	1.37	1.31
22	BA	2447	G	N9-C4	7.71	1.44	1.38
22	BA	984	A	N9-C4	-6.87	1.33	1.37
22	BA	1142	A	C8-N7	6.70	1.36	1.31

The worst 5 of 3765 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2447	G	C6-N1-C2	-18.49	114.00	125.10
22	BA	919	U	N1-C2-O2	18.00	135.40	122.80
22	BA	919	U	C2-N1-C1'	16.54	137.55	117.70
22	BA	302	C	N1-C1'-C2'	-16.46	92.60	114.00
22	BA	805	G	P-O3'-C3'	15.12	137.85	119.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
51	B3	29	ARG	Peptide
25	BD	9	VAL	Peptide
32	BK	15	GLY	Peptide
35	BN	101	GLY	Peptide

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AB	1704	0	1732	221	0
1	CB	1704	0	1732	174	0
2	AC	1624	0	1699	112	0
2	CC	1624	0	1699	143	0
3	AD	1643	0	1710	151	0
3	CD	1643	0	1710	152	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	AE	1105	0	1148	132	0
4	CE	1105	0	1148	99	0
5	AF	817	0	808	73	0
5	CF	817	0	808	66	0
6	AG	1181	0	1240	87	0
6	CG	1174	0	1230	136	0
7	AH	979	0	1034	74	0
7	CH	979	0	1034	88	0
8	AI	1022	0	1070	83	0
8	CI	1022	0	1070	98	0
9	AJ	786	0	828	74	0
9	CJ	786	0	828	97	0
10	AK	877	0	887	89	0
10	CK	877	0	887	78	0
11	AL	955	0	1019	89	0
11	CL	955	0	1019	89	0
12	AM	883	0	944	74	0
12	CM	876	0	937	107	0
13	AN	774	0	827	76	0
13	CN	769	0	822	82	0
14	AO	714	0	737	54	0
14	CO	714	0	737	36	0
15	AP	649	0	666	52	0
15	CP	638	0	656	67	0
16	AQ	648	0	691	75	0
16	CQ	648	0	691	61	0
17	AR	455	0	478	25	0
17	CR	455	0	478	35	0
18	AS	637	0	665	52	0
18	CS	637	0	665	75	0
19	AT	665	0	714	72	0
19	CT	665	0	714	52	0
20	AU	425	0	449	88	0
20	CU	425	0	449	80	0
21	AA	32895	0	16553	1203	0
22	BA	61274	0	30819	1932	0
22	DA	60995	0	30679	3174	0
23	BB	2529	0	1281	63	0
24	BC	2082	0	2157	213	0
24	DC	2082	0	2157	210	0
25	BD	1565	0	1616	186	0
25	DD	1565	0	1616	179	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	BE	1552	0	1619	127	0
26	DE	1552	0	1619	172	0
27	BF	1410	0	1447	124	0
27	DF	1420	0	1460	170	0
28	BG	1323	0	1374	169	0
28	DG	1323	0	1374	137	0
29	BH	1111	0	1148	107	0
29	DH	1111	0	1148	102	0
30	BI	1032	0	1088	108	0
30	DI	1032	0	1088	77	0
31	BJ	1129	0	1162	154	0
31	DJ	1129	0	1162	141	0
32	BK	938	0	1012	99	0
32	DK	938	0	1012	111	0
33	BL	1045	0	1117	117	0
33	DL	1045	0	1117	115	0
34	BM	1074	0	1157	102	0
34	DM	1074	0	1157	96	0
35	BN	960	0	1000	82	0
35	DN	960	0	1000	122	0
36	BO	892	0	923	74	0
36	DO	892	0	923	75	0
37	BP	917	0	965	131	0
37	DP	917	0	965	112	0
38	BQ	947	0	1022	124	0
38	DQ	947	0	1022	131	0
39	BR	816	0	839	91	0
39	DR	816	0	839	91	0
40	BS	857	0	922	67	0
40	DS	857	0	922	76	0
41	BT	738	0	807	117	0
41	DT	738	0	807	98	0
42	BU	779	0	834	57	0
42	DU	779	0	834	89	0
43	BV	753	0	780	45	0
43	DV	753	0	780	64	0
44	BW	596	0	610	187	0
44	DW	596	0	610	111	0
45	BX	625	0	655	61	0
45	DX	625	0	655	63	0
46	BY	509	0	543	55	0
46	DY	509	0	543	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	BZ	449	0	491	39	0
47	DZ	449	0	491	43	0
48	B0	444	0	461	22	0
48	D0	444	0	461	53	0
49	B1	409	0	440	44	0
49	D1	409	0	440	31	0
50	B2	377	0	418	29	0
50	D2	377	0	418	41	0
51	B3	504	0	574	41	0
51	D3	504	0	574	58	0
52	B4	302	0	340	32	0
52	D4	302	0	340	29	0
53	CA	32831	0	16521	1452	0
54	DB	2507	0	1270	121	0
55	AA	43	0	0	0	0
55	BA	137	0	0	0	0
55	BB	4	0	0	0	0
55	CA	42	0	0	0	0
55	DA	135	0	0	0	0
55	DB	1	0	0	0	0
55	DJ	1	0	0	0	0
56	B4	1	0	0	0	0
56	D4	1	0	0	0	0
57	AA	195	0	0	2	0
57	AE	1	0	0	0	0
57	AL	3	0	0	0	0
57	AN	6	0	0	0	0
57	AT	2	0	0	0	0
57	AU	1	0	0	0	0
57	B0	1	0	0	0	0
57	B2	1	0	0	0	0
57	B3	3	0	0	0	0
57	B4	3	0	0	0	0
57	BA	610	0	0	24	0
57	BB	20	0	0	1	0
57	BC	10	0	0	0	0
57	BD	2	0	0	1	0
57	BL	4	0	0	1	0
57	BN	3	0	0	0	0
57	BQ	1	0	0	0	0
57	BT	2	0	0	1	0
57	CA	192	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	CE	5	0	0	0	0
57	CI	1	0	0	0	0
57	CL	1	0	0	0	0
57	CN	3	0	0	0	0
57	CT	3	0	0	0	0
57	CU	2	0	0	0	0
57	D2	1	0	0	1	0
57	D3	1	0	0	0	0
57	D4	4	0	0	0	0
57	DA	599	0	0	9	0
57	DB	4	0	0	0	0
57	DC	13	0	0	1	0
57	DD	4	0	0	0	0
57	DE	3	0	0	0	0
57	DJ	3	0	0	0	0
57	DL	5	0	0	0	0
57	DN	2	0	0	2	0
57	DT	2	0	0	1	0
57	DU	1	0	0	0	0
57	DV	1	0	0	0	0
All	All	284450	0	190838	15808	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 33.

The worst 5 of 15808 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
38:BQ:63:ARG:NH1	38:BQ:96:ASP:HA	1.49	1.26
22:DA:1439:A:C2	22:DA:1552:A:C6	2.32	1.17
22:DA:1439:A:N1	22:DA:1552:A:C5	2.12	1.17
27:BF:35:LEU:HB3	27:BF:153:ILE:HG22	1.19	1.16
33:BL:93:ASN:HD22	33:BL:94:THR:N	1.44	1.16

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AB	216/241 (90%)	131 (61%)	49 (23%)	36 (17%)	0	1
1	CB	216/241 (90%)	149 (69%)	47 (22%)	20 (9%)	1	8
2	AC	204/233 (88%)	151 (74%)	35 (17%)	18 (9%)	1	8
2	CC	204/233 (88%)	144 (71%)	41 (20%)	19 (9%)	1	8
3	AD	203/206 (98%)	140 (69%)	36 (18%)	27 (13%)	0	2
3	CD	203/206 (98%)	142 (70%)	39 (19%)	22 (11%)	1	5
4	AE	148/167 (89%)	107 (72%)	25 (17%)	16 (11%)	1	5
4	CE	148/167 (89%)	111 (75%)	21 (14%)	16 (11%)	1	5
5	AF	98/135 (73%)	74 (76%)	15 (15%)	9 (9%)	1	8
5	CF	98/135 (73%)	68 (69%)	18 (18%)	12 (12%)	1	3
6	AG	149/179 (83%)	108 (72%)	34 (23%)	7 (5%)	4	27
6	CG	148/179 (83%)	99 (67%)	35 (24%)	14 (10%)	1	7
7	AH	127/130 (98%)	93 (73%)	30 (24%)	4 (3%)	7	41
7	CH	127/130 (98%)	96 (76%)	20 (16%)	11 (9%)	1	8
8	AI	125/130 (96%)	84 (67%)	31 (25%)	10 (8%)	1	10
8	CI	125/130 (96%)	90 (72%)	21 (17%)	14 (11%)	1	4
9	AJ	96/103 (93%)	67 (70%)	18 (19%)	11 (12%)	1	4
9	CJ	96/103 (93%)	55 (57%)	24 (25%)	17 (18%)	0	1
10	AK	115/129 (89%)	85 (74%)	21 (18%)	9 (8%)	1	11
10	CK	115/129 (89%)	85 (74%)	22 (19%)	8 (7%)	2	13
11	AL	121/124 (98%)	87 (72%)	20 (16%)	14 (12%)	1	4
11	CL	121/124 (98%)	85 (70%)	29 (24%)	7 (6%)	3	21
12	AM	112/118 (95%)	89 (80%)	16 (14%)	7 (6%)	2	18
12	CM	111/118 (94%)	60 (54%)	38 (34%)	13 (12%)	1	4
13	AN	92/101 (91%)	56 (61%)	24 (26%)	12 (13%)	0	3
13	CN	91/101 (90%)	60 (66%)	26 (29%)	5 (6%)	3	23
14	AO	86/89 (97%)	63 (73%)	20 (23%)	3 (4%)	6	37
14	CO	86/89 (97%)	62 (72%)	20 (23%)	4 (5%)	4	27
15	AP	80/82 (98%)	58 (72%)	14 (18%)	8 (10%)	1	6
15	CP	78/82 (95%)	50 (64%)	17 (22%)	11 (14%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	AQ	78/84 (93%)	51 (65%)	15 (19%)	12 (15%)	0	1
16	CQ	78/84 (93%)	59 (76%)	10 (13%)	9 (12%)	1	4
17	AR	53/75 (71%)	40 (76%)	11 (21%)	2 (4%)	5	34
17	CR	53/75 (71%)	39 (74%)	12 (23%)	2 (4%)	5	34
18	AS	77/92 (84%)	59 (77%)	9 (12%)	9 (12%)	1	4
18	CS	77/92 (84%)	46 (60%)	24 (31%)	7 (9%)	1	8
19	AT	83/87 (95%)	56 (68%)	20 (24%)	7 (8%)	1	9
19	CT	83/87 (95%)	59 (71%)	16 (19%)	8 (10%)	1	7
20	AU	49/71 (69%)	25 (51%)	13 (26%)	11 (22%)	0	0
20	CU	49/71 (69%)	21 (43%)	11 (22%)	17 (35%)	0	0
24	BC	269/273 (98%)	194 (72%)	50 (19%)	25 (9%)	1	8
24	DC	269/273 (98%)	174 (65%)	63 (23%)	32 (12%)	1	4
25	BD	207/209 (99%)	146 (70%)	27 (13%)	34 (16%)	0	1
25	DD	207/209 (99%)	132 (64%)	43 (21%)	32 (16%)	0	1
26	BE	199/201 (99%)	155 (78%)	24 (12%)	20 (10%)	1	6
26	DE	199/201 (99%)	130 (65%)	46 (23%)	23 (12%)	1	4
27	BF	175/179 (98%)	134 (77%)	25 (14%)	16 (9%)	1	8
27	DF	176/179 (98%)	98 (56%)	43 (24%)	35 (20%)	0	0
28	BG	174/177 (98%)	111 (64%)	38 (22%)	25 (14%)	0	2
28	DG	174/177 (98%)	106 (61%)	38 (22%)	30 (17%)	0	1
29	BH	147/149 (99%)	68 (46%)	47 (32%)	32 (22%)	0	0
29	DH	147/149 (99%)	75 (51%)	54 (37%)	18 (12%)	1	3
30	BI	139/142 (98%)	84 (60%)	41 (30%)	14 (10%)	1	6
30	DI	139/142 (98%)	81 (58%)	39 (28%)	19 (14%)	0	2
31	BJ	140/142 (99%)	107 (76%)	21 (15%)	12 (9%)	1	8
31	DJ	140/142 (99%)	91 (65%)	38 (27%)	11 (8%)	1	11
32	BK	120/123 (98%)	86 (72%)	15 (12%)	19 (16%)	0	1
32	DK	120/123 (98%)	80 (67%)	20 (17%)	20 (17%)	0	1
33	BL	141/144 (98%)	101 (72%)	32 (23%)	8 (6%)	3	22
33	DL	141/144 (98%)	81 (57%)	40 (28%)	20 (14%)	0	2
34	BM	134/136 (98%)	97 (72%)	22 (16%)	15 (11%)	1	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	DM	134/136 (98%)	92 (69%)	29 (22%)	13 (10%)	1	7
35	BN	118/127 (93%)	92 (78%)	17 (14%)	9 (8%)	2	12
35	DN	118/127 (93%)	72 (61%)	30 (25%)	16 (14%)	0	2
36	BO	114/117 (97%)	91 (80%)	12 (10%)	11 (10%)	1	7
36	DO	114/117 (97%)	77 (68%)	30 (26%)	7 (6%)	2	19
37	BP	112/115 (97%)	77 (69%)	18 (16%)	17 (15%)	0	1
37	DP	112/115 (97%)	68 (61%)	27 (24%)	17 (15%)	0	1
38	BQ	115/118 (98%)	100 (87%)	9 (8%)	6 (5%)	3	25
38	DQ	115/118 (98%)	80 (70%)	25 (22%)	10 (9%)	1	8
39	BR	101/103 (98%)	80 (79%)	13 (13%)	8 (8%)	1	11
39	DR	101/103 (98%)	70 (69%)	21 (21%)	10 (10%)	1	7
40	BS	108/110 (98%)	86 (80%)	16 (15%)	6 (6%)	3	23
40	DS	108/110 (98%)	76 (70%)	23 (21%)	9 (8%)	1	9
41	BT	91/100 (91%)	52 (57%)	24 (26%)	15 (16%)	0	1
41	DT	91/100 (91%)	46 (50%)	31 (34%)	14 (15%)	0	1
42	BU	100/104 (96%)	69 (69%)	15 (15%)	16 (16%)	0	1
42	DU	100/104 (96%)	51 (51%)	26 (26%)	23 (23%)	0	0
43	BV	92/94 (98%)	77 (84%)	13 (14%)	2 (2%)	10	53
43	DV	92/94 (98%)	61 (66%)	23 (25%)	8 (9%)	1	8
44	BW	77/85 (91%)	30 (39%)	24 (31%)	23 (30%)	0	0
44	DW	77/85 (91%)	33 (43%)	27 (35%)	17 (22%)	0	0
45	BX	75/78 (96%)	56 (75%)	14 (19%)	5 (7%)	2	16
45	DX	75/78 (96%)	47 (63%)	20 (27%)	8 (11%)	1	5
46	BY	61/63 (97%)	38 (62%)	16 (26%)	7 (12%)	1	4
46	DY	61/63 (97%)	42 (69%)	14 (23%)	5 (8%)	1	10
47	BZ	56/59 (95%)	45 (80%)	9 (16%)	2 (4%)	5	36
47	DZ	56/59 (95%)	34 (61%)	16 (29%)	6 (11%)	1	5
48	B0	54/57 (95%)	41 (76%)	9 (17%)	4 (7%)	2	12
48	D0	54/57 (95%)	39 (72%)	8 (15%)	7 (13%)	0	3
49	B1	48/55 (87%)	36 (75%)	7 (15%)	5 (10%)	1	5
49	D1	48/55 (87%)	37 (77%)	7 (15%)	4 (8%)	1	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	B2	44/46 (96%)	39 (89%)	4 (9%)	1 (2%)	10	52
50	D2	44/46 (96%)	31 (70%)	10 (23%)	3 (7%)	2	15
51	B3	62/65 (95%)	53 (86%)	5 (8%)	4 (6%)	2	17
51	D3	62/65 (95%)	39 (63%)	18 (29%)	5 (8%)	1	10
52	B4	36/38 (95%)	31 (86%)	2 (6%)	3 (8%)	1	9
52	D4	36/38 (95%)	23 (64%)	7 (19%)	6 (17%)	0	1
All	All	11238/11970 (94%)	7646 (68%)	2332 (21%)	1260 (11%)	1	4

5 of 1260 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AB	18	GLN
1	AB	20	ARG
1	AB	40	ILE
1	AB	75	ALA
1	AB	119	GLN

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	
1	AB	180/199 (90%)	138 (77%)	42 (23%)	1	5
1	CB	180/199 (90%)	155 (86%)	25 (14%)	5	24
2	AC	170/190 (90%)	139 (82%)	31 (18%)	2	12
2	CC	170/190 (90%)	152 (89%)	18 (11%)	10	38
3	AD	172/173 (99%)	144 (84%)	28 (16%)	3	15
3	CD	172/173 (99%)	138 (80%)	34 (20%)	2	9
4	AE	113/126 (90%)	94 (83%)	19 (17%)	3	14
4	CE	113/126 (90%)	93 (82%)	20 (18%)	3	13
5	AF	87/116 (75%)	74 (85%)	13 (15%)	4	20
5	CF	87/116 (75%)	74 (85%)	13 (15%)	4	20
6	AG	124/147 (84%)	109 (88%)	15 (12%)	7	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	CG	123/147 (84%)	99 (80%)	24 (20%)	2	10
7	AH	104/105 (99%)	88 (85%)	16 (15%)	4	18
7	CH	104/105 (99%)	90 (86%)	14 (14%)	6	26
8	AI	105/107 (98%)	88 (84%)	17 (16%)	3	15
8	CI	105/107 (98%)	91 (87%)	14 (13%)	6	27
9	AJ	86/90 (96%)	72 (84%)	14 (16%)	3	15
9	CJ	86/90 (96%)	77 (90%)	9 (10%)	10	39
10	AK	90/99 (91%)	71 (79%)	19 (21%)	1	8
10	CK	90/99 (91%)	78 (87%)	12 (13%)	6	27
11	AL	103/104 (99%)	81 (79%)	22 (21%)	1	7
11	CL	103/104 (99%)	84 (82%)	19 (18%)	2	11
12	AM	92/96 (96%)	88 (96%)	4 (4%)	40	81
12	CM	91/96 (95%)	80 (88%)	11 (12%)	7	32
13	AN	79/84 (94%)	73 (92%)	6 (8%)	19	60
13	CN	79/84 (94%)	67 (85%)	12 (15%)	4	19
14	AO	76/77 (99%)	69 (91%)	7 (9%)	13	47
14	CO	76/77 (99%)	70 (92%)	6 (8%)	18	58
15	AP	65/65 (100%)	54 (83%)	11 (17%)	3	14
15	CP	65/65 (100%)	53 (82%)	12 (18%)	2	11
16	AQ	74/78 (95%)	61 (82%)	13 (18%)	3	13
16	CQ	74/78 (95%)	63 (85%)	11 (15%)	4	20
17	AR	48/65 (74%)	45 (94%)	3 (6%)	25	69
17	CR	48/65 (74%)	46 (96%)	2 (4%)	40	82
18	AS	70/79 (89%)	62 (89%)	8 (11%)	8	35
18	CS	70/79 (89%)	62 (89%)	8 (11%)	8	35
19	AT	65/66 (98%)	48 (74%)	17 (26%)	1	2
19	CT	65/66 (98%)	54 (83%)	11 (17%)	3	14
20	AU	44/61 (72%)	32 (73%)	12 (27%)	0	2
20	CU	44/61 (72%)	34 (77%)	10 (23%)	1	6
24	BC	216/218 (99%)	173 (80%)	43 (20%)	2	9
24	DC	216/218 (99%)	188 (87%)	28 (13%)	6	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	BD	164/164 (100%)	136 (83%)	28 (17%)	3	14
25	DD	164/164 (100%)	140 (85%)	24 (15%)	5	21
26	BE	165/165 (100%)	125 (76%)	40 (24%)	1	4
26	DE	165/165 (100%)	150 (91%)	15 (9%)	14	47
27	BF	148/150 (99%)	128 (86%)	20 (14%)	6	26
27	DF	149/150 (99%)	122 (82%)	27 (18%)	2	12
28	BG	137/138 (99%)	107 (78%)	30 (22%)	1	7
28	DG	137/138 (99%)	119 (87%)	18 (13%)	6	28
29	BH	114/114 (100%)	96 (84%)	18 (16%)	4	16
29	DH	114/114 (100%)	96 (84%)	18 (16%)	4	16
30	BI	109/110 (99%)	91 (84%)	18 (16%)	3	14
30	DI	109/110 (99%)	102 (94%)	7 (6%)	25	69
31	BJ	116/116 (100%)	89 (77%)	27 (23%)	1	5
31	DJ	116/116 (100%)	104 (90%)	12 (10%)	10	40
32	BK	103/104 (99%)	84 (82%)	19 (18%)	2	11
32	DK	103/104 (99%)	87 (84%)	16 (16%)	4	17
33	BL	102/103 (99%)	79 (78%)	23 (22%)	1	6
33	DL	102/103 (99%)	88 (86%)	14 (14%)	5	25
34	BM	109/109 (100%)	87 (80%)	22 (20%)	2	9
34	DM	109/109 (100%)	99 (91%)	10 (9%)	13	47
35	BN	100/103 (97%)	83 (83%)	17 (17%)	3	14
35	DN	100/103 (97%)	85 (85%)	15 (15%)	4	19
36	BO	86/87 (99%)	69 (80%)	17 (20%)	2	9
36	DO	86/87 (99%)	78 (91%)	8 (9%)	13	46
37	BP	99/100 (99%)	78 (79%)	21 (21%)	1	8
37	DP	99/100 (99%)	90 (91%)	9 (9%)	14	47
38	BQ	89/90 (99%)	74 (83%)	15 (17%)	3	14
38	DQ	89/90 (99%)	78 (88%)	11 (12%)	7	30
39	BR	84/84 (100%)	65 (77%)	19 (23%)	1	6
39	DR	84/84 (100%)	71 (84%)	13 (16%)	4	17
40	BS	93/93 (100%)	73 (78%)	20 (22%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	DS	93/93 (100%)	76 (82%)	17 (18%)	2	12
41	BT	80/84 (95%)	61 (76%)	19 (24%)	1	4
41	DT	80/84 (95%)	74 (92%)	6 (8%)	19	61
42	BU	83/85 (98%)	66 (80%)	17 (20%)	2	8
42	DU	83/85 (98%)	74 (89%)	9 (11%)	9	37
43	BV	78/78 (100%)	61 (78%)	17 (22%)	1	7
43	DV	78/78 (100%)	66 (85%)	12 (15%)	4	18
44	BW	59/63 (94%)	42 (71%)	17 (29%)	0	1
44	DW	59/63 (94%)	44 (75%)	15 (25%)	1	3
45	BX	67/68 (98%)	53 (79%)	14 (21%)	1	8
45	DX	67/68 (98%)	58 (87%)	9 (13%)	6	26
46	BY	55/55 (100%)	43 (78%)	12 (22%)	1	7
46	DY	55/55 (100%)	52 (94%)	3 (6%)	30	75
47	BZ	48/49 (98%)	32 (67%)	16 (33%)	0	0
47	DZ	48/49 (98%)	41 (85%)	7 (15%)	5	21
48	B0	47/48 (98%)	43 (92%)	4 (8%)	15	53
48	D0	47/48 (98%)	40 (85%)	7 (15%)	4	20
49	B1	45/49 (92%)	36 (80%)	9 (20%)	2	9
49	D1	45/49 (92%)	41 (91%)	4 (9%)	14	49
50	B2	38/38 (100%)	31 (82%)	7 (18%)	2	11
50	D2	38/38 (100%)	34 (90%)	4 (10%)	10	39
51	B3	51/52 (98%)	44 (86%)	7 (14%)	5	25
51	D3	51/52 (98%)	42 (82%)	9 (18%)	3	13
52	B4	34/34 (100%)	30 (88%)	4 (12%)	8	33
52	D4	34/34 (100%)	29 (85%)	5 (15%)	4	21
All	All	9331/9756 (96%)	7837 (84%)	1494 (16%)	3	16

5 of 1494 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
39	BR	10	LYS
49	B1	41	VAL
39	DR	75	VAL

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Mol	Chain	Res	Type
40	BS	4	ILE
43	BV	41	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 333 such sidechains are listed below:

Mol	Chain	Res	Type
42	BU	52	ASN
2	CC	184	ASN
42	DU	45	GLN
43	BV	51	GLN
48	B0	4	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1532/1533 (99%)	471 (30%)	241 (15%)
22	BA	2850/2903 (98%)	800 (28%)	404 (14%)
22	DA	2838/2903 (97%)	1022 (36%)	515 (18%)
23	BB	117/118 (99%)	29 (24%)	19 (16%)
53	CA	1529/1530 (99%)	512 (33%)	238 (15%)
54	DB	116/117 (99%)	36 (31%)	19 (16%)
All	All	8982/9104 (98%)	2870 (31%)	1436 (15%)

5 of 2870 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	5	U
21	AA	6	G
21	AA	7	A
21	AA	8	A
21	AA	9	G

5 of 1436 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	BB	24	G
53	CA	874	G
22	DA	2311	A
53	CA	15	G
53	CA	366	A

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 365 ligands modelled in this entry, 365 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AB	218/241 (90%)	0.04	7 (3%) 45 9	85, 115, 146, 164	0
1	CB	218/241 (90%)	0.12	3 (1%) 72 22	90, 125, 152, 170	0
2	AC	206/233 (88%)	-0.24	0 100 100	57, 83, 116, 147	0
2	CC	206/233 (88%)	0.19	1 (0%) 88 46	83, 129, 170, 188	0
3	AD	205/206 (99%)	-0.20	3 (1%) 70 21	50, 87, 137, 176	0
3	CD	205/206 (99%)	-0.26	1 (0%) 88 46	41, 63, 102, 148	0
4	AE	150/167 (89%)	-0.22	0 100 100	51, 70, 116, 147	0
4	CE	150/167 (89%)	-0.10	0 100 100	65, 87, 122, 144	0
5	AF	100/135 (74%)	-0.13	0 100 100	60, 90, 125, 142	0
5	CF	100/135 (74%)	-0.04	0 100 100	65, 113, 147, 158	0
6	AG	151/179 (84%)	-0.05	1 (0%) 84 38	69, 108, 139, 157	0
6	CG	150/179 (83%)	1.08	31 (20%) 1 1	98, 173, 223, 233	0
7	AH	129/130 (99%)	-0.38	0 100 100	49, 71, 106, 133	0
7	CH	129/130 (99%)	-0.17	0 100 100	63, 100, 133, 159	0
8	AI	127/130 (97%)	0.13	6 (4%) 30 6	56, 115, 166, 189	0
8	CI	127/130 (97%)	0.64	11 (8%) 10 3	127, 174, 225, 239	0
9	AJ	98/103 (95%)	0.00	2 (2%) 62 17	59, 97, 152, 160	0
9	CJ	98/103 (95%)	0.90	13 (13%) 4 1	122, 160, 189, 201	0
10	AK	117/129 (90%)	-0.11	0 100 100	43, 88, 124, 137	0
10	CK	117/129 (90%)	-0.02	0 100 100	57, 99, 130, 151	0
11	AL	123/124 (99%)	-0.21	2 (1%) 68 20	33, 54, 96, 135	0
11	CL	123/124 (99%)	-0.00	1 (0%) 83 35	47, 74, 110, 135	0
12	AM	114/118 (96%)	0.01	1 (0%) 81 32	70, 117, 155, 177	0
12	CM	113/118 (95%)	1.45	27 (23%) 1 1	220, 351, 413, 434	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AN	96/101 (95%)	-0.11	0 100 100	59, 86, 136, 158	0
13	CN	95/101 (94%)	0.84	10 (10%) 7 2	102, 191, 256, 269	0
14	AO	88/89 (98%)	-0.28	0 100 100	48, 75, 106, 128	0
14	CO	88/89 (98%)	0.01	1 (1%) 77 27	72, 109, 141, 167	0
15	AP	82/82 (100%)	-0.18	3 (3%) 39 8	55, 79, 129, 174	0
15	CP	80/82 (97%)	0.09	0 100 100	64, 96, 133, 152	0
16	AQ	80/84 (95%)	0.02	2 (2%) 54 12	38, 73, 112, 144	0
16	CQ	80/84 (95%)	0.38	3 (3%) 38 7	54, 96, 117, 131	0
17	AR	55/75 (73%)	0.03	1 (1%) 65 18	56, 80, 129, 146	0
17	CR	55/75 (73%)	0.13	0 100 100	57, 89, 131, 170	0
18	AS	79/92 (85%)	0.09	1 (1%) 74 24	79, 110, 152, 161	0
18	CS	79/92 (85%)	1.44	22 (27%) 1 1	250, 307, 359, 371	0
19	AT	85/87 (97%)	-0.11	0 100 100	51, 81, 114, 133	0
19	CT	85/87 (97%)	0.49	3 (3%) 42 8	79, 125, 161, 177	0
20	AU	51/71 (71%)	0.16	0 100 100	60, 104, 138, 148	0
20	CU	51/71 (71%)	0.08	0 100 100	63, 97, 143, 153	0
21	AA	1533/1533 (100%)	-0.60	22 (1%) 72 22	34, 72, 169, 235	0
22	BA	2854/2903 (98%)	-0.59	52 (1%) 65 18	13, 33, 142, 320	0
22	DA	2841/2903 (97%)	0.25	102 (3%) 41 8	59, 119, 216, 320	0
23	BB	118/118 (100%)	-0.69	0 100 100	18, 47, 75, 99	0
24	BC	271/273 (99%)	-0.31	2 (0%) 84 38	20, 43, 83, 142	0
24	DC	271/273 (99%)	0.12	3 (1%) 77 27	63, 94, 128, 153	0
25	BD	209/209 (100%)	-0.46	0 100 100	13, 29, 72, 96	0
25	DD	209/209 (100%)	0.14	1 (0%) 88 46	68, 108, 141, 168	0
26	BE	201/201 (100%)	-0.44	0 100 100	15, 42, 87, 124	0
26	DE	201/201 (100%)	0.63	13 (6%) 18 4	89, 191, 252, 282	0
27	BF	177/179 (98%)	-0.22	0 100 100	32, 67, 116, 132	0
27	DF	178/179 (99%)	1.01	26 (14%) 3 1	125, 209, 220, 232	0
28	BG	176/177 (99%)	-0.30	0 100 100	27, 57, 103, 128	0
28	DG	176/177 (99%)	0.71	13 (7%) 14 3	120, 165, 207, 220	0
29	BH	149/149 (100%)	1.10	42 (28%) 1 1	42, 178, 213, 217	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
29	DH	149/149 (100%)	1.33	38 (25%) 1 1	104, 173, 208, 219	0
30	BI	141/142 (99%)	1.64	42 (29%) 1 1	199, 245, 286, 294	0
30	DI	141/142 (99%)	2.86	83 (58%) 0 0	264, 305, 323, 331	0
31	BJ	142/142 (100%)	-0.47	0 100 100	12, 25, 57, 111	0
31	DJ	142/142 (100%)	0.08	0 100 100	76, 110, 134, 153	0
32	BK	122/123 (99%)	-0.46	0 100 100	20, 32, 76, 121	0
32	DK	122/123 (99%)	0.00	1 (0%) 83 35	71, 93, 127, 142	0
33	BL	143/144 (99%)	-0.46	0 100 100	13, 38, 74, 100	0
33	DL	143/144 (99%)	0.62	8 (5%) 24 5	80, 150, 189, 202	0
34	BM	136/136 (100%)	-0.50	0 100 100	14, 30, 61, 99	0
34	DM	136/136 (100%)	0.03	0 100 100	73, 117, 143, 161	0
35	BN	120/127 (94%)	-0.48	0 100 100	14, 28, 44, 97	0
35	DN	120/127 (94%)	0.33	1 (0%) 83 35	89, 121, 152, 171	0
36	BO	116/117 (99%)	-0.38	0 100 100	30, 46, 73, 101	0
36	DO	116/117 (99%)	0.88	13 (11%) 6 2	146, 178, 207, 216	0
37	BP	114/115 (99%)	-0.39	0 100 100	22, 39, 90, 131	0
37	DP	114/115 (99%)	0.18	3 (2%) 53 11	80, 108, 135, 143	0
38	BQ	117/118 (99%)	-0.48	0 100 100	9, 22, 46, 96	0
38	DQ	117/118 (99%)	0.39	2 (1%) 67 19	87, 112, 154, 191	0
39	BR	103/103 (100%)	-0.44	0 100 100	11, 33, 75, 91	0
39	DR	103/103 (100%)	0.69	6 (5%) 22 5	85, 135, 170, 190	0
40	BS	110/110 (100%)	-0.52	0 100 100	14, 23, 57, 118	0
40	DS	110/110 (100%)	0.47	7 (6%) 19 4	76, 120, 154, 170	0
41	BT	93/100 (93%)	-0.15	0 100 100	28, 51, 112, 140	0
41	DT	93/100 (93%)	0.81	9 (9%) 8 2	132, 189, 223, 233	0
42	BU	102/104 (98%)	-0.20	0 100 100	29, 54, 100, 155	0
42	DU	102/104 (98%)	1.20	21 (20%) 1 1	153, 202, 250, 283	0
43	BV	94/94 (100%)	-0.49	0 100 100	17, 39, 79, 105	0
43	DV	94/94 (100%)	0.21	1 (1%) 77 27	113, 143, 165, 179	0
44	BW	79/85 (92%)	-0.22	0 100 100	18, 39, 94, 127	0
44	DW	79/85 (92%)	0.74	4 (5%) 27 5	99, 157, 191, 201	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
45	BX	77/78 (98%)	-0.33	0 100 100	23, 43, 80, 104	0
45	DX	77/78 (98%)	0.34	2 (2%) 53 11	84, 124, 170, 177	0
46	BY	63/63 (100%)	-0.17	0 100 100	41, 68, 113, 128	0
46	DY	63/63 (100%)	0.83	6 (9%) 8 2	180, 226, 268, 278	0
47	BZ	58/59 (98%)	-0.46	0 100 100	13, 27, 56, 97	0
47	DZ	58/59 (98%)	0.40	1 (1%) 67 19	97, 143, 180, 187	0
48	B0	56/57 (98%)	-0.55	0 100 100	12, 29, 61, 113	0
48	D0	56/57 (98%)	0.65	2 (3%) 41 8	84, 128, 163, 172	0
49	B1	50/55 (90%)	-0.20	0 100 100	29, 50, 91, 116	0
49	D1	50/55 (90%)	0.99	6 (12%) 5 1	110, 143, 159, 168	0
50	B2	46/46 (100%)	-0.43	0 100 100	20, 30, 49, 131	0
50	D2	46/46 (100%)	0.49	1 (2%) 59 14	87, 115, 137, 147	0
51	B3	64/65 (98%)	-0.51	0 100 100	15, 30, 43, 62	0
51	D3	64/65 (98%)	0.76	7 (10%) 6 2	93, 126, 150, 169	0
52	B4	38/38 (100%)	-0.38	0 100 100	19, 33, 62, 87	0
52	D4	38/38 (100%)	0.60	2 (5%) 25 5	84, 127, 158, 161	0
53	CA	1530/1530 (100%)	-0.00	68 (4%) 33 7	44, 100, 246, 325	0
54	DB	117/117 (100%)	0.30	3 (2%) 53 11	108, 175, 209, 221	0
All	All	20431/21074 (96%)	-0.01	769 (3%) 38 7	9, 93, 219, 434	0

The worst 5 of 769 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	BA	2154	A	14.9
53	CA	209	U	13.2
30	BI	2	LYS	12.8
29	DH	92	GLY	12.4
30	DI	2	LYS	10.6

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
55	MG	DJ	201	1/1	4.07	779.80	242,242,242,242	0
55	MG	DA	3064	1/1	3.11	275.86	204,204,204,204	0
55	MG	CA	1624	1/1	0.77	102.18	120,120,120,120	0
55	MG	DA	3110	1/1	1.11	90.83	181,181,181,181	0
55	MG	DA	3065	1/1	2.72	87.12	221,221,221,221	0
55	MG	DA	3015	1/1	0.81	77.40	183,183,183,183	0
55	MG	BA	3026	1/1	0.56	62.08	152,152,152,152	0
55	MG	DA	3075	1/1	1.51	55.58	207,207,207,207	0
55	MG	DA	3129	1/1	1.07	55.43	194,194,194,194	0
55	MG	CA	1619	1/1	0.44	52.82	180,180,180,180	0
55	MG	BB	201	1/1	0.36	38.05	187,187,187,187	0
55	MG	DA	3063	1/1	1.08	37.07	191,191,191,191	0
55	MG	BA	3120	1/1	0.24	36.45	156,156,156,156	0
55	MG	BA	3071	1/1	0.36	34.56	132,132,132,132	0
55	MG	BA	3057	1/1	0.63	31.45	219,219,219,219	0
55	MG	DA	3020	1/1	0.63	31.19	207,207,207,207	0
55	MG	BA	3060	1/1	0.32	28.99	129,129,129,129	0
55	MG	BA	3015	1/1	0.40	28.48	221,221,221,221	0
55	MG	CA	1614	1/1	0.69	28.34	178,178,178,178	0
55	MG	AA	1619	1/1	0.43	26.45	165,165,165,165	0
55	MG	DA	3005	1/1	0.81	23.19	208,208,208,208	0
55	MG	BA	3035	1/1	0.34	22.26	168,168,168,168	0
55	MG	DA	3061	1/1	0.48	20.58	160,160,160,160	0
55	MG	BA	3056	1/1	0.37	20.54	187,187,187,187	0
55	MG	AA	1636	1/1	0.60	20.38	164,164,164,164	0
55	MG	DA	3079	1/1	0.44	19.96	184,184,184,184	0
55	MG	CA	1612	1/1	0.34	17.13	117,117,117,117	0
55	MG	DA	3060	1/1	0.29	16.98	198,198,198,198	0
55	MG	BA	3132	1/1	0.37	16.77	202,202,202,202	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
55	MG	BA	3062	1/1	0.36	16.31	193,193,193,193	0
55	MG	BA	3014	1/1	0.25	15.94	64,64,64,64	0
55	MG	DA	3002	1/1	1.15	15.60	179,179,179,179	0
55	MG	BA	3072	1/1	0.33	15.02	94,94,94,94	0
55	MG	BA	3037	1/1	0.29	14.54	171,171,171,171	0
55	MG	AA	1627	1/1	0.24	12.58	86,86,86,86	0
55	MG	DA	3027	1/1	1.41	12.46	195,195,195,195	0
55	MG	BA	3125	1/1	0.60	11.69	162,162,162,162	0
55	MG	BA	3020	1/1	0.29	11.25	16,16,16,16	0
55	MG	DA	3059	1/1	0.50	11.16	188,188,188,188	0
55	MG	CA	1620	1/1	0.27	10.94	172,172,172,172	0
55	MG	DA	3013	1/1	0.57	10.80	211,211,211,211	0
55	MG	DA	3042	1/1	0.36	10.68	139,139,139,139	0
55	MG	BA	3077	1/1	0.22	10.58	90,90,90,90	0
55	MG	BA	3058	1/1	0.22	10.17	164,164,164,164	0
55	MG	CA	1625	1/1	0.29	10.14	118,118,118,118	0
55	MG	BA	3061	1/1	0.19	9.33	171,171,171,171	0
55	MG	AA	1611	1/1	0.23	9.29	176,176,176,176	0
55	MG	BA	3137	1/1	0.35	8.87	188,188,188,188	0
55	MG	DA	3039	1/1	0.41	8.12	220,220,220,220	0
55	MG	AA	1628	1/1	0.31	7.70	96,96,96,96	0
55	MG	DA	3098	1/1	0.44	7.63	158,158,158,158	0
55	MG	CA	1628	1/1	1.00	7.57	204,204,204,204	0
55	MG	BA	3105	1/1	0.23	7.47	16,16,16,16	0
55	MG	DA	3058	1/1	0.36	7.26	171,171,171,171	0
55	MG	BA	3088	1/1	0.20	6.96	81,81,81,81	0
55	MG	BA	3134	1/1	0.51	6.94	137,137,137,137	0
55	MG	CA	1615	1/1	0.27	6.83	136,136,136,136	0
55	MG	DA	3132	1/1	0.80	6.79	216,216,216,216	0
55	MG	BA	3045	1/1	0.18	6.26	21,21,21,21	0
55	MG	DA	3131	1/1	1.27	5.94	204,204,204,204	0
55	MG	CA	1603	1/1	0.20	5.80	169,169,169,169	0
55	MG	CA	1627	1/1	0.25	5.61	166,166,166,166	0
55	MG	DA	3022	1/1	0.24	5.56	155,155,155,155	0
55	MG	AA	1626	1/1	0.19	5.50	39,39,39,39	0
55	MG	DA	3029	1/1	0.63	5.33	205,205,205,205	0
55	MG	BA	3110	1/1	0.21	5.30	11,11,11,11	0
55	MG	BA	3038	1/1	0.17	5.20	30,30,30,30	0
55	MG	DA	3127	1/1	0.34	5.12	97,97,97,97	0
55	MG	BA	3136	1/1	0.18	4.79	150,150,150,150	0
55	MG	DA	3109	1/1	0.43	4.42	165,165,165,165	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
55	MG	BA	3028	1/1	0.20	4.29	100,100,100,100	0
55	MG	CA	1626	1/1	0.20	4.08	40,40,40,40	0
55	MG	BA	3084	1/1	0.15	3.72	58,58,58,58	0
55	MG	DA	3007	1/1	0.24	3.48	198,198,198,198	0
55	MG	BA	3103	1/1	0.15	3.45	60,60,60,60	0
55	MG	DA	3021	1/1	0.23	3.37	66,66,66,66	0
55	MG	DA	3101	1/1	0.37	3.31	127,127,127,127	0
55	MG	DA	3134	1/1	0.44	3.13	198,198,198,198	0
55	MG	BA	3011	1/1	0.20	2.82	120,120,120,120	0
55	MG	AA	1622	1/1	0.15	2.81	30,30,30,30	0
55	MG	DA	3115	1/1	0.21	2.68	151,151,151,151	0
55	MG	CA	1610	1/1	0.17	2.54	145,145,145,145	0
55	MG	AA	1615	1/1	0.18	2.53	164,164,164,164	0
55	MG	BA	3049	1/1	0.17	2.50	104,104,104,104	0
55	MG	AA	1641	1/1	0.19	2.48	131,131,131,131	0
55	MG	BA	3127	1/1	0.16	2.47	43,43,43,43	0
55	MG	AA	1609	1/1	0.17	2.27	71,71,71,71	0
55	MG	BA	3092	1/1	0.17	2.19	75,75,75,75	0
55	MG	BA	3117	1/1	0.18	2.13	23,23,23,23	0
55	MG	DA	3070	1/1	0.37	2.13	209,209,209,209	0
55	MG	BA	3109	1/1	0.15	2.03	13,13,13,13	0
55	MG	DA	3116	1/1	0.24	2.03	154,154,154,154	0
55	MG	BA	3040	1/1	0.14	2.03	27,27,27,27	0
55	MG	DA	3104	1/1	0.21	2.00	109,109,109,109	0
55	MG	AA	1642	1/1	0.15	1.99	40,40,40,40	0
55	MG	DA	3085	1/1	0.37	1.97	169,169,169,169	0
55	MG	BA	3041	1/1	0.16	1.89	19,19,19,19	0
55	MG	CA	1640	1/1	0.20	1.73	161,161,161,161	0
55	MG	BA	3098	1/1	0.21	1.71	60,60,60,60	0
55	MG	BA	3089	1/1	0.14	1.63	134,134,134,134	0
55	MG	BA	3106	1/1	0.15	1.40	37,37,37,37	0
55	MG	DA	3072	1/1	0.24	1.36	80,80,80,80	0
55	MG	DA	3050	1/1	0.18	1.29	209,209,209,209	0
55	MG	BA	3108	1/1	0.16	1.22	30,30,30,30	0
55	MG	DA	3126	1/1	0.41	1.22	164,164,164,164	0
55	MG	DA	3121	1/1	0.23	1.18	97,97,97,97	0
55	MG	AA	1606	1/1	0.16	1.01	38,38,38,38	0
55	MG	BA	3126	1/1	0.14	0.91	21,21,21,21	0
55	MG	CA	1637	1/1	0.18	0.72	100,100,100,100	0
55	MG	DA	3100	1/1	0.18	0.64	171,171,171,171	0
55	MG	DA	3107	1/1	0.30	0.61	169,169,169,169	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CA	1631	1/1	0.18	0.57	92,92,92,92	0
55	MG	DA	3130	1/1	0.42	0.56	102,102,102,102	0
55	MG	BA	3093	1/1	0.13	0.54	110,110,110,110	0
55	MG	DA	3034	1/1	0.24	0.54	105,105,105,105	0
55	MG	DA	3135	1/1	0.24	0.52	162,162,162,162	0
55	MG	BA	3042	1/1	0.14	0.45	18,18,18,18	0
55	MG	DA	3124	1/1	0.31	0.44	165,165,165,165	0
55	MG	BA	3112	1/1	0.14	0.44	121,121,121,121	0
55	MG	AA	1629	1/1	0.17	0.44	58,58,58,58	0
55	MG	BA	3004	1/1	0.16	0.31	155,155,155,155	0
55	MG	DA	3087	1/1	0.19	0.29	87,87,87,87	0
55	MG	CA	1605	1/1	0.15	0.28	48,48,48,48	0
55	MG	CA	1623	1/1	0.20	0.28	96,96,96,96	0
55	MG	DA	3048	1/1	0.18	0.26	128,128,128,128	0
55	MG	BA	3076	1/1	0.15	0.23	16,16,16,16	0
55	MG	CA	1636	1/1	0.25	0.18	171,171,171,171	0
55	MG	DA	3086	1/1	0.23	0.17	122,122,122,122	0
55	MG	BA	3075	1/1	0.27	0.14	119,119,119,119	0
55	MG	BA	3047	1/1	0.16	0.12	20,20,20,20	0
55	MG	DA	3038	1/1	0.21	-0.00	97,97,97,97	0
55	MG	BA	3131	1/1	0.16	-0.05	17,17,17,17	0
55	MG	CA	1621	1/1	0.16	-0.06	40,40,40,40	0
55	MG	DA	3014	1/1	0.22	-0.18	151,151,151,151	0
55	MG	BA	3029	1/1	0.15	-0.19	43,43,43,43	0
55	MG	DA	3128	1/1	0.20	-0.21	153,153,153,153	0
55	MG	DA	3096	1/1	0.21	-0.24	107,107,107,107	0
55	MG	DA	3077	1/1	0.19	-0.25	159,159,159,159	0
55	MG	CA	1607	1/1	0.15	-0.34	154,154,154,154	0
55	MG	BA	3031	1/1	0.13	-0.35	11,11,11,11	0
55	MG	DA	3006	1/1	0.21	-0.35	200,200,200,200	0
55	MG	DA	3076	1/1	0.21	-0.39	167,167,167,167	0
55	MG	BA	3001	1/1	0.12	-0.39	109,109,109,109	0
55	MG	DA	3025	1/1	0.21	-0.40	108,108,108,108	0
55	MG	DA	3105	1/1	0.17	-0.40	62,62,62,62	0
55	MG	BA	3133	1/1	0.18	-0.40	103,103,103,103	0
55	MG	AA	1618	1/1	0.13	-0.42	68,68,68,68	0
55	MG	CA	1639	1/1	0.17	-0.43	149,149,149,149	0
55	MG	DA	3106	1/1	0.19	-0.44	69,69,69,69	0
55	MG	BA	3034	1/1	0.13	-0.45	8,8,8,8	0
55	MG	DA	3078	1/1	0.18	-0.45	68,68,68,68	0
55	MG	DA	3094	1/1	0.20	-0.46	172,172,172,172	0
55	MG	AA	1635	1/1	0.13	-0.49	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	1603	1/1	0.12	-0.50	124,124,124,124	0
55	MG	DA	3052	1/1	0.16	-0.55	110,110,110,110	0
55	MG	BA	3114	1/1	0.14	-0.55	86,86,86,86	0
55	MG	DA	3122	1/1	0.17	-0.56	113,113,113,113	0
55	MG	DA	3018	1/1	0.18	-0.60	194,194,194,194	0
55	MG	BA	3002	1/1	0.13	-0.61	81,81,81,81	0
55	MG	AA	1612	1/1	0.10	-0.63	60,60,60,60	0
55	MG	AA	1640	1/1	0.12	-0.64	109,109,109,109	0
55	MG	BA	3013	1/1	0.13	-0.67	8,8,8,8	0
55	MG	CA	1632	1/1	0.15	-0.67	160,160,160,160	0
55	MG	DA	3028	1/1	0.17	-0.68	162,162,162,162	0
55	MG	AA	1633	1/1	0.10	-0.70	78,78,78,78	0
55	MG	DA	3035	1/1	0.15	-0.70	87,87,87,87	0
55	MG	DA	3017	1/1	0.23	-0.72	86,86,86,86	0
55	MG	CA	1633	1/1	0.08	-0.72	61,61,61,61	0
55	MG	DA	3037	1/1	0.18	-0.75	176,176,176,176	0
55	MG	AA	1630	1/1	0.09	-0.77	163,163,163,163	0
55	MG	CA	1611	1/1	0.16	-0.78	108,108,108,108	0
55	MG	DA	3032	1/1	0.18	-0.78	71,71,71,71	0
55	MG	BA	3083	1/1	0.12	-0.81	42,42,42,42	0
55	MG	AA	1623	1/1	0.10	-0.81	70,70,70,70	0
55	MG	CA	1617	1/1	0.22	-0.84	220,220,220,220	0
55	MG	DA	3011	1/1	0.18	-0.85	126,126,126,126	0
55	MG	CA	1616	1/1	0.23	-0.89	192,192,192,192	0
55	MG	DA	3009	1/1	0.18	-0.91	107,107,107,107	0
55	MG	BA	3085	1/1	0.12	-0.92	116,116,116,116	0
55	MG	DA	3084	1/1	0.16	-0.92	178,178,178,178	0
55	MG	BB	203	1/1	0.10	-0.92	37,37,37,37	0
55	MG	AA	1602	1/1	0.13	-0.92	121,121,121,121	0
55	MG	DA	3092	1/1	0.20	-0.94	157,157,157,157	0
55	MG	DA	3045	1/1	0.17	-0.96	102,102,102,102	0
56	ZN	D4	101	1/1	0.08	-0.97	156,156,156,156	0
55	MG	CA	1602	1/1	0.14	-0.97	120,120,120,120	0
55	MG	BA	3122	1/1	0.06	-0.99	64,64,64,64	0
55	MG	CA	1638	1/1	0.16	-1.03	155,155,155,155	0
55	MG	AA	1637	1/1	0.08	-1.05	85,85,85,85	0
55	MG	DA	3031	1/1	0.15	-1.05	113,113,113,113	0
55	MG	DA	3089	1/1	0.13	-1.07	169,169,169,169	0
55	MG	DA	3081	1/1	0.15	-1.08	141,141,141,141	0
55	MG	DA	3111	1/1	0.15	-1.09	166,166,166,166	0
55	MG	DA	3041	1/1	0.17	-1.11	77,77,77,77	0
55	MG	BA	3130	1/1	0.12	-1.12	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	3027	1/1	0.13	-1.17	31,31,31,31	0
55	MG	AA	1620	1/1	0.11	-1.19	107,107,107,107	0
55	MG	BA	3007	1/1	0.09	-1.21	67,67,67,67	0
55	MG	BA	3023	1/1	0.11	-1.21	11,11,11,11	0
55	MG	BA	3050	1/1	0.12	-1.23	16,16,16,16	0
55	MG	DA	3073	1/1	0.14	-1.23	141,141,141,141	0
55	MG	BA	3107	1/1	0.12	-1.23	11,11,11,11	0
55	MG	BA	3008	1/1	0.12	-1.24	17,17,17,17	0
55	MG	DA	3019	1/1	0.15	-1.25	161,161,161,161	0
55	MG	BA	3024	1/1	0.12	-1.29	16,16,16,16	0
55	MG	BA	3116	1/1	0.12	-1.29	133,133,133,133	0
55	MG	DA	3044	1/1	0.15	-1.33	138,138,138,138	0
55	MG	BA	3046	1/1	0.13	-1.33	23,23,23,23	0
55	MG	CA	1601	1/1	0.09	-1.34	124,124,124,124	0
55	MG	DA	3026	1/1	0.17	-1.35	145,145,145,145	0
55	MG	DA	3074	1/1	0.12	-1.35	194,194,194,194	0
55	MG	DA	3099	1/1	0.14	-1.39	142,142,142,142	0
55	MG	BA	3025	1/1	0.11	-1.39	21,21,21,21	0
55	MG	DA	3125	1/1	0.17	-1.40	77,77,77,77	0
55	MG	BA	3012	1/1	0.13	-1.44	8,8,8,8	0
55	MG	DA	3049	1/1	0.15	-1.50	99,99,99,99	0
55	MG	DA	3036	1/1	0.11	-1.52	97,97,97,97	0
55	MG	BA	3003	1/1	0.10	-1.54	63,63,63,63	0
55	MG	CA	1608	1/1	0.15	-1.55	60,60,60,60	0
55	MG	BA	3063	1/1	0.10	-1.56	42,42,42,42	0
55	MG	CA	1629	1/1	0.10	-1.57	174,174,174,174	0
55	MG	BB	202	1/1	0.10	-1.64	67,67,67,67	0
55	MG	BA	3101	1/1	0.11	-1.64	27,27,27,27	0
55	MG	BA	3135	1/1	0.11	-1.65	12,12,12,12	0
55	MG	BA	3123	1/1	0.13	-1.66	10,10,10,10	0
55	MG	DA	3097	1/1	0.15	-1.68	110,110,110,110	0
55	MG	BA	3086	1/1	0.12	-1.68	45,45,45,45	0
55	MG	AA	1639	1/1	0.09	-1.69	96,96,96,96	0
55	MG	DA	3004	1/1	0.17	-1.72	118,118,118,118	0
55	MG	BA	3017	1/1	0.12	-1.74	9,9,9,9	0
55	MG	DA	3012	1/1	0.19	-1.83	75,75,75,75	0
55	MG	DB	201	1/1	0.08	-1.83	117,117,117,117	0
55	MG	DA	3090	1/1	0.12	-1.87	90,90,90,90	0
56	ZN	B4	101	1/1	0.08	-1.93	51,51,51,51	0
55	MG	AA	1624	1/1	0.09	-1.94	101,101,101,101	0
55	MG	DA	3046	1/1	0.12	-1.94	173,173,173,173	0
55	MG	AA	1616	1/1	0.09	-1.96	126,126,126,126	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3001	1/1	0.08	-2.00	109,109,109,109	0
55	MG	CA	1635	1/1	0.14	-2.00	76,76,76,76	0
55	MG	DA	3091	1/1	0.14	-2.04	95,95,95,95	0
55	MG	DA	3053	1/1	0.14	-2.04	59,59,59,59	0
55	MG	AA	1607	1/1	0.10	-2.05	62,62,62,62	0
55	MG	CA	1630	1/1	0.08	-2.06	121,121,121,121	0
55	MG	DA	3088	1/1	0.17	-2.06	160,160,160,160	0
55	MG	BA	3032	1/1	0.10	-2.06	31,31,31,31	0
55	MG	DA	3119	1/1	0.08	-2.07	86,86,86,86	0
55	MG	AA	1613	1/1	0.11	-2.08	102,102,102,102	0
55	MG	BA	3070	1/1	0.10	-2.08	164,164,164,164	0
55	MG	AA	1604	1/1	0.10	-2.13	98,98,98,98	0
55	MG	CA	1618	1/1	0.10	-2.16	90,90,90,90	0
55	MG	DA	3108	1/1	0.12	-2.16	103,103,103,103	0
55	MG	DA	3033	1/1	0.14	-2.21	113,113,113,113	0
55	MG	CA	1622	1/1	0.07	-2.29	169,169,169,169	0
55	MG	BA	3087	1/1	0.11	-2.30	13,13,13,13	0
55	MG	DA	3112	1/1	0.11	-2.31	148,148,148,148	0
55	MG	BA	3100	1/1	0.10	-2.36	47,47,47,47	0
55	MG	DA	3051	1/1	0.14	-2.37	140,140,140,140	0
55	MG	BA	3065	1/1	0.08	-2.38	26,26,26,26	0
55	MG	DA	3102	1/1	0.18	-2.40	83,83,83,83	0
55	MG	DA	3095	1/1	0.13	-2.46	114,114,114,114	0
55	MG	BA	3036	1/1	0.13	-2.48	11,11,11,11	0
55	MG	BA	3129	1/1	0.10	-2.48	31,31,31,31	0
55	MG	BA	3030	1/1	0.10	-2.48	57,57,57,57	0
55	MG	CA	1634	1/1	0.10	-2.57	112,112,112,112	0
55	MG	AA	1621	1/1	0.08	-2.57	139,139,139,139	0
55	MG	DA	3120	1/1	0.10	-2.61	84,84,84,84	0
55	MG	DA	3054	1/1	0.11	-2.63	75,75,75,75	0
55	MG	BA	3022	1/1	0.05	-2.65	37,37,37,37	0
55	MG	DA	3040	1/1	0.17	-2.67	117,117,117,117	0
55	MG	DA	3023	1/1	0.12	-2.69	71,71,71,71	0
55	MG	BA	3113	1/1	0.10	-2.71	60,60,60,60	0
55	MG	BA	3074	1/1	0.07	-2.72	59,59,59,59	0
55	MG	DA	3066	1/1	0.09	-2.76	94,94,94,94	0
55	MG	DA	3067	1/1	0.09	-2.79	70,70,70,70	0
55	MG	BA	3073	1/1	0.11	-2.79	12,12,12,12	0
55	MG	BA	3079	1/1	0.07	-2.79	99,99,99,99	0
55	MG	BA	3119	1/1	0.10	-2.80	88,88,88,88	0
55	MG	BA	3048	1/1	0.09	-2.80	144,144,144,144	0
55	MG	DA	3117	1/1	0.12	-2.82	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	3124	1/1	0.09	-2.89	39,39,39,39	0
55	MG	DA	3080	1/1	0.10	-2.92	74,74,74,74	0
55	MG	DA	3071	1/1	0.11	-2.96	64,64,64,64	0
55	MG	AA	1601	1/1	0.09	-2.96	82,82,82,82	0
55	MG	BA	3066	1/1	0.09	-2.99	18,18,18,18	0
55	MG	DA	3113	1/1	0.09	-3.06	59,59,59,59	0
55	MG	BA	3115	1/1	0.13	-3.08	49,49,49,49	0
55	MG	BA	3121	1/1	0.10	-3.16	12,12,12,12	0
55	MG	BA	3043	1/1	0.05	-3.17	17,17,17,17	0
55	MG	BA	3018	1/1	0.07	-3.20	35,35,35,35	0
55	MG	DA	3047	1/1	0.11	-3.29	82,82,82,82	0
55	MG	DA	3118	1/1	0.13	-3.33	77,77,77,77	0
55	MG	CA	1642	1/1	0.06	-3.33	78,78,78,78	0
55	MG	DA	3068	1/1	0.08	-3.36	65,65,65,65	0
55	MG	DA	3083	1/1	0.14	-3.41	144,144,144,144	0
55	MG	DA	3123	1/1	0.08	-3.43	99,99,99,99	0
55	MG	BA	3051	1/1	0.07	-3.51	71,71,71,71	0
55	MG	BA	3078	1/1	0.06	-3.53	26,26,26,26	0
55	MG	CA	1604	1/1	0.07	-3.56	71,71,71,71	0
55	MG	BA	3091	1/1	0.08	-3.57	47,47,47,47	0
55	MG	DA	3057	1/1	0.15	-3.59	104,104,104,104	0
55	MG	CA	1641	1/1	0.07	-3.64	68,68,68,68	0
55	MG	AA	1608	1/1	0.09	-3.70	106,106,106,106	0
55	MG	DA	3103	1/1	0.13	-3.71	62,62,62,62	0
55	MG	BA	3006	1/1	0.06	-3.75	32,32,32,32	0
55	MG	DA	3062	1/1	0.07	-3.79	113,113,113,113	0
55	MG	BA	3059	1/1	0.06	-3.81	36,36,36,36	0
55	MG	AA	1617	1/1	0.11	-3.82	83,83,83,83	0
55	MG	BA	3095	1/1	0.09	-3.94	38,38,38,38	0
55	MG	AA	1614	1/1	0.06	-4.00	55,55,55,55	0
55	MG	DA	3024	1/1	0.04	-4.00	85,85,85,85	0
55	MG	DA	3069	1/1	0.07	-4.07	79,79,79,79	0
55	MG	DA	3082	1/1	0.12	-4.07	83,83,83,83	0
55	MG	BA	3052	1/1	0.08	-4.23	25,25,25,25	0
55	MG	DA	3055	1/1	0.06	-4.29	75,75,75,75	0
55	MG	BA	3054	1/1	0.09	-4.31	14,14,14,14	0
55	MG	AA	1643	1/1	0.05	-4.41	35,35,35,35	0
55	MG	BA	3064	1/1	0.09	-4.48	38,38,38,38	0
55	MG	AA	1632	1/1	0.06	-4.52	81,81,81,81	0
55	MG	BA	3068	1/1	0.10	-4.52	11,11,11,11	0
55	MG	DA	3016	1/1	0.14	-4.53	169,169,169,169	0
55	MG	BA	3005	1/1	0.09	-4.56	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	1631	1/1	0.06	-4.56	165,165,165,165	0
55	MG	BA	3021	1/1	0.08	-4.56	17,17,17,17	0
55	MG	BA	3081	1/1	0.07	-4.74	32,32,32,32	0
55	MG	AA	1610	1/1	0.07	-4.81	33,33,33,33	0
55	MG	BA	3102	1/1	0.07	-4.97	36,36,36,36	0
55	MG	DA	3133	1/1	0.09	-5.03	84,84,84,84	0
55	MG	BA	3009	1/1	0.08	-5.04	13,13,13,13	0
55	MG	DA	3056	1/1	0.14	-5.10	103,103,103,103	0
55	MG	BB	204	1/1	0.09	-5.17	40,40,40,40	0
55	MG	BA	3082	1/1	0.07	-5.19	30,30,30,30	0
55	MG	BA	3016	1/1	0.06	-5.20	64,64,64,64	0
55	MG	BA	3069	1/1	0.06	-5.38	14,14,14,14	0
55	MG	BA	3118	1/1	0.06	-5.54	13,13,13,13	0
55	MG	DA	3043	1/1	0.15	-5.64	104,104,104,104	0
55	MG	DA	3114	1/1	0.10	-5.78	95,95,95,95	0
55	MG	BA	3067	1/1	0.09	-5.79	21,21,21,21	0
55	MG	BA	3019	1/1	0.07	-6.18	39,39,39,39	0
55	MG	BA	3033	1/1	0.09	-6.25	9,9,9,9	0
55	MG	BA	3080	1/1	0.07	-6.26	31,31,31,31	0
55	MG	BA	3094	1/1	0.06	-6.34	37,37,37,37	0
55	MG	AA	1634	1/1	0.08	-6.45	59,59,59,59	0
55	MG	CA	1613	1/1	0.07	-6.51	96,96,96,96	0
55	MG	BA	3055	1/1	0.08	-6.51	25,25,25,25	0
55	MG	AA	1625	1/1	0.05	-7.02	67,67,67,67	0
55	MG	CA	1609	1/1	0.11	-7.26	83,83,83,83	0
55	MG	CA	1606	1/1	0.11	-7.52	64,64,64,64	0
55	MG	BA	3111	1/1	0.06	-7.70	47,47,47,47	0
55	MG	AA	1605	1/1	0.06	-7.73	123,123,123,123	0
55	MG	BA	3097	1/1	0.06	-7.95	18,18,18,18	0
55	MG	DA	3008	1/1	0.11	-8.74	100,100,100,100	0
55	MG	DA	3093	1/1	0.16	-8.75	121,121,121,121	0
55	MG	BA	3044	1/1	0.07	-9.05	34,34,34,34	0
55	MG	BA	3010	1/1	0.07	-9.72	29,29,29,29	0
55	MG	BA	3053	1/1	0.09	-11.54	30,30,30,30	0
55	MG	BA	3128	1/1	0.09	-11.92	18,18,18,18	0
55	MG	DA	3030	1/1	0.14	-12.92	144,144,144,144	0
55	MG	AA	1638	1/1	0.09	-14.02	29,29,29,29	0
55	MG	BA	3104	1/1	0.09	-14.16	22,22,22,22	0
55	MG	BA	3099	1/1	0.09	-17.00	82,82,82,82	0
55	MG	BA	3090	1/1	0.05	-17.28	28,28,28,28	0
55	MG	BA	3039	1/1	0.08	-17.68	9,9,9,9	0
55	MG	BA	3096	1/1	0.04	-20.37	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3010	1/1	1.06	-	200,200,200,200	0
55	MG	DA	3003	1/1	1.01	-	210,210,210,210	0

6.5 Other polymers ⓘ

There are no such residues in this entry.