



wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 07:17 PM BST

PDB ID : 4V64
Title : Crystal structure of the bacterial ribosome from Escherichia coli in complex with hygromycin B.
Authors : Borovinskaya, M.A.; Shoji, S.; Fredrick, K.; Cate, J.H.D.
Deposited on : 2008-06-11
Resolution : 3.50 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>

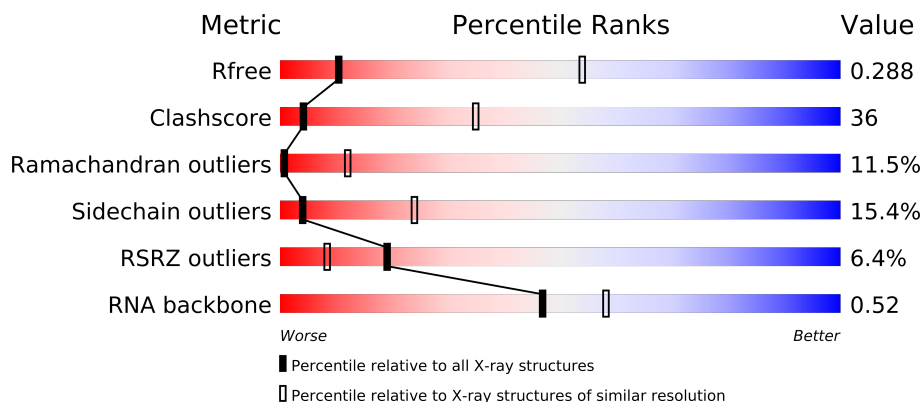
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.50 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	1243 (3.70-3.30)
Clashscore	79885	1039 (3.66-3.34)
Ramachandran outliers	78287	1000 (3.66-3.34)
Sidechain outliers	78261	1000 (3.66-3.34)
RSRZ outliers	66119	1243 (3.70-3.30)
RNA backbone	1838	1007 (4.22-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	AA	1542	
1	CA	1542	
2	AC	232	
2	CC	232	
3	AD	205	
3	CD	205	
4	AE	166	
4	CE	166	
5	AF	135	
5	CF	135	
6	AG	178	
6	CG	178	

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Mol	Chain	Length	Quality of chain
7	AH	129	
7	CH	129	
8	AI	129	
8	CI	129	
9	AJ	103	
9	CJ	103	
10	AK	128	
10	CK	128	
11	AL	123	
11	CL	123	
12	AM	117	
12	CM	117	
13	AN	100	
13	CN	100	
14	AO	89	
14	CO	89	
15	AP	82	
15	CP	82	
16	AQ	83	
16	CQ	83	
17	AR	74	
17	CR	74	
18	AS	91	
18	CS	91	
19	AT	86	
19	CT	86	
20	AB	240	
20	CB	240	
21	AU	71	
21	CU	71	
22	BA	120	
22	DA	120	
23	BB	2904	
23	DB	2904	
24	BV	94	
24	DV	94	
25	BC	273	
25	DC	273	
26	BD	209	
26	DD	209	
27	BE	201	
27	DE	201	

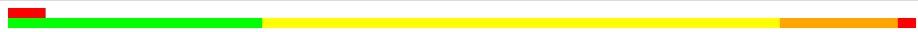
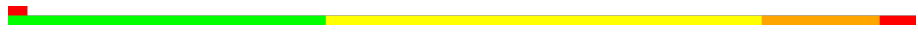
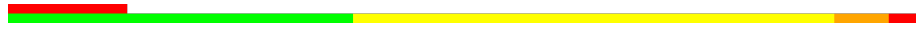

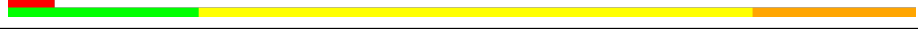

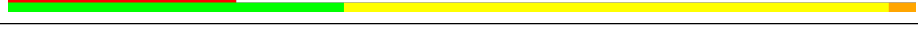

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Mol	Chain	Length	Quality of chain
28	BF	178	
28	DF	178	
29	BG	176	
29	DG	176	
30	BH	149	
30	DH	149	
31	BJ	142	
31	DJ	142	
32	BK	123	
32	DK	123	
33	BL	144	
33	DL	144	
34	BM	136	
34	DM	136	
35	BN	127	
35	DN	127	
36	BO	117	
36	DO	117	
37	BP	114	
37	DP	114	
38	BQ	117	
38	DQ	117	
39	BR	103	
39	DR	103	
40	BS	110	
40	DS	110	
41	BT	100	
41	DT	100	
42	BU	103	
42	DU	103	
43	BW	84	
43	DW	84	
44	BX	63	
44	DX	63	
45	BY	58	
45	DY	58	
46	BZ	78	
46	DZ	78	
47	B0	56	
47	D0	56	
48	B1	54	
48	D1	54	

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Mol	Chain	Length	Quality of chain
49	B2	46	
49	D2	46	
50	B3	64	
50	D3	64	
51	B4	38	
51	D4	38	
52	BI	141	
52	DI	141	

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

Mol	Type	Chain	Res	Geometry	Electron density
53	MG	AA	2012	-	X
53	MG	AA	2013	-	X
53	MG	AA	2021	-	X
53	MG	AA	2023	-	X
53	MG	AA	2035	-	X
53	MG	AA	2037	-	X
53	MG	AA	2045	-	X
53	MG	AA	2055	-	X
53	MG	AA	2057	-	X
53	MG	BB	3022	-	X
53	MG	BB	3028	-	X
53	MG	BB	3033	-	X
53	MG	BB	3039	-	X
53	MG	CA	2011	-	X
53	MG	CA	2020	-	X
53	MG	CA	2021	-	X
53	MG	CA	2038	-	X
53	MG	CA	2045	-	X
53	MG	DB	3003	-	X
53	MG	DB	3058	-	X
53	MG	DB	3099	-	X
54	HYG	CA	2062	-	X

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 284077 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

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

- Molecule 2 is a 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	150	Total	C	N	O	S	0	0	0
			1174	730	226	214	4			
6	CG	152	Total	C	N	O	S	0	0	0
			1196	745	230	217	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	96	Total	C	N	O	S	0	0	0
			774	483	160	128	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
			715	440	146	128	1			
14	CO	88	Total	C	N	O	S	0	0	0
			715	440	146	128	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	81	Total	C	N	O	S	0	0	0
			656	417	122	114	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	80	Total	C	N	O	S	0	0	0
			644	413	121	108	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 S2.

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

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

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

- Molecule 22 is a RNA chain called 5S ribosomal RNA.

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

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

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

- Molecule 24 is a protein called 50S ribosomal protein L25.

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

- Molecule 25 is a protein called 50S ribosomal protein L2.

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

- Molecule 26 is a protein called 50S ribosomal protein L3.

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

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

- Molecule 27 is a protein called 50S ribosomal protein L4.

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

- Molecule 28 is a protein called 50S ribosomal protein L5.

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

- Molecule 29 is a protein called 50S ribosomal protein L6.

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

- Molecule 30 is a protein called 50S ribosomal protein L9.

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

- 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	121	Total	C	N	O	S	0	0	0
			930	582	179	164	5			
32	DK	121	Total	C	N	O	S	0	0	0
			930	582	179	164	5			

- 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	S	0	0	0
			947	604	192	151				
38	DQ	117	Total	C	N	O	S	0	0	0
			947	604	192	151				

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BT	93	Total	C	N	O	S	0	0	0
			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	S	0	0	0
			779	492	146	141				

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

- Molecule 43 is a protein called 50S ribosomal protein L27.

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

- Molecule 44 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BX	63	Total	C	N	O	S			
			509	313	99	95	2	0	0	0
44	DX	63	Total	C	N	O	S			
			509	313	99	95	2	0	0	0

- Molecule 45 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BY	58	Total	C	N	O	S			
			449	281	87	79	2	0	0	0
45	DY	58	Total	C	N	O	S			
			449	281	87	79	2	0	0	0

- Molecule 46 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BZ	77	Total	C	N	O	S			
			625	388	129	106	2	0	0	0
46	DZ	77	Total	C	N	O	S			
			625	388	129	106	2	0	0	0

- Molecule 47 is a protein called 50S ribosomal protein L32.

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

- Molecule 48 is a protein called 50S ribosomal protein L33.

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

- Molecule 49 is a protein called 50S ribosomal protein L34.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L36.

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

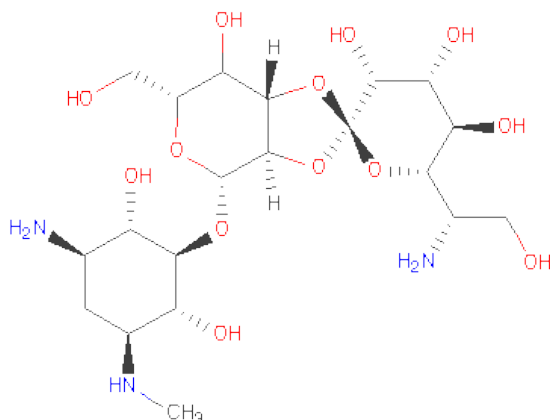
- Molecule 52 is a protein called 50S ribosomal protein L11.

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

- Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
53	BB	110	Total	Mg	0	0
			110	110		
53	CA	61	Total	Mg	0	0
			61	61		
53	AE	1	Total	Mg	0	0
			1	1		
53	AA	58	Total	Mg	0	0
			58	58		
53	AN	1	Total	Mg	0	0
			1	1		
53	CE	1	Total	Mg	0	0
			1	1		
53	DB	111	Total	Mg	0	0
			111	111		

- Molecule 54 is HYGROMYCIN B (three-letter code: HYG) (formula: C₂₀H₃₇N₃O₁₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
54	AA	1	Total	C	N	O	0	0
			36	20	3	13		
54	CA	1	Total	C	N	O	0	0
			36	20	3	13		

- Molecule 55 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	B4	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	D4	1	Total 1	Zn 1	0	0

- Molecule 56 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AA	282	Total 282	O 282	0	0
56	AE	4	Total 4	O 4	0	0
56	AK	2	Total 2	O 2	0	0
56	AL	5	Total 5	O 5	0	0
56	AN	4	Total 4	O 4	0	0
56	AT	3	Total 3	O 3	0	0
56	BB	492	Total 492	O 492	0	0
56	BC	8	Total 8	O 8	0	0
56	BD	1	Total 1	O 1	0	0
56	BE	2	Total 2	O 2	0	0
56	BH	1	Total 1	O 1	0	0
56	BL	2	Total 2	O 2	0	0
56	B2	1	Total 1	O 1	0	0
56	CA	294	Total 294	O 294	0	0
56	CE	4	Total 4	O 4	0	0
56	CI	1	Total 1	O 1	0	0
56	CK	1	Total 1	O 1	0	0
56	CL	3	Total 3	O 3	0	0

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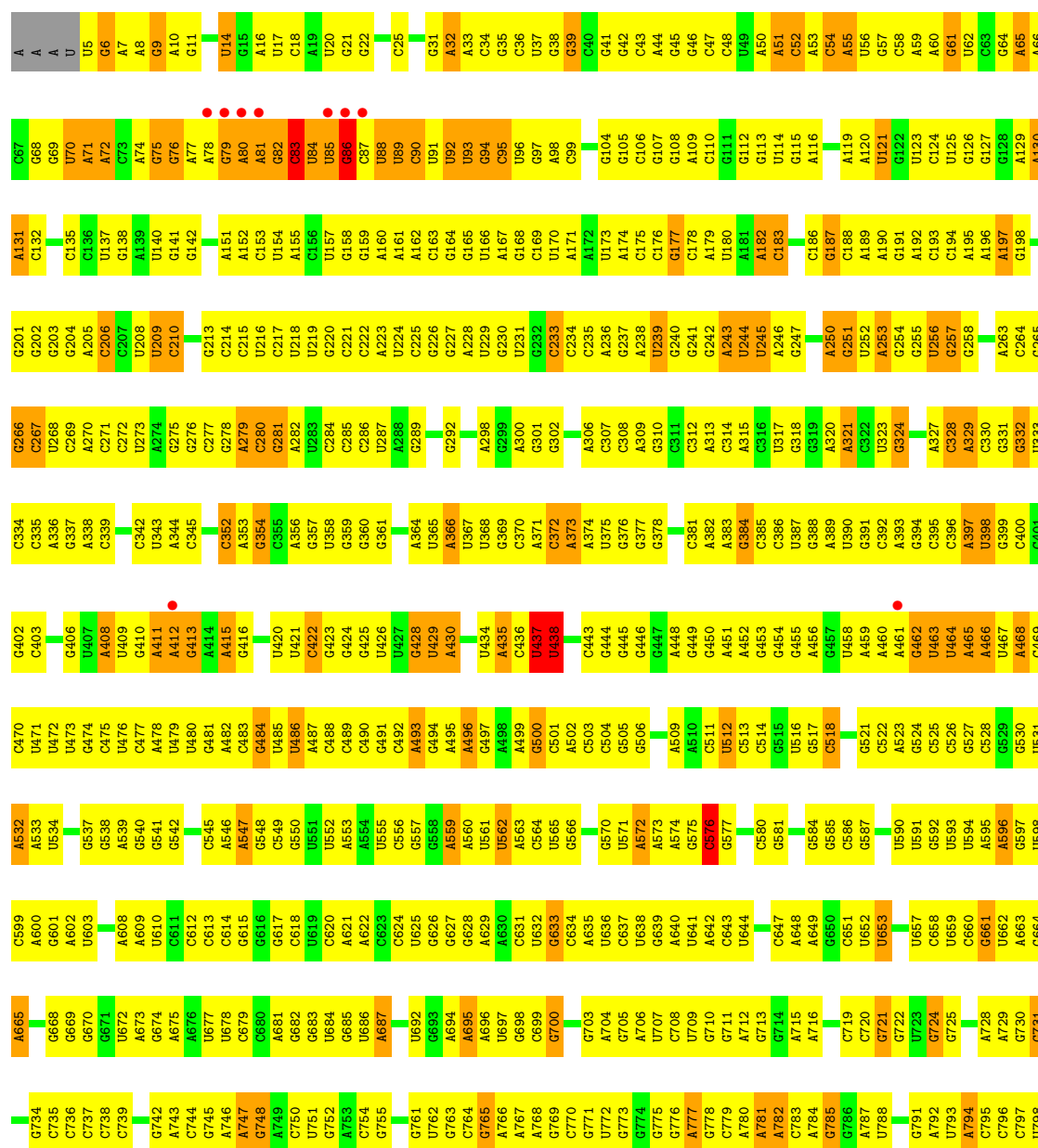
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	CN	3	Total 3	O 3	0	0
56	CT	1	Total 1	O 1	0	0
56	DB	499	Total 499	O 499	0	0
56	DC	5	Total 5	O 5	0	0
56	DD	1	Total 1	O 1	0	0
56	DE	1	Total 1	O 1	0	0
56	DL	5	Total 5	O 5	0	0
56	DP	1	Total 1	O 1	0	0
56	D2	1	Total 1	O 1	0	0

3 Residue-property plots

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

• Molecule 1: 16S ribosomal RNA

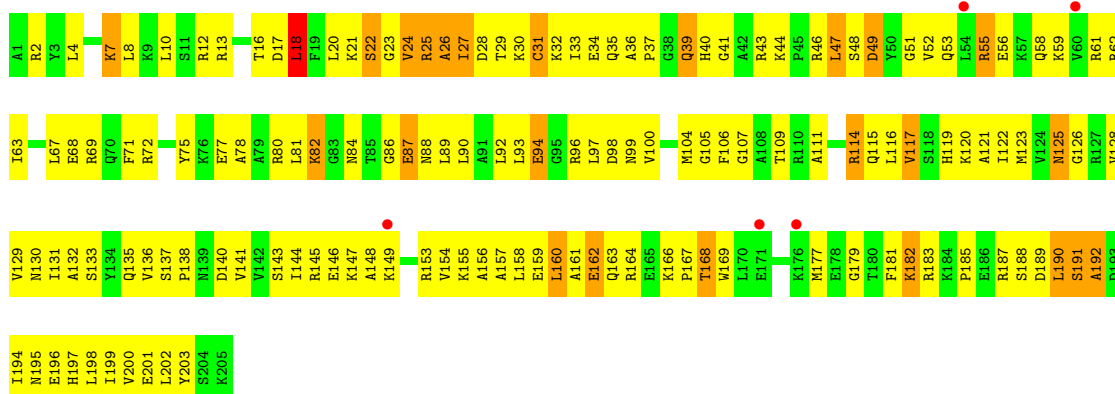
Chain AA: 



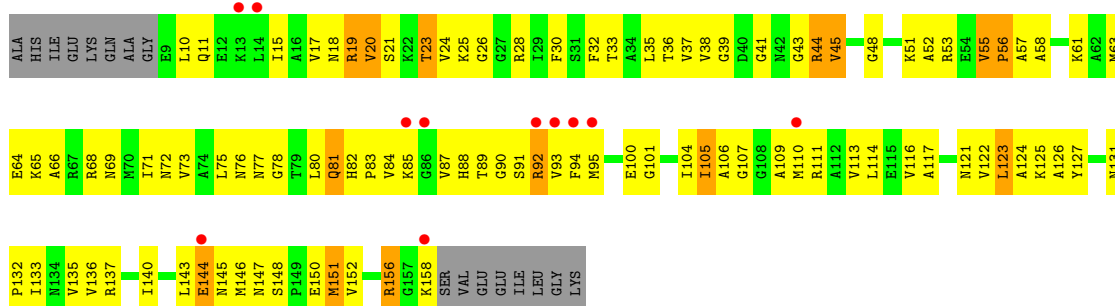
G1185	G1057	A996	C931	A860	U793	G724	C660	A595	G529	U464	A397	G332	A263	G201
G1186	G1058	U997	C934	G861	A794	G725	G661	A596	G530	A465	U998	U333	C264	G202
G1187	G1059	C998	A935	U862	C796		U662	G597	U531	A466	C999	C334	G265	G203
A1191	G1060	C999	A936	U863	C797	A728	A663	U598	A532	U467	C400	C335	G266	G204
U1194	G1061	A1000	C937	A864	C798	A729	G664	C599	A533	A468	C401	A336	C267	A205
C1195	G1062	C1001	A938	A865	G730	G730	A665	A600	U534	C469	G402	G337	U268	C206
G1127	G1063	G1002	A938	C966	G731			G601		C470	C403	A338	C269	C207
G1128	G1064	G1003	G939	G867			G668	A602	G537	U471	C406	C339	A270	U208
G1129	U1065	A1004	C940	C868	G734	G734	G669	A603	G538	U472	U406	U340	C271	U209
A1197	C1066	A1005	G941	U804	C735	C735	U670	U603	A539	U473	U407	C341	C272	C210
G1131		G1006			C736		G671	A607	G540	G474	U408	C342	U273	
G1069	U1067	U1007	G945	U875	C737		U672	A608	G541	C475	U409	U343	A274	G213
U1070	U1008	U1008	A946	C876	C738		U673	A609	G542	U476	G410	G275	G275	G214
C1071	C1071	U1009	G947	G877	C739		G674	U610	U543	C477	A411	G276	G276	C215
U1135	G1072	C1010	C948	A878			A675	C611	G544		A412	G277	C277	U216
C1136	U1073	U1011	A949	C879	G742		U676	C612	G545	U478	A413	G278	G278	C217
G1074	G1074	A1012	U950	C880	A743		U677	C613	A546	U479	A414	C352	C217	
G1077		A1014	G951	G881	C744		U678	C614	A547	G481	A415	A353	A279	U218
U1078	U1078	A1016	U952	U813	G745		C679	G615	G548	A482	G416	C355	G280	U219
G1079	U1079	G1015	G953	C883	A746		G680	G616	C549	C483		A356	G281	G220
C1141	U1078	A1016	G954	U884	A747		A681	G617	G550	G484	U420	U357	A282	C221
G1142	U1080	U1017	U955	C885	G748		G682	C618	G551	U485	U421	U358	U283	C222
G1143	A1081	G1018	U956	G886	A749		U683	G619	U552	U486	U422	C284	C285	A223
U1211	A1082	U1019	U957	C887	C750		U684	C620	A553	C487	G423	G360	C286	C224
A1145		G1020	A958	A889	U751		G685	A621	G554	G488	G424	G361	U287	G226
A1146	U1085	A1021	A959				U686	A622	U555	C489	G425	G362	A288	G227
C1214	U1086	A1022	U960	C893	C754		A687	C623	C556	C490	U426	A363	G289	A228
G1215	G1087	U1023	U961	G894	G755		G688	C624	A559	G491	U427	A364		U229
C1217	U1088	G1024			G756			U625	A560	C492	U428	U365	G292	G230
C1218	G1089	U1025	A964	G898	U762		U692	G626	A561	G494	U429	U367	A298	U231
A1219	U1090	G1026	U965	C899	G763		G693	G627	A562	A495	U430	U368	C299	G232
A1151	U1091	C1027	U966	A900	C764		A694	G628	A563	A496		G369	A300	C233
A1152	U1091	C1027	C967	A901	C765		A695	A629	C564	G497	U434	C370	C234	C235
G1153	C1092	C1028	U968	G902	A766		U696	C631	U565	A498	U435	A371	A236	A236
	A1093	U1029	A969	G903	C767		C698	U632	C566		C436	C372	G302	G237
U1159	U1094	C1031	C970	U904	A768		C699	G633	G500	G500	U437	A373	A306	A238
G1160	U1095	G1032	C971	U905	C769		C699	G634	G570	C501	U438	A374	C307	U239
G1161	C1096	G1033	C972	A906	C770		G700	A635	U571	A502	U439	U375	C308	G240
C1162	C1097	G1034	G973	A907	G771		U701	U636	A572	C503		G376	A309	G241
A1163	U1098	A1035	A974	A908	U772		A702	C637	A573	C504	C443	G377	G310	G242
G1164	G1099	A1036	A975	A909	C773		G703	U638	A574	G505	G444	G378	C311	A243
U1165	C1100	C1037	G976	C910	G774		A704	U639	G575	G506	G445	G379	G312	U244
G1166	A1101	C1037	G977	C910	G775		G705	G639	G576		G446	C380	A313	U245
C1230	C1102	U1038	A977		G776		A706	A640	G577		G447	C381	C314	A246
G1231	C1103	G1039	A978	A914	G777		U707	U641	G578	C511	A448	C382	A315	G247
	U1168	U1040	C979	A915	A777		C708	A642	A579	U512	G449	A383	U317	
C1234	U1169	G1041	C980	U916	G778		U709	C643	C580	U516	G450	G384	G318	A250
U1235	A1105	A1042	U981	G917	C779		G710	U644	G581	G517	G451	C385	A320	G251
A1236	U1171	G1106	U982	A918	A780		G711		G581	G518	G452	G386	A321	U252
C1237	G1043		U983	A919	A781		G712		G584		G453	G387	A322	A253
A1238	U1044		A983	U920	A782		A713		G585	G521	G454	U388	G322	G254
U1239	C1045		C984	U921	C783		G714		G586	C522	G455	U389	U323	G255
U1240	A1111	A1046	C985	U922	A784		G715		G587	G523	G456	U390	G324	U256
C1242	C1112	G1047	U986	A923	G785		A716		G588	G524	G457	G391	G257	G257
G1243	G1113	G1048	U987	C924	G786				G589	A523	U458	G392	G258	G258
C1244	C1114	U1049	G988	G925	A787		C719		U590	G525	G459	C393	C328	G259
G1245	U1179	G1050	U991	G926	U788		C720		U591	C526	A460	G394	A329	G260
A1246	U1116		U992	C927	U789		G721		G592	G527	A461	G395	C330	U261
U1247	A1117		U993	G928	A790		G722		U594	C528	U463		G331	A262
A1248	U1118	C1120	A994	G929	G791		U723							
C1249	U1183		G995	C930	A792									

[illegible]

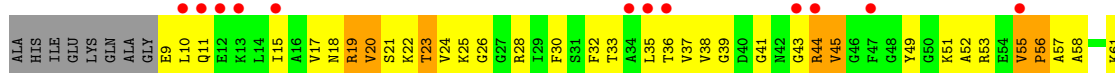
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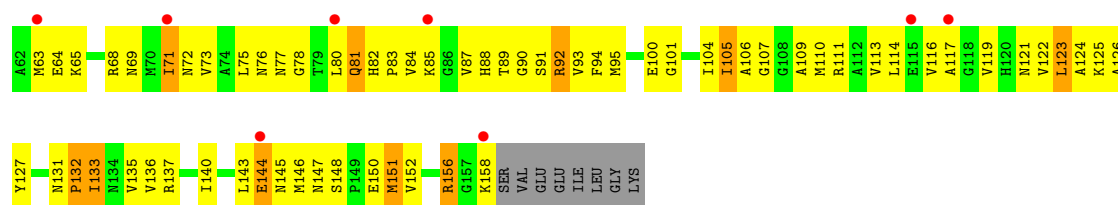


- Chain AE:



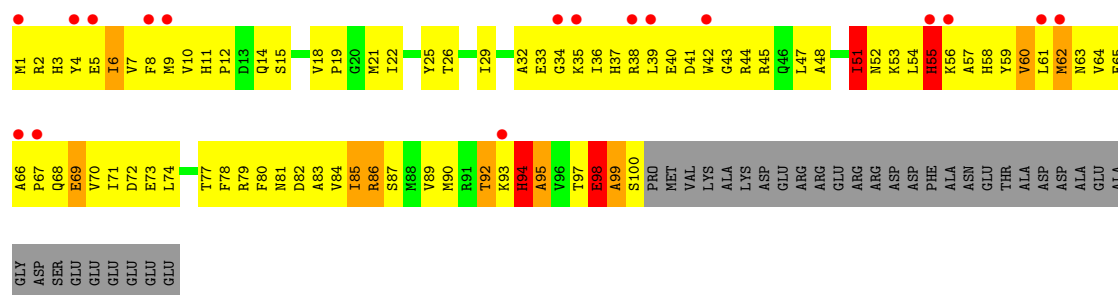
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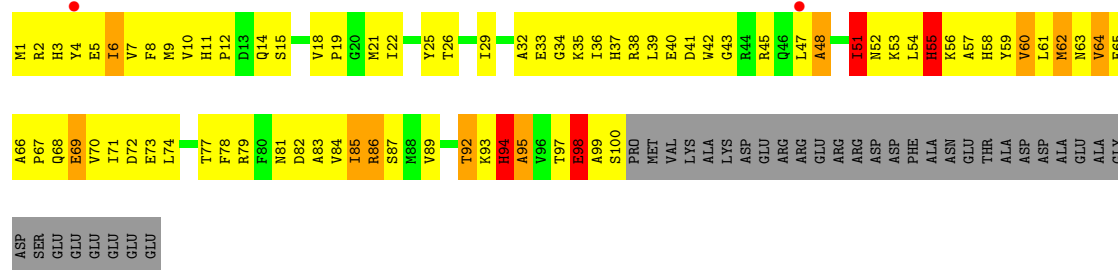
• Molecule 5: 30S ribosomal protein S6

Chain AF:



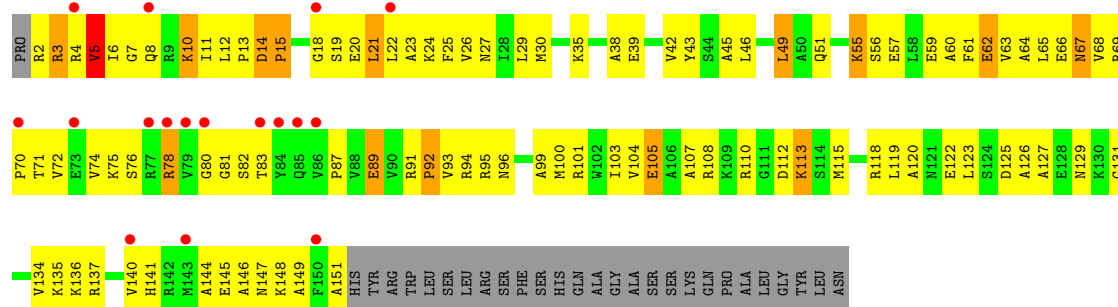
• Molecule 5: 30S ribosomal protein S6

Chain CF:



• Molecule 6: 30S ribosomal protein S7

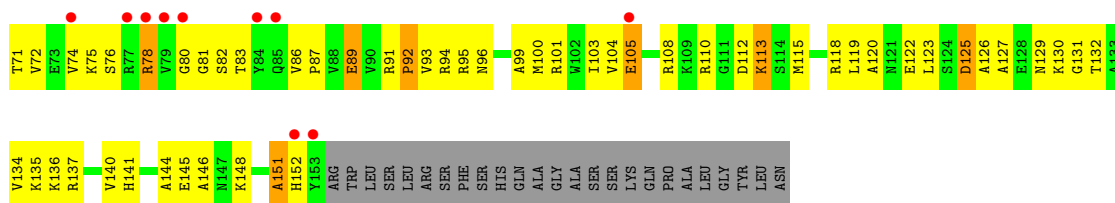
Chain AG:



• Molecule 6: 30S ribosomal protein S7

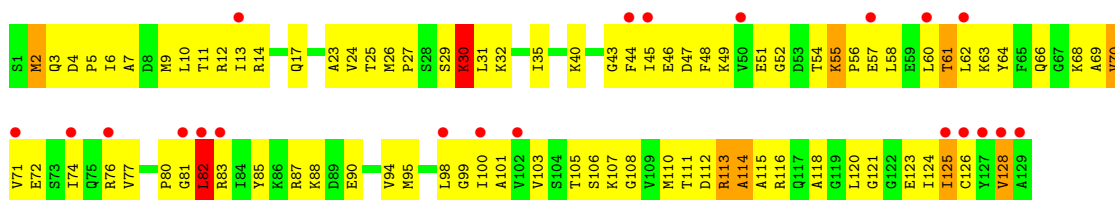
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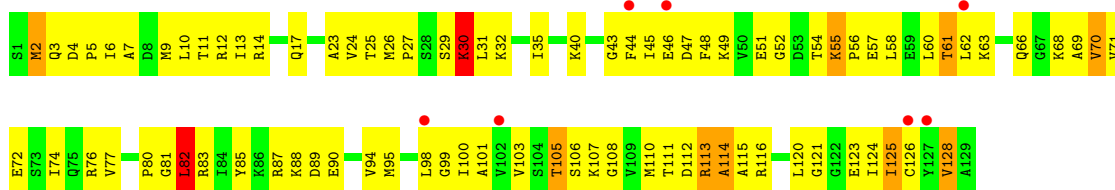
• Molecule 7: 30S ribosomal protein S8

Chain AH:



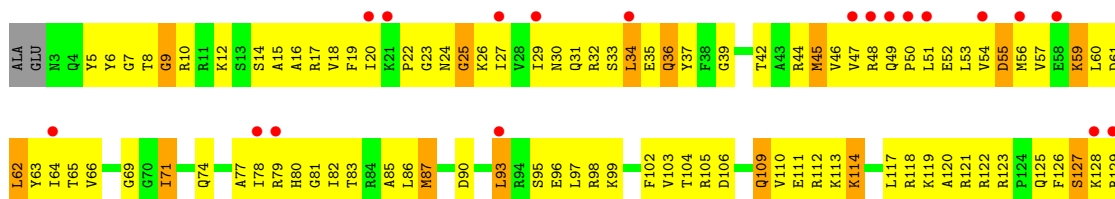
• Molecule 7: 30S ribosomal protein S8

Chain CH:



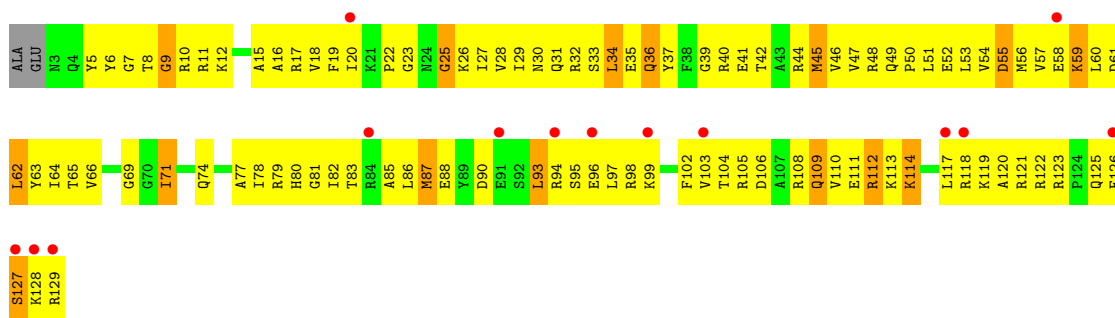
• Molecule 8: 30S ribosomal protein S9

Chain AI:



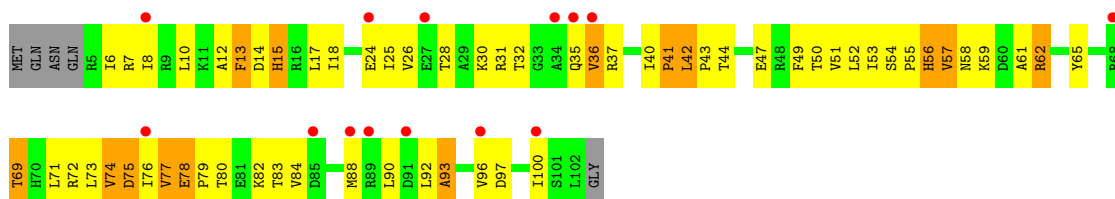
• Molecule 8: 30S ribosomal protein S9

Chain CI:



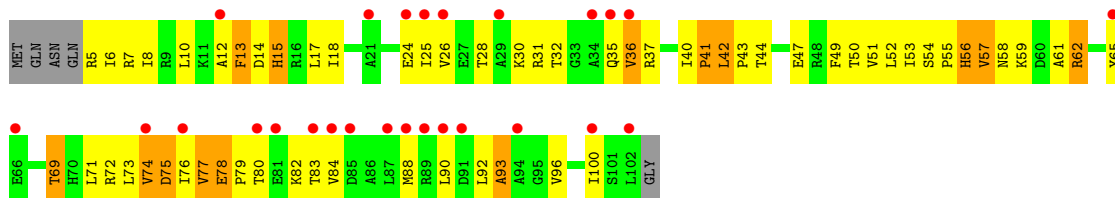
• Molecule 9: 30S ribosomal protein S10

Chain AJ:



- Molecule 9: 30S ribosomal protein S10

Chain CJ:



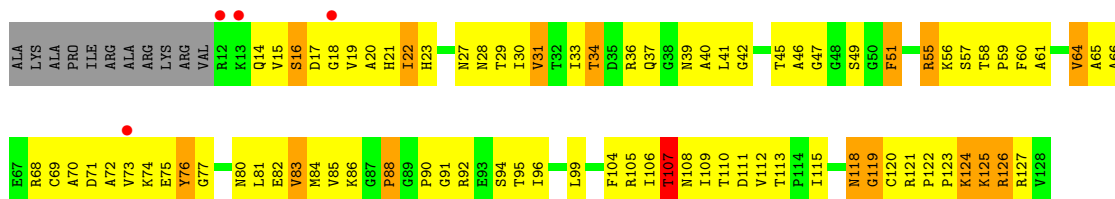
- Molecule 10: 30S ribosomal protein S11

Chain AK:



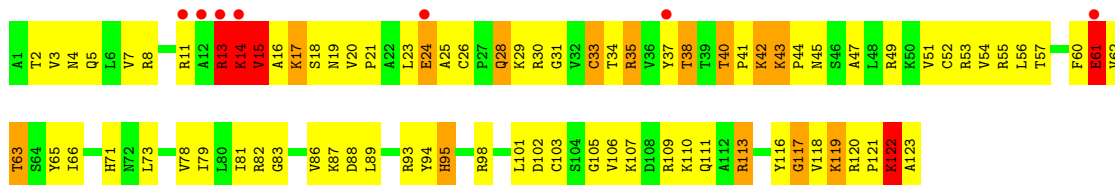
- Molecule 10: 30S ribosomal protein S11

Chain CK:



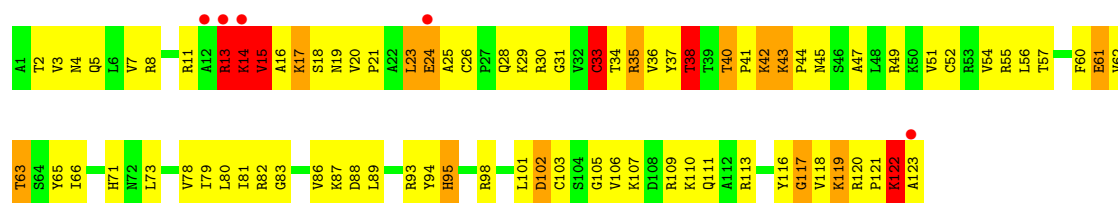
- Molecule 11: 30S ribosomal protein S12

Chain AL:



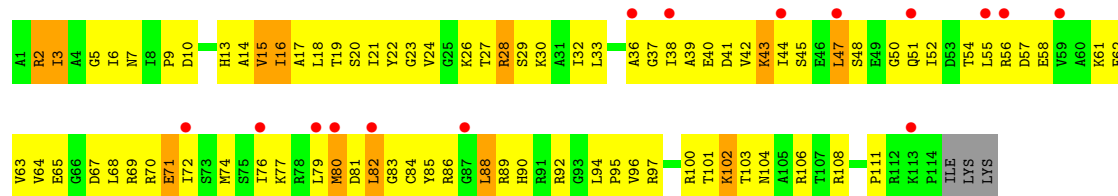
- Molecule 11: 30S ribosomal protein S12

Chain CL:



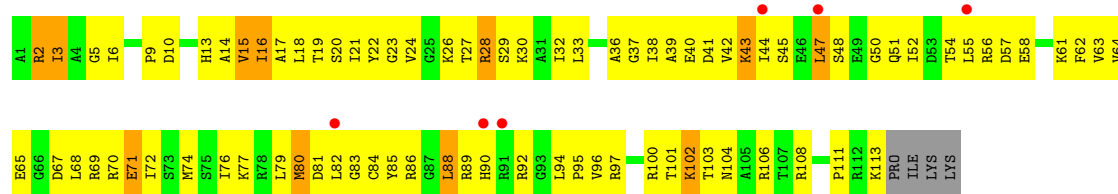
• Molecule 12: 30S ribosomal protein S13

Chain AM:



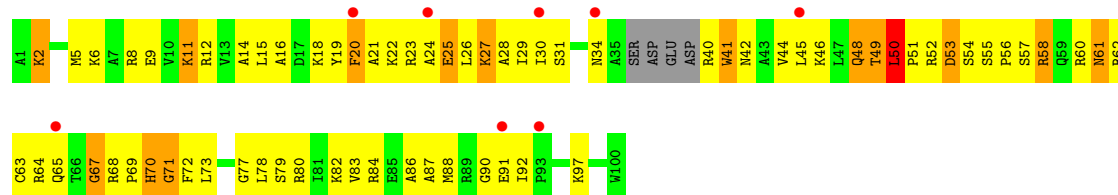
• Molecule 12: 30S ribosomal protein S13

Chain CM:



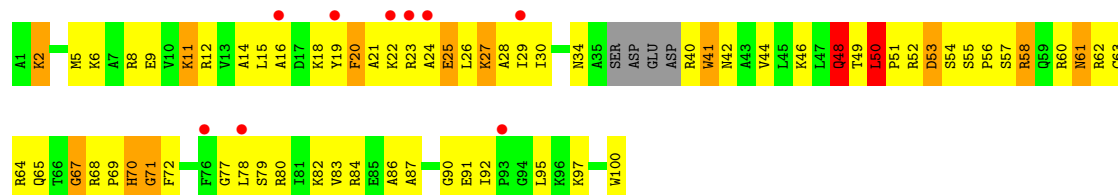
• Molecule 13: 30S ribosomal protein S14

Chain AN:



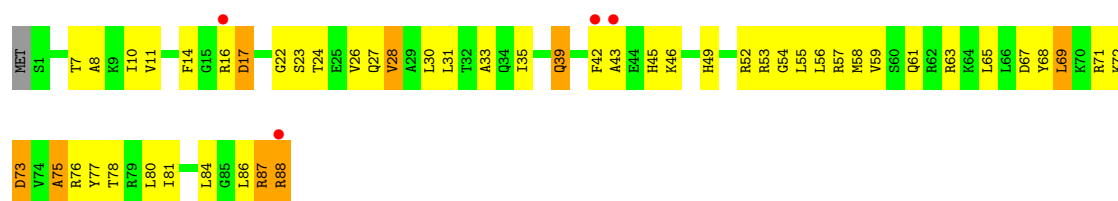
• Molecule 13: 30S ribosomal protein S14

Chain CN:



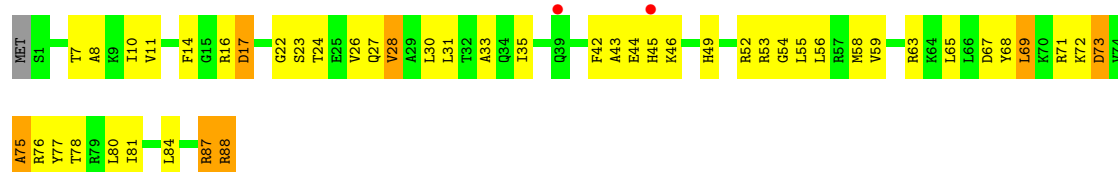
• Molecule 14: 30S ribosomal protein S15

Chain AO:



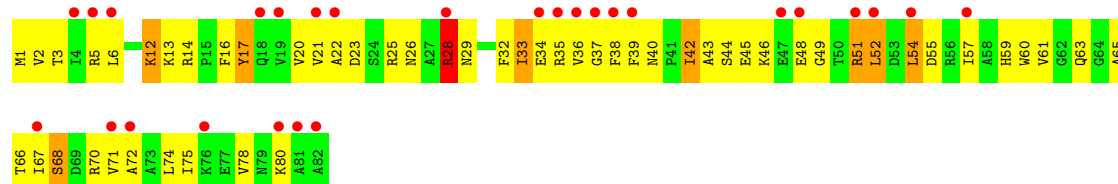
• Molecule 14: 30S ribosomal protein S15

Chain CO:



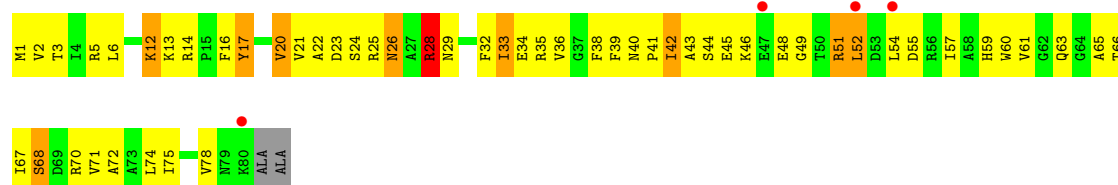
• Molecule 15: 30S ribosomal protein S16

Chain AP:



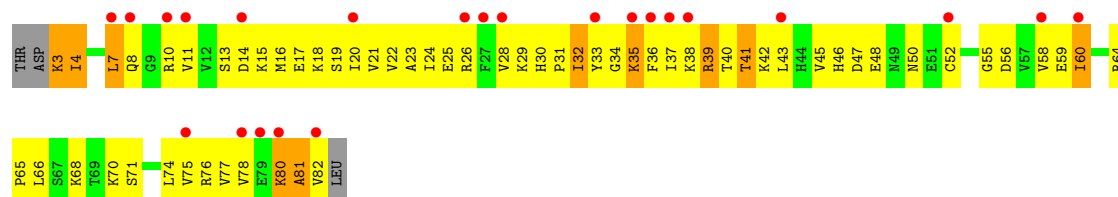
• Molecule 15: 30S ribosomal protein S16

Chain CP:



• Molecule 16: 30S ribosomal protein S17

Chain AQ:

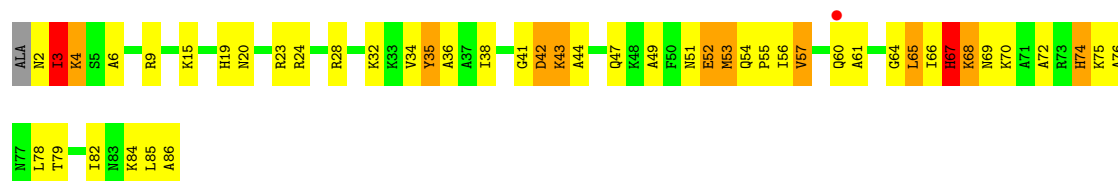


• Molecule 16: 30S ribosomal protein S17

Chain CQ:

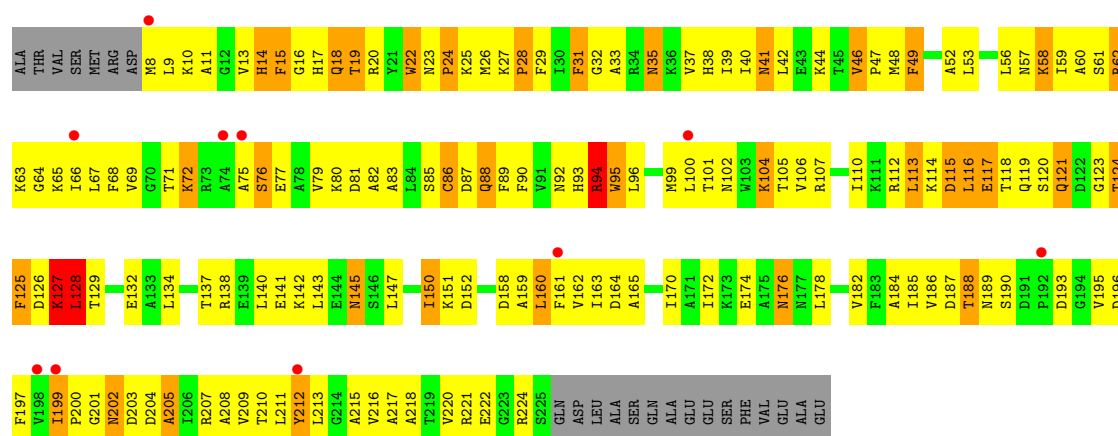






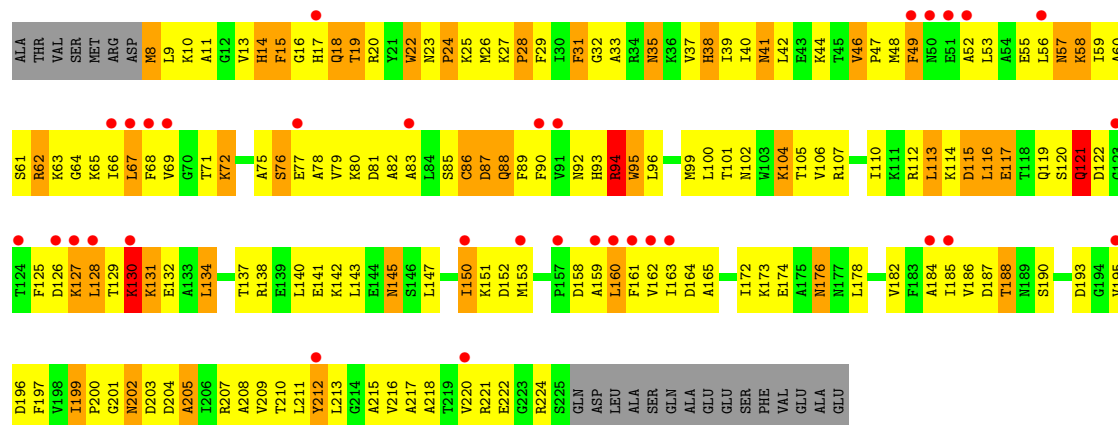
• Molecule 20: 30S ribosomal protein S2

Chain AB:



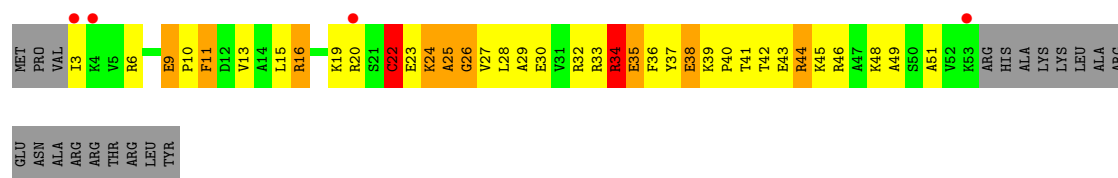
• Molecule 20: 30S ribosomal protein S2

Chain CB:



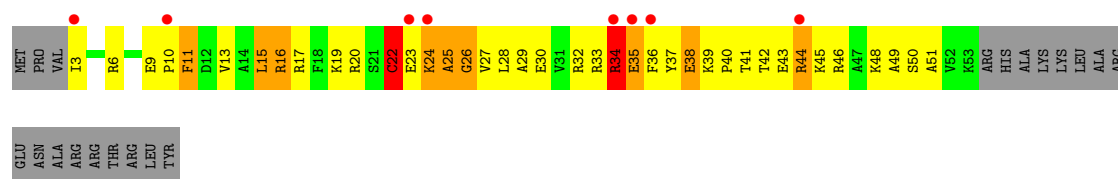
• Molecule 21: 30S ribosomal protein S21

Chain AU:



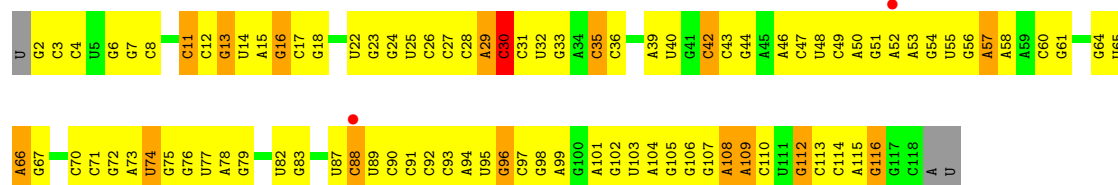
• Molecule 21: 30S ribosomal protein S21

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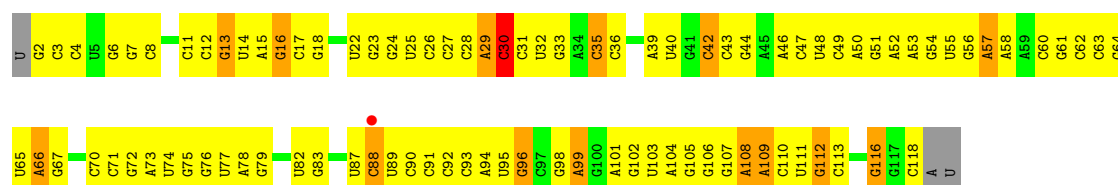
• Molecule 22: 5S ribosomal RNA

Chain BA:



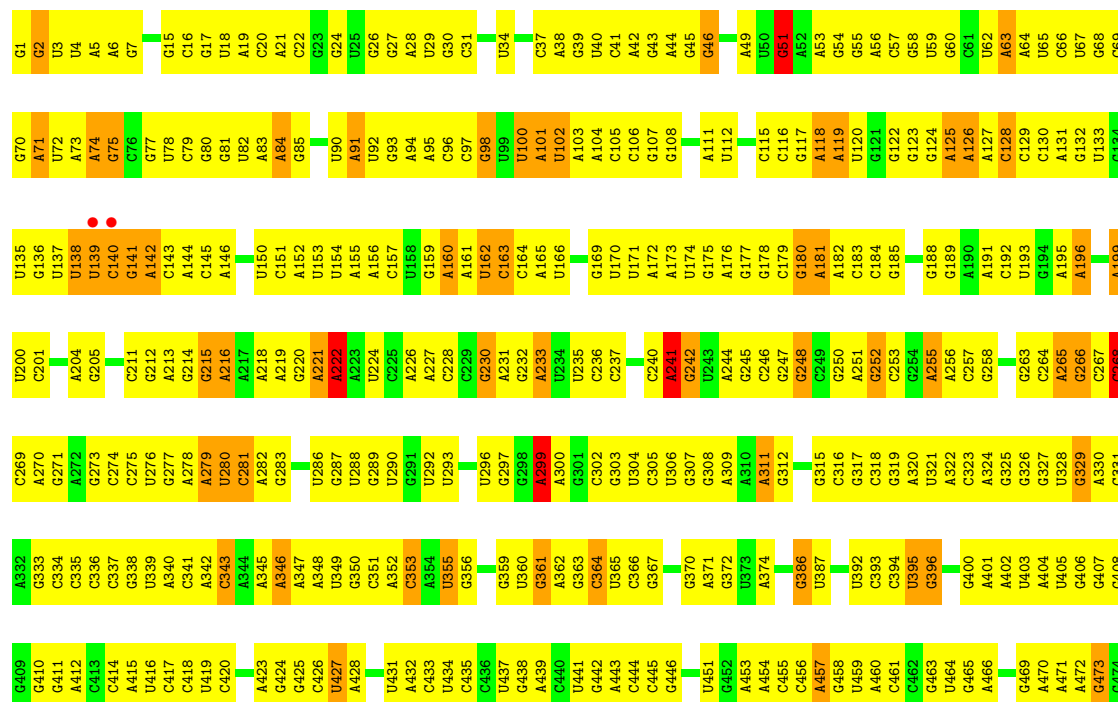
• Molecule 22: 5S ribosomal RNA

Chain DA:



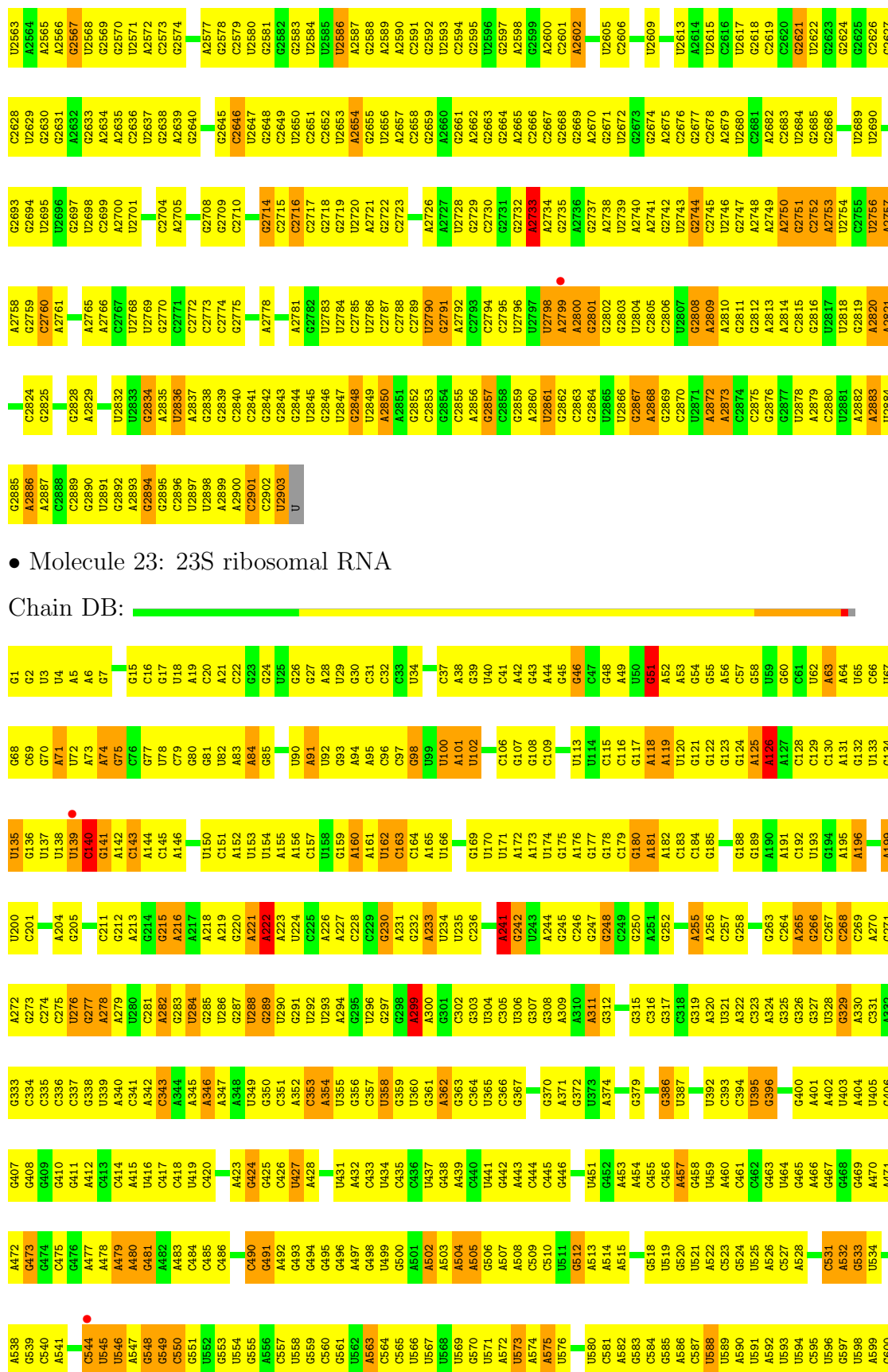
• Molecule 23: 23S ribosomal RNA

Chain BB:



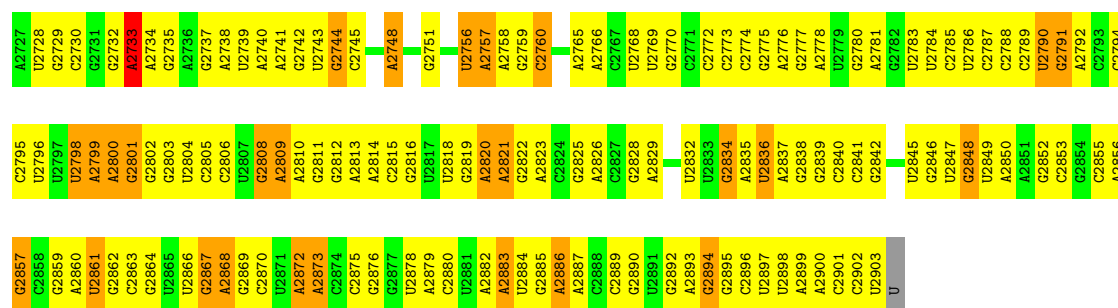
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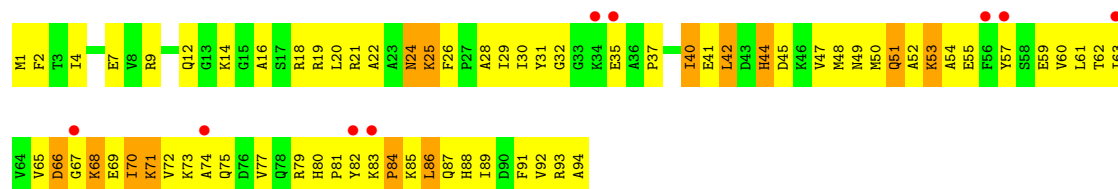
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G2148	U2149	U2150	U2151	C2152	C2153	A2154	U2155	U2156	U2157	A2158	U2159	U2160	U2161	U2162	U2163	U2164	U2165	U2166	U2167	U2168	U2169	U2170	U2171	U2172	U2173	U2174	U2175	U2176	U2177	U2178	U2179	U2180	U2181	U2182	U2183	U2184	U2185	U2186	U2187	U2188	U2189	U2190	U2191	U2192	U2193	U2194	U2195	U2196	U2197	U2198	U2199	U2200	U2201	U2202	U2203	U2204	U2205	U2206	U2207	U2208	U2209																						
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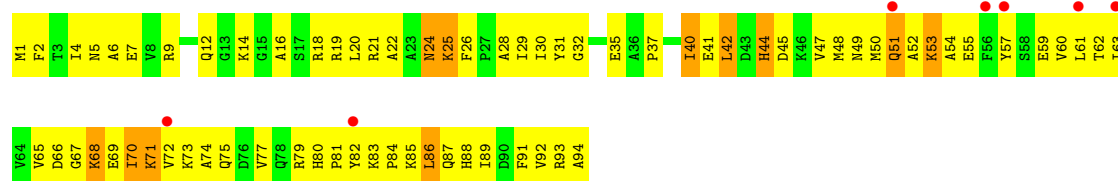
- Molecule 24: 50S ribosomal protein L25

Chain BV:



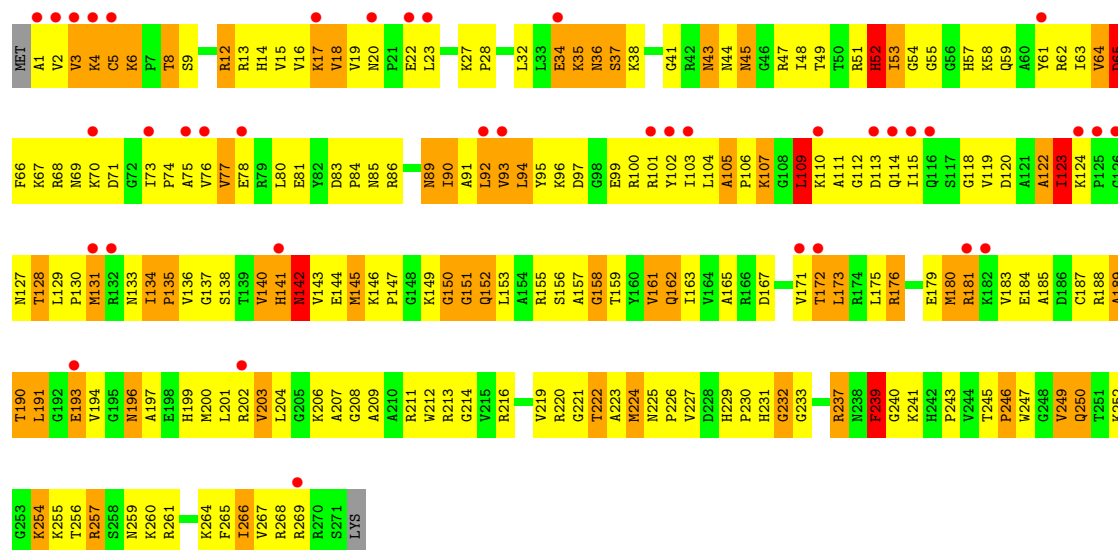
- Molecule 24: 50S ribosomal protein L25

Chain DV:



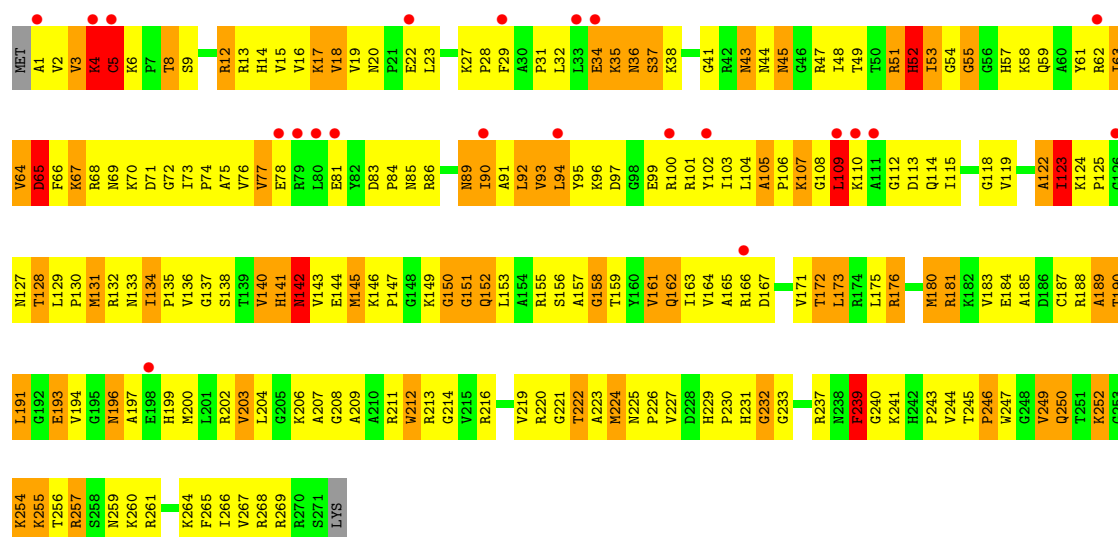
- Molecule 25: 50S ribosomal protein L2

Chain BC:



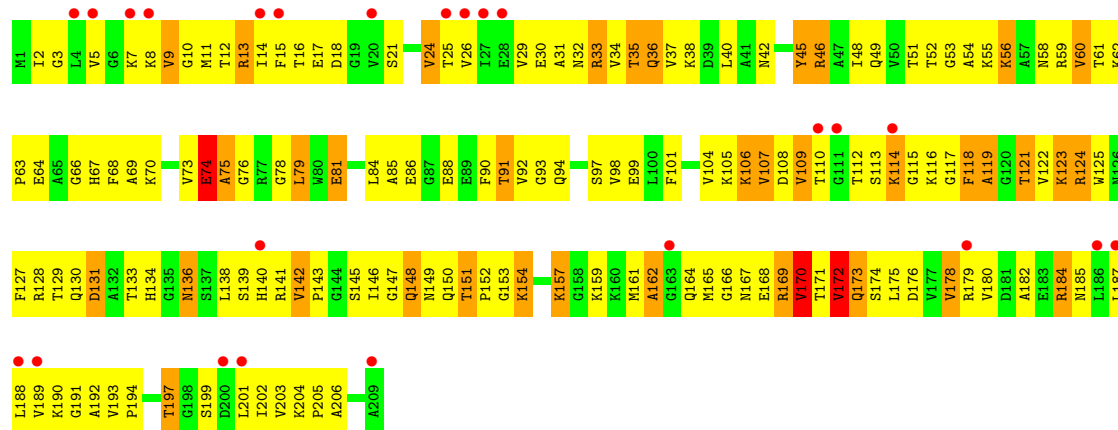
- Molecule 25: 50S ribosomal protein L2

Chain DC:



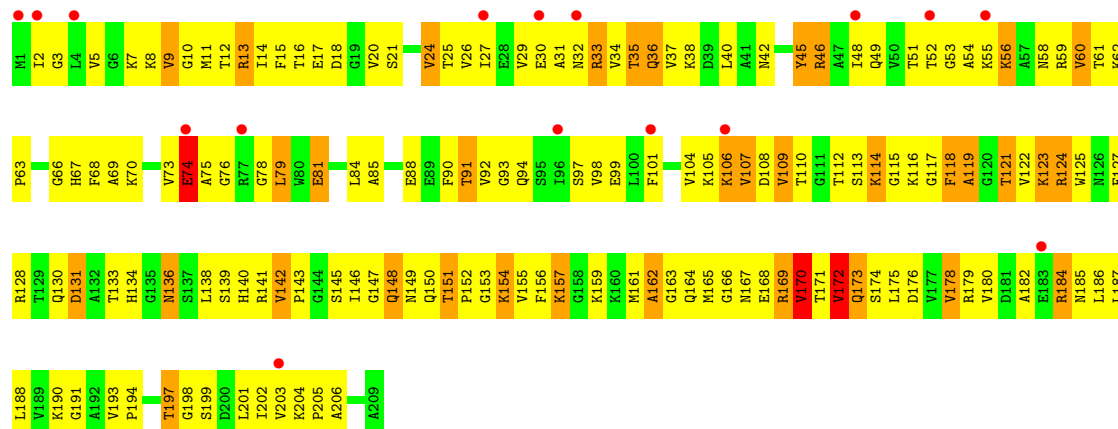
- Molecule 26: 50S ribosomal protein L3

Chain BD:



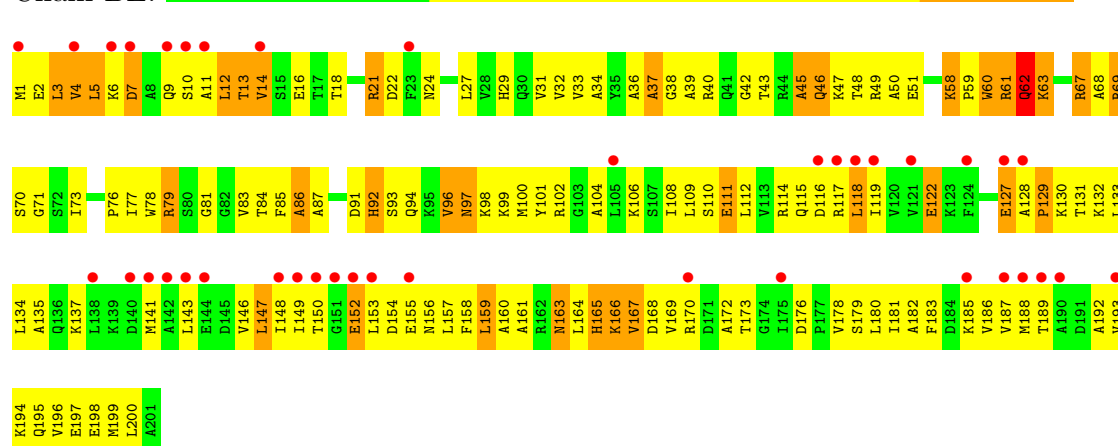
- Molecule 26: 50S ribosomal protein L3

Chain DD:



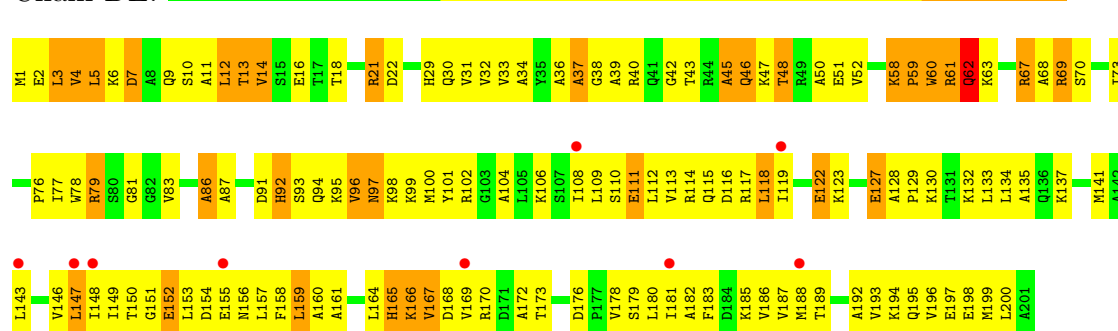
- Molecule 27: 50S ribosomal protein L4

Chain BE:



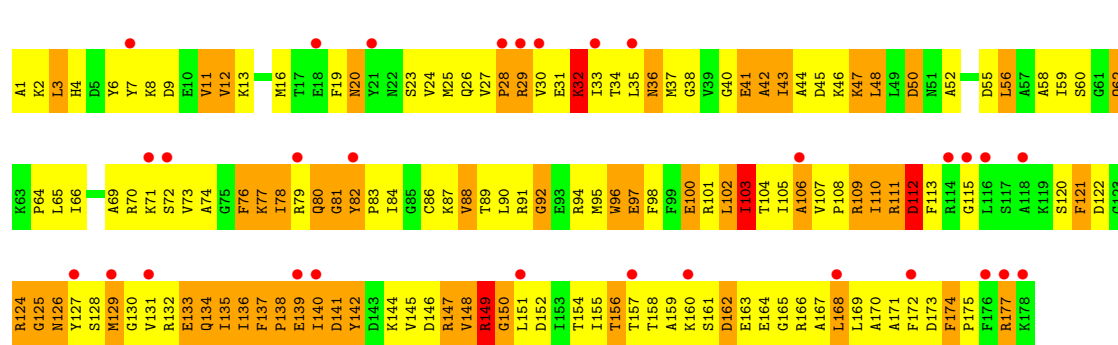
- Molecule 27: 50S ribosomal protein L4

Chain DE:



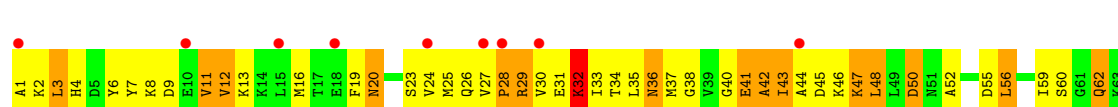
- Molecule 28: 50S ribosomal protein L5

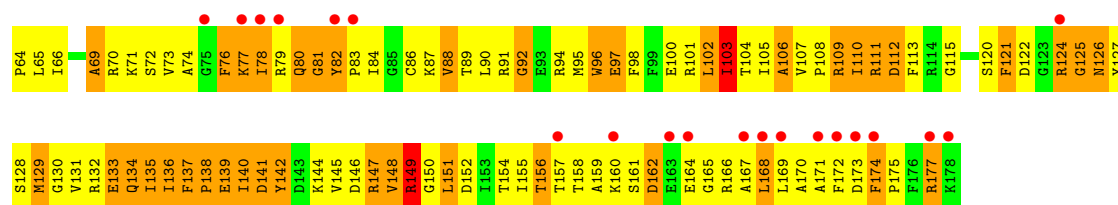
Chain BF:



- Molecule 28: 50S ribosomal protein L5

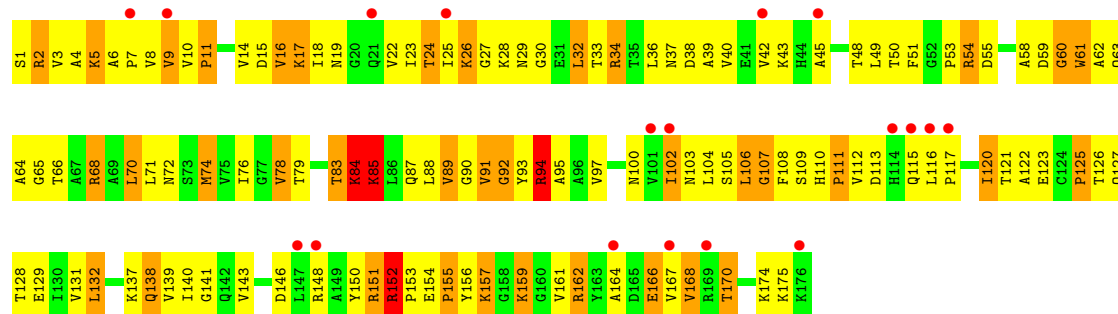
Chain DF:





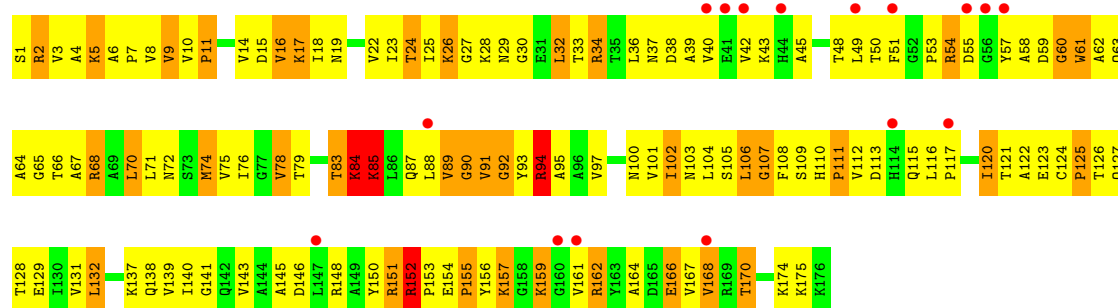
• Molecule 29: 50S ribosomal protein L6

Chain BG:



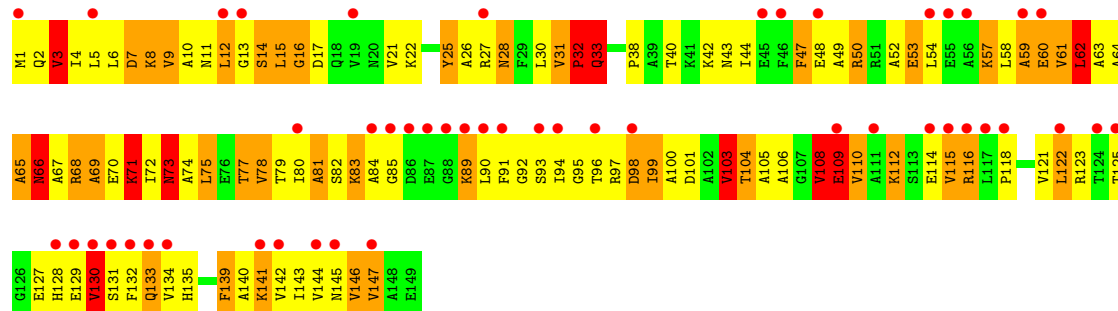
• Molecule 29: 50S ribosomal protein L6

Chain DG:



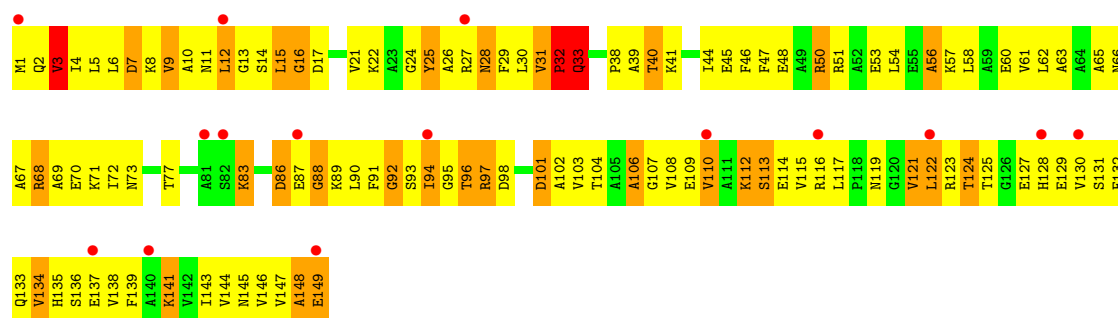
• Molecule 30: 50S ribosomal protein L9

Chain BH:



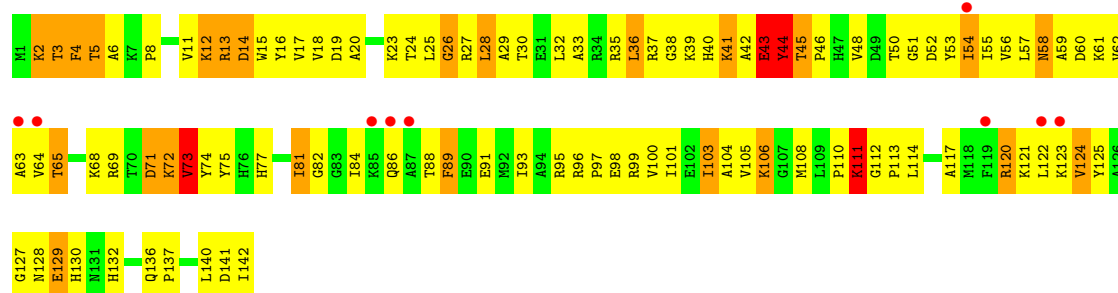
• Molecule 30: 50S ribosomal protein L9

Chain DH:



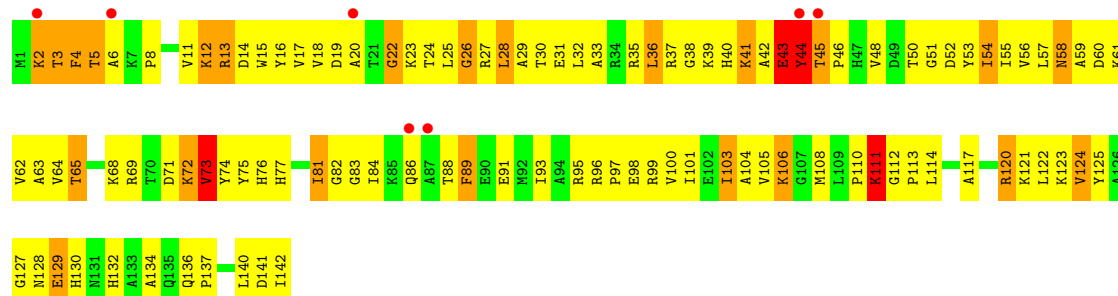
- Molecule 31: 50S ribosomal protein L13

Chain BJ:



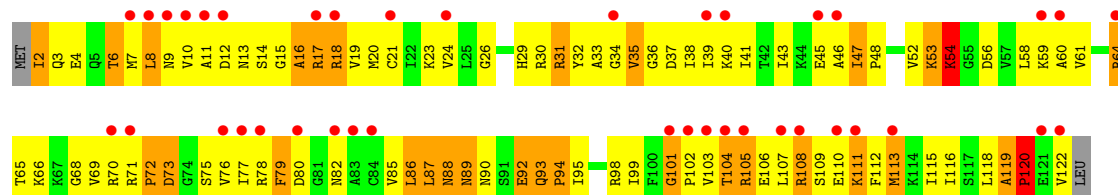
- Molecule 31: 50S ribosomal protein L13

Chain DJ:



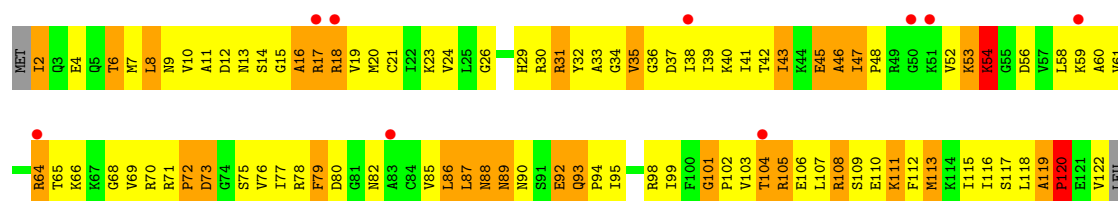
- Molecule 32: 50S ribosomal protein L14

Chain BK:



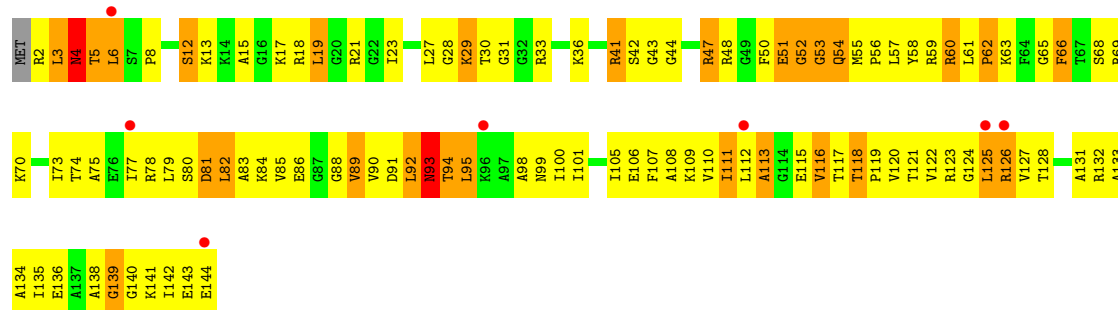
- Molecule 32: 50S ribosomal protein L14

Chain DK:



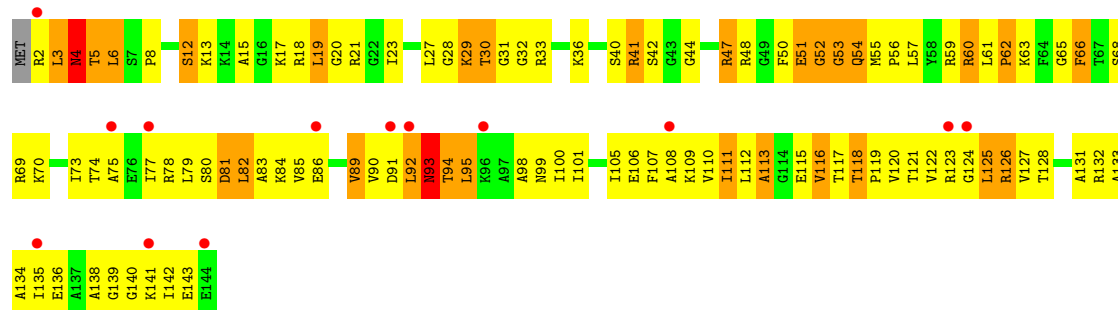
• Molecule 33: 50S ribosomal protein L15

Chain BL:



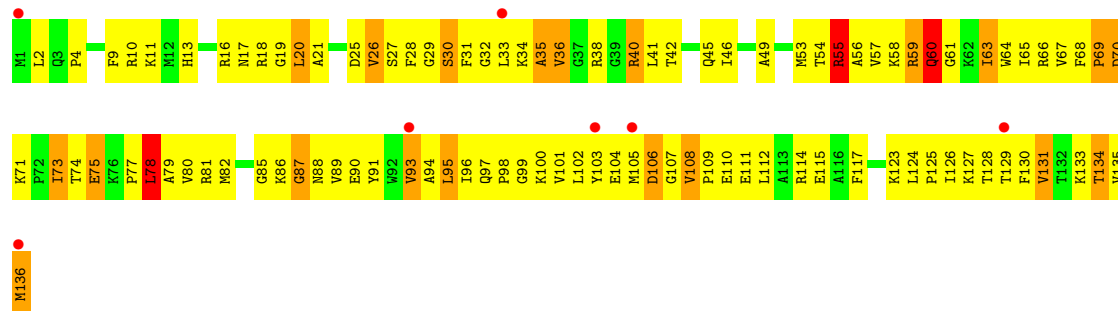
• Molecule 33: 50S ribosomal protein L15

Chain DL:



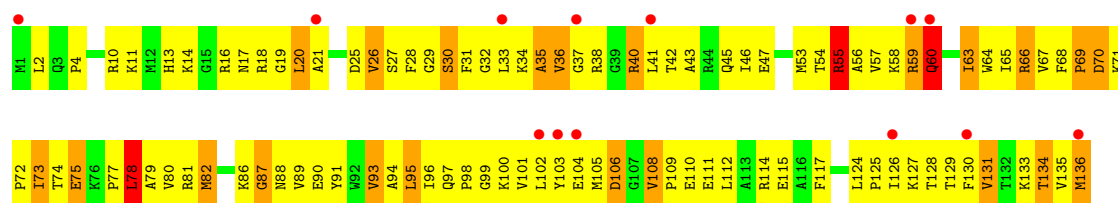
• Molecule 34: 50S ribosomal protein L16

Chain BM:



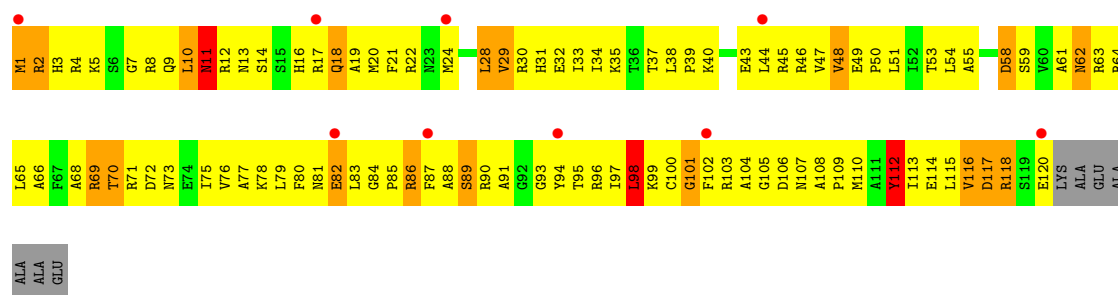
• Molecule 34: 50S ribosomal protein L16

Chain DM:



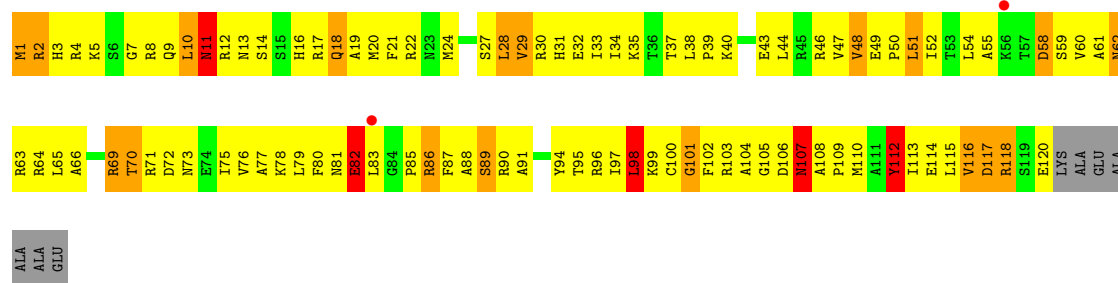
• Molecule 35: 50S ribosomal protein L17

Chain BN:



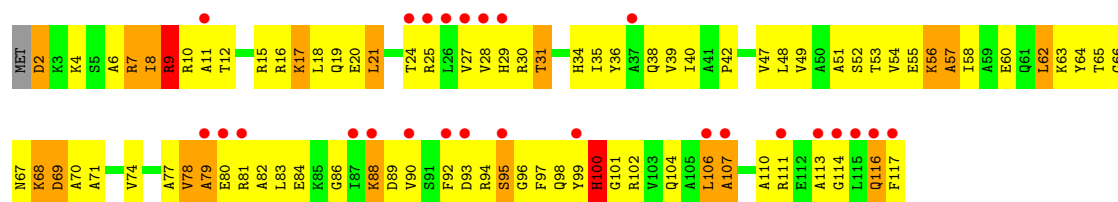
• Molecule 35: 50S ribosomal protein L17

Chain DN:



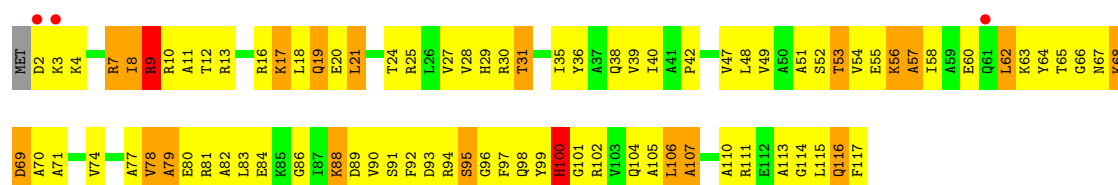
• Molecule 36: 50S ribosomal protein L18

Chain BO:



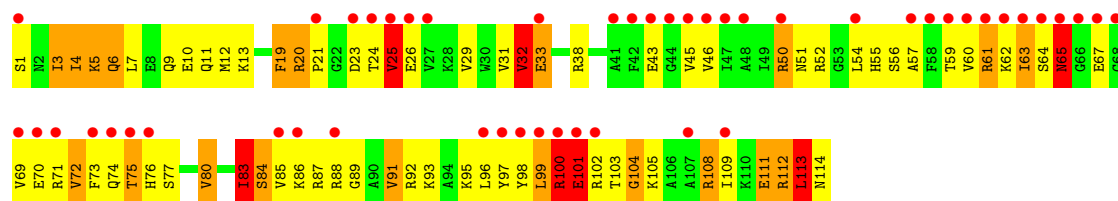
• Molecule 36: 50S ribosomal protein L18

Chain DO:



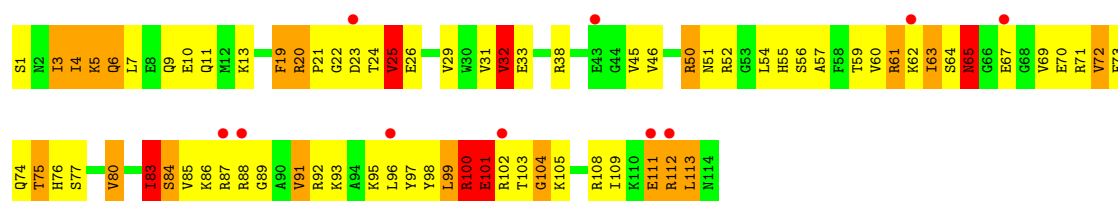
- Molecule 37: 50S ribosomal protein L19

Chain BP:



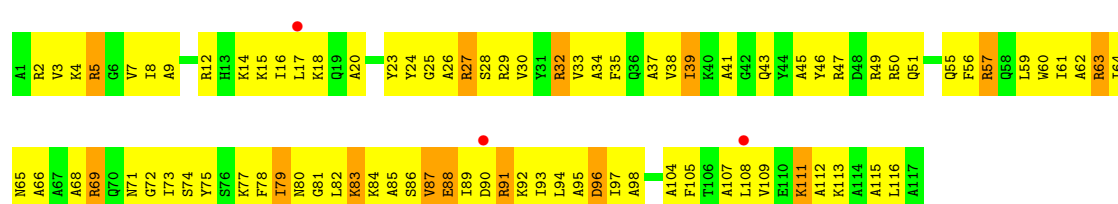
- Molecule 37: 50S ribosomal protein L19

Chain DP:



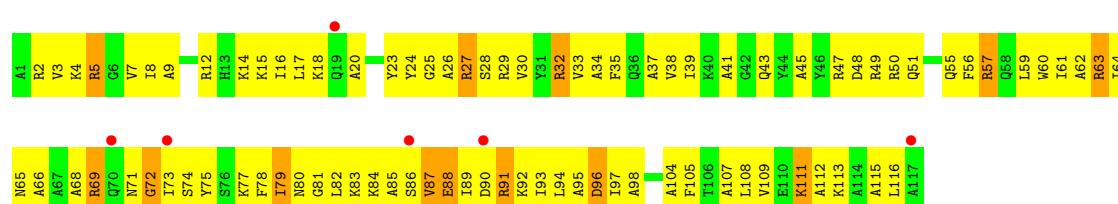
- Molecule 38: 50S ribosomal protein L20

Chain BQ:



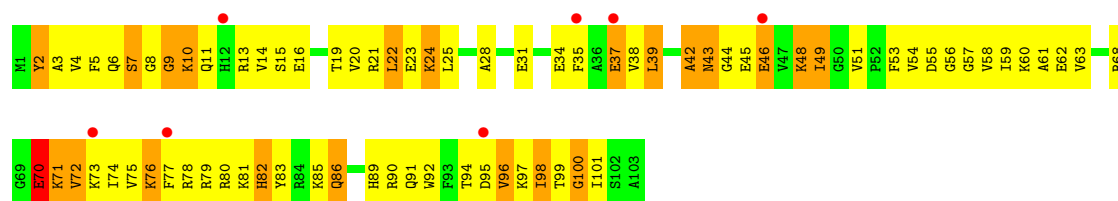
- Molecule 38: 50S ribosomal protein L20

Chain DQ:



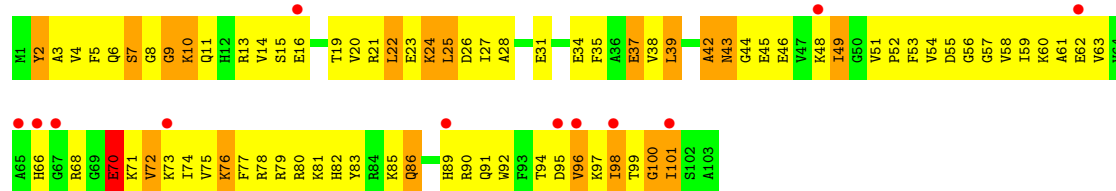
- Molecule 39: 50S ribosomal protein L21

Chain BR:



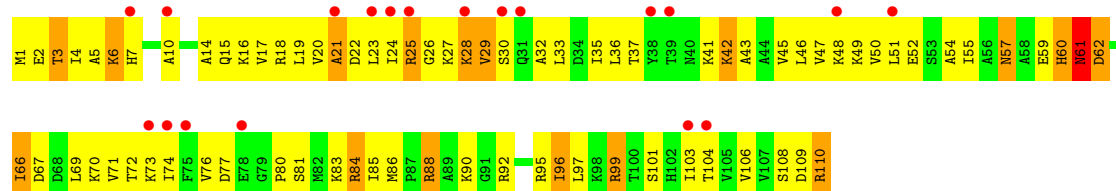
- Molecule 39: 50S ribosomal protein L21

Chain DR:



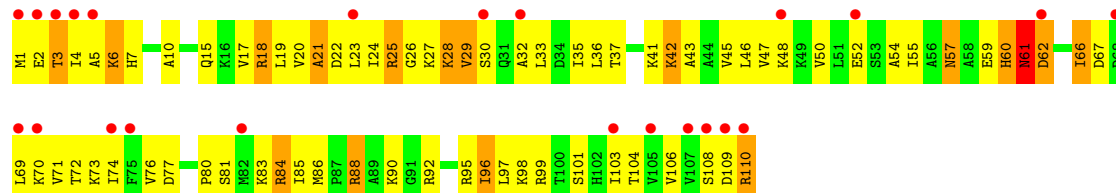
- Molecule 40: 50S ribosomal protein L22

Chain BS:



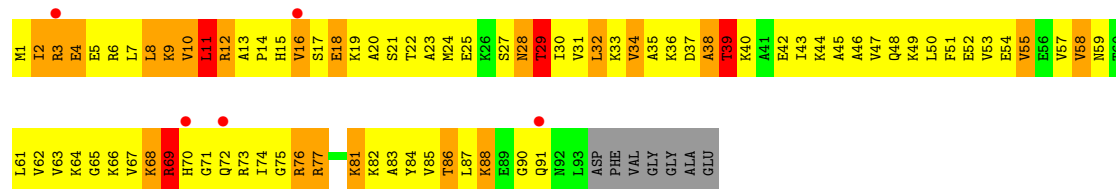
- Molecule 40: 50S ribosomal protein L22

Chain DS:



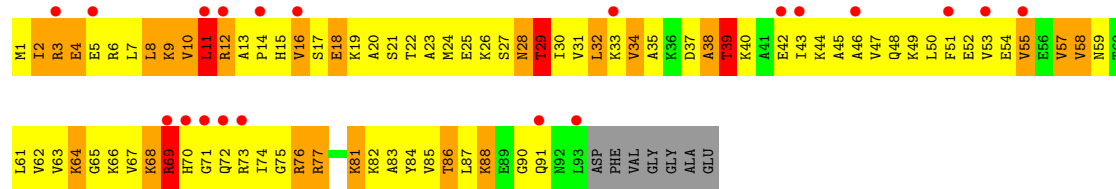
- Molecule 41: 50S ribosomal protein L23

Chain BT:



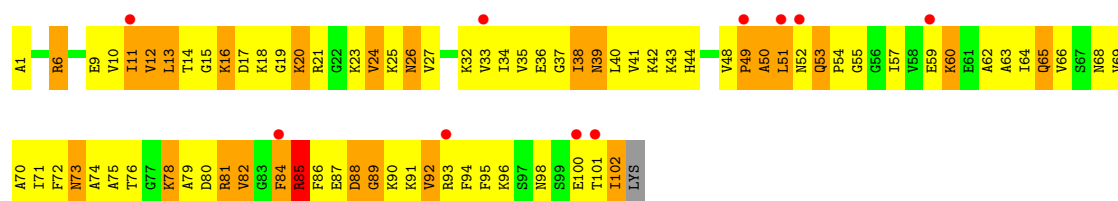
- Molecule 41: 50S ribosomal protein L23

Chain DT:



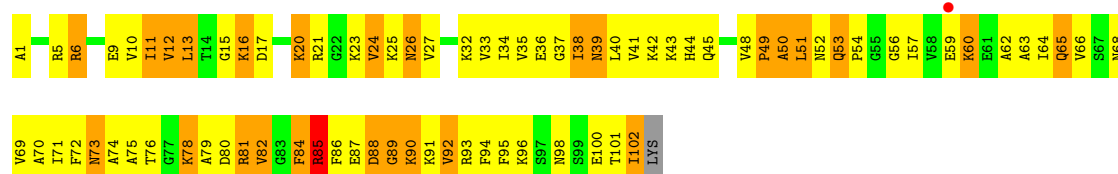
- Molecule 42: 50S ribosomal protein L24

Chain BU:



• Molecule 42: 50S ribosomal protein L24

Chain DU:



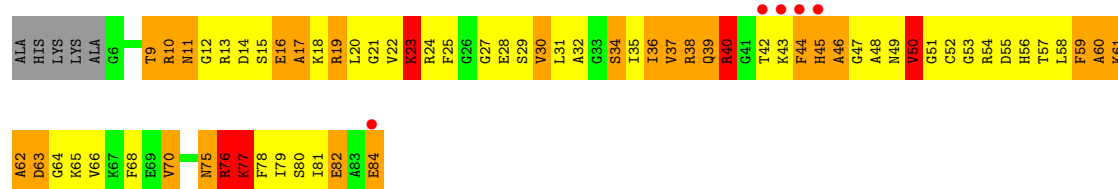
• Molecule 43: 50S ribosomal protein L27

Chain BW:



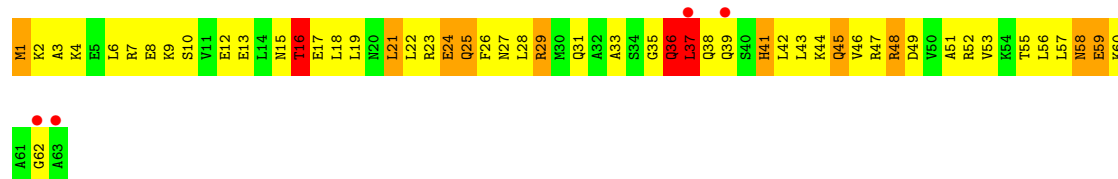
• Molecule 43: 50S ribosomal protein L27

Chain DW:



• Molecule 44: 50S ribosomal protein L29

Chain BX:



• Molecule 44: 50S ribosomal protein L29

Chain DX:





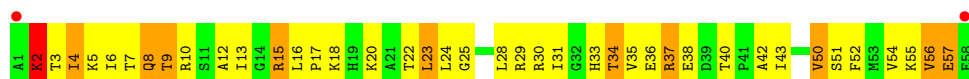
- Molecule 45: 50S ribosomal protein L30

Chain BY:



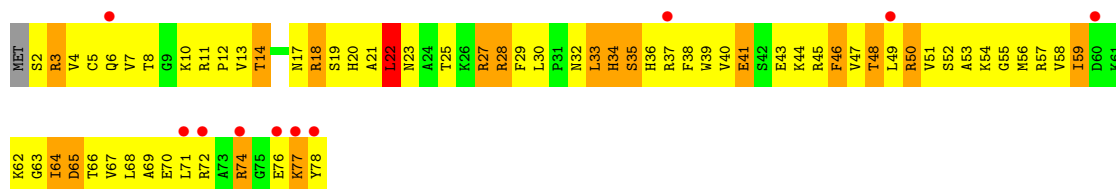
- Molecule 45: 50S ribosomal protein L30

Chain DY:



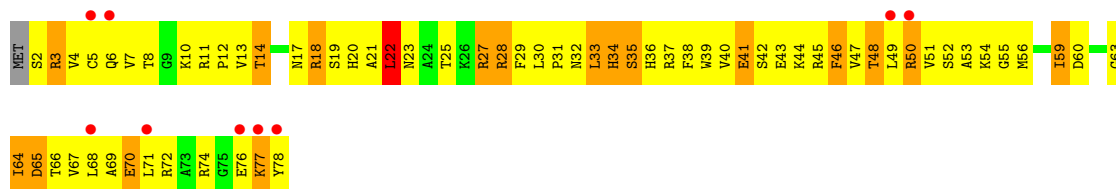
- Molecule 46: 50S ribosomal protein L28

Chain BZ:



- Molecule 46: 50S ribosomal protein L28

Chain DZ:



- Molecule 47: 50S ribosomal protein L32

Chain B0:



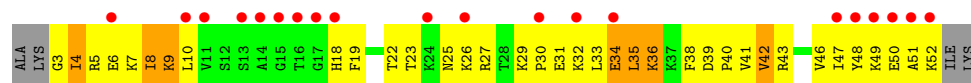
- Molecule 47: 50S ribosomal protein L32

Chain D0:



- Molecule 48: 50S ribosomal protein L33

Chain B1: 



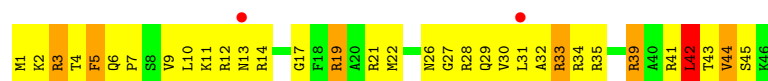
- Molecule 48: 50S ribosomal protein L33

Chain D1: 



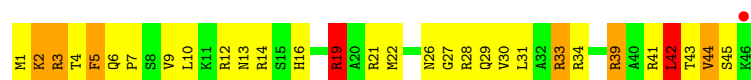
- Molecule 49: 50S ribosomal protein L34

Chain B2: 



- Molecule 49: 50S ribosomal protein L34

Chain D2: 



- Molecule 50: 50S ribosomal protein L35

Chain B3: 



- Molecule 50: 50S ribosomal protein L35

Chain D3: 



- Molecule 51: 50S ribosomal protein L36

Chain B4: 



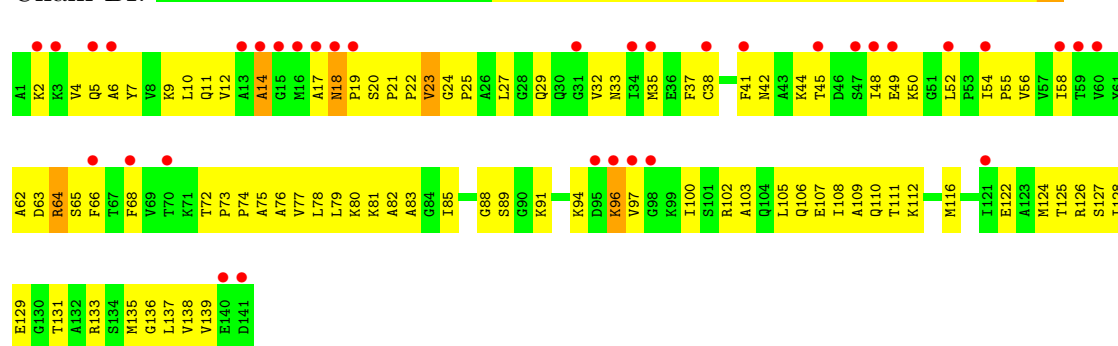
- Molecule 51: 50S ribosomal protein L36

Chain D4: 



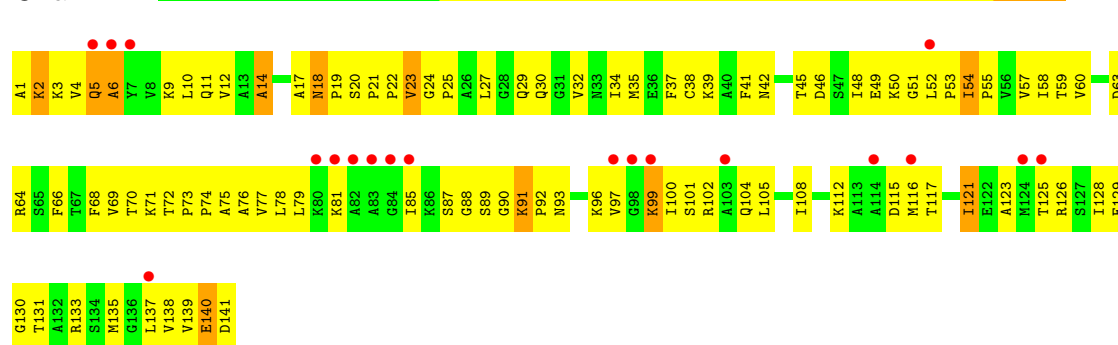
- Molecule 52: 50S ribosomal protein L11

Chain BI:



- Molecule 52: 50S ribosomal protein L11

Chain DI:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.70Å 379.50Å 739.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.00 – 3.50 137.77 – 3.50	Depositor EDS
% Data completeness (in resolution range)	62.1 (70.00-3.50) 62.3 (137.77-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 3.49Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.269 , 0.318 0.252 , 0.288	Depositor DCC
R_{free} test set	22229 reflections (5.14%)	DCC
Wilson B-factor (Å ²)	117.9	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 26.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 454411 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	284077	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% 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, HYG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AA	0.26	1/36762 (0.0%)	0.77	13/57350 (0.0%)
1	CA	0.26	1/36762 (0.0%)	0.77	17/57350 (0.0%)
2	AC	0.23	0/1651	0.44	0/2225
2	CC	0.23	0/1651	0.44	0/2225
3	AD	0.23	0/1665	0.43	0/2227
3	CD	0.23	0/1665	0.43	0/2227
4	AE	0.23	0/1118	0.45	0/1504
4	CE	0.23	0/1118	0.45	0/1504
5	AF	0.24	0/835	0.44	0/1128
5	CF	0.24	0/835	0.44	0/1128
6	AG	0.23	0/1187	0.45	0/1591
6	CG	0.23	0/1211	0.44	0/1624
7	AH	0.23	0/989	0.45	0/1326
7	CH	0.23	0/989	0.45	0/1326
8	AI	0.24	0/1034	0.44	0/1375
8	CI	0.24	0/1034	0.44	0/1375
9	AJ	0.22	0/796	0.47	0/1077
9	CJ	0.22	0/796	0.47	0/1077
10	AK	0.24	0/893	0.46	0/1205
10	CK	0.24	0/893	0.46	0/1205
11	AL	0.22	0/969	0.47	0/1300
11	CL	0.22	0/969	0.47	0/1300
12	AM	0.21	0/892	0.45	0/1193
12	CM	0.21	0/884	0.45	0/1181
13	AN	0.24	0/785	0.43	0/1043
13	CN	0.24	0/785	0.43	0/1043
14	AO	0.22	0/723	0.44	0/966
14	CO	0.22	0/723	0.44	0/966
15	AP	0.25	0/659	0.45	0/884
15	CP	0.25	0/648	0.44	0/870
16	AQ	0.24	0/657	0.46	0/881
16	CQ	0.24	0/665	0.48	0/892

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AR	0.23	0/462	0.44	0/621
17	CR	0.23	0/462	0.44	0/621
18	AS	0.25	0/652	0.45	0/877
18	CS	0.25	0/660	0.46	0/888
19	AT	0.23	0/671	0.41	0/888
19	CT	0.24	0/671	0.41	0/888
20	AB	0.25	0/1735	0.44	0/2338
20	CB	0.25	0/1735	0.44	0/2338
21	AU	0.26	0/430	0.46	0/570
21	CU	0.26	0/430	0.46	0/570
22	BA	0.24	0/2803	0.75	2/4371 (0.0%)
22	DA	0.25	0/2803	0.75	1/4371 (0.0%)
23	BB	0.27	7/68314 (0.0%)	0.78	41/106569 (0.0%)
23	DB	0.28	7/68314 (0.0%)	0.78	49/106569 (0.0%)
24	BV	0.25	0/766	0.43	0/1025
24	DV	0.25	0/766	0.43	0/1025
25	BC	0.22	0/2121	0.47	0/2852
25	DC	0.22	0/2121	0.47	0/2852
26	BD	0.24	0/1586	0.46	0/2134
26	DD	0.24	0/1586	0.47	0/2134
27	BE	0.23	0/1571	0.49	0/2113
27	DE	0.24	0/1571	0.49	0/2113
28	BF	0.26	0/1444	0.51	0/1937
28	DF	0.26	0/1444	0.51	0/1937
29	BG	0.23	0/1343	0.46	0/1816
29	DG	0.23	0/1343	0.46	0/1816
30	BH	0.25	0/1122	0.46	0/1515
30	DH	0.25	0/1122	0.46	0/1515
31	BJ	0.23	0/1152	0.47	0/1551
31	DJ	0.23	0/1152	0.47	0/1551
32	BK	0.24	0/939	0.52	0/1258
32	DK	0.23	0/939	0.52	0/1258
33	BL	0.23	0/1054	0.47	0/1403
33	DL	0.23	0/1054	0.47	0/1403
34	BM	0.25	0/1093	0.47	0/1460
34	DM	0.25	0/1093	0.47	0/1460
35	BN	0.24	0/973	0.51	0/1301
35	DN	0.24	0/973	0.51	0/1301
36	BO	0.23	0/902	0.47	0/1209
36	DO	0.23	0/902	0.48	0/1209
37	BP	0.24	0/929	0.48	0/1242
37	DP	0.24	0/929	0.48	0/1242
38	BQ	0.25	0/960	0.46	0/1278

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DQ	0.25	0/960	0.46	0/1278
39	BR	0.25	0/829	0.48	0/1107
39	DR	0.25	0/829	0.48	0/1107
40	BS	0.22	0/864	0.49	0/1156
40	DS	0.22	0/864	0.49	0/1156
41	BT	0.23	0/744	0.52	0/994
41	DT	0.23	0/744	0.52	0/994
42	BU	0.25	0/787	0.45	0/1051
42	DU	0.25	0/787	0.45	0/1051
43	BW	0.28	0/603	0.48	0/797
43	DW	0.27	0/603	0.48	0/797
44	BX	0.23	0/510	0.51	0/677
44	DX	0.23	0/510	0.51	0/677
45	BY	0.23	0/453	0.49	0/605
45	DY	0.23	0/453	0.49	0/605
46	BZ	0.25	0/635	0.51	0/848
46	DZ	0.25	0/635	0.51	0/848
47	B0	0.22	0/450	0.52	0/599
47	D0	0.22	0/450	0.52	0/599
48	B1	0.27	0/416	0.47	0/554
48	D1	0.27	0/416	0.47	0/554
49	B2	0.25	0/380	0.49	0/498
49	D2	0.26	0/380	0.49	0/498
50	B3	0.24	0/513	0.46	0/676
50	D3	0.24	0/513	0.46	0/676
51	B4	0.22	0/303	0.46	0/397
51	D4	0.22	0/303	0.46	0/397
52	BI	0.24	0/1046	0.46	0/1410
52	DI	0.25	0/1046	0.47	0/1410
All	All	0.26	16/306361 (0.0%)	0.70	123/457973 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	13
1	CA	0	13
23	BB	0	36
23	DB	0	38
All	All	0	100

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	DB	1086	A	C5-C6	-16.14	1.26	1.41
23	BB	1086	A	C5-C6	-16.11	1.26	1.41
23	BB	1088	A	C6-N1	-10.49	1.28	1.35
23	DB	1088	A	C6-N1	-10.45	1.28	1.35
23	DB	1060	U	C2-N3	7.89	1.43	1.37

The worst 5 of 123 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	BB	2791	G	O5'-P-OP1	-31.87	72.45	110.70
23	DB	2791	G	O5'-P-OP2	-31.41	73.01	110.70
23	DB	2204	G	O5'-P-OP1	-29.65	75.12	110.70
1	AA	1213	A	O5'-P-OP2	-29.58	75.21	110.70
23	BB	2204	G	O5'-P-OP2	-28.34	76.69	110.70

There are no chirality outliers.

5 of 100 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	187	G	Sidechain
1	AA	281	G	Sidechain
1	AA	324	G	Sidechain
1	AA	437	U	Sidechain
1	AA	83	C	Sidechain

5.2 Close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32831	0	16521	1355	0
1	CA	32831	0	16521	1385	0
2	AC	1624	0	1699	137	0
2	CC	1624	0	1699	145	0
3	AD	1643	0	1710	166	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	CD	1643	0	1710	156	0
4	AE	1105	0	1148	105	0
4	CE	1105	0	1148	115	0
5	AF	817	0	808	98	0
5	CF	817	0	808	88	0
6	AG	1174	0	1230	118	0
6	CG	1196	0	1246	110	0
7	AH	979	0	1034	93	0
7	CH	979	0	1034	93	0
8	AI	1022	0	1070	153	0
8	CI	1022	0	1070	151	0
9	AJ	786	0	828	78	0
9	CJ	786	0	828	84	0
10	AK	877	0	887	100	0
10	CK	877	0	887	101	0
11	AL	955	0	1019	90	0
11	CL	955	0	1019	94	0
12	AM	883	0	944	110	0
12	CM	876	0	937	109	0
13	AN	774	0	827	96	0
13	CN	774	0	827	90	0
14	AO	715	0	742	48	0
14	CO	715	0	742	41	0
15	AP	649	0	666	53	0
15	CP	638	0	656	55	0
16	AQ	648	0	691	73	0
16	CQ	656	0	702	73	0
17	AR	455	0	478	34	0
17	CR	455	0	478	34	0
18	AS	637	0	665	101	0
18	CS	644	0	675	98	0
19	AT	665	0	714	49	0
19	CT	665	0	714	49	0
20	AB	1704	0	1732	205	0
20	CB	1704	0	1732	208	0
21	AU	425	0	449	75	0
21	CU	425	0	449	68	0
22	BA	2507	0	1270	109	0
22	DA	2507	0	1270	111	0
23	BB	60995	0	30678	2412	0
23	DB	60995	0	30677	2498	0
24	BV	753	0	780	89	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	DV	753	0	780	90	0
25	BC	2082	0	2157	261	0
25	DC	2082	0	2157	274	0
26	BD	1565	0	1616	216	0
26	DD	1565	0	1616	220	0
27	BE	1552	0	1619	180	0
27	DE	1552	0	1619	170	0
28	BF	1420	0	1460	236	0
28	DF	1420	0	1460	238	0
29	BG	1323	0	1374	163	0
29	DG	1323	0	1374	161	0
30	BH	1111	0	1148	176	0
30	DH	1111	0	1148	146	0
31	BJ	1129	0	1162	150	0
31	DJ	1129	0	1162	154	0
32	BK	930	0	1000	122	0
32	DK	930	0	1000	134	0
33	BL	1045	0	1117	150	0
33	DL	1045	0	1117	155	0
34	BM	1074	0	1157	114	0
34	DM	1074	0	1157	112	0
35	BN	960	0	1000	135	0
35	DN	960	0	1000	129	0
36	BO	892	0	923	97	0
36	DO	892	0	923	104	0
37	BP	917	0	965	112	0
37	DP	917	0	965	113	0
38	BQ	947	0	1022	156	0
38	DQ	947	0	1022	167	0
39	BR	816	0	839	123	0
39	DR	816	0	839	138	0
40	BS	857	0	922	93	0
40	DS	857	0	922	93	0
41	BT	738	0	807	127	0
41	DT	738	0	807	122	0
42	BU	779	0	834	132	0
42	DU	779	0	834	121	0
43	BW	596	0	610	128	0
43	DW	596	0	610	137	0
44	BX	509	0	543	54	0
44	DX	509	0	543	50	0
45	BY	449	0	491	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	DY	449	0	491	50	0
46	BZ	625	0	652	89	0
46	DZ	625	0	652	92	0
47	B0	444	0	461	40	0
47	D0	444	0	461	42	0
48	B1	409	0	440	57	0
48	D1	409	0	440	44	0
49	B2	377	0	418	43	0
49	D2	377	0	418	43	0
50	B3	504	0	574	40	0
50	D3	504	0	574	40	0
51	B4	302	0	340	40	0
51	D4	302	0	340	35	0
52	BI	1032	0	1088	111	0
52	DI	1032	0	1088	182	0
53	AA	58	0	0	0	0
53	AE	1	0	0	0	0
53	AN	1	0	0	0	0
53	BB	110	0	0	0	0
53	CA	61	0	0	0	0
53	CE	1	0	0	0	0
53	DB	111	0	0	0	0
54	AA	36	0	37	2	0
54	CA	36	0	37	1	0
55	B4	1	0	0	0	0
55	D4	1	0	0	0	0
56	AA	282	0	0	4	0
56	AE	4	0	0	0	0
56	AK	2	0	0	0	0
56	AL	5	0	0	0	0
56	AN	4	0	0	0	0
56	AT	3	0	0	0	0
56	B2	1	0	0	0	0
56	BB	492	0	0	5	0
56	BC	8	0	0	0	0
56	BD	1	0	0	0	0
56	BE	2	0	0	0	0
56	BH	1	0	0	0	0
56	BL	2	0	0	0	0
56	CA	294	0	0	0	0
56	CE	4	0	0	0	0
56	CI	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	CK	1	0	0	0	0
56	CL	3	0	0	0	0
56	CN	3	0	0	0	0
56	CT	1	0	0	0	0
56	D2	1	0	0	0	0
56	DB	499	0	0	8	0
56	DC	5	0	0	0	0
56	DD	1	0	0	0	0
56	DE	1	0	0	0	0
56	DL	5	0	0	1	0
56	DP	1	0	0	0	0
All	All	284077	0	190751	17232	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 36.

The worst 5 of 17232 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:DB:1099:G:H8	52:DI:3:LYS:N	1.38	1.20
23:BB:855:G:H21	43:BW:23:LYS:HG2	1.08	1.15
42:DU:85:ARG:HD3	42:DU:86:PHE:H	1.13	1.14
41:DT:5:GLU:HA	41:DT:8:LEU:HB2	1.25	1.13
42:BU:85:ARG:HD3	42:BU:86:PHE:H	1.11	1.12

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AC	204/232 (88%)	147 (72%)	40 (20%)	17 (8%)	1	20
2	CC	204/232 (88%)	148 (72%)	40 (20%)	16 (8%)	1	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AD	203/205 (99%)	136 (67%)	52 (26%)	15 (7%)	2	24
3	CD	203/205 (99%)	134 (66%)	54 (27%)	15 (7%)	2	24
4	AE	148/166 (89%)	117 (79%)	27 (18%)	4 (3%)	8	56
4	CE	148/166 (89%)	117 (79%)	25 (17%)	6 (4%)	4	44
5	AF	98/135 (73%)	66 (67%)	21 (21%)	11 (11%)	1	13
5	CF	98/135 (73%)	67 (68%)	21 (21%)	10 (10%)	1	14
6	AG	148/178 (83%)	122 (82%)	18 (12%)	8 (5%)	3	35
6	CG	150/178 (84%)	124 (83%)	20 (13%)	6 (4%)	5	44
7	AH	127/129 (98%)	92 (72%)	26 (20%)	9 (7%)	2	25
7	CH	127/129 (98%)	90 (71%)	28 (22%)	9 (7%)	2	25
8	AI	125/129 (97%)	88 (70%)	29 (23%)	8 (6%)	2	29
8	CI	125/129 (97%)	88 (70%)	29 (23%)	8 (6%)	2	29
9	AJ	96/103 (93%)	69 (72%)	17 (18%)	10 (10%)	1	14
9	CJ	96/103 (93%)	68 (71%)	18 (19%)	10 (10%)	1	14
10	AK	115/128 (90%)	81 (70%)	26 (23%)	8 (7%)	2	26
10	CK	115/128 (90%)	80 (70%)	27 (24%)	8 (7%)	2	26
11	AL	121/123 (98%)	78 (64%)	29 (24%)	14 (12%)	1	12
11	CL	121/123 (98%)	79 (65%)	28 (23%)	14 (12%)	1	12
12	AM	112/117 (96%)	72 (64%)	36 (32%)	4 (4%)	5	49
12	CM	111/117 (95%)	69 (62%)	38 (34%)	4 (4%)	5	49
13	AN	92/100 (92%)	57 (62%)	25 (27%)	10 (11%)	1	13
13	CN	92/100 (92%)	56 (61%)	26 (28%)	10 (11%)	1	13
14	AO	86/89 (97%)	65 (76%)	16 (19%)	5 (6%)	3	32
14	CO	86/89 (97%)	65 (76%)	16 (19%)	5 (6%)	3	32
15	AP	80/82 (98%)	56 (70%)	15 (19%)	9 (11%)	1	12
15	CP	78/82 (95%)	53 (68%)	15 (19%)	10 (13%)	0	10
16	AQ	78/83 (94%)	56 (72%)	17 (22%)	5 (6%)	2	29
16	CQ	79/83 (95%)	56 (71%)	17 (22%)	6 (8%)	2	23
17	AR	53/74 (72%)	41 (77%)	10 (19%)	2 (4%)	5	46
17	CR	53/74 (72%)	41 (77%)	10 (19%)	2 (4%)	5	46
18	AS	77/91 (85%)	58 (75%)	17 (22%)	2 (3%)	8	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	CS	78/91 (86%)	58 (74%)	18 (23%)	2 (3%)	8	57
19	AT	83/86 (96%)	59 (71%)	19 (23%)	5 (6%)	2	31
19	CT	83/86 (96%)	59 (71%)	19 (23%)	5 (6%)	2	31
20	AB	216/240 (90%)	143 (66%)	53 (24%)	20 (9%)	1	18
20	CB	216/240 (90%)	148 (68%)	46 (21%)	22 (10%)	1	14
21	AU	49/71 (69%)	28 (57%)	14 (29%)	7 (14%)	0	7
21	CU	49/71 (69%)	28 (57%)	14 (29%)	7 (14%)	0	7
24	BV	92/94 (98%)	63 (68%)	23 (25%)	6 (6%)	2	29
24	DV	92/94 (98%)	62 (67%)	24 (26%)	6 (6%)	2	29
25	BC	269/273 (98%)	158 (59%)	65 (24%)	46 (17%)	0	4
25	DC	269/273 (98%)	158 (59%)	65 (24%)	46 (17%)	0	4
26	BD	207/209 (99%)	121 (58%)	56 (27%)	30 (14%)	0	7
26	DD	207/209 (99%)	123 (59%)	52 (25%)	32 (16%)	0	5
27	BE	199/201 (99%)	120 (60%)	56 (28%)	23 (12%)	1	12
27	DE	199/201 (99%)	120 (60%)	56 (28%)	23 (12%)	1	12
28	BF	176/178 (99%)	103 (58%)	39 (22%)	34 (19%)	0	3
28	DF	176/178 (99%)	101 (57%)	41 (23%)	34 (19%)	0	3
29	BG	174/176 (99%)	105 (60%)	37 (21%)	32 (18%)	0	3
29	DG	174/176 (99%)	105 (60%)	36 (21%)	33 (19%)	0	3
30	BH	147/149 (99%)	68 (46%)	43 (29%)	36 (24%)	0	1
30	DH	147/149 (99%)	88 (60%)	32 (22%)	27 (18%)	0	3
31	BJ	140/142 (99%)	85 (61%)	39 (28%)	16 (11%)	1	12
31	DJ	140/142 (99%)	83 (59%)	40 (29%)	17 (12%)	1	11
32	BK	119/123 (97%)	70 (59%)	28 (24%)	21 (18%)	0	4
32	DK	119/123 (97%)	69 (58%)	27 (23%)	23 (19%)	0	3
33	BL	141/144 (98%)	75 (53%)	40 (28%)	26 (18%)	0	3
33	DL	141/144 (98%)	75 (53%)	40 (28%)	26 (18%)	0	3
34	BM	134/136 (98%)	77 (58%)	38 (28%)	19 (14%)	0	7
34	DM	134/136 (98%)	78 (58%)	35 (26%)	21 (16%)	0	5
35	BN	118/127 (93%)	73 (62%)	33 (28%)	12 (10%)	1	14
35	DN	118/127 (93%)	73 (62%)	32 (27%)	13 (11%)	1	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	BO	114/117 (97%)	83 (73%)	21 (18%)	10 (9%)	1	19
36	DO	114/117 (97%)	83 (73%)	20 (18%)	11 (10%)	1	17
37	BP	112/114 (98%)	59 (53%)	35 (31%)	18 (16%)	0	5
37	DP	112/114 (98%)	58 (52%)	36 (32%)	18 (16%)	0	5
38	BQ	115/117 (98%)	79 (69%)	27 (24%)	9 (8%)	1	22
38	DQ	115/117 (98%)	75 (65%)	32 (28%)	8 (7%)	2	26
39	BR	101/103 (98%)	60 (59%)	31 (31%)	10 (10%)	1	15
39	DR	101/103 (98%)	61 (60%)	29 (29%)	11 (11%)	1	13
40	BS	108/110 (98%)	75 (69%)	21 (19%)	12 (11%)	1	13
40	DS	108/110 (98%)	75 (69%)	20 (18%)	13 (12%)	1	11
41	BT	91/100 (91%)	47 (52%)	25 (28%)	19 (21%)	0	2
41	DT	91/100 (91%)	47 (52%)	23 (25%)	21 (23%)	0	1
42	BU	100/103 (97%)	53 (53%)	35 (35%)	12 (12%)	1	11
42	DU	100/103 (97%)	51 (51%)	35 (35%)	14 (14%)	0	8
43	BW	77/84 (92%)	29 (38%)	23 (30%)	25 (32%)	0	0
43	DW	77/84 (92%)	29 (38%)	22 (29%)	26 (34%)	0	0
44	BX	61/63 (97%)	37 (61%)	14 (23%)	10 (16%)	0	5
44	DX	61/63 (97%)	37 (61%)	14 (23%)	10 (16%)	0	5
45	BY	56/58 (97%)	40 (71%)	11 (20%)	5 (9%)	1	18
45	DY	56/58 (97%)	40 (71%)	11 (20%)	5 (9%)	1	18
46	BZ	75/78 (96%)	47 (63%)	20 (27%)	8 (11%)	1	13
46	DZ	75/78 (96%)	48 (64%)	19 (25%)	8 (11%)	1	13
47	B0	54/56 (96%)	33 (61%)	16 (30%)	5 (9%)	1	18
47	D0	54/56 (96%)	33 (61%)	16 (30%)	5 (9%)	1	18
48	B1	48/54 (89%)	34 (71%)	12 (25%)	2 (4%)	4	43
48	D1	48/54 (89%)	34 (71%)	12 (25%)	2 (4%)	4	43
49	B2	44/46 (96%)	31 (70%)	9 (20%)	4 (9%)	1	18
49	D2	44/46 (96%)	30 (68%)	8 (18%)	6 (14%)	0	8
50	B3	62/64 (97%)	41 (66%)	15 (24%)	6 (10%)	1	16
50	D3	62/64 (97%)	42 (68%)	14 (23%)	6 (10%)	1	16
51	B4	36/38 (95%)	21 (58%)	10 (28%)	5 (14%)	0	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	D4	36/38 (95%)	21 (58%)	9 (25%)	6 (17%)	0	5
52	BI	139/141 (99%)	119 (86%)	16 (12%)	4 (3%)	7	54
52	DI	139/141 (99%)	115 (83%)	19 (14%)	5 (4%)	5	49
All	All	11241/11918 (94%)	7279 (65%)	2673 (24%)	1289 (12%)	1	12

5 of 1289 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AC	112	ALA
2	AC	180	ASP
2	AC	205	GLU
4	AE	20	VAL
5	AF	98	GLU

5.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AC	170/189 (90%)	144 (85%)	26 (15%)	4	25
2	CC	170/189 (90%)	145 (85%)	25 (15%)	4	26
3	AD	172/172 (100%)	148 (86%)	24 (14%)	5	28
3	CD	172/172 (100%)	149 (87%)	23 (13%)	6	31
4	AE	113/125 (90%)	100 (88%)	13 (12%)	8	39
4	CE	113/125 (90%)	98 (87%)	15 (13%)	6	31
5	AF	87/116 (75%)	76 (87%)	11 (13%)	7	34
5	CF	87/116 (75%)	75 (86%)	12 (14%)	5	29
6	AG	123/146 (84%)	108 (88%)	15 (12%)	7	36
6	CG	125/146 (86%)	108 (86%)	17 (14%)	5	30
7	AH	104/104 (100%)	96 (92%)	8 (8%)	18	64
7	CH	104/104 (100%)	96 (92%)	8 (8%)	18	64
8	AI	105/106 (99%)	94 (90%)	11 (10%)	10	46
8	CI	105/106 (99%)	93 (89%)	12 (11%)	8	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	AJ	86/90 (96%)	79 (92%)	7 (8%)	17	61
9	CJ	86/90 (96%)	80 (93%)	6 (7%)	21	68
10	AK	90/98 (92%)	77 (86%)	13 (14%)	5	27
10	CK	90/98 (92%)	77 (86%)	13 (14%)	5	27
11	AL	103/103 (100%)	85 (82%)	18 (18%)	3	17
11	CL	103/103 (100%)	84 (82%)	19 (18%)	2	14
12	AM	92/95 (97%)	82 (89%)	10 (11%)	9	43
12	CM	91/95 (96%)	82 (90%)	9 (10%)	11	49
13	AN	79/83 (95%)	67 (85%)	12 (15%)	4	25
13	CN	79/83 (95%)	67 (85%)	12 (15%)	4	25
14	AO	76/77 (99%)	69 (91%)	7 (9%)	13	53
14	CO	76/77 (99%)	70 (92%)	6 (8%)	18	62
15	AP	65/65 (100%)	57 (88%)	8 (12%)	7	35
15	CP	65/65 (100%)	57 (88%)	8 (12%)	7	35
16	AQ	74/77 (96%)	65 (88%)	9 (12%)	7	36
16	CQ	75/77 (97%)	65 (87%)	10 (13%)	6	31
17	AR	48/64 (75%)	46 (96%)	2 (4%)	40	84
17	CR	48/64 (75%)	46 (96%)	2 (4%)	40	84
18	AS	70/78 (90%)	52 (74%)	18 (26%)	1	5
18	CS	71/78 (91%)	53 (75%)	18 (25%)	1	5
19	AT	65/65 (100%)	53 (82%)	12 (18%)	2	13
19	CT	65/65 (100%)	53 (82%)	12 (18%)	2	13
20	AB	180/198 (91%)	152 (84%)	28 (16%)	4	23
20	CB	180/198 (91%)	150 (83%)	30 (17%)	3	19
21	AU	44/61 (72%)	35 (80%)	9 (20%)	2	10
21	CU	44/61 (72%)	35 (80%)	9 (20%)	2	10
24	BV	78/78 (100%)	68 (87%)	10 (13%)	6	33
24	DV	78/78 (100%)	69 (88%)	9 (12%)	8	39
25	BC	216/218 (99%)	178 (82%)	38 (18%)	3	16
25	DC	216/218 (99%)	175 (81%)	41 (19%)	2	13
26	BD	164/164 (100%)	140 (85%)	24 (15%)	5	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	DD	164/164 (100%)	140 (85%)	24 (15%)	5	27
27	BE	165/165 (100%)	146 (88%)	19 (12%)	8	39
27	DE	165/165 (100%)	146 (88%)	19 (12%)	8	39
28	BF	149/149 (100%)	114 (76%)	35 (24%)	1	7
28	DF	149/149 (100%)	115 (77%)	34 (23%)	1	7
29	BG	137/137 (100%)	116 (85%)	21 (15%)	4	25
29	DG	137/137 (100%)	116 (85%)	21 (15%)	4	25
30	BH	114/114 (100%)	77 (68%)	37 (32%)	0	3
30	DH	114/114 (100%)	93 (82%)	21 (18%)	2	14
31	BJ	116/116 (100%)	98 (84%)	18 (16%)	4	24
31	DJ	116/116 (100%)	98 (84%)	18 (16%)	4	24
32	BK	102/104 (98%)	79 (78%)	23 (22%)	1	8
32	DK	102/104 (98%)	79 (78%)	23 (22%)	1	8
33	BL	102/103 (99%)	89 (87%)	13 (13%)	6	33
33	DL	102/103 (99%)	90 (88%)	12 (12%)	8	38
34	BM	109/109 (100%)	88 (81%)	21 (19%)	2	12
34	DM	109/109 (100%)	88 (81%)	21 (19%)	2	12
35	BN	100/103 (97%)	82 (82%)	18 (18%)	2	15
35	DN	100/103 (97%)	81 (81%)	19 (19%)	2	13
36	BO	86/87 (99%)	69 (80%)	17 (20%)	2	11
36	DO	86/87 (99%)	69 (80%)	17 (20%)	2	11
37	BP	99/99 (100%)	80 (81%)	19 (19%)	2	12
37	DP	99/99 (100%)	81 (82%)	18 (18%)	2	14
38	BQ	89/89 (100%)	79 (89%)	10 (11%)	9	41
38	DQ	89/89 (100%)	79 (89%)	10 (11%)	9	41
39	BR	84/84 (100%)	68 (81%)	16 (19%)	2	13
39	DR	84/84 (100%)	70 (83%)	14 (17%)	3	19
40	BS	93/93 (100%)	81 (87%)	12 (13%)	6	33
40	DS	93/93 (100%)	82 (88%)	11 (12%)	8	38
41	BT	80/84 (95%)	62 (78%)	18 (22%)	1	8
41	DT	80/84 (95%)	62 (78%)	18 (22%)	1	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	BU	83/84 (99%)	67 (81%)	16 (19%)	2	12
42	DU	83/84 (99%)	67 (81%)	16 (19%)	2	12
43	BW	59/62 (95%)	42 (71%)	17 (29%)	0	4
43	DW	59/62 (95%)	42 (71%)	17 (29%)	0	4
44	BX	55/55 (100%)	42 (76%)	13 (24%)	1	7
44	DX	55/55 (100%)	42 (76%)	13 (24%)	1	7
45	BY	48/48 (100%)	40 (83%)	8 (17%)	3	19
45	DY	48/48 (100%)	40 (83%)	8 (17%)	3	19
46	BZ	67/68 (98%)	54 (81%)	13 (19%)	2	12
46	DZ	67/68 (98%)	53 (79%)	14 (21%)	1	10
47	B0	47/47 (100%)	39 (83%)	8 (17%)	3	18
47	D0	47/47 (100%)	40 (85%)	7 (15%)	4	26
48	B1	45/48 (94%)	40 (89%)	5 (11%)	9	42
48	D1	45/48 (94%)	41 (91%)	4 (9%)	14	56
49	B2	38/38 (100%)	32 (84%)	6 (16%)	4	23
49	D2	38/38 (100%)	32 (84%)	6 (16%)	4	23
50	B3	51/51 (100%)	46 (90%)	5 (10%)	12	50
50	D3	51/51 (100%)	46 (90%)	5 (10%)	12	50
51	B4	34/34 (100%)	32 (94%)	2 (6%)	28	75
51	D4	34/34 (100%)	32 (94%)	2 (6%)	28	75
52	BI	109/109 (100%)	108 (99%)	1 (1%)	87	97
52	DI	109/109 (100%)	103 (94%)	6 (6%)	30	77
All	All	9333/9704 (96%)	7895 (85%)	1438 (15%)	4	24

5 of 1438 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
43	BW	38	ARG
6	CG	49	LEU
41	DT	24	MET
44	BX	28	LEU
2	CC	35	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 346 such sidechains are listed below:

Mol	Chain	Res	Type
44	BX	25	GLN
6	CG	129	ASN
42	DU	26	ASN
45	BY	48	ASN
2	CC	7	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1529/1542 (99%)	257 (16%)	27 (1%)
1	CA	1529/1542 (99%)	240 (15%)	27 (1%)
22	BA	116/120 (96%)	22 (18%)	0
22	DA	116/120 (96%)	22 (18%)	0
23	BB	2837/2904 (97%)	460 (16%)	17 (0%)
23	DB	2837/2904 (97%)	460 (16%)	21 (0%)
All	All	8964/9132 (98%)	1461 (16%)	92 (1%)

5 of 1461 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	9	G
1	AA	14	U
1	AA	32	A
1	AA	39	G

5 of 92 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	BB	2756	U
1	CA	372	C
23	DB	2282	G
23	BB	2808	G
1	CA	243	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 347 ligands modelled in this entry, 345 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
54	HYG	AA	2059	-	39,39,39	1.21	3 (7%)	60,60,60	1.49	8 (13%)
54	HYG	CA	2062	-	39,39,39	1.23	4 (10%)	60,60,60	1.48	7 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	HYG	AA	2059	-	-	1/14/87/87	0/4/4/4
54	HYG	CA	2062	-	-	1/14/87/87	0/4/4/4

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	AA	2059	HYG	C27-C33	2.76	1.56	1.52
54	CA	2062	HYG	C27-C33	2.75	1.56	1.52
54	CA	2062	HYG	O22-C17	-2.32	1.38	1.43
54	CA	2062	HYG	C16-C15	2.11	1.57	1.53
54	CA	2062	HYG	C3-C4	2.07	1.56	1.53

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	AA	2059	HYG	C23-O28-C27	4.74	115.86	111.78
54	CA	2062	HYG	C23-O28-C27	4.72	115.84	111.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	CA	2062	HYG	O8-C1-C2	-4.31	101.78	109.86
54	AA	2059	HYG	O8-C1-C2	-4.29	101.81	109.86
54	CA	2062	HYG	O22-C17-C16	4.20	122.21	111.36

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	CA	2062	HYG	C26-C27-C33-N36
54	AA	2059	HYG	C26-C27-C33-N36

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1530/1542 (99%)	-0.61	11 (0%) 84 56	16, 85, 158, 180	0
1	CA	1530/1542 (99%)	-0.63	5 (0%) 91 76	8, 57, 142, 180	0
2	AC	206/232 (88%)	1.47	56 (27%) 1 2	8, 89, 145, 180	0
2	CC	206/232 (88%)	0.68	14 (6%) 17 8	15, 81, 138, 180	0
3	AD	205/205 (100%)	0.79	25 (12%) 5 3	19, 97, 160, 180	0
3	CD	205/205 (100%)	0.44	5 (2%) 56 26	5, 63, 135, 180	0
4	AE	150/166 (90%)	0.64	11 (7%) 15 7	5, 76, 136, 167	0
4	CE	150/166 (90%)	0.93	20 (13%) 4 3	5, 62, 135, 175	0
5	AF	100/135 (74%)	1.00	17 (17%) 2 2	13, 81, 137, 180	0
5	CF	100/135 (74%)	0.62	2 (2%) 62 30	14, 78, 126, 166	0
6	AG	150/178 (84%)	0.64	17 (11%) 6 4	41, 110, 166, 180	0
6	CG	152/178 (85%)	0.39	10 (6%) 18 8	27, 98, 156, 177	0
7	AH	129/129 (100%)	0.87	21 (16%) 2 2	26, 91, 148, 180	0
7	CH	129/129 (100%)	0.43	7 (5%) 25 10	5, 53, 117, 153	0
8	AI	127/129 (98%)	0.75	19 (14%) 3 3	32, 103, 160, 180	0
8	CI	127/129 (98%)	0.79	14 (11%) 6 4	32, 103, 162, 180	0
9	AJ	98/103 (95%)	0.99	14 (14%) 3 3	34, 106, 162, 180	0
9	CJ	98/103 (95%)	1.22	26 (26%) 1 2	42, 107, 156, 180	0
10	AK	117/128 (91%)	0.22	1 (0%) 81 51	5, 71, 122, 174	0
10	CK	117/128 (91%)	0.39	4 (3%) 43 19	5, 57, 112, 179	0
11	AL	123/123 (100%)	0.52	7 (5%) 23 10	15, 82, 132, 153	0
11	CL	123/123 (100%)	0.30	5 (4%) 35 15	5, 44, 109, 165	0
12	AM	114/117 (97%)	0.96	15 (13%) 4 3	68, 130, 178, 180	0
12	CM	113/117 (96%)	0.38	6 (5%) 25 10	32, 108, 156, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AN	96/100 (96%)	0.70	8 (8%) 11 6	32, 103, 161, 180	0
13	CN	96/100 (96%)	0.51	9 (9%) 9 5	38, 99, 137, 171	0
14	AO	88/89 (98%)	0.71	4 (4%) 32 14	35, 83, 132, 180	0
14	CO	88/89 (98%)	0.24	2 (2%) 57 27	8, 54, 111, 165	0
15	AP	82/82 (100%)	1.67	27 (32%) 1 1	43, 99, 163, 180	0
15	CP	80/82 (97%)	0.52	4 (5%) 28 12	5, 51, 143, 164	0
16	AQ	80/83 (96%)	1.28	23 (28%) 1 1	49, 106, 156, 177	0
16	CQ	81/83 (97%)	0.39	0 100 100	5, 51, 121, 157	0
17	AR	55/74 (74%)	0.50	3 (5%) 24 10	16, 78, 142, 152	0
17	CR	55/74 (74%)	0.60	1 (1%) 65 33	13, 69, 132, 149	0
18	AS	79/91 (86%)	0.88	13 (16%) 2 2	67, 128, 175, 180	0
18	CS	80/91 (87%)	0.65	9 (11%) 6 4	49, 113, 171, 180	0
19	AT	85/86 (98%)	0.60	7 (8%) 12 6	43, 100, 153, 175	0
19	CT	85/86 (98%)	0.13	1 (1%) 75 42	14, 58, 121, 177	0
20	AB	218/240 (90%)	0.41	10 (4%) 31 14	30, 102, 152, 180	0
20	CB	218/240 (90%)	0.96	33 (15%) 3 3	26, 106, 160, 180	0
21	AU	51/71 (71%)	0.75	4 (7%) 13 7	26, 102, 172, 180	0
21	CU	51/71 (71%)	1.14	8 (15%) 3 2	19, 85, 151, 180	0
22	BA	117/120 (97%)	-0.63	2 (1%) 67 34	43, 83, 131, 173	0
22	DA	117/120 (97%)	-0.66	1 (0%) 81 51	32, 75, 118, 180	0
23	BB	2841/2904 (97%)	-0.40	15 (0%) 88 64	6, 56, 146, 180	0
23	DB	2841/2904 (97%)	-0.42	7 (0%) 93 80	5, 40, 139, 180	0
24	BV	94/94 (100%)	0.66	9 (9%) 8 5	11, 96, 146, 176	0
24	DV	94/94 (100%)	0.42	7 (7%) 14 7	14, 86, 143, 180	0
25	BC	271/273 (99%)	0.97	39 (14%) 3 3	7, 48, 104, 170	0
25	DC	271/273 (99%)	0.63	22 (8%) 12 6	5, 28, 81, 120	0
26	BD	209/209 (100%)	0.75	24 (11%) 5 4	5, 73, 138, 180	0
26	DD	209/209 (100%)	0.64	16 (7%) 13 7	5, 42, 118, 180	0
27	BE	201/201 (100%)	1.17	39 (19%) 2 2	5, 65, 142, 180	0
27	DE	201/201 (100%)	0.47	9 (4%) 32 14	5, 67, 135, 180	0
28	BF	178/178 (100%)	1.01	30 (16%) 2 2	50, 116, 175, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å²)	Q<0.9
28	DF	178/178 (100%)	0.97	29 (16%) 2 2	7, 101, 172, 180	0
29	BG	176/176 (100%)	0.81	18 (10%) 7 5	23, 102, 155, 180	0
29	DG	176/176 (100%)	0.56	16 (9%) 9 5	24, 90, 161, 180	0
30	BH	149/149 (100%)	1.65	49 (32%) 1 1	14, 117, 177, 180	0
30	DH	149/149 (100%)	0.81	15 (10%) 7 5	11, 100, 156, 180	0
31	BJ	142/142 (100%)	0.68	9 (6%) 19 8	6, 80, 141, 171	0
31	DJ	142/142 (100%)	0.75	7 (4%) 28 12	5, 60, 119, 165	0
32	BK	121/123 (98%)	1.73	39 (32%) 1 1	5, 73, 135, 180	0
32	DK	121/123 (98%)	0.82	9 (7%) 14 7	5, 35, 102, 145	0
33	BL	143/144 (99%)	0.44	7 (4%) 28 12	10, 64, 128, 180	0
33	DL	143/144 (99%)	0.61	13 (9%) 9 5	5, 54, 118, 162	0
34	BM	136/136 (100%)	0.34	7 (5%) 27 11	8, 70, 129, 172	0
34	DM	136/136 (100%)	0.85	13 (9%) 8 5	5, 51, 114, 168	0
35	BN	120/127 (94%)	0.70	9 (7%) 14 7	7, 67, 132, 163	0
35	DN	120/127 (94%)	0.39	2 (1%) 67 34	5, 42, 86, 145	0
36	BO	116/117 (99%)	1.22	26 (22%) 1 2	27, 87, 135, 156	0
36	DO	116/117 (99%)	0.36	3 (2%) 53 24	17, 78, 142, 180	0
37	BP	114/114 (100%)	1.82	49 (42%) 1 1	20, 85, 149, 178	0
37	DP	114/114 (100%)	0.70	10 (8%) 10 6	5, 48, 107, 159	0
38	BQ	117/117 (100%)	0.29	3 (2%) 53 24	5, 63, 127, 180	0
38	DQ	117/117 (100%)	0.57	6 (5%) 27 11	5, 48, 116, 150	0
39	BR	103/103 (100%)	0.65	7 (6%) 17 8	16, 82, 145, 158	0
39	DR	103/103 (100%)	0.93	12 (11%) 5 4	5, 73, 136, 180	0
40	BS	110/110 (100%)	1.02	19 (17%) 2 2	5, 53, 116, 142	0
40	DS	110/110 (100%)	1.12	23 (20%) 1 2	5, 42, 116, 146	0
41	BT	93/100 (93%)	0.59	5 (5%) 25 10	6, 72, 139, 179	0
41	DT	93/100 (93%)	1.14	20 (21%) 1 2	11, 64, 156, 180	0
42	BU	102/103 (99%)	0.94	10 (9%) 8 5	5, 78, 144, 178	0
42	DU	102/103 (99%)	0.45	1 (0%) 79 47	10, 90, 154, 180	0
43	BW	79/84 (94%)	0.94	13 (16%) 2 2	10, 79, 157, 163	0
43	DW	79/84 (94%)	0.69	5 (6%) 19 8	5, 75, 131, 174	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BX	63/63 (100%)	0.44	4 (6%) 19 8	9, 74, 146, 179	0
44	DX	63/63 (100%)	0.60	4 (6%) 19 8	17, 96, 147, 180	0
45	BY	58/58 (100%)	0.54	3 (5%) 26 11	14, 78, 135, 170	0
45	DY	58/58 (100%)	0.45	2 (3%) 43 19	10, 73, 129, 160	0
46	BZ	77/78 (98%)	1.02	10 (12%) 4 3	5, 49, 121, 160	0
46	DZ	77/78 (98%)	0.61	9 (11%) 5 4	5, 42, 107, 141	0
47	B0	56/56 (100%)	0.77	4 (7%) 16 7	5, 77, 144, 166	0
47	D0	56/56 (100%)	0.31	2 (3%) 41 18	8, 52, 128, 160	0
48	B1	50/54 (92%)	2.02	20 (40%) 1 1	51, 99, 149, 165	0
48	D1	50/54 (92%)	1.52	12 (24%) 1 2	43, 93, 138, 171	0
49	B2	46/46 (100%)	0.50	2 (4%) 34 14	7, 49, 103, 135	0
49	D2	46/46 (100%)	0.57	1 (2%) 59 28	5, 28, 99, 180	0
50	B3	64/64 (100%)	0.95	8 (12%) 5 3	16, 56, 110, 137	0
50	D3	64/64 (100%)	0.49	4 (6%) 19 8	5, 43, 112, 152	0
51	B4	38/38 (100%)	0.42	2 (5%) 25 10	33, 92, 143, 146	0
51	D4	38/38 (100%)	0.44	0 100 100	5, 68, 112, 150	0
52	BI	141/141 (100%)	1.34	35 (24%) 1 2	67, 169, 180, 180	0
52	DI	141/141 (100%)	1.00	19 (13%) 4 3	91, 160, 180, 180	0
All	All	20417/21050 (96%)	0.22	1313 (6%) 19 8	5, 70, 153, 180	0

The worst 5 of 1313 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	DA	88	C	9.2
30	BH	45	GLU	9.1
48	D1	52	LYS	9.1
15	AP	80	LYS	9.0
15	AP	81	ALA	8.2

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
53	MG	AA	2055	1/1	0.34	21.57	102,102,102,102	0
53	MG	AA	2013	1/1	0.08	15.00	122,122,122,122	0
53	MG	AA	2035	1/1	0.30	14.70	137,137,137,137	0
53	MG	AA	2012	1/1	0.16	13.39	84,84,84,84	0
53	MG	CA	2011	1/1	0.48	12.41	132,132,132,132	0
53	MG	AA	2045	1/1	0.46	10.80	92,92,92,92	0
53	MG	AA	2021	1/1	0.30	8.99	5,5,5,5	1
53	MG	CA	2021	1/1	0.27	8.98	125,125,125,125	0
53	MG	BB	3033	1/1	0.21	7.47	125,125,125,125	0
53	MG	AA	2057	1/1	0.18	6.07	141,141,141,141	0
53	MG	CA	2038	1/1	0.16	5.45	128,128,128,128	0
53	MG	DB	3099	1/1	0.23	5.03	7,7,7,7	0
53	MG	CA	2020	1/1	0.26	4.92	73,73,73,73	0
53	MG	AA	2023	1/1	0.17	4.45	66,66,66,66	1
53	MG	CA	2045	1/1	0.17	4.28	48,48,48,48	0
53	MG	DB	3058	1/1	0.26	3.97	151,151,151,151	0
53	MG	BB	3028	1/1	0.21	3.16	86,86,86,86	0
53	MG	BB	3039	1/1	0.19	3.02	7,7,7,7	0
54	HYG	CA	2062	36/36	0.24	2.98	45,45,45,45	0
53	MG	BB	3022	1/1	0.31	2.72	34,34,34,34	0
53	MG	DB	3003	1/1	0.24	2.26	63,63,63,63	0
53	MG	AA	2050	1/1	0.19	1.96	105,105,105,105	0
53	MG	AA	2037	1/1	0.53	1.83	138,138,138,138	0
53	MG	BB	3097	1/1	0.14	1.40	114,114,114,114	0
53	MG	CA	2027	1/1	0.11	1.39	50,50,50,50	1
53	MG	DB	3091	1/1	0.20	1.38	13,13,13,13	0
53	MG	DB	3037	1/1	0.17	1.27	28,28,28,28	0
53	MG	BB	3086	1/1	0.24	1.10	42,42,42,42	0
53	MG	DB	3093	1/1	0.18	1.05	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	AA	2033	1/1	0.11	1.04	99,99,99,99	0
53	MG	BB	3083	1/1	0.23	1.03	12,12,12,12	0
53	MG	DB	3077	1/1	0.22	0.99	54,54,54,54	0
53	MG	CA	2032	1/1	0.15	0.89	33,33,33,33	0
54	HYG	AA	2059	36/36	0.26	0.89	52,52,52,52	0
53	MG	AA	2058	1/1	0.18	0.79	86,86,86,86	0
53	MG	AA	2024	1/1	0.17	0.74	5,5,5,5	1
53	MG	DB	3040	1/1	0.19	0.71	5,5,5,5	0
53	MG	AA	2038	1/1	0.13	0.61	71,71,71,71	0
53	MG	BB	3017	1/1	0.18	0.59	34,34,34,34	0
53	MG	BB	3042	1/1	0.14	0.58	168,168,168,168	0
53	MG	BB	3093	1/1	0.25	0.39	71,71,71,71	0
53	MG	DB	3011	1/1	0.19	0.38	17,17,17,17	0
53	MG	DB	3101	1/1	0.18	0.37	5,5,5,5	0
53	MG	CA	2036	1/1	0.19	0.33	101,101,101,101	0
53	MG	DB	3066	1/1	0.09	0.30	146,146,146,146	0
53	MG	DB	3098	1/1	0.23	0.27	44,44,44,44	0
53	MG	AA	2030	1/1	0.13	0.26	99,99,99,99	0
53	MG	BB	3062	1/1	0.17	0.25	14,14,14,14	0
53	MG	DB	3097	1/1	0.14	0.21	38,38,38,38	0
53	MG	BB	3044	1/1	0.16	0.18	53,53,53,53	0
53	MG	DB	3063	1/1	0.17	0.13	43,43,43,43	0
53	MG	DB	3060	1/1	0.20	0.02	112,112,112,112	0
53	MG	DB	3021	1/1	0.20	-0.02	11,11,11,11	0
53	MG	DB	3007	1/1	0.18	-0.02	18,18,18,18	0
53	MG	AA	2014	1/1	0.17	-0.04	112,112,112,112	0
53	MG	BB	3104	1/1	0.18	-0.07	36,36,36,36	0
53	MG	BB	3075	1/1	0.20	-0.08	40,40,40,40	0
53	MG	DB	3012	1/1	0.18	-0.08	9,9,9,9	0
53	MG	CE	201	1/1	0.15	-0.10	127,127,127,127	0
53	MG	BB	3011	1/1	0.20	-0.15	5,5,5,5	0
53	MG	AA	2018	1/1	0.10	-0.16	131,131,131,131	0
53	MG	DB	3038	1/1	0.16	-0.16	5,5,5,5	0
53	MG	DB	3051	1/1	0.20	-0.19	23,23,23,23	0
53	MG	DB	3110	1/1	0.17	-0.26	21,21,21,21	0
53	MG	DB	3059	1/1	0.16	-0.31	180,180,180,180	0
53	MG	BB	3090	1/1	0.12	-0.36	112,112,112,112	0
53	MG	AA	2004	1/1	0.14	-0.38	56,56,56,56	0
53	MG	AA	2031	1/1	0.10	-0.39	58,58,58,58	0
53	MG	AA	2039	1/1	0.11	-0.51	64,64,64,64	0
53	MG	AN	201	1/1	0.12	-0.51	69,69,69,69	0
53	MG	BB	3099	1/1	0.22	-0.52	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	AA	2017	1/1	0.13	-0.60	87,87,87,87	0
53	MG	DB	3023	1/1	0.12	-0.62	32,32,32,32	0
53	MG	DB	3084	1/1	0.18	-0.65	5,5,5,5	0
53	MG	AA	2034	1/1	0.12	-0.68	68,68,68,68	0
53	MG	AA	2025	1/1	0.17	-0.71	58,58,58,58	0
53	MG	AA	2003	1/1	0.18	-0.74	39,39,39,39	0
53	MG	CA	2016	1/1	0.08	-0.77	53,53,53,53	0
53	MG	BB	3005	1/1	0.19	-0.77	5,5,5,5	0
53	MG	DB	3089	1/1	0.16	-0.78	7,7,7,7	0
53	MG	BB	3081	1/1	0.19	-0.80	46,46,46,46	0
53	MG	BB	3082	1/1	0.18	-0.81	46,46,46,46	0
53	MG	DB	3095	1/1	0.17	-0.89	89,89,89,89	0
53	MG	AA	2022	1/1	0.09	-0.91	82,82,82,82	0
53	MG	BB	3110	1/1	0.12	-0.95	23,23,23,23	0
53	MG	CA	2039	1/1	0.11	-0.96	16,16,16,16	0
53	MG	CA	2053	1/1	0.08	-0.96	30,30,30,30	0
53	MG	CA	2050	1/1	0.12	-1.02	8,8,8,8	0
53	MG	AA	2006	1/1	0.07	-1.02	60,60,60,60	0
53	MG	DB	3031	1/1	0.17	-1.04	8,8,8,8	0
53	MG	AA	2011	1/1	0.07	-1.05	85,85,85,85	0
53	MG	BB	3040	1/1	0.15	-1.07	26,26,26,26	0
53	MG	CA	2058	1/1	0.12	-1.12	106,106,106,106	0
53	MG	BB	3077	1/1	0.11	-1.14	36,36,36,36	0
53	MG	BB	3105	1/1	0.11	-1.16	20,20,20,20	0
53	MG	DB	3100	1/1	0.17	-1.16	13,13,13,13	0
53	MG	BB	3098	1/1	0.16	-1.17	35,35,35,35	0
53	MG	BB	3036	1/1	0.12	-1.21	42,42,42,42	0
53	MG	BB	3085	1/1	0.15	-1.21	103,103,103,103	0
53	MG	BB	3070	1/1	0.17	-1.22	37,37,37,37	0
53	MG	CA	2014	1/1	0.10	-1.23	47,47,47,47	0
53	MG	CA	2035	1/1	0.08	-1.24	89,89,89,89	0
53	MG	DB	3030	1/1	0.17	-1.25	6,6,6,6	0
53	MG	BB	3045	1/1	0.10	-1.26	31,31,31,31	0
53	MG	DB	3057	1/1	0.06	-1.26	71,71,71,71	0
53	MG	CA	2040	1/1	0.12	-1.37	48,48,48,48	0
53	MG	BB	3012	1/1	0.13	-1.40	32,32,32,32	0
53	MG	DB	3025	1/1	0.14	-1.42	5,5,5,5	0
53	MG	BB	3023	1/1	0.17	-1.44	5,5,5,5	0
53	MG	BB	3109	1/1	0.10	-1.45	54,54,54,54	0
53	MG	CA	2012	1/1	0.08	-1.54	93,93,93,93	0
53	MG	BB	3108	1/1	0.14	-1.55	47,47,47,47	0
53	MG	BB	3034	1/1	0.10	-1.56	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	BB	3037	1/1	0.11	-1.56	23,23,23,23	0
53	MG	CA	2019	1/1	0.08	-1.58	73,73,73,73	0
53	MG	CA	2033	1/1	0.13	-1.61	56,56,56,56	0
53	MG	DB	3027	1/1	0.15	-1.61	6,6,6,6	0
53	MG	DB	3078	1/1	0.07	-1.62	27,27,27,27	0
53	MG	BB	3013	1/1	0.11	-1.62	43,43,43,43	0
53	MG	CA	2007	1/1	0.03	-1.63	46,46,46,46	0
53	MG	AA	2032	1/1	0.07	-1.64	62,62,62,62	0
53	MG	DB	3064	1/1	0.04	-1.66	20,20,20,20	0
53	MG	CA	2022	1/1	0.09	-1.68	63,63,63,63	0
53	MG	CA	2015	1/1	0.12	-1.69	149,149,149,149	0
53	MG	CA	2013	1/1	0.08	-1.69	73,73,73,73	0
53	MG	BB	3059	1/1	0.14	-1.70	26,26,26,26	0
53	MG	DB	3082	1/1	0.11	-1.70	30,30,30,30	0
53	MG	AA	2010	1/1	0.04	-1.70	60,60,60,60	0
53	MG	DB	3094	1/1	0.03	-1.72	29,29,29,29	0
53	MG	CA	2060	1/1	0.07	-1.77	80,80,80,80	0
53	MG	BB	3084	1/1	0.16	-1.78	24,24,24,24	0
53	MG	DB	3052	1/1	0.11	-1.79	100,100,100,100	0
53	MG	CA	2017	1/1	0.10	-1.80	5,5,5,5	0
53	MG	DB	3087	1/1	0.12	-1.80	53,53,53,53	0
53	MG	DB	3047	1/1	0.16	-1.84	14,14,14,14	0
53	MG	BB	3010	1/1	0.09	-1.84	44,44,44,44	0
53	MG	DB	3092	1/1	0.10	-1.88	66,66,66,66	0
53	MG	AA	2028	1/1	0.12	-1.90	100,100,100,100	0
53	MG	BB	3092	1/1	0.05	-1.91	54,54,54,54	0
53	MG	DB	3096	1/1	0.14	-1.91	6,6,6,6	0
53	MG	DB	3020	1/1	0.15	-1.96	5,5,5,5	0
53	MG	CA	2037	1/1	0.07	-1.99	94,94,94,94	0
53	MG	DB	3034	1/1	0.18	-2.04	52,52,52,52	0
53	MG	BB	3049	1/1	0.12	-2.04	10,10,10,10	0
53	MG	BB	3024	1/1	0.13	-2.05	15,15,15,15	0
53	MG	AA	2049	1/1	0.04	-2.06	75,75,75,75	0
53	MG	AA	2009	1/1	0.10	-2.09	7,7,7,7	0
53	MG	DB	3086	1/1	0.13	-2.09	11,11,11,11	0
53	MG	BB	3080	1/1	0.14	-2.11	39,39,39,39	0
53	MG	DB	3088	1/1	0.13	-2.11	25,25,25,25	0
53	MG	BB	3027	1/1	0.17	-2.11	33,33,33,33	0
55	ZN	B4	101	1/1	0.06	-2.11	80,80,80,80	0
53	MG	BB	3101	1/1	0.08	-2.12	24,24,24,24	0
53	MG	BB	3100	1/1	0.09	-2.17	129,129,129,129	0
53	MG	AA	2040	1/1	0.05	-2.20	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	DB	3069	1/1	0.17	-2.20	11,11,11,11	0
53	MG	AA	2026	1/1	0.06	-2.21	65,65,65,65	0
53	MG	BB	3073	1/1	0.08	-2.22	39,39,39,39	0
53	MG	DB	3013	1/1	0.14	-2.23	51,51,51,51	0
53	MG	AA	2007	1/1	0.06	-2.24	31,31,31,31	0
53	MG	DB	3019	1/1	0.12	-2.25	5,5,5,5	0
53	MG	BB	3106	1/1	0.10	-2.25	62,62,62,62	0
53	MG	CA	2054	1/1	0.09	-2.27	104,104,104,104	0
53	MG	AA	2053	1/1	0.07	-2.31	79,79,79,79	0
55	ZN	D4	101	1/1	0.10	-2.31	46,46,46,46	0
53	MG	BB	3025	1/1	0.10	-2.32	30,30,30,30	0
53	MG	BB	3107	1/1	0.11	-2.35	6,6,6,6	0
53	MG	DB	3055	1/1	0.14	-2.36	26,26,26,26	0
53	MG	BB	3054	1/1	0.06	-2.36	77,77,77,77	0
53	MG	AA	2019	1/1	0.06	-2.39	107,107,107,107	0
53	MG	DB	3022	1/1	0.09	-2.40	25,25,25,25	0
53	MG	BB	3087	1/1	0.14	-2.43	57,57,57,57	0
53	MG	AA	2047	1/1	0.07	-2.44	100,100,100,100	0
53	MG	DB	3081	1/1	0.12	-2.44	18,18,18,18	0
53	MG	BB	3102	1/1	0.10	-2.44	20,20,20,20	0
53	MG	BB	3031	1/1	0.11	-2.45	41,41,41,41	0
53	MG	CA	2047	1/1	0.06	-2.46	121,121,121,121	0
53	MG	CA	2024	1/1	0.03	-2.47	29,29,29,29	0
53	MG	DB	3079	1/1	0.15	-2.47	28,28,28,28	0
53	MG	CA	2002	1/1	0.10	-2.54	5,5,5,5	0
53	MG	AA	2008	1/1	0.07	-2.57	125,125,125,125	0
53	MG	CA	2046	1/1	0.09	-2.60	57,57,57,57	0
53	MG	AA	2029	1/1	0.05	-2.61	39,39,39,39	0
53	MG	BB	3004	1/1	0.05	-2.63	32,32,32,32	0
53	MG	AA	2027	1/1	0.07	-2.63	36,36,36,36	0
53	MG	BB	3103	1/1	0.09	-2.65	5,5,5,5	0
53	MG	DB	3074	1/1	0.09	-2.67	12,12,12,12	0
53	MG	CA	2010	1/1	0.07	-2.67	33,33,33,33	0
53	MG	BB	3051	1/1	0.13	-2.68	35,35,35,35	0
53	MG	BB	3096	1/1	0.13	-2.75	34,34,34,34	0
53	MG	DB	3111	1/1	0.11	-2.77	38,38,38,38	0
53	MG	AA	2046	1/1	0.08	-2.82	5,5,5,5	0
53	MG	BB	3095	1/1	0.07	-2.83	33,33,33,33	0
53	MG	DB	3068	1/1	0.13	-2.85	5,5,5,5	0
53	MG	DB	3050	1/1	0.05	-2.87	90,90,90,90	0
53	MG	BB	3055	1/1	0.15	-2.87	17,17,17,17	0
53	MG	AA	2043	1/1	0.05	-2.89	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	DB	3085	1/1	0.12	-2.89	5,5,5,5	0
53	MG	BB	3038	1/1	0.06	-2.91	71,71,71,71	0
53	MG	DB	3070	1/1	0.07	-2.91	45,45,45,45	0
53	MG	AA	2042	1/1	0.08	-2.92	69,69,69,69	0
53	MG	AA	2036	1/1	0.05	-2.96	31,31,31,31	0
53	MG	BB	3071	1/1	0.09	-2.99	26,26,26,26	0
53	MG	CA	2005	1/1	0.11	-3.02	24,24,24,24	0
53	MG	BB	3007	1/1	0.12	-3.05	82,82,82,82	0
53	MG	BB	3016	1/1	0.11	-3.05	38,38,38,38	0
53	MG	DB	3015	1/1	0.08	-3.09	33,33,33,33	0
53	MG	CA	2004	1/1	0.09	-3.15	8,8,8,8	0
53	MG	DB	3048	1/1	0.07	-3.17	28,28,28,28	0
53	MG	CA	2008	1/1	0.08	-3.22	93,93,93,93	0
53	MG	DB	3062	1/1	0.04	-3.25	77,77,77,77	0
53	MG	CA	2051	1/1	0.06	-3.26	39,39,39,39	0
53	MG	BB	3091	1/1	0.09	-3.28	16,16,16,16	0
53	MG	BB	3048	1/1	0.09	-3.33	44,44,44,44	0
53	MG	AA	2015	1/1	0.05	-3.33	24,24,24,24	0
53	MG	DB	3073	1/1	0.10	-3.35	14,14,14,14	0
53	MG	BB	3046	1/1	0.11	-3.35	22,22,22,22	0
53	MG	CA	2056	1/1	0.05	-3.36	5,5,5,5	0
53	MG	BB	3021	1/1	0.08	-3.36	30,30,30,30	0
53	MG	CA	2059	1/1	0.06	-3.38	94,94,94,94	0
53	MG	DB	3109	1/1	0.07	-3.45	9,9,9,9	0
53	MG	DB	3005	1/1	0.15	-3.50	10,10,10,10	0
53	MG	AA	2056	1/1	0.08	-3.50	124,124,124,124	0
53	MG	BB	3066	1/1	0.10	-3.56	23,23,23,23	0
53	MG	DB	3006	1/1	0.12	-3.57	5,5,5,5	0
53	MG	BB	3056	1/1	0.08	-3.58	26,26,26,26	0
53	MG	BB	3014	1/1	0.07	-3.58	50,50,50,50	0
53	MG	DB	3067	1/1	0.08	-3.60	5,5,5,5	0
53	MG	BB	3026	1/1	0.09	-3.63	39,39,39,39	0
53	MG	CA	2044	1/1	0.08	-3.66	59,59,59,59	0
53	MG	CA	2042	1/1	0.06	-3.66	58,58,58,58	0
53	MG	AA	2052	1/1	0.07	-3.67	78,78,78,78	0
53	MG	BB	3003	1/1	0.06	-3.67	32,32,32,32	0
53	MG	DB	3105	1/1	0.13	-3.71	23,23,23,23	0
53	MG	CA	2028	1/1	0.06	-3.79	75,75,75,75	0
53	MG	DB	3076	1/1	0.12	-3.80	5,5,5,5	0
53	MG	BB	3008	1/1	0.10	-3.82	89,89,89,89	0
53	MG	CA	2061	1/1	0.10	-3.85	23,23,23,23	0
53	MG	BB	3069	1/1	0.11	-3.85	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	DB	3017	1/1	0.09	-3.87	13,13,13,13	0
53	MG	DB	3008	1/1	0.16	-3.88	6,6,6,6	0
53	MG	DB	3090	1/1	0.08	-3.89	37,37,37,37	0
53	MG	BB	3068	1/1	0.13	-3.90	53,53,53,53	0
53	MG	AA	2044	1/1	0.10	-4.01	112,112,112,112	0
53	MG	DB	3049	1/1	0.06	-4.03	36,36,36,36	0
53	MG	BB	3001	1/1	0.10	-4.14	51,51,51,51	0
53	MG	DB	3041	1/1	0.12	-4.16	29,29,29,29	0
53	MG	AA	2001	1/1	0.06	-4.20	35,35,35,35	0
53	MG	DB	3004	1/1	0.10	-4.21	6,6,6,6	0
53	MG	CA	2049	1/1	0.06	-4.24	74,74,74,74	0
53	MG	BB	3032	1/1	0.10	-4.25	56,56,56,56	0
53	MG	CA	2009	1/1	0.05	-4.26	67,67,67,67	0
53	MG	BB	3061	1/1	0.04	-4.26	48,48,48,48	0
53	MG	BB	3089	1/1	0.14	-4.27	56,56,56,56	0
53	MG	BB	3018	1/1	0.13	-4.28	32,32,32,32	0
53	MG	DB	3065	1/1	0.06	-4.28	37,37,37,37	0
53	MG	DB	3075	1/1	0.10	-4.29	57,57,57,57	0
53	MG	BB	3006	1/1	0.11	-4.32	5,5,5,5	0
53	MG	DB	3080	1/1	0.08	-4.34	10,10,10,10	0
53	MG	BB	3035	1/1	0.12	-4.35	15,15,15,15	0
53	MG	DB	3032	1/1	0.10	-4.39	63,63,63,63	0
53	MG	CA	2043	1/1	0.04	-4.41	19,19,19,19	0
53	MG	BB	3009	1/1	0.05	-4.44	46,46,46,46	0
53	MG	BB	3064	1/1	0.06	-4.47	35,35,35,35	0
53	MG	DB	3103	1/1	0.12	-4.50	27,27,27,27	0
53	MG	BB	3060	1/1	0.14	-4.51	19,19,19,19	0
53	MG	BB	3065	1/1	0.06	-4.52	29,29,29,29	0
53	MG	DB	3042	1/1	0.08	-4.53	6,6,6,6	0
53	MG	DB	3036	1/1	0.09	-4.57	30,30,30,30	0
53	MG	DB	3024	1/1	0.11	-4.58	63,63,63,63	0
53	MG	AA	2054	1/1	0.09	-4.62	110,110,110,110	0
53	MG	DB	3056	1/1	0.09	-4.62	5,5,5,5	0
53	MG	CA	2006	1/1	0.09	-4.64	95,95,95,95	0
53	MG	DB	3014	1/1	0.04	-4.78	5,5,5,5	0
53	MG	CA	2041	1/1	0.05	-4.80	46,46,46,46	0
53	MG	AA	2020	1/1	0.04	-4.82	5,5,5,5	0
53	MG	AA	2051	1/1	0.07	-4.82	41,41,41,41	0
53	MG	BB	3067	1/1	0.11	-4.84	44,44,44,44	0
53	MG	BB	3058	1/1	0.08	-4.89	22,22,22,22	0
53	MG	DB	3045	1/1	0.07	-4.90	57,57,57,57	0
53	MG	DB	3061	1/1	0.08	-4.91	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	DB	3107	1/1	0.08	-4.92	10,10,10,10	0
53	MG	BB	3043	1/1	0.08	-4.95	104,104,104,104	0
53	MG	BB	3074	1/1	0.06	-4.95	28,28,28,28	0
53	MG	AA	2005	1/1	0.09	-5.05	69,69,69,69	0
53	MG	DB	3035	1/1	0.05	-5.05	55,55,55,55	0
53	MG	CA	2001	1/1	0.05	-5.06	5,5,5,5	0
53	MG	CA	2018	1/1	0.03	-5.18	6,6,6,6	0
53	MG	DB	3104	1/1	0.12	-5.26	33,33,33,33	0
53	MG	DB	3016	1/1	0.06	-5.31	15,15,15,15	0
53	MG	DB	3026	1/1	0.08	-5.44	34,34,34,34	0
53	MG	CA	2031	1/1	0.05	-5.48	28,28,28,28	0
53	MG	DB	3043	1/1	0.09	-5.57	5,5,5,5	0
53	MG	CA	2030	1/1	0.06	-5.60	7,7,7,7	0
53	MG	CA	2048	1/1	0.06	-5.80	58,58,58,58	0
53	MG	BB	3029	1/1	0.08	-5.80	14,14,14,14	0
53	MG	DB	3046	1/1	0.08	-5.81	24,24,24,24	0
53	MG	AA	2002	1/1	0.04	-5.82	99,99,99,99	0
53	MG	BB	3078	1/1	0.07	-5.84	70,70,70,70	0
53	MG	AA	2041	1/1	0.06	-5.91	83,83,83,83	0
53	MG	BB	3088	1/1	0.07	-5.92	28,28,28,28	0
53	MG	DB	3106	1/1	0.12	-5.94	23,23,23,23	0
53	MG	DB	3044	1/1	0.10	-5.98	24,24,24,24	0
53	MG	BB	3072	1/1	0.09	-6.07	17,17,17,17	0
53	MG	DB	3033	1/1	0.08	-6.10	9,9,9,9	0
53	MG	DB	3102	1/1	0.07	-6.13	12,12,12,12	0
53	MG	CA	2003	1/1	0.04	-6.13	35,35,35,35	0
53	MG	DB	3001	1/1	0.12	-6.18	5,5,5,5	0
53	MG	BB	3002	1/1	0.08	-6.23	5,5,5,5	0
53	MG	BB	3094	1/1	0.09	-6.23	28,28,28,28	0
53	MG	CA	2057	1/1	0.08	-6.31	99,99,99,99	0
53	MG	BB	3019	1/1	0.07	-6.46	22,22,22,22	0
53	MG	CA	2025	1/1	0.12	-6.64	50,50,50,50	0
53	MG	DB	3039	1/1	0.05	-6.71	22,22,22,22	0
53	MG	AE	201	1/1	0.09	-7.06	144,144,144,144	0
53	MG	BB	3020	1/1	0.09	-7.47	26,26,26,26	0
53	MG	BB	3052	1/1	0.07	-7.48	38,38,38,38	0
53	MG	DB	3071	1/1	0.07	-7.52	16,16,16,16	0
53	MG	BB	3079	1/1	0.06	-7.55	19,19,19,19	0
53	MG	DB	3018	1/1	0.10	-7.68	22,22,22,22	0
53	MG	CA	2034	1/1	0.10	-8.19	6,6,6,6	0
53	MG	DB	3053	1/1	0.06	-8.22	35,35,35,35	0
53	MG	BB	3041	1/1	0.12	-8.53	7,7,7,7	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	BB	3015	1/1	0.11	-8.80	13,13,13,13	0
53	MG	DB	3083	1/1	0.13	-8.85	85,85,85,85	0
53	MG	BB	3050	1/1	0.11	-8.96	28,28,28,28	0
53	MG	DB	3002	1/1	0.06	-9.46	12,12,12,12	0
53	MG	CA	2029	1/1	0.06	-10.60	23,23,23,23	1
53	MG	DB	3010	1/1	0.06	-10.77	8,8,8,8	0
53	MG	DB	3072	1/1	0.11	-10.99	18,18,18,18	0
53	MG	CA	2055	1/1	0.06	-11.27	11,11,11,11	0
53	MG	DB	3009	1/1	0.06	-11.49	29,29,29,29	0
53	MG	DB	3054	1/1	0.04	-12.45	19,19,19,19	0
53	MG	DB	3108	1/1	0.07	-12.64	37,37,37,37	0
53	MG	BB	3047	1/1	0.07	-12.83	75,75,75,75	0
53	MG	BB	3030	1/1	0.04	-13.23	35,35,35,35	0
53	MG	BB	3063	1/1	0.08	-16.84	11,11,11,11	0
53	MG	AA	2016	1/1	0.05	-17.34	89,89,89,89	0
53	MG	BB	3053	1/1	0.06	-17.79	28,28,28,28	0
53	MG	BB	3076	1/1	0.08	-19.80	38,38,38,38	0
53	MG	DB	3028	1/1	0.05	-27.23	24,24,24,24	0
53	MG	BB	3057	1/1	0.13	-33.00	28,28,28,28	0
53	MG	DB	3029	1/1	0.12	-93.00	88,88,88,88	0
53	MG	AA	2048	1/1	0.04	-109.00	99,99,99,99	0
53	MG	CA	2052	1/1	0.06	-	73,73,73,73	0
53	MG	CA	2023	1/1	0.38	-	137,137,137,137	0
53	MG	CA	2026	1/1	0.18	-	26,26,26,26	1

6.5 Other polymers ⓘ

There are no such residues in this entry.