



wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 06:34 PM BST

PDB ID : 4V56
Title : Crystal structure of the bacterial ribosome from Escherichia coli in complex with spectinomycin.
Authors : Borovinskaya, M.A.; Shoji, S.; Holton, J.M.; Fredrick, K.; Cate, J.H.D.
Deposited on : 2007-07-21
Resolution : 3.93 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>

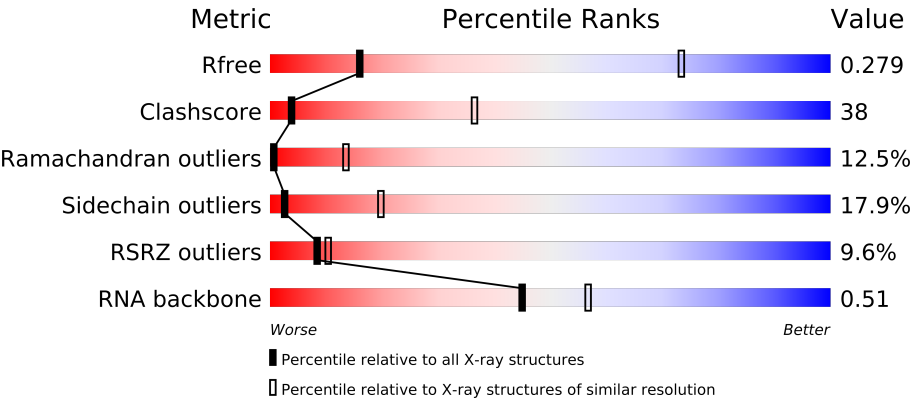
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.93 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	1009 (4.42-3.44)
Clashscore	79885	1184 (4.38-3.50)
Ramachandran outliers	78287	1128 (4.38-3.50)
Sidechain outliers	78261	1116 (4.38-3.50)
RSRZ outliers	66119	1009 (4.42-3.44)
RNA backbone	1838	1018 (5.00-2.80)

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	AP	82	
13	CP	82	
14	AQ	83	
14	CQ	83	
15	AR	74	
15	CR	74	
16	AS	91	
16	CS	91	
17	AT	86	
17	CT	86	
18	AB	240	
18	CB	240	
19	AU	70	
19	CU	70	
20	AO	89	
20	CO	89	
21	AN	100	
21	CN	100	
22	BA	120	
22	DA	120	
23	BB	2904	
23	DB	2904	
24	BI	141	
24	DI	141	
25	BC	272	
25	DC	272	
26	BD	209	
26	DD	209	
27	BK	123	
27	DK	123	

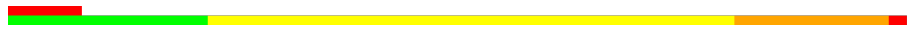
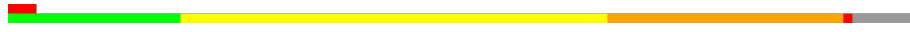

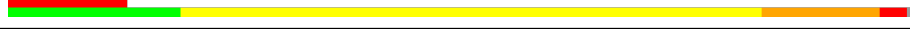


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Mol	Chain	Length	Quality of chain
28	BP	114	
28	DP	114	
29	BE	201	
29	DE	201	
30	BY	58	
30	DY	58	
31	B0	56	
31	D0	56	
32	B4	38	
32	D4	38	
33	B1	54	
33	D1	54	
34	B3	64	
34	D3	64	
35	BV	94	
35	DV	94	
36	B2	46	
36	D2	46	
37	BL	144	
37	DL	144	
38	BM	136	
38	DM	136	
39	BX	63	
39	DX	63	
40	BH	149	
40	DH	149	
41	BJ	142	
41	DJ	142	
42	BN	127	
42	DN	127	
43	BO	117	
43	DO	117	
44	BQ	117	
44	DQ	117	
45	BS	110	
45	DS	110	
46	BU	103	
46	DU	103	
47	BF	178	
47	DF	178	
48	BG	176	
48	DG	176	

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Mol	Chain	Length	Quality of chain
49	BR	103	
49	DR	103	
50	BT	100	
50	DT	100	
51	BZ	78	
51	DZ	78	
52	BW	84	
52	DW	84	

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	1622	-	X
53	MG	AA	1623	-	X
53	MG	AA	1624	-	X
53	MG	AA	1626	-	X
53	MG	AA	1632	-	X
53	MG	AA	1647	-	X
53	MG	AA	1657	-	X
53	MG	AA	1659	-	X
53	MG	BB	3017	-	X
53	MG	BB	3028	-	X
53	MG	BB	3033	-	X
53	MG	BB	3036	-	X
53	MG	BB	3039	-	X
53	MG	BB	3047	-	X
53	MG	BB	3087	-	X
53	MG	CA	1612	-	X
53	MG	CA	1613	-	X
53	MG	CA	1616	-	X
53	MG	CA	1617	-	X
53	MG	CA	1632	-	X
53	MG	CA	1649	-	X
53	MG	CA	1654	-	X
53	MG	CA	1656	-	X
53	MG	DB	3029	-	X
53	MG	DB	3037	-	X
53	MG	DB	3052	-	X
53	MG	DB	3054	-	X
53	MG	DB	3066	-	X

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 284033 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	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 S16.

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

- Molecule 14 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AQ	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			
14	CQ	81	Total	C	N	O	S	0	0	0
			657	417	122	115	3			

- Molecule 15 is a protein called 30S ribosomal protein S18.

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

- Molecule 16 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AS	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			
16	CS	80	Total	C	N	O	S	0	0	0
			644	413	121	108	2			

- Molecule 17 is a protein called 30S ribosomal protein S20.

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

- Molecule 18 is a protein called 30S ribosomal protein S2.

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

- Molecule 19 is a protein called 30S ribosomal protein S21.

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

- Molecule 20 is a protein called 30S ribosomal protein S15.

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

- Molecule 21 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			
21	CN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			

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

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			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	120	U	-	INSERTION	GB 85674274
DA	120	U	-	INSERTION	GB 85674274

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

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			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BB	2903	U	-	INSERTION	GB 85674274
BB	2904	U	-	INSERTION	GB 85674274
DB	2903	U	-	INSERTION	GB 85674274
DB	2904	U	-	INSERTION	GB 85674274

- Molecule 24 is a protein called 50S ribosomal protein L11.

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

- 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			
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 L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BK	121	Total	C	N	O	S	0	0	0
			930	582	179	164	5			
27	DK	121	Total	C	N	O	S	0	0	0
			930	582	179	164	5			

- Molecule 28 is a protein called 50S ribosomal protein L19.

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

- Molecule 29 is a protein called 50S ribosomal protein L4.

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

- Molecule 30 is a protein called 50S ribosomal protein L30.

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

- Molecule 31 is a protein called 50S ribosomal protein L32.

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

- Molecule 32 is a protein called 50S ribosomal protein L36.

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

- Molecule 33 is a protein called 50S ribosomal protein L33.

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

- Molecule 34 is a protein called 50S ribosomal protein L35.

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

- Molecule 35 is a protein called 50S ribosomal protein L25.

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

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

- Molecule 36 is a protein called 50S ribosomal protein L34.

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

- Molecule 37 is a protein called 50S ribosomal protein L15.

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

- Molecule 38 is a protein called 50S ribosomal protein L16.

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

- Molecule 39 is a protein called 50S ribosomal protein L29.

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

- Molecule 40 is a protein called 50S ribosomal protein L9.

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

- Molecule 41 is a protein called 50S ribosomal protein L13.

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

- Molecule 42 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BN	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			
42	DN	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			

- Molecule 43 is a protein called 50S ribosomal protein L18.

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

- Molecule 44 is a protein called 50S ribosomal protein L20.

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

- Molecule 45 is a protein called 50S ribosomal protein L22.

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

- Molecule 46 is a protein called 50S ribosomal protein L24.

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

- Molecule 47 is a protein called 50S ribosomal protein L5.

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

- Molecule 48 is a protein called 50S ribosomal protein L6.

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

- Molecule 49 is a protein called 50S ribosomal protein L21.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	BT	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			
50	DT	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			

- Molecule 51 is a protein called 50S ribosomal protein L28.

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

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

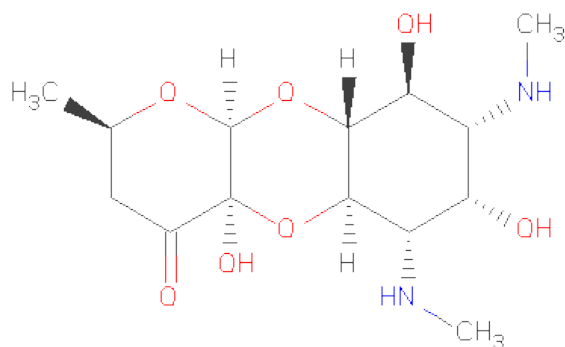
- Molecule 52 is a protein called 50S ribosomal protein L27.

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

- 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	58	Total	Mg	0	0
			58	58		
53	AA	60	Total	Mg	0	0
			60	60		
53	CE	1	Total	Mg	0	0
			1	1		
53	DN	1	Total	Mg	0	0
			1	1		
53	DB	110	Total	Mg	0	0
			110	110		

- Molecule 54 is SPECTINOMYCIN (three-letter code: SCM) (formula: C₁₄H₂₄N₂O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
54	AA	1	Total	C	N	O	0	0
			23	14	2	7		
54	CA	1	Total	C	N	O	0	0
			23	14	2	7		

- 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		
55	D4	1	Total	Zn	0	0
			1	1		

- Molecule 56 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AA	288	Total	O	0	0
			288	288		
56	AE	3	Total	O	0	0
			3	3		
56	AK	1	Total	O	0	0
			1	1		
56	AL	4	Total	O	0	0
			4	4		
56	AP	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AT	1	Total 1	O 1	0	0
56	AN	2	Total 2	O 2	0	0
56	BB	494	Total 494	O 494	0	0
56	BC	4	Total 4	O 4	0	0
56	BE	3	Total 3	O 3	0	0
56	BL	4	Total 4	O 4	0	0
56	BH	1	Total 1	O 1	0	0
56	BT	1	Total 1	O 1	0	0
56	CA	275	Total 275	O 275	0	0
56	CE	4	Total 4	O 4	0	0
56	CK	1	Total 1	O 1	0	0
56	CL	5	Total 5	O 5	0	0
56	CP	1	Total 1	O 1	0	0
56	CT	2	Total 2	O 2	0	0
56	CN	5	Total 5	O 5	0	0
56	DB	500	Total 500	O 500	0	0
56	DC	3	Total 3	O 3	0	0
56	DD	1	Total 1	O 1	0	0
56	DP	1	Total 1	O 1	0	0
56	DE	1	Total 1	O 1	0	0
56	DL	3	Total 3	O 3	0	0

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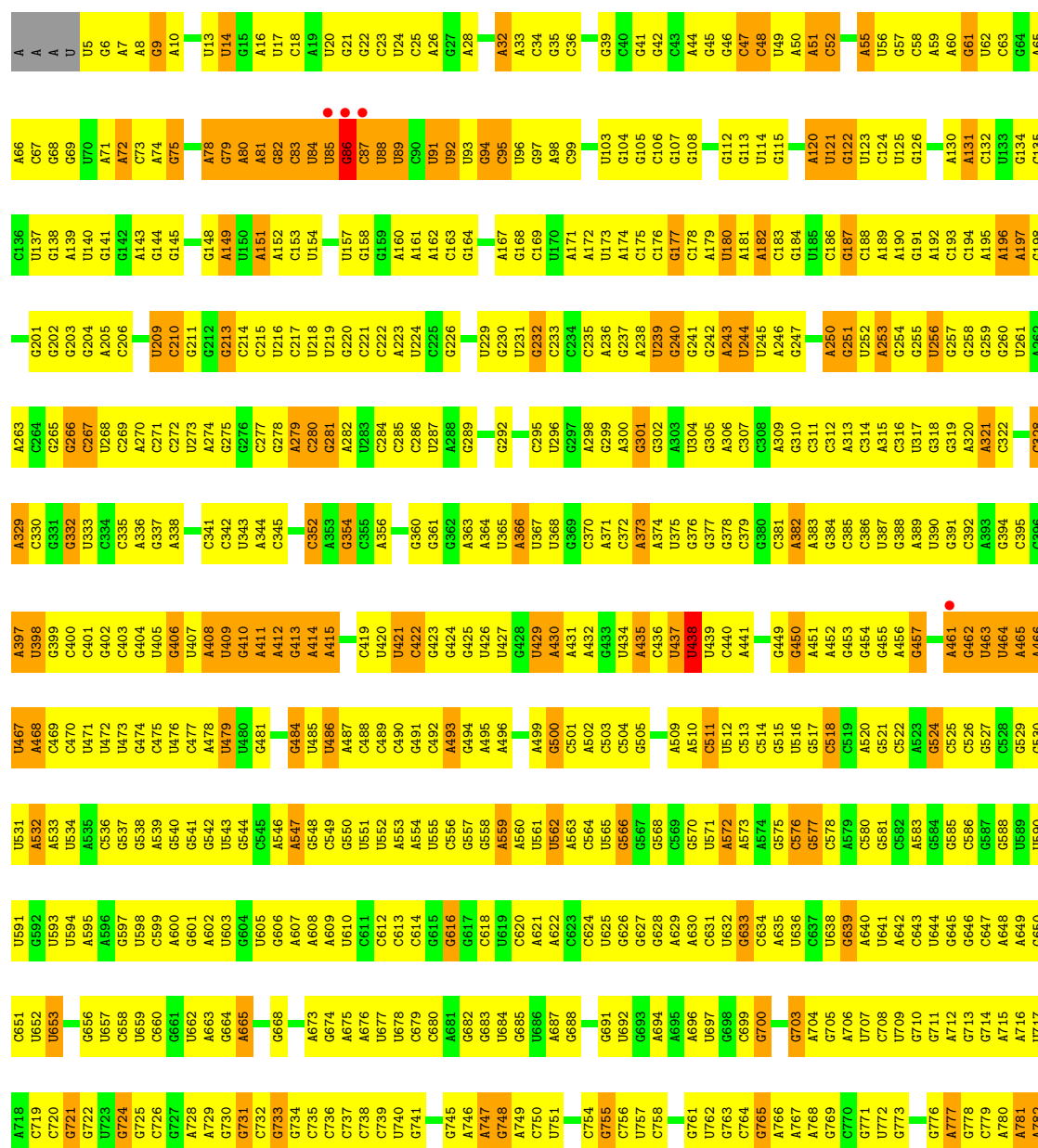
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	DJ	1	Total 1	O 1	0	0
56	DN	2	Total 2	O 2	0	0
56	DR	1	Total 1	O 1	0	0

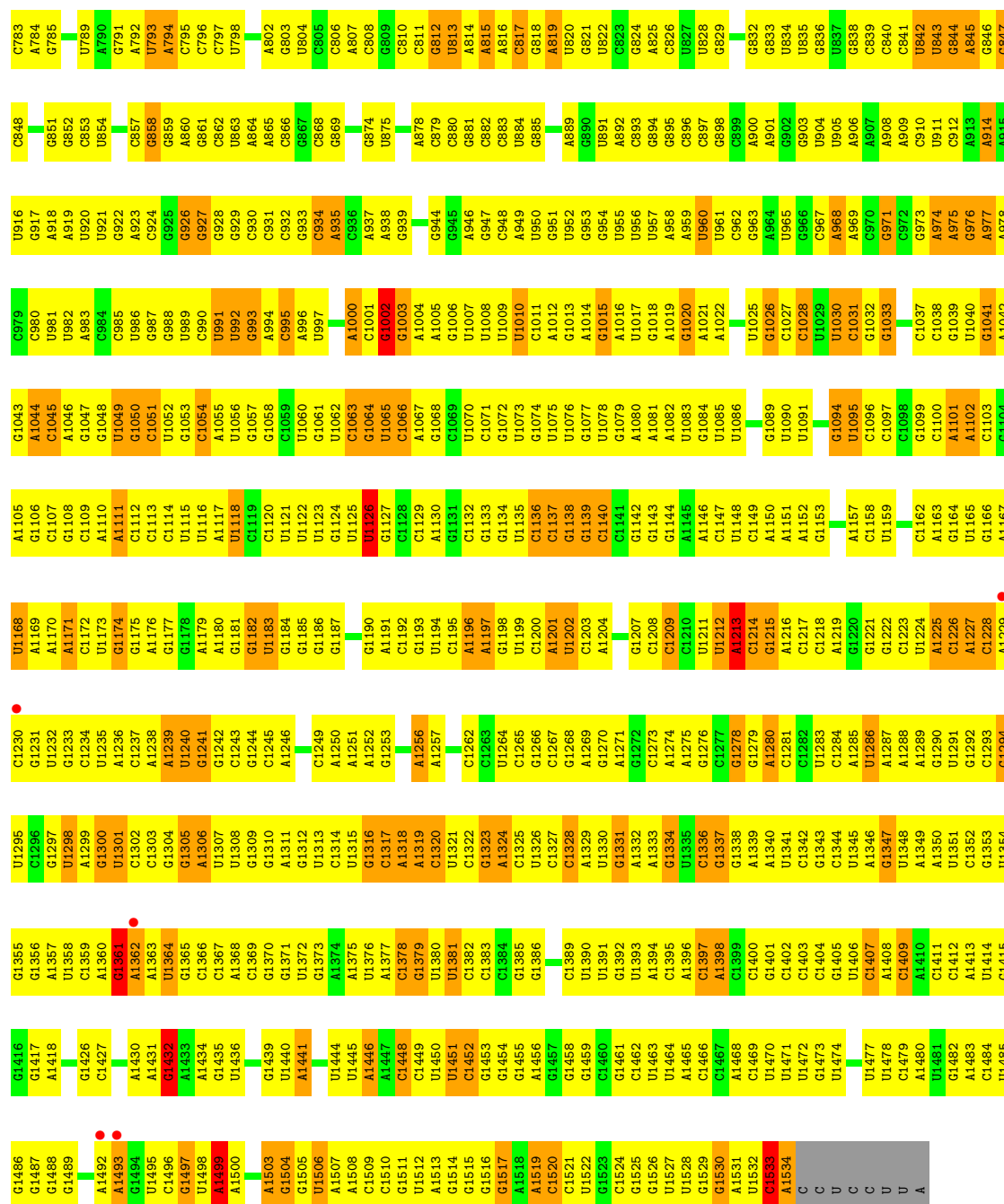
3 Residue-property plots

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

• Molecule 1: 16S rRNA

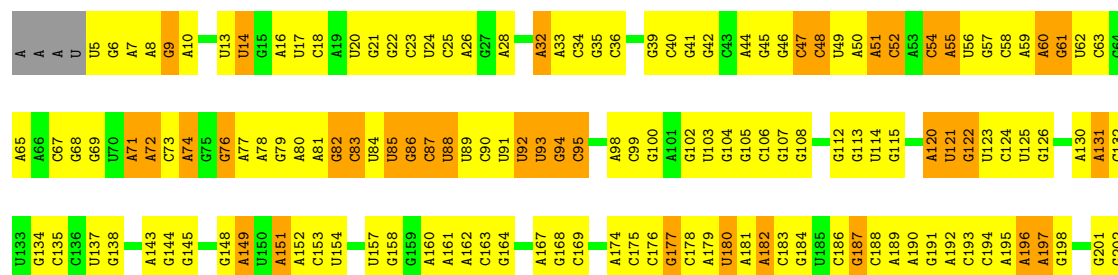
Chain AA: 



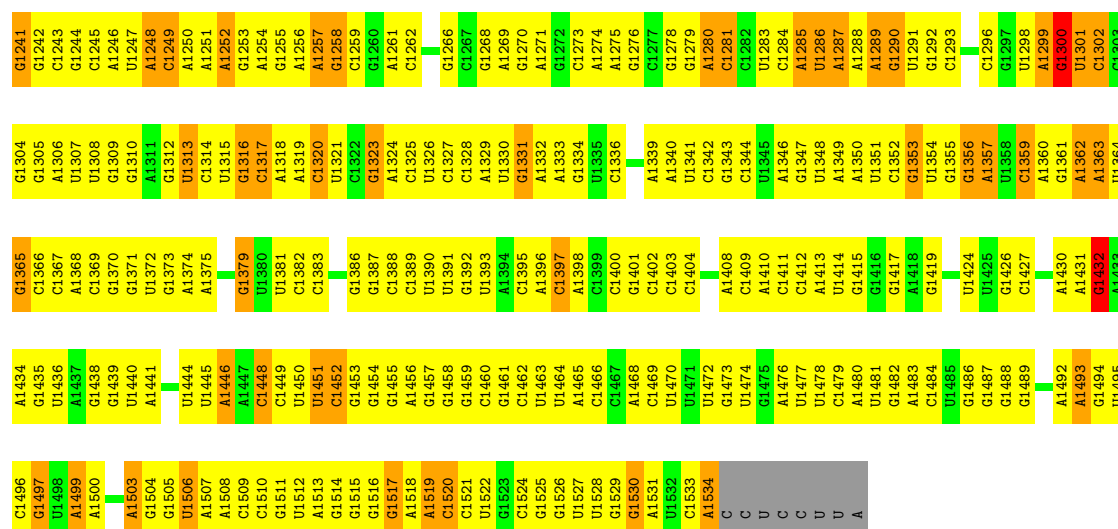


• Molecule 1: 16S rRNA

Chain CA:

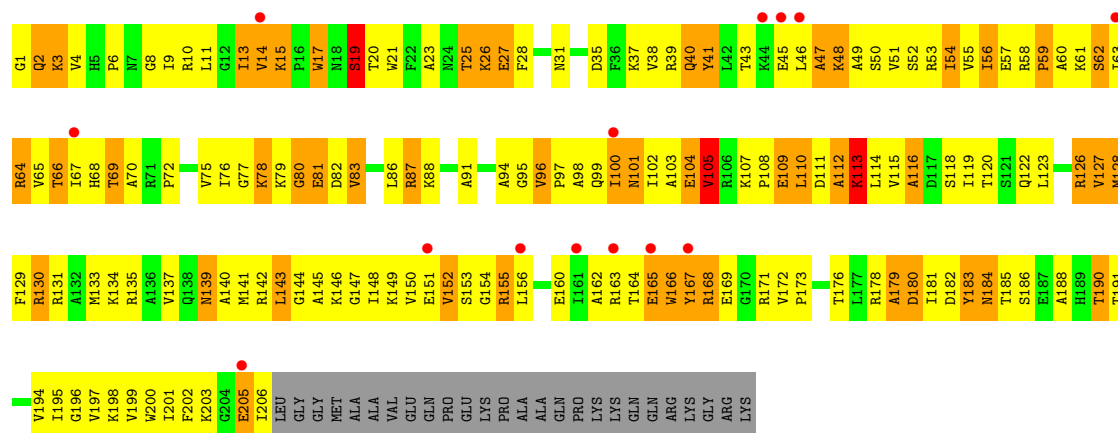


G1175	G1176	G1177	G1178	A1179	A1180	G1181	G1182	G1184	G1190	G1191	G1192	G1193	A1196	A1197	G1198	G1199	C1200	A1201	U1202	C1203	G1206	G1207	C1208	C1209	C1210	C1211	U1212	C1213	C1214	C1215	U1216	C1217	U1218	U1219	G2200	G2201	G2210	G2211	G2212	G2213	G2214	G2215	U2216	C2217	U2218	U2219	G2220	G2221	G2222	G2223	U2224	G2225	G2226	U2229	G2300	G2301	U2302	G2303	G2304	G2305	G2306	G2307	G2308	G2309	G2310	G2311	G2312	G2313	G2314	G2315	G2316	G2317	G2318	G2319	G2320	G2321	G2322	G2323	G2324	G2325	G2326	G2327	G2328	G2329	G2330	G2331	G2332	G2333	G2334	G2335	A336	A337	A338	G341	G342	G343	G344	G345	G346	G347	C352	A353	G354	G355	G356	G361	G362	A363	A364	U365	U366	G428	U429	A430	U431	G432	A433	G434	G435	A371	U434	A435	A373	A374	U437	U438	A441	G449	G450	A451	A452	A453	G454	G455	A456	G457	A461	G462	U463	U464	A465	A466	G467	U468	U469	A471	U472	U473	G474	G475	C476	C477	U478	U479	U480	G481	A482	C483	G484	U485	U486	A487	U488	C489	C490	G491	C492	C493	G494	A495	A496	A499	G500	C501	G502	C503	C504	G505	A509	C510	C511	U512	C513	C514	G515	G516	G517	C518	C519	A520	G521	C522	A523	G524	C525	C526	G527	C528	U529	G530	C531	U532	U533	A534	A535	C536	G537	G538	A539	G540	G541	G542	U543	G544	C545	A546	A547	U548	U549	G550	U551	U552	A553	A554	U555	G556	G557	G558	A559	A560	U561	U562	A563	G564	U565	G566	G567	A568	G569	U570	U571	A572	C573	C574	A575	G576	G577	C578	A579	C580	G581	C582	A583	G584	G585	C586	G587	C588	G589	G590	G591	U592	U593	U594	A595	A596	A597	G598	G599	G600	G601	G602	U603	G604	G605	G606	A607	G608	A609	C612	C613	U614	G615	G616	G617	G618	U619	G620	A621	A622	U623	A624	G625	A626	U627	A628	U629	A630	G631	G632	U633	G634	A635	U636	G637	G638	G639	A640	U641	U642	G643	C644	G645	G646	C647	A648	G649	G650	C651	U652	U653	G656	U657	C658	U659	G660	G661	U662	G663	G664	G665	G666	G667	G668	U672	A673	G674	A675	C676	C677	C678	C679	C680	A681	G682	G683	U684	G685	U686	A687	G688	G689	G690	G691	U692	G693	A694	A695	U696	G697	G698	G699	G700	U701	A702	G703	A704	G705	U706	U707	C708	U709	G710	G711	A712	G713	G714	A715	A716	U717	C719	G720	G721	U722	U723	G724	G725	A728	G729	G730	G731	C732	G733	G734	G735	G736	C737	C738	C739	U740	G741	G745	A746	G747	G748	A749	C750	A753	G754	G755	C756	G757	C758	G761	U762	G763	C764	G765	A766	G767	G768	G769	C770	G771	U772	G773	G776	A777	G778	C779	A780	U781	G782	A783	C784	U785	A786	G787	U788	A789	G790	G791	G792	U793	A794	G795	C796	C797	U798	A802	G803	U804	C805	C806	A807	C808	U809	C810	C811	G812	U813	A814	A815	U816	C817	G818	A819	U820	G821	U822	C823	G824	A825	C826	U827	G828	U829	G832	G833	U834	U835	C836	U837	U838	A839	A840	C841	U842	U843	G844	A845	U846	A847	A848	U849	G850	C851	U852	A853	U854	G855	U856	C857	G858	A859	U860	G861	G862	U863	A864	G865	C866	G867	U868	A869	G870	G871	G872	G873	G874	G875	G876	G877	A878	C879	G880	G881	C882	G883	U884	G885	A889	G890	U891	A892	C893	U894	G895	U896	U897	G898	C899	A900	U901	G902	U903	G904	U905	A906	U907	A908	A909	C910	U911	C912	A913	A914	U915	U916	G917	A918	A919	U920	U921	G922	A923	G924	G925	G926	U927	G928	G929	G930	C931	G932	G933	G934	A935	G936	U937	A938	G939	G940	G941	A942	A946	G947	G948	U949	U950	G951	U952	G953	G954	U955	U956	U957	A958	A959	U960	U961	C962	G963	A964	U965	G966	U967	A968	A969	C970	G971	C972	U973	A974	U975	G976	A977	U978	A979	U980	U981	U982	U983	U984	C985	U986	U987	U988	U989	U990	U991	U992	U993	U994	U995	U996	U997	U998	U999	U1000	U1001	U1002	U1003	U1004	U1005	U1006	U1007	U1008	U1009	U1010	U1011	U1012	U1013	U1014	U1015	U1016	U1017	U1018	U1019	U1020	U1021	U1022	U1023	U1024	U1025	U1026	U1027	U1028	U1029	U1030	U1031	U1032	U1033	U1034	U1035	U1036	U1037	U1038	U1039	U1040	U1041	U1042	U1043	U1044	U1045	U1046	U1047	U1048	U1049	U1050	U1051	U1052	U1053	U1054	U1055	U1056	U1057	U1058	U1059	U1060	U1061	U1062	U1063	U1064	U1065	U1066	U1067	U1068	U1069	U1070	U1071	U1072	U1073	U1074	U1075	U1076	U1077	U1078	U1079	U1080	U1081	U1082	U1083	U1084	U1085	U1086	U1087	U1088	U1089	U1090	U1091	U1092	U1093	U1094	U1095	U1096	U1097	U1098	U1099	U1100	U1101	U1102	U1103	U1104	U1105	U1106	U1107	U1108	U1109	U1110	U1111	U1112	U1113	U1114	U1115	U1116	U1117	U1118	U1119	U1120	U1121	U1122	U1123	U1124	U1125	U1126	U1127	U1128	U1129	U1130	U1131	U1132	U1133	U1134	U1135	U1136	U1137	U1138	U1139	U1140	U1141	U1142	U1143	U1144	U1145	U1146	U1147	U1148	U1149	U1150	U1151	U1152	U1153	U1154	U1155	U1156	U1157	U1158	U1159	U1160	U1161	U1162	U1163	U1164	U1165	U1166	U1167	U1168	U1169	U1170	U1171	U1172	U1173	U1174	U1175	U1176	U1177	U1178	U1179	U1180	U1181	U1182	U1183	U1184	U1185	U1186	U1187	U1188	U1189	U1190	U1191	U1192	U1193	U1194	U1195	U1196	U1197	U1198	U1199	U1200	U1201	U1202	U1203	U1204	U1205	U1206	U1207	U1208	U1209	U1210	U1211	U1212	U1213	U1214	U1215	U1216	U1217	U1218	U1219	U1220	U1221	U1222	U1223	U1224	U1225	U1226	U1227	U1228	U1229	U1230	U1231	U1232	U1233	U1234	U1235	U1236	U1237	U1238	U1239	U1240	U1241	U1242	U1243	U1244	U1245	U1246	U1247	U1248	U1249	U1250	U1251	U1252	U1253	U1254	U1255	U1256	U1257	U1258	U1259	U1260	U1261	U1262	U1263	U1264	U1265	U1266	U1267	U1268	U1269	U1270	U1271	U1272	U1273	U1274	U1275	U1276	U1277	U1278	U1279	U1280	U1281	U1282	U1283	U1284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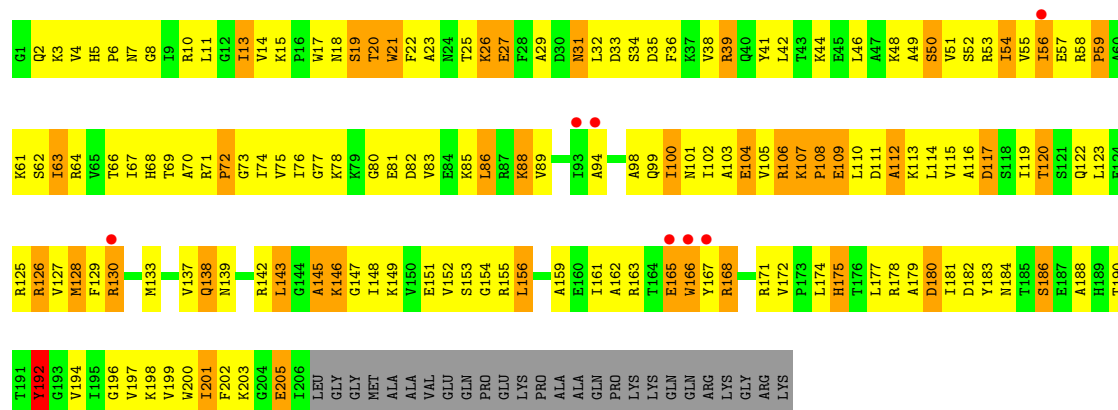
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Chain AC:



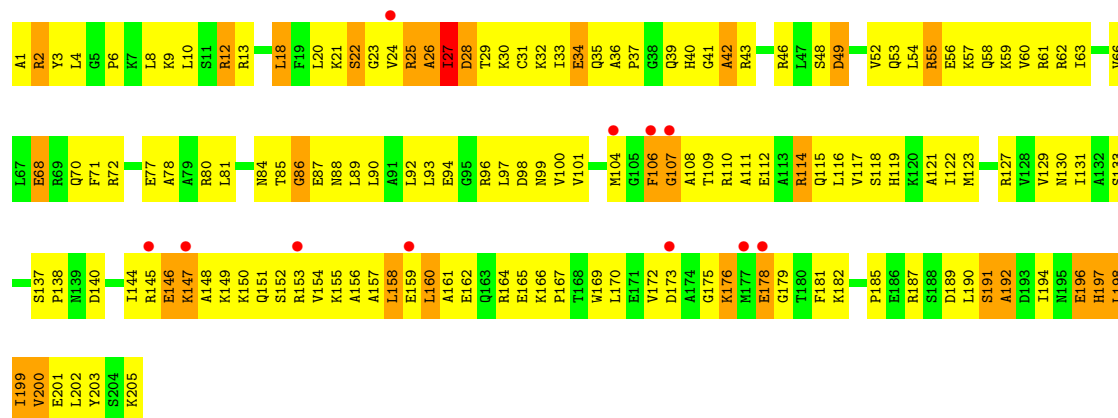
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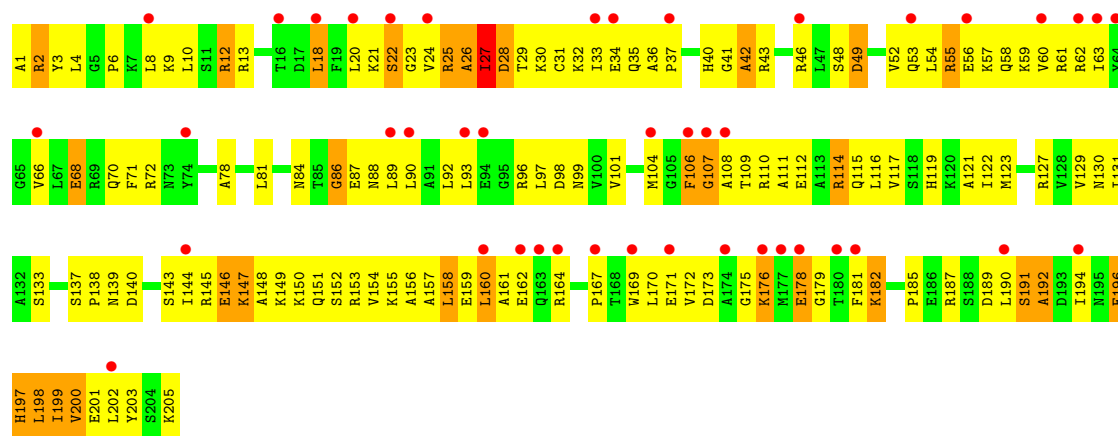
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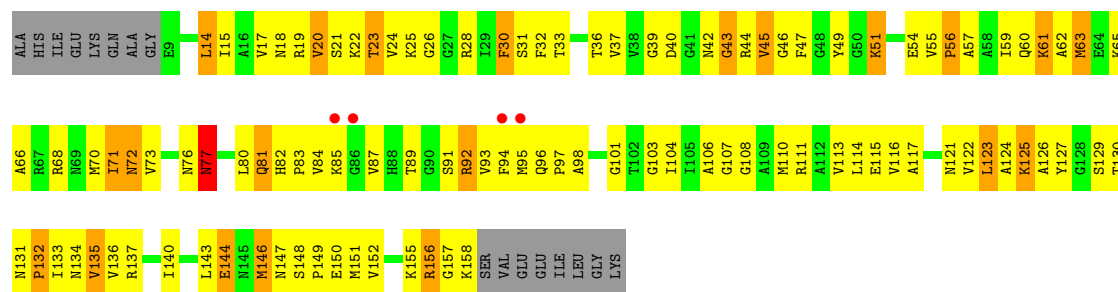
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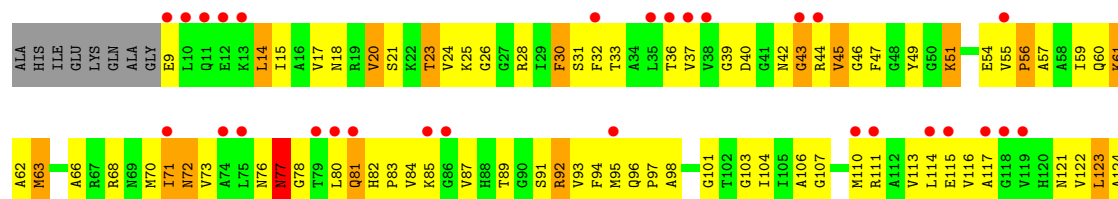
• Molecule 4: 30S ribosomal protein S5

Chain AE:



• Molecule 4: 30S ribosomal protein S5

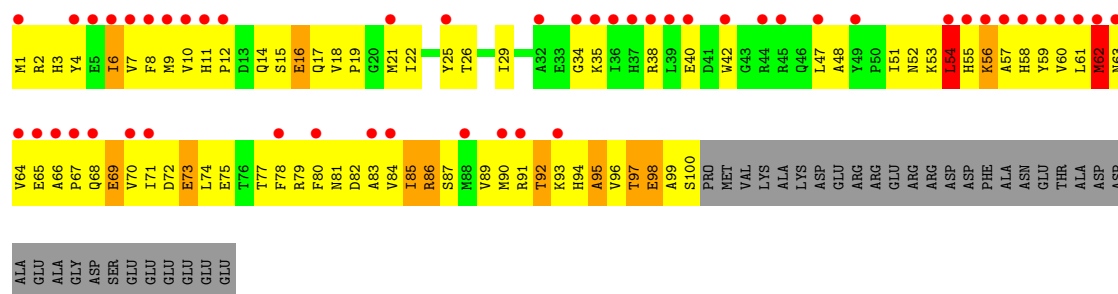
Chain CE:





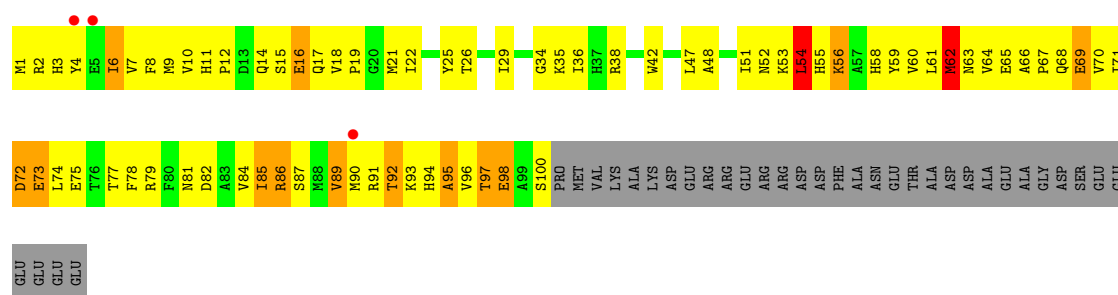
• Molecule 5: 30S ribosomal protein S6

Chain AF:



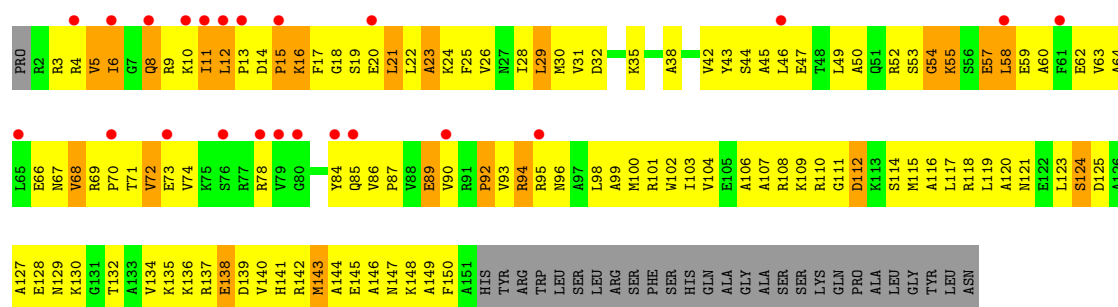
• Molecule 5: 30S ribosomal protein S6

Chain CF:



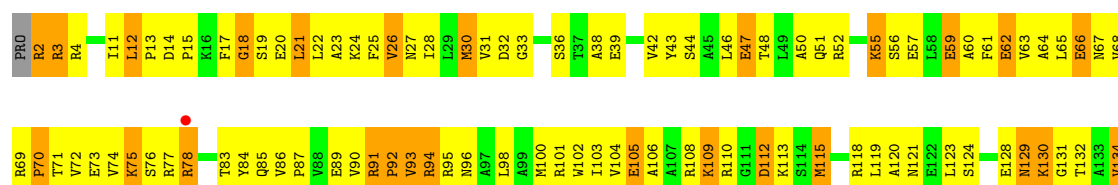
• Molecule 6: 30S ribosomal protein S7

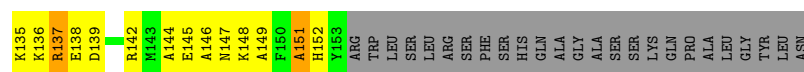
Chain AG:



• Molecule 6: 30S ribosomal protein S7

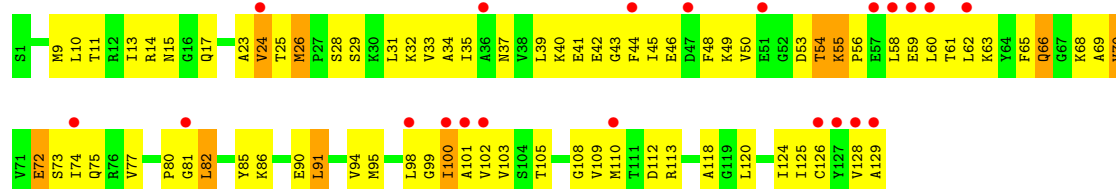
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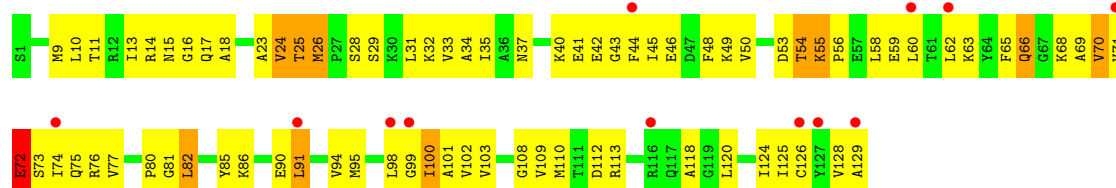
• Molecule 7: 30S ribosomal protein S8

Chain AH:



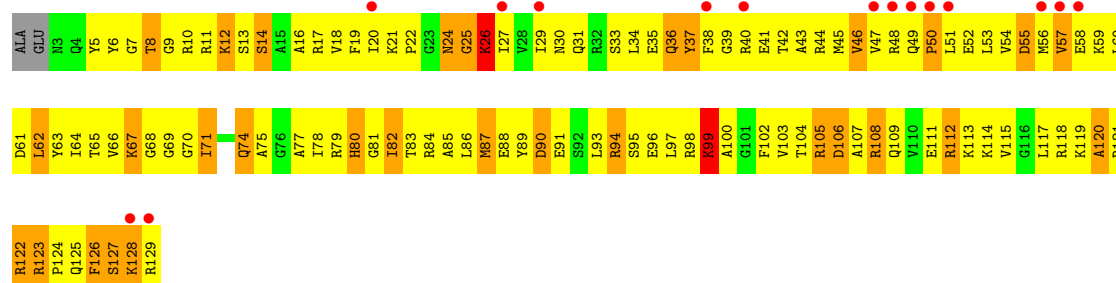
• Molecule 7: 30S ribosomal protein S8

Chain CH:



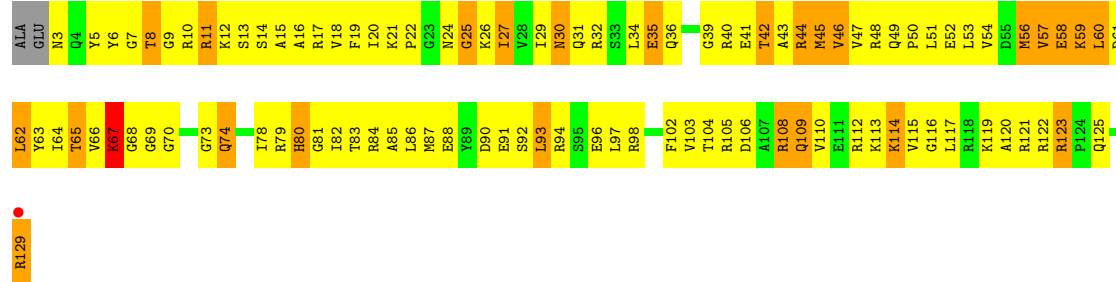
• Molecule 8: 30S ribosomal protein S9

Chain AI:



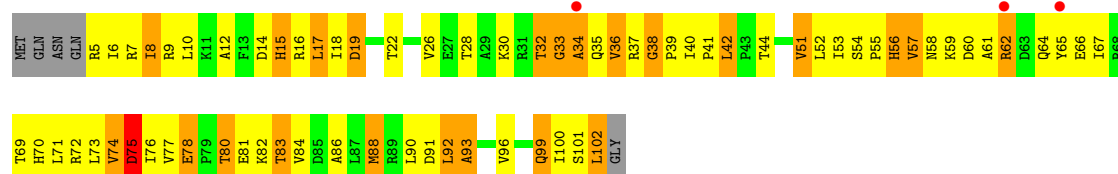
• Molecule 8: 30S ribosomal protein S9

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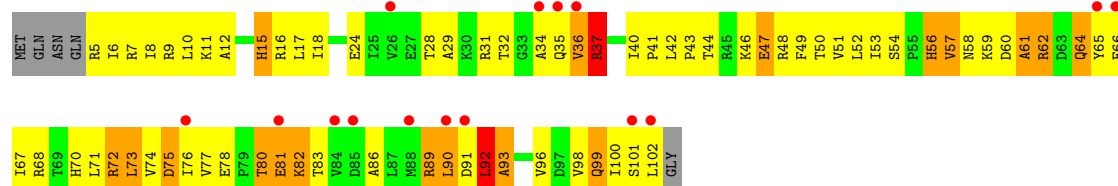
• Molecule 9: 30S ribosomal protein S10

Chain AJ:



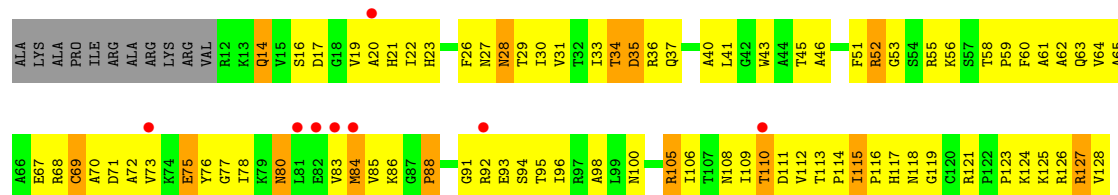
• Molecule 9: 30S ribosomal protein S10

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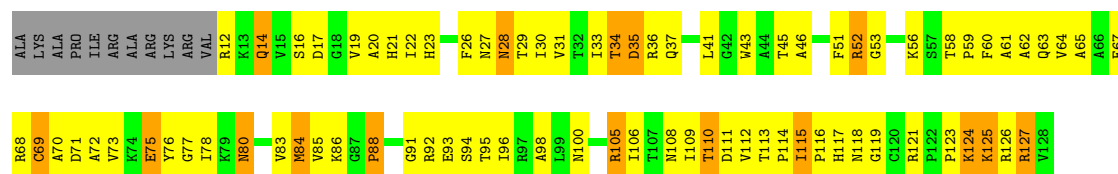
• Molecule 10: 30S ribosomal protein S11

Chain AK:



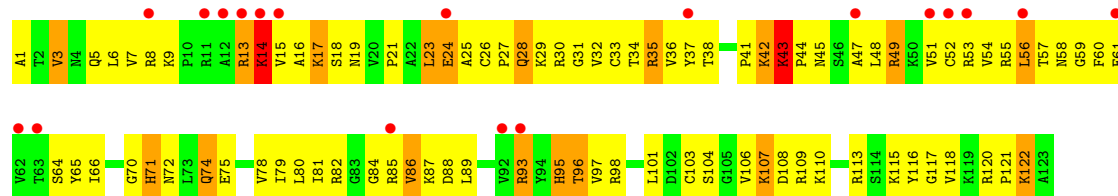
• Molecule 10: 30S ribosomal protein S11

Chain CK:



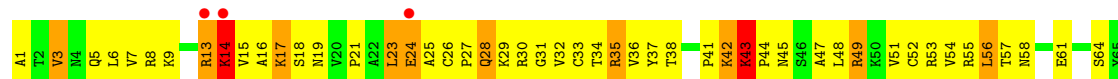
• Molecule 11: 30S ribosomal protein S12

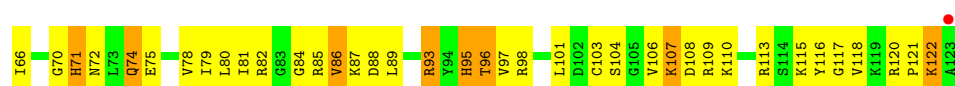
Chain AL:



• Molecule 11: 30S ribosomal protein S12

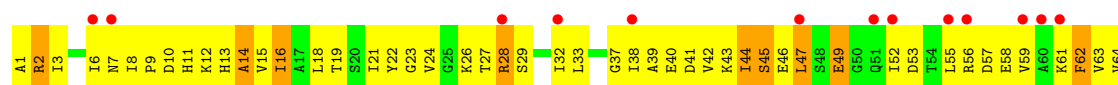
Chain CL:





• Molecule 12: 30S ribosomal protein S13

Chain AM:



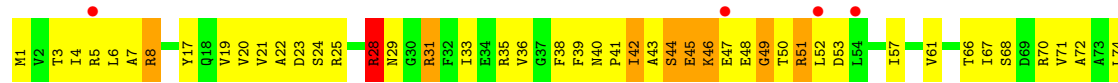
• Molecule 12: 30S ribosomal protein S13

Chain CM:



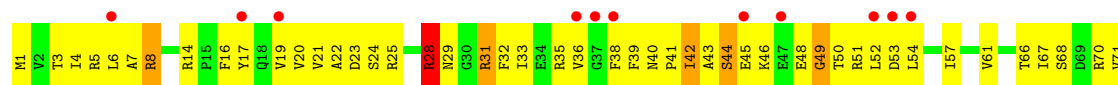
• Molecule 13: 30S ribosomal protein S16

Chain AP:



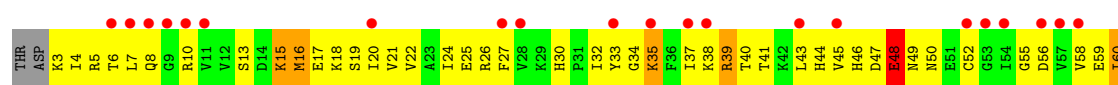
• Molecule 13: 30S ribosomal protein S16

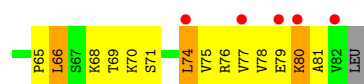
Chain CP:



• Molecule 14: 30S ribosomal protein S17

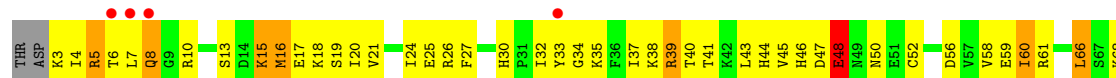
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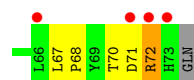
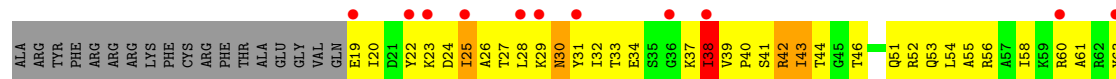
- Molecule 14: 30S ribosomal protein S17

Chain CQ:



- Molecule 15: 30S ribosomal protein S18

Chain AR:



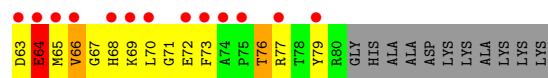
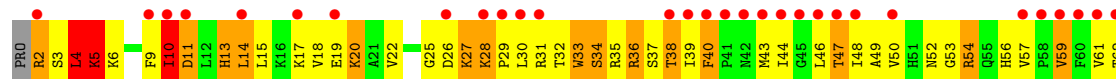
- Molecule 15: 30S ribosomal protein S18

Chain CR:



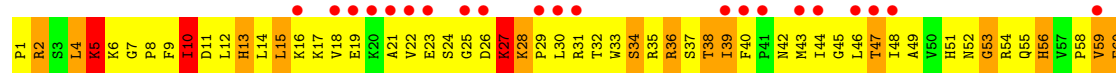
- Molecule 16: 30S ribosomal protein S19

Chain AS:



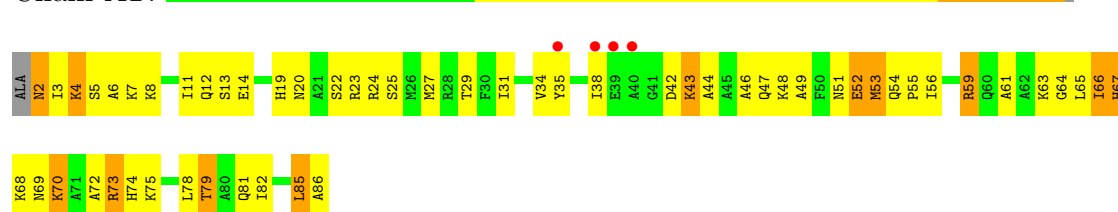
- Molecule 16: 30S ribosomal protein S19

Chain CS:



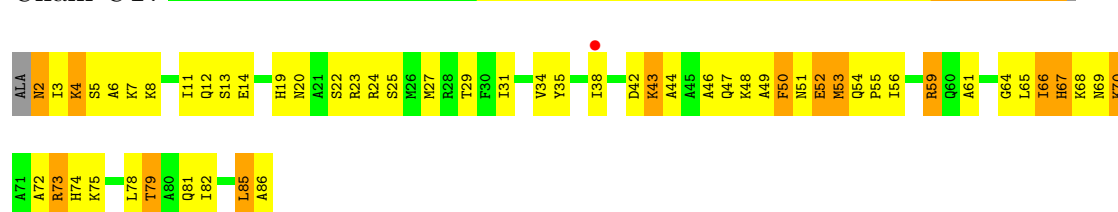
- Molecule 17: 30S ribosomal protein S20

Chain AT:



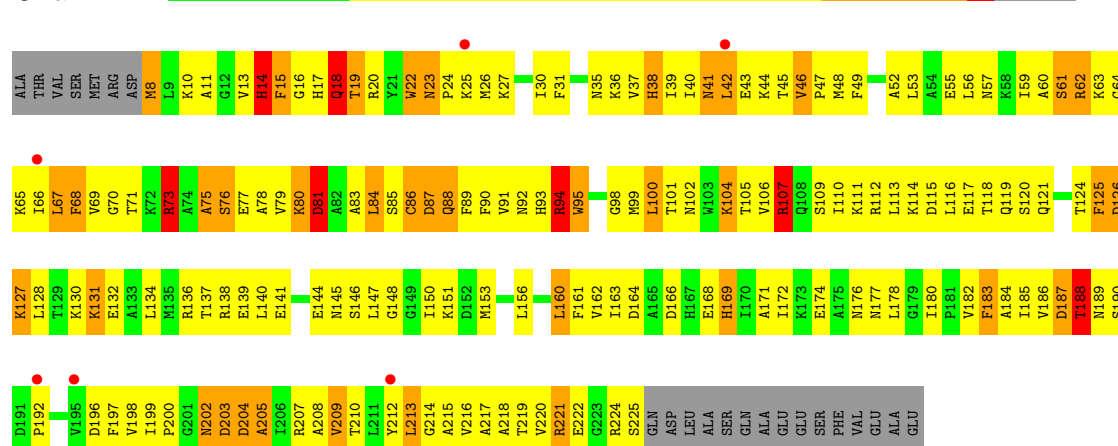
- Molecule 17: 30S ribosomal protein S20

Chain CT:



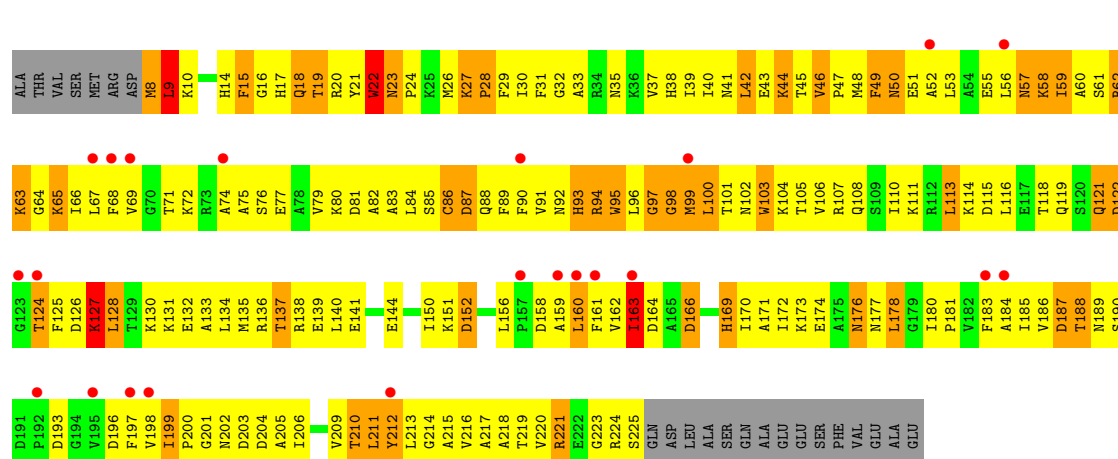
- Molecule 18: 30S ribosomal protein S2

Chain AB:

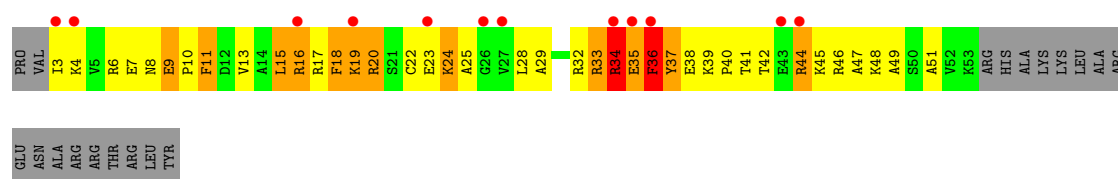


- Molecule 18: 30S ribosomal protein S2

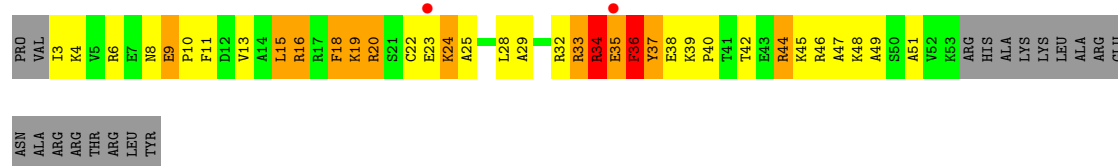
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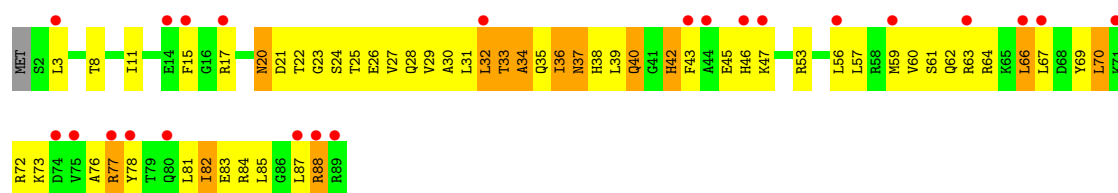
- Molecule 19: 30S ribosomal protein S21

Chain AU: 

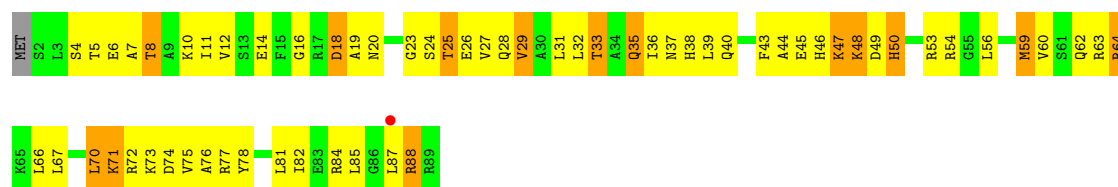
- Molecule 19: 30S ribosomal protein S21

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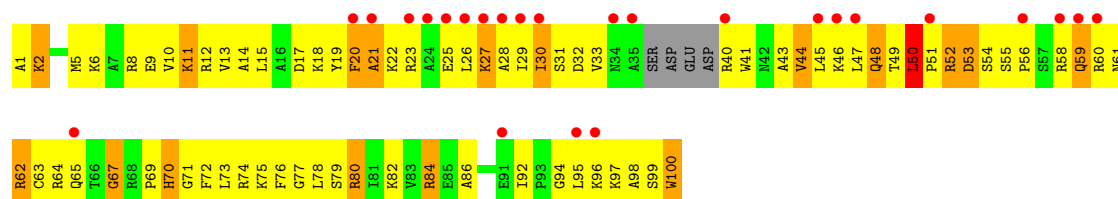
- Molecule 20: 30S ribosomal protein S15

Chain AO: 

- Molecule 20: 30S ribosomal protein S15

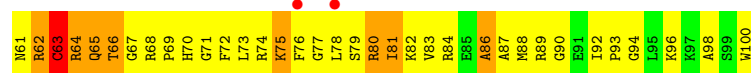
Chain CO: 

- Molecule 21: 30S ribosomal protein S14

Chain AN: 

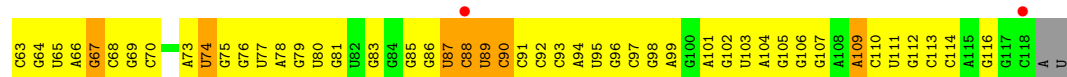
- Molecule 21: 30S ribosomal protein S14

Chain CN: 



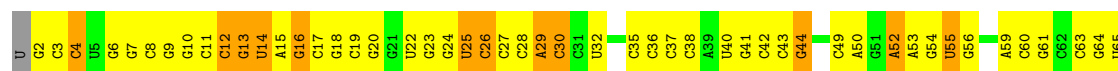
• Molecule 22: 5S rRNA

Chain BA:



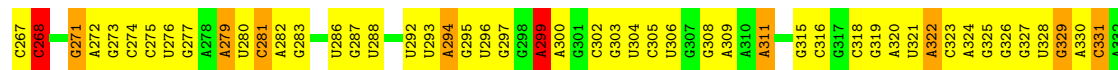
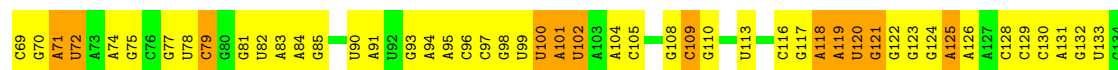
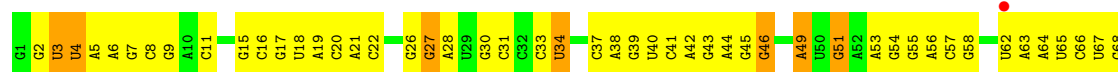
• Molecule 22: 5S rRNA

Chain DA:



• Molecule 23: 23S rRNA

Chain BB:



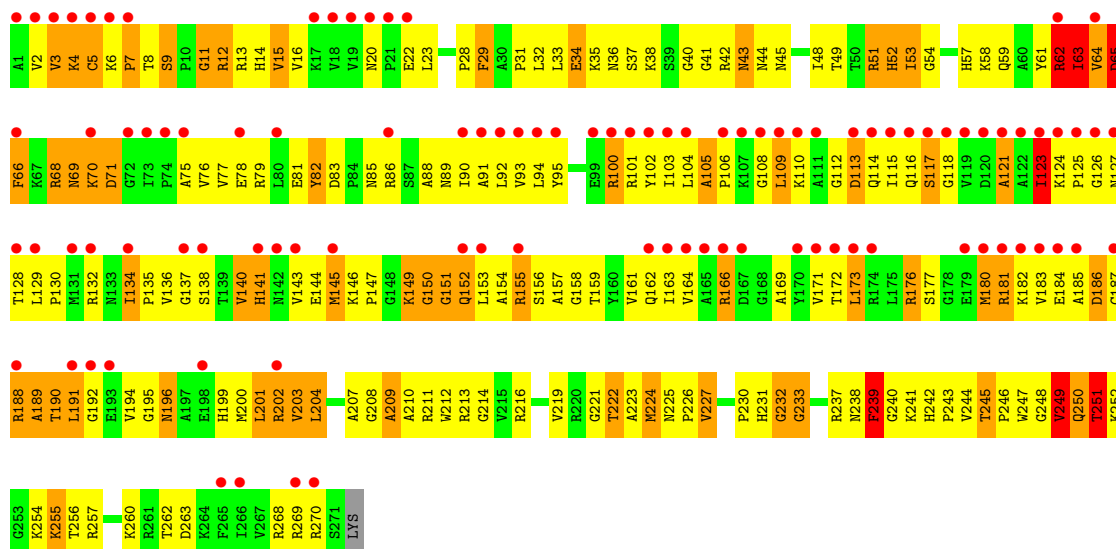


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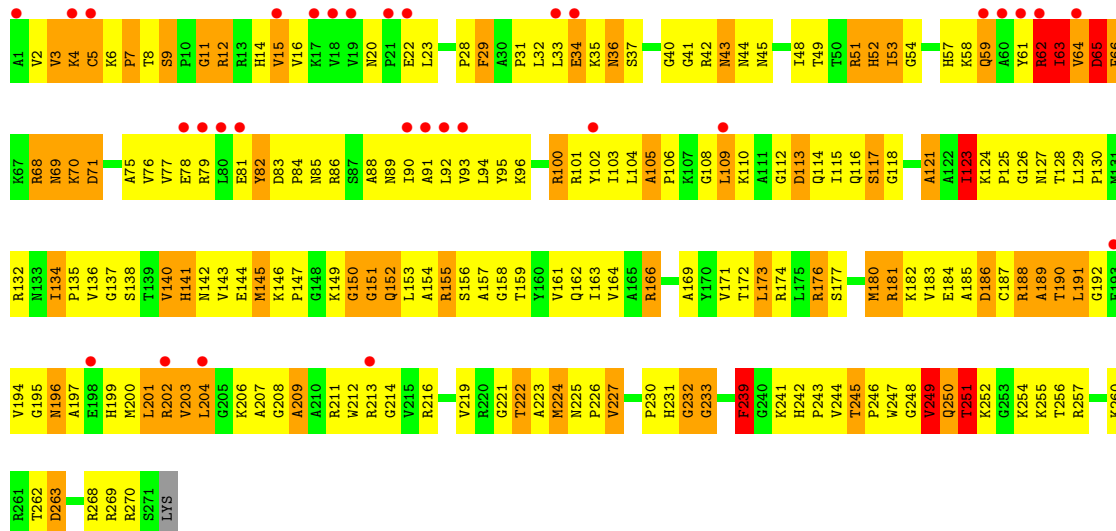
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C2533	C2334	U2274	G2332	C2336	C2333	U2274	G2157	A	U2075	U2004	C1939	C1869	C1806	U1748	C1686	C1625
C2534	C2335	U2275	G2333	C2337	C2334	U2275	G2157	A	U2076	U2005	C1940	C1870	C1807	U1749	C1687	A1626
C2535	C2336	U2276	G2334	C2338	C2335	U2276	G2157	A	U2077	U2006	C1941	C1871	C1808	U1750	C1688	
C2536	C2337	U2277	G2335	C2339	C2336	U2277	G2157	A	U2078	U2007	C1942	C1872	C1809	U1751	C1689	
C2537	C2338	U2278	G2336	C2340	C2337	U2278	G2157	A	U2079	U2008	C1943	C1873	C1810	U1752	C1690	
C2538	C2339	U2279	G2337	C2341	C2338	U2279	G2157	A	U2080	U2009	C1944	C1874	C1811	U1753	C1691	
C2539	C2340	U2280	G2338	C2342	C2339	U2280	G2157	A	U2081	U2010	C1945	C1875	C1812	U1754	C1692	
C2540	C2341	U2281	G2339	C2343	C2340	U2281	G2157	A	U2082	U2011	C1946	C1876	C1813	U1755	C1693	
C2541	C2342	U2282	G2340	C2344	C2341	U2282	G2157	A	U2083	U2012	C1947	C1877	C1814	U1756	C1694	
C2542	C2343	U2283	G2341	C2345	C2342	U2283	G2157	A	U2084	U2013	C1948	C1878	C1815	U1757	C1695	
C2543	C2344	U2284	G2342	C2346	C2343	U2284	G2157	A	U2085	U2014	C1949	C1879	C1816	U1758	C1696	
C2544	C2345	U2285	G2343	C2347	C2344	U2285	G2157	A	U2086	U2015	C1950	C1880	C1817	U1759	C1697	
C2545	C2346	U2286	G2344	C2348	C2345	U2286	G2157	A	U2087	U2016	C1951	C1881	C1818	U1760	C1698	
C2546	C2347	U2287	G2345	C2349	C2346	U2287	G2157	A	U2088	U2017	C1952	C1882	C1819	U1761	C1699	
C2547	C2348	U2288	G2346	C2350	C2347	U2288	G2157	A	U2089	U2018	C1953	C1883	C1820	U1762	C1700	
C2548	C2349	U2289	G2347	C2351	C2348	U2289	G2157	A	U2090	U2019	C1954	C1884	C1821	U1763	C1701	
C2549	C2350	U2290	G2348	C2352	C2349	U2290	G2157	A	U2091	U2020	C1955	C1885	C1822	U1764	C1702	
C2550	C2351	U2291	G2349	C2353	C2350	U2291	G2157	A	U2092	U2021	C1956	C1886	C1823	U1765	C1703	
C2551	C2352	U2292	G2350	C2354	C2351	U2292	G2157	A	U2093	U2022	C1957	C1887	C1824	U1766	C1704	
C2552	C2353	U2293	G2351	C2355	C2352	U2293	G2157	A	U2094	U2023	C1958	C1888	C1825	U1767	C1705	
C2553	C2354	U2294	G2352	C2356	C2353	U2294	G2157	A	U2095	U2024	C1959	C1889	C1826	U1768	C1706	
C2554	C2355	U2295	G2353	C2357	C2354	U2295	G2157	A	U2096	U2025	C1960	C1890	C1827	U1769	C1707	
C2555	C2356	U2296	G2354	C2358	C2355	U2296	G2157	A	U2097	U2026	C1961	C1891	C1828	U1770	C1708	
C2556	C2357	U2297	G2355	C2359	C2356	U2297	G2157	A	U2098	U2027	C1962	C1892	C1829	U1771	C1709	
C2557	C2358	U2298	G2356	C2360	C2357	U2298	G2157	A	U2099	U2028	C1963	C1893	C1830	U1772	C1710	
C2558	C2359	U2299	G2357	C2361	C2358	U2299	G2157	A	U2100	U2029	C1964	C1894	C1831	U1773	C1711	
C2559	C2360	U2300	G2358	C2362	C2359	U2300	G2157	A	U2101	U2030	C1965	C1895	C1832	U1774	C1712	
C2560	C2361	U2301	G2359	C2363	C2360	U2301	G21									





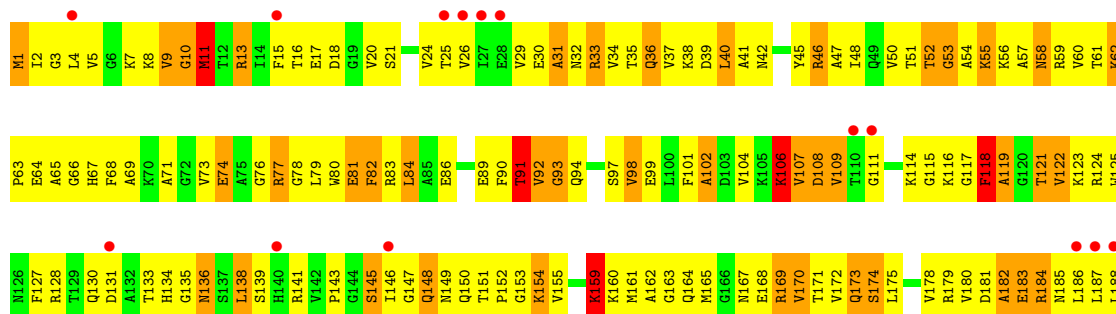
• Molecule 25: 50S ribosomal protein L2

Chain DC:



• Molecule 26: 50S ribosomal protein L3

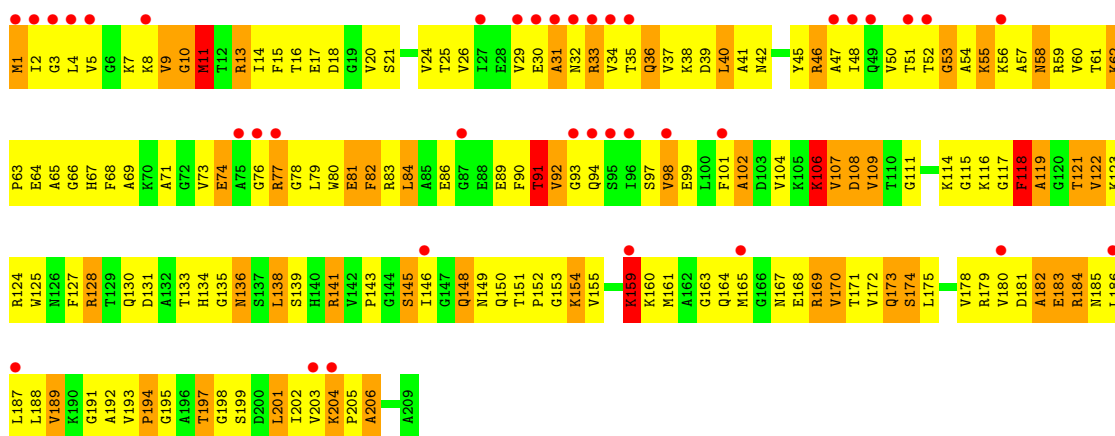
Chain BD:





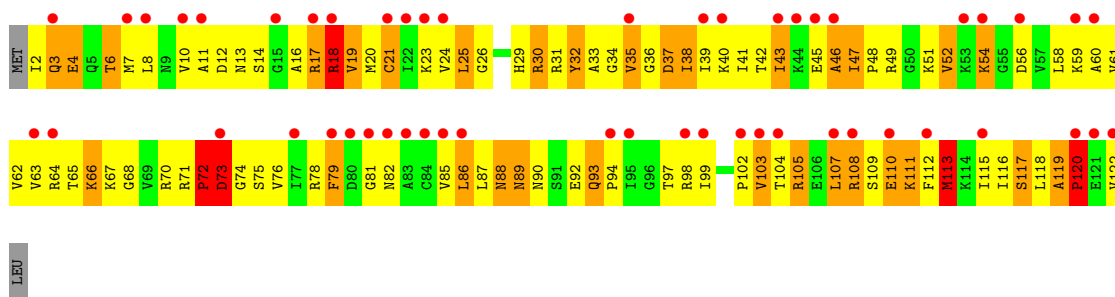
• Molecule 26: 50S ribosomal protein L3

Chain DD:



• Molecule 27: 50S ribosomal protein L14

Chain BK:



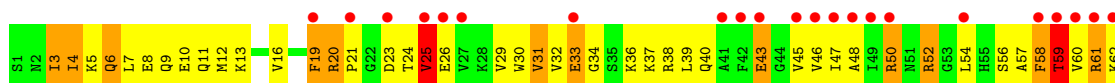
• Molecule 27: 50S ribosomal protein L14

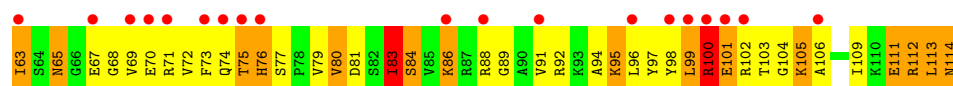
Chain DK:



• Molecule 28: 50S ribosomal protein L19

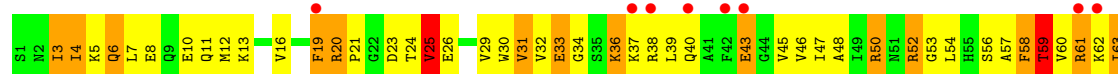
Chain BP:





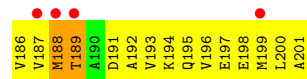
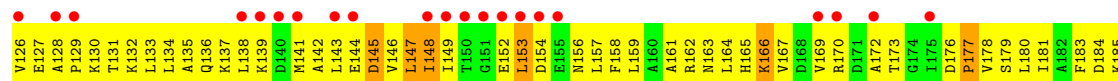
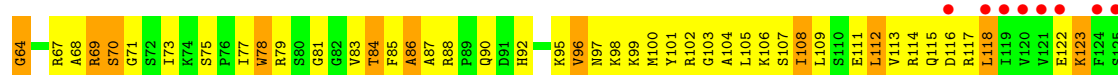
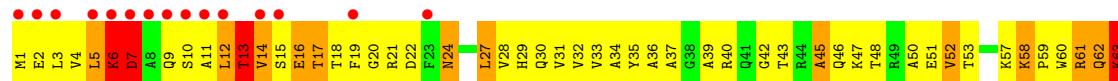
• Molecule 28: 50S ribosomal protein L19

Chain DP:



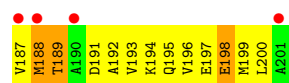
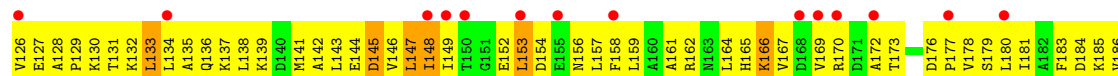
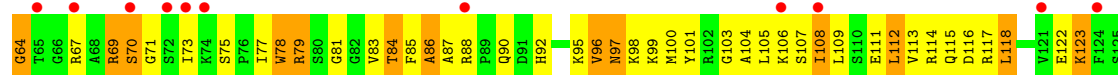
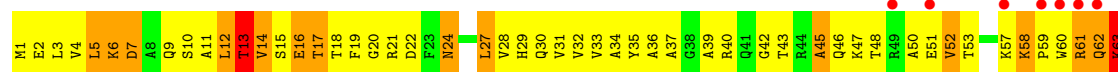
• Molecule 29: 50S ribosomal protein L4

Chain BE:



• Molecule 29: 50S ribosomal protein L4

Chain DE:



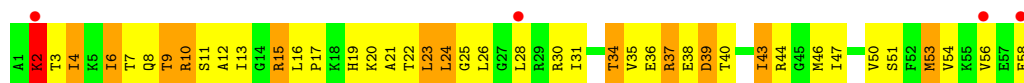
• Molecule 30: 50S ribosomal protein L30

Chain BY:



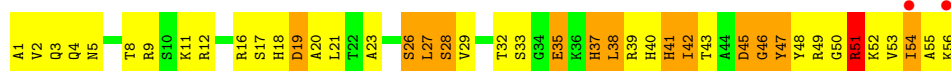
- Molecule 30: 50S ribosomal protein L30

Chain DY:



- Molecule 31: 50S ribosomal protein L32

Chain B0:



- Molecule 31: 50S ribosomal protein L32

Chain D0:



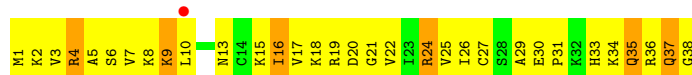
- Molecule 32: 50S ribosomal protein L36

Chain B4:



- Molecule 32: 50S ribosomal protein L36

Chain D4:



- Molecule 33: 50S ribosomal protein L33

Chain B1:



- Molecule 33: 50S ribosomal protein L33

Chain D1:



- Molecule 34: 50S ribosomal protein L35

Chain B3:



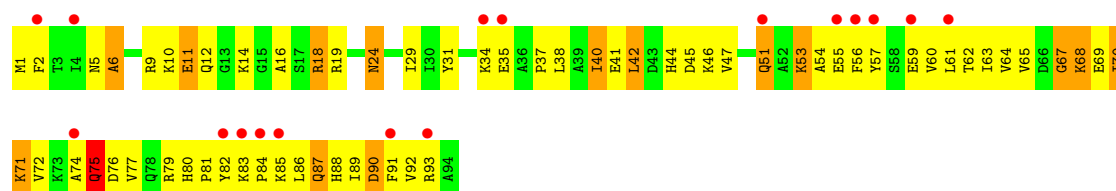
- Molecule 34: 50S ribosomal protein L35

Chain D3:



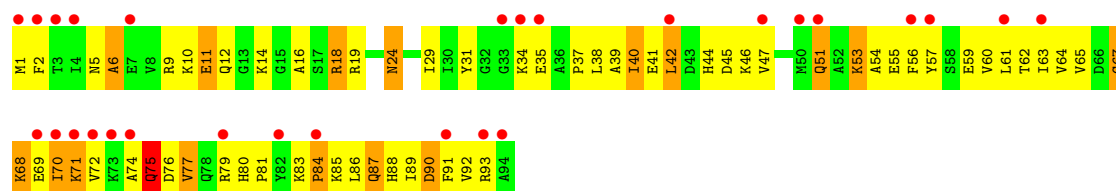
- Molecule 35: 50S ribosomal protein L25

Chain BV:



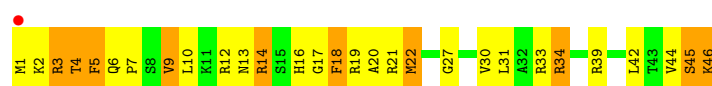
- Molecule 35: 50S ribosomal protein L25

Chain DV:



- Molecule 36: 50S ribosomal protein L34

Chain B2:



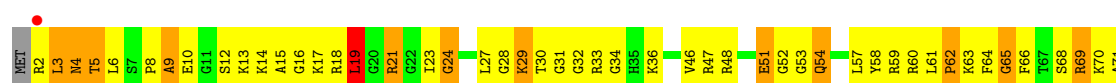
- Molecule 36: 50S ribosomal protein L34

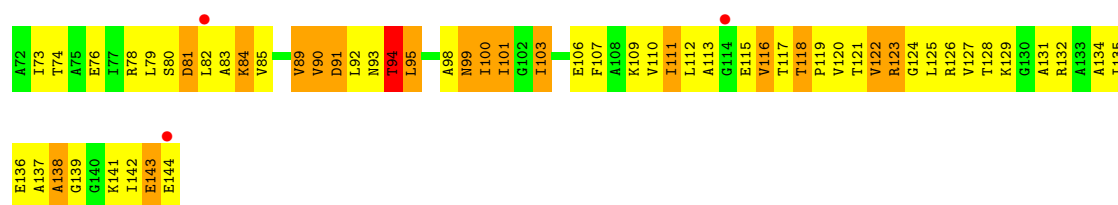
Chain D2:



- Molecule 37: 50S ribosomal protein L15

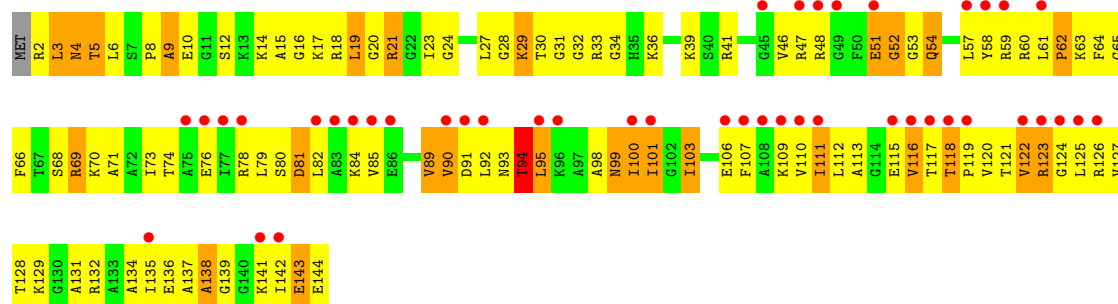
Chain BL:





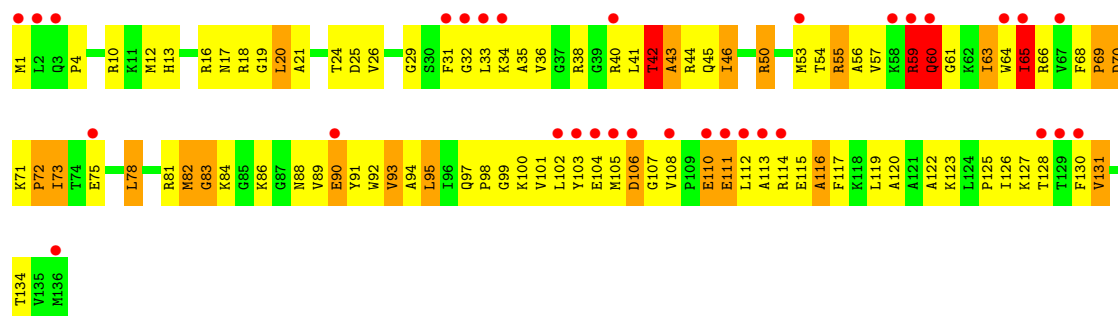
• Molecule 37: 50S ribosomal protein L15

Chain DL:



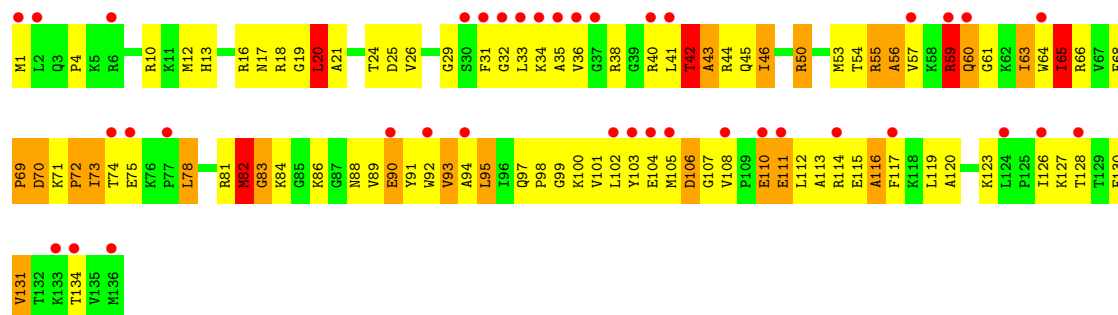
• Molecule 38: 50S ribosomal protein L16

Chain BM:



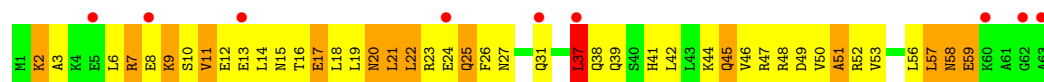
• Molecule 38: 50S ribosomal protein L16

Chain DM:



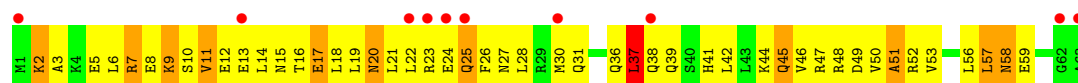
• Molecule 39: 50S ribosomal protein L29

Chain BX:



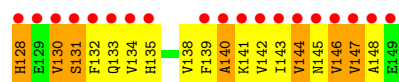
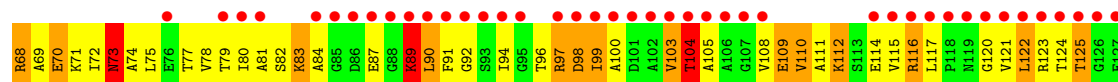
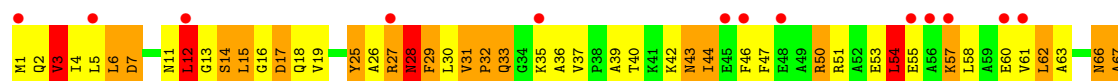
- Molecule 39: 50S ribosomal protein L29

Chain DX:



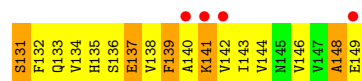
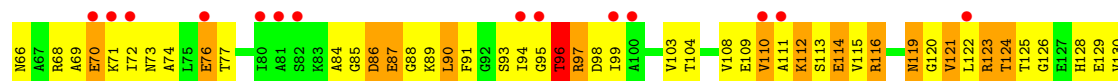
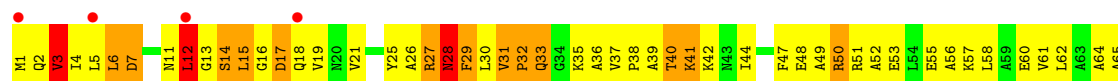
- Molecule 40: 50S ribosomal protein L9

Chain BH:



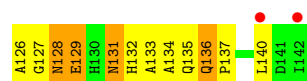
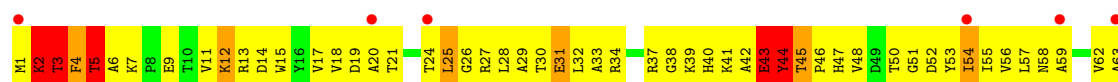
- Molecule 40: 50S ribosomal protein L9

Chain DH:



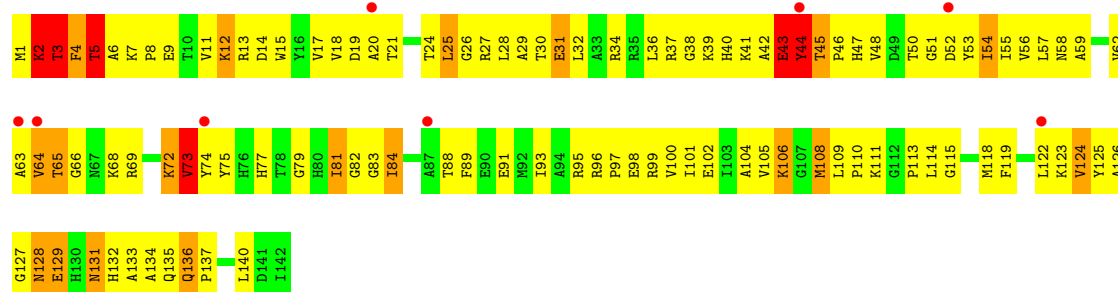
- Molecule 41: 50S ribosomal protein L13

Chain BJ:



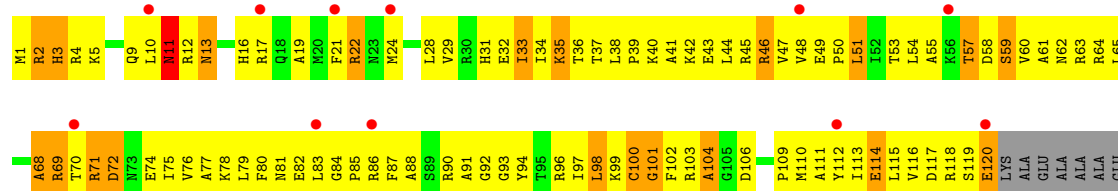
- Molecule 41: 50S ribosomal protein L13

Chain DJ:



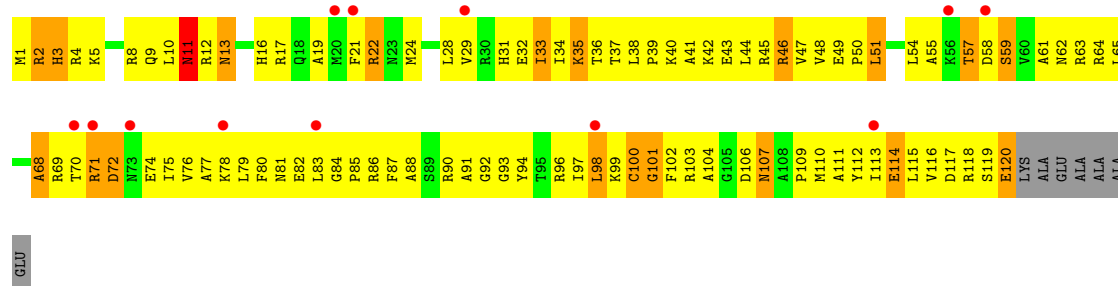
- Molecule 42: 50S ribosomal protein L17

Chain BN:



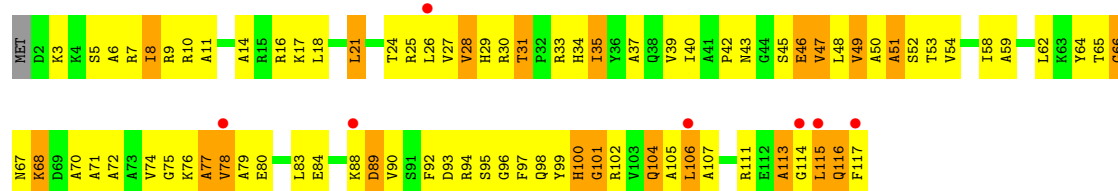
- Molecule 42: 50S ribosomal protein L17

Chain DN:



- Molecule 43: 50S ribosomal protein L18

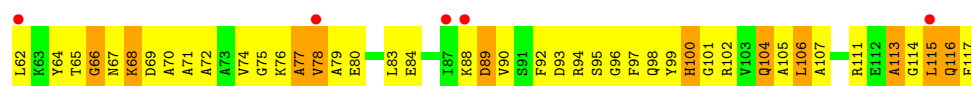
Chain BO:



- Molecule 43: 50S ribosomal protein L18

Chain DO:





• Molecule 44: 50S ribosomal protein L20

Chain BQ:



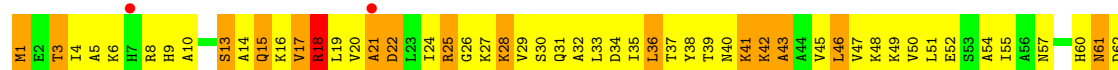
• Molecule 44: 50S ribosomal protein L20

Chain DQ:



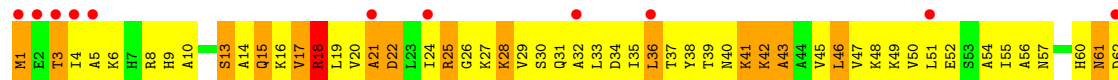
• Molecule 45: 50S ribosomal protein L22

Chain BS:



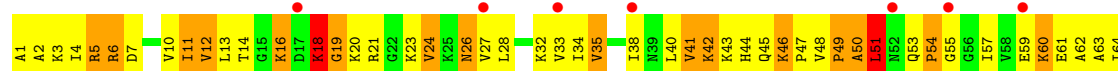
• Molecule 45: 50S ribosomal protein L22

Chain DS:



• Molecule 46: 50S ribosomal protein L24

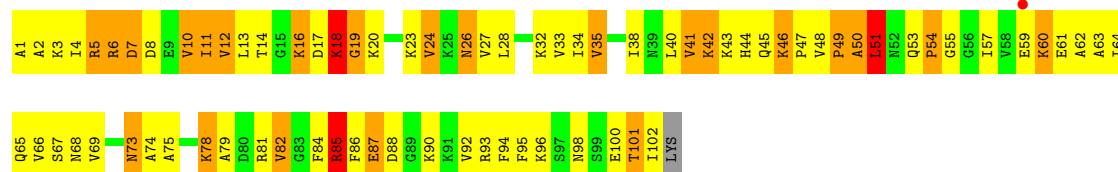
Chain BU:





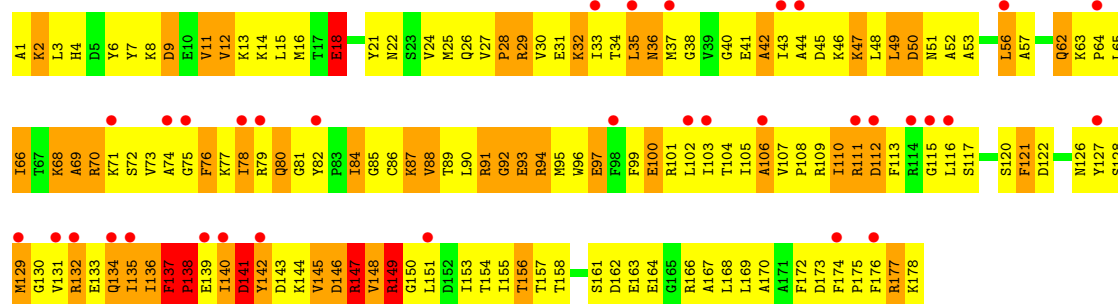
- Molecule 46: 50S ribosomal protein L24

Chain DU:



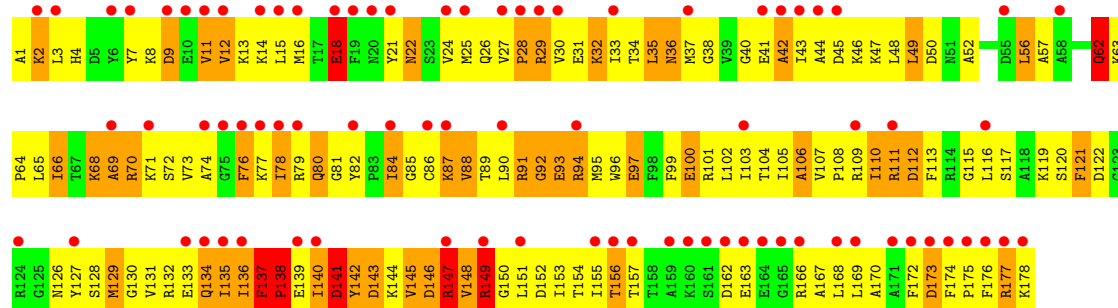
- Molecule 47: 50S ribosomal protein L5

Chain BF:



- Molecule 47: 50S ribosomal protein L5

Chain DF:





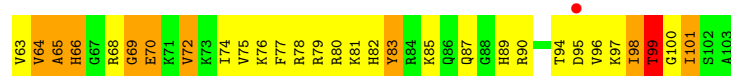
• Molecule 48: 50S ribosomal protein L6

Chain DG:



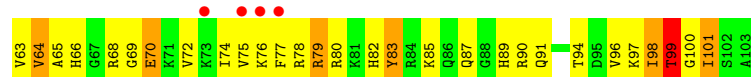
• Molecule 49: 50S ribosomal protein L21

Chain BR:



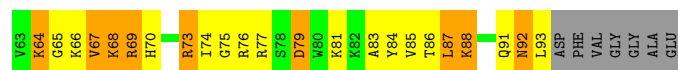
• Molecule 49: 50S ribosomal protein L21

Chain DR:



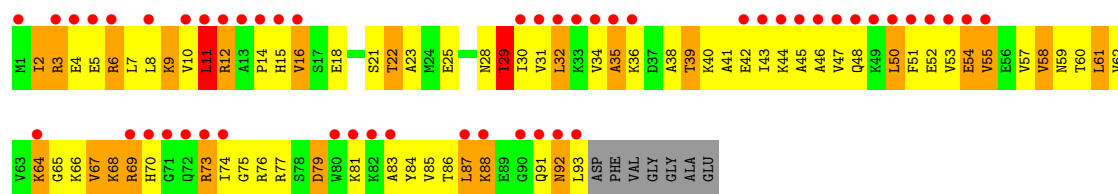
• Molecule 50: 50S ribosomal protein L23

Chain BT:



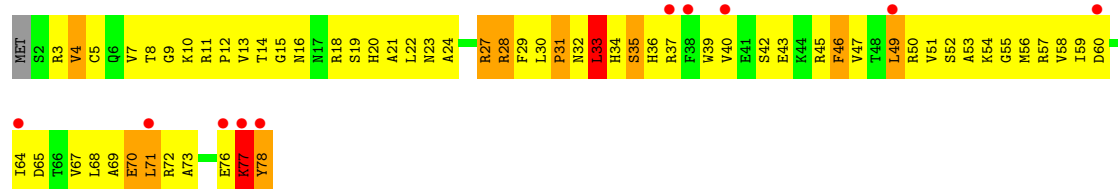
• Molecule 50: 50S ribosomal protein L23

Chain DT:



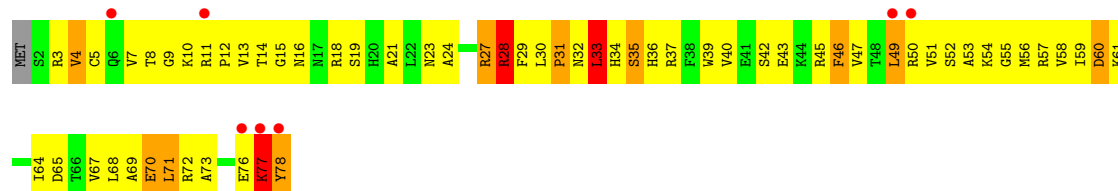
- Molecule 51: 50S ribosomal protein L28

Chain BZ:



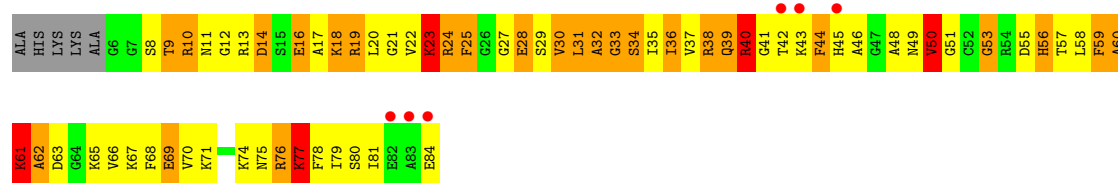
- Molecule 51: 50S ribosomal protein L28

Chain DZ:



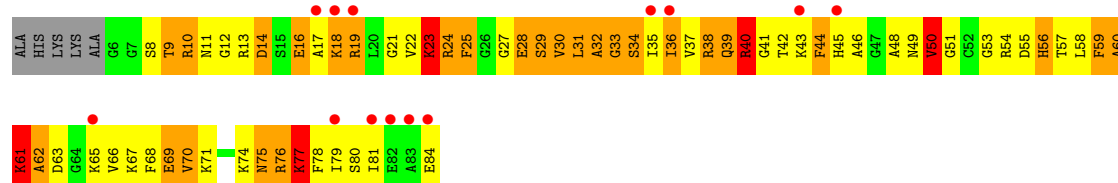
- Molecule 52: 50S ribosomal protein L27

Chain BW:



- Molecule 52: 50S ribosomal protein L27

Chain DW:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.85Å 379.20Å 739.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.00 – 3.93 182.94 – 3.94	Depositor EDS
% Data completeness (in resolution range)	(Not available) (70.00-3.93) 76.0 (182.94-3.94)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 3.89Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.258 , 0.311 0.245 , 0.279	Depositor DCC
R_{free} test set	19247 reflections (5.18%)	DCC
Wilson B-factor (Å ²)	149.7	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 31.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 390843 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	284033	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SCM, ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AA	0.27	2/36762 (0.0%)	0.76	12/57350 (0.0%)
1	CA	0.31	1/36762 (0.0%)	0.77	11/57350 (0.0%)
2	AC	0.23	0/1651	0.45	0/2225
2	CC	0.23	0/1651	0.46	0/2225
3	AD	0.23	0/1665	0.44	0/2227
3	CD	0.23	0/1665	0.44	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	0.45	0/1128
5	CF	0.24	0/835	0.45	0/1128
6	AG	0.23	0/1187	0.45	0/1591
6	CG	0.23	0/1211	0.45	0/1624
7	AH	0.23	0/989	0.44	0/1326
7	CH	0.23	0/989	0.44	0/1326
8	AI	0.24	0/1034	0.44	0/1375
8	CI	0.24	0/1034	0.45	0/1375
9	AJ	0.22	0/796	0.48	0/1077
9	CJ	0.22	0/796	0.48	0/1077
10	AK	0.24	0/893	0.44	0/1205
10	CK	0.24	0/893	0.44	0/1205
11	AL	0.22	0/969	0.48	0/1300
11	CL	0.22	0/969	0.48	0/1300
12	AM	0.21	0/892	0.45	0/1193
12	CM	0.21	0/884	0.45	0/1181
13	AP	0.25	0/659	0.45	0/884
13	CP	0.25	0/648	0.44	0/870
14	AQ	0.23	0/657	0.46	0/881
14	CQ	0.24	0/666	0.46	0/892
15	AR	0.23	0/462	0.46	0/621
15	CR	0.23	0/462	0.46	0/621
16	AS	0.25	0/652	0.46	0/877
16	CS	0.25	0/660	0.49	0/888

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AT	0.23	0/671	0.40	0/888
17	CT	0.23	0/671	0.40	0/888
18	AB	0.25	0/1735	0.45	0/2338
18	CB	0.25	0/1735	0.45	0/2338
19	AU	0.26	0/430	0.46	0/570
19	CU	0.25	0/430	0.46	0/570
20	AO	0.22	0/722	0.45	0/964
20	CO	0.23	0/722	0.44	0/964
21	AN	0.24	0/785	0.44	0/1043
21	CN	0.24	0/785	0.46	0/1043
22	BA	0.23	0/2803	0.74	1/4371 (0.0%)
22	DA	0.24	0/2803	0.75	1/4371 (0.0%)
23	BB	0.28	5/68314 (0.0%)	0.77	33/106569 (0.0%)
23	DB	0.28	5/68314 (0.0%)	0.77	33/106569 (0.0%)
24	BI	0.24	0/1046	0.46	0/1410
24	DI	0.25	0/1046	0.47	0/1410
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	0.48	0/2134
26	DD	0.24	0/1586	0.48	0/2134
27	BK	0.24	0/939	0.53	0/1258
27	DK	0.24	0/939	0.53	0/1258
28	BP	0.24	0/929	0.49	0/1242
28	DP	0.24	0/929	0.49	0/1242
29	BE	0.24	0/1571	0.48	0/2113
29	DE	0.24	0/1571	0.48	0/2113
30	BY	0.24	0/453	0.49	0/605
30	DY	0.23	0/453	0.49	0/605
31	B0	0.23	0/450	0.51	0/599
31	D0	0.23	0/450	0.51	0/599
32	B4	0.22	0/303	0.49	0/397
32	D4	0.23	0/303	0.49	0/397
33	B1	0.27	0/416	0.48	0/554
33	D1	0.27	0/416	0.48	0/554
34	B3	0.24	0/513	0.46	0/676
34	D3	0.24	0/513	0.46	0/676
35	BV	0.25	0/766	0.43	0/1025
35	DV	0.25	0/766	0.43	0/1025
36	B2	0.26	0/380	0.47	0/498
36	D2	0.26	0/380	0.47	0/498
37	BL	0.24	0/1054	0.48	0/1403
37	DL	0.24	0/1054	0.48	0/1403
38	BM	0.25	0/1093	0.47	0/1460

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DM	0.25	0/1093	0.47	0/1460
39	BX	0.24	0/510	0.50	0/677
39	DX	0.23	0/510	0.50	0/677
40	BH	0.25	0/1122	0.47	0/1515
40	DH	0.25	0/1122	0.47	0/1515
41	BJ	0.23	0/1152	0.47	0/1551
41	DJ	0.23	0/1152	0.47	0/1551
42	BN	0.24	0/973	0.49	0/1301
42	DN	0.24	0/973	0.49	0/1301
43	BO	0.23	0/902	0.47	0/1209
43	DO	0.23	0/902	0.47	0/1209
44	BQ	0.25	0/960	0.47	0/1278
44	DQ	0.25	0/960	0.47	0/1278
45	BS	0.22	0/864	0.50	0/1156
45	DS	0.22	0/864	0.50	0/1156
46	BU	0.25	0/787	0.45	0/1051
46	DU	0.25	0/787	0.45	0/1051
47	BF	0.26	0/1444	0.49	0/1937
47	DF	0.26	0/1444	0.49	0/1937
48	BG	0.23	0/1343	0.47	0/1816
48	DG	0.23	0/1343	0.47	0/1816
49	BR	0.26	0/829	0.48	0/1107
49	DR	0.25	0/829	0.48	0/1107
50	BT	0.23	0/744	0.51	0/994
50	DT	0.23	0/744	0.51	0/994
51	BZ	0.25	0/635	0.49	0/848
51	DZ	0.25	0/635	0.50	0/848
52	BW	0.28	0/603	0.49	0/797
52	DW	0.28	0/603	0.49	0/797
All	All	0.27	13/306360 (0.0%)	0.70	91/457969 (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	15
1	CA	0	19
23	BB	0	37
23	DB	0	37
All	All	0	108

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	DB	1086	A	C5-C6	-16.20	1.26	1.41
23	BB	1086	A	C5-C6	-16.10	1.26	1.41
23	DB	1088	A	C6-N1	-10.51	1.28	1.35
23	BB	1088	A	C6-N1	-10.50	1.28	1.35
23	BB	1060	U	C2-N3	7.92	1.43	1.37

The worst 5 of 91 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	DB	2204	G	O5'-P-OP1	-30.02	74.68	110.70
23	BB	2204	G	O5'-P-OP2	-28.49	76.52	110.70
23	DB	2791	G	O5'-P-OP2	-28.43	76.59	110.70
23	BB	2791	G	O5'-P-OP1	-27.42	77.80	110.70
23	DB	2204	G	O5'-P-OP2	17.65	131.88	110.70

There are no chirality outliers.

5 of 108 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	187	G	Sidechain
1	AA	281	G	Sidechain
1	AA	437	U	Sidechain
1	AA	438	U	Sidechain
1	AA	450	G	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	1458	0
1	CA	32831	0	16521	1414	0
2	AC	1624	0	1699	205	0
2	CC	1624	0	1699	191	0
3	AD	1643	0	1710	179	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	CD	1643	0	1710	177	0
4	AE	1105	0	1148	129	0
4	CE	1105	0	1148	121	0
5	AF	817	0	808	89	0
5	CF	817	0	808	91	0
6	AG	1174	0	1230	146	0
6	CG	1196	0	1246	133	0
7	AH	979	0	1034	89	0
7	CH	979	0	1034	91	0
8	AI	1022	0	1070	180	0
8	CI	1022	0	1070	146	0
9	AJ	786	0	828	85	0
9	CJ	786	0	828	103	0
10	AK	877	0	887	110	0
10	CK	877	0	887	100	0
11	AL	955	0	1019	96	0
11	CL	955	0	1019	97	0
12	AM	883	0	944	135	0
12	CM	876	0	937	138	0
13	AP	649	0	666	65	0
13	CP	638	0	656	66	0
14	AQ	648	0	691	63	0
14	CQ	657	0	702	62	0
15	AR	455	0	478	35	0
15	CR	455	0	478	37	0
16	AS	637	0	665	97	0
16	CS	644	0	675	115	0
17	AT	665	0	714	60	0
17	CT	665	0	714	61	0
18	AB	1704	0	1732	209	0
18	CB	1704	0	1732	229	0
19	AU	425	0	449	57	0
19	CU	425	0	449	54	0
20	AO	714	0	734	63	0
20	CO	714	0	734	62	0
21	AN	774	0	827	102	0
21	CN	774	0	827	114	0
22	BA	2507	0	1270	116	0
22	DA	2507	0	1270	111	0
23	BB	60995	0	30679	2412	0
23	DB	60995	0	30678	2455	0
24	BI	1032	0	1088	109	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	DI	1032	0	1088	168	0
25	BC	2082	0	2157	234	0
25	DC	2082	0	2157	239	0
26	BD	1565	0	1616	234	0
26	DD	1565	0	1616	239	0
27	BK	930	0	1000	153	0
27	DK	930	0	1000	154	0
28	BP	917	0	965	126	0
28	DP	917	0	965	132	0
29	BE	1552	0	1619	208	0
29	DE	1552	0	1619	202	0
30	BY	449	0	491	59	0
30	DY	449	0	491	53	0
31	B0	444	0	461	48	0
31	D0	444	0	461	44	0
32	B4	302	0	340	42	0
32	D4	302	0	340	43	0
33	B1	409	0	440	54	0
33	D1	409	0	440	50	0
34	B3	504	0	574	47	0
34	D3	504	0	574	52	0
35	BV	753	0	780	83	0
35	DV	753	0	780	86	0
36	B2	377	0	418	37	0
36	D2	377	0	418	43	0
37	BL	1045	0	1117	138	0
37	DL	1045	0	1117	144	0
38	BM	1074	0	1157	123	0
38	DM	1074	0	1157	119	0
39	BX	509	0	543	46	0
39	DX	509	0	543	50	0
40	BH	1111	0	1148	172	0
40	DH	1111	0	1148	147	0
41	BJ	1129	0	1162	134	0
41	DJ	1129	0	1162	141	0
42	BN	960	0	1000	137	0
42	DN	960	0	1000	133	0
43	BO	892	0	923	91	0
43	DO	892	0	923	94	0
44	BQ	947	0	1022	150	0
44	DQ	947	0	1022	143	0
45	BS	857	0	922	97	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	DS	857	0	922	98	0
46	BU	779	0	834	116	0
46	DU	779	0	834	114	0
47	BF	1420	0	1460	264	0
47	DF	1420	0	1460	249	0
48	BG	1323	0	1374	187	0
48	DG	1323	0	1374	178	0
49	BR	816	0	839	105	0
49	DR	816	0	839	112	0
50	BT	738	0	807	115	0
50	DT	738	0	807	110	0
51	BZ	625	0	652	75	0
51	DZ	625	0	652	71	0
52	BW	596	0	610	122	0
52	DW	596	0	610	130	0
53	AA	60	0	0	0	0
53	BB	110	0	0	0	0
53	CA	58	0	0	0	0
53	CE	1	0	0	0	0
53	DB	110	0	0	0	0
53	DN	1	0	0	0	0
54	AA	23	0	24	2	0
54	CA	23	0	24	1	0
55	B4	1	0	0	0	0
55	D4	1	0	0	0	0
56	AA	288	0	0	6	0
56	AE	3	0	0	1	0
56	AK	1	0	0	0	0
56	AL	4	0	0	0	0
56	AN	2	0	0	0	0
56	AP	1	0	0	0	0
56	AT	1	0	0	0	0
56	BB	494	0	0	4	0
56	BC	4	0	0	0	0
56	BE	3	0	0	0	0
56	BH	1	0	0	0	0
56	BL	4	0	0	0	0
56	BT	1	0	0	0	0
56	CA	275	0	0	4	0
56	CE	4	0	0	0	0
56	CK	1	0	0	0	0
56	CL	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	CN	5	0	0	0	0
56	CP	1	0	0	0	0
56	CT	2	0	0	0	0
56	DB	500	0	0	9	0
56	DC	3	0	0	0	0
56	DD	1	0	0	0	0
56	DE	1	0	0	0	0
56	DJ	1	0	0	0	0
56	DL	3	0	0	0	0
56	DN	2	0	0	0	0
56	DP	1	0	0	0	0
56	DR	1	0	0	0	0
All	All	284033	0	190711	17874	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 38.

The worst 5 of 17874 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:DB:1099:G:H8	24:DI:3:LYS:N	1.36	1.21
23:BB:855:G:H21	52:BW:23:LYS:HG2	1.11	1.13
23:DB:322:A:H5'	23:DB:340:A:H1'	1.32	1.12
2:AC:70:ALA:HA	2:AC:105:VAL:HG21	1.26	1.11
23:BB:1205:A:H62	29:BE:165:HIS:HB2	1.11	1.10

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%)	112 (55%)	56 (28%)	36 (18%)	0 5
2	CC	204/232 (88%)	134 (66%)	48 (24%)	22 (11%)	1 17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AD	203/205 (99%)	133 (66%)	58 (29%)	12 (6%)	2	38
3	CD	203/205 (99%)	132 (65%)	58 (29%)	13 (6%)	2	36
4	AE	148/166 (89%)	109 (74%)	30 (20%)	9 (6%)	2	37
4	CE	148/166 (89%)	108 (73%)	31 (21%)	9 (6%)	2	37
5	AF	98/135 (73%)	62 (63%)	27 (28%)	9 (9%)	1	24
5	CF	98/135 (73%)	64 (65%)	25 (26%)	9 (9%)	1	24
6	AG	148/178 (83%)	98 (66%)	44 (30%)	6 (4%)	4	49
6	CG	150/178 (84%)	101 (67%)	36 (24%)	13 (9%)	1	25
7	AH	127/129 (98%)	86 (68%)	35 (28%)	6 (5%)	4	45
7	CH	127/129 (98%)	85 (67%)	36 (28%)	6 (5%)	4	45
8	AI	125/129 (97%)	84 (67%)	25 (20%)	16 (13%)	0	13
8	CI	125/129 (97%)	89 (71%)	30 (24%)	6 (5%)	4	44
9	AJ	96/103 (93%)	61 (64%)	18 (19%)	17 (18%)	0	5
9	CJ	96/103 (93%)	62 (65%)	21 (22%)	13 (14%)	0	11
10	AK	115/128 (90%)	85 (74%)	26 (23%)	4 (4%)	6	55
10	CK	115/128 (90%)	84 (73%)	25 (22%)	6 (5%)	3	42
11	AL	121/123 (98%)	71 (59%)	34 (28%)	16 (13%)	0	12
11	CL	121/123 (98%)	72 (60%)	33 (27%)	16 (13%)	0	12
12	AM	112/117 (96%)	69 (62%)	36 (32%)	7 (6%)	2	37
12	CM	111/117 (95%)	77 (69%)	23 (21%)	11 (10%)	1	20
13	AP	80/82 (98%)	53 (66%)	18 (22%)	9 (11%)	1	16
13	CP	78/82 (95%)	53 (68%)	19 (24%)	6 (8%)	1	29
14	AQ	78/83 (94%)	61 (78%)	14 (18%)	3 (4%)	5	52
14	CQ	79/83 (95%)	62 (78%)	15 (19%)	2 (2%)	9	62
15	AR	53/74 (72%)	33 (62%)	17 (32%)	3 (6%)	3	39
15	CR	53/74 (72%)	33 (62%)	16 (30%)	4 (8%)	2	30
16	AS	77/91 (85%)	49 (64%)	21 (27%)	7 (9%)	1	24
16	CS	78/91 (86%)	51 (65%)	20 (26%)	7 (9%)	1	24
17	AT	83/86 (96%)	62 (75%)	16 (19%)	5 (6%)	2	38
17	CT	83/86 (96%)	63 (76%)	14 (17%)	6 (7%)	2	32
18	AB	216/240 (90%)	140 (65%)	53 (24%)	23 (11%)	1	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	CB	216/240 (90%)	135 (62%)	59 (27%)	22 (10%)	1	19
19	AU	49/70 (70%)	29 (59%)	13 (26%)	7 (14%)	0	10
19	CU	49/70 (70%)	29 (59%)	15 (31%)	5 (10%)	1	19
20	AO	86/89 (97%)	55 (64%)	24 (28%)	7 (8%)	1	27
20	CO	86/89 (97%)	50 (58%)	29 (34%)	7 (8%)	1	27
21	AN	92/100 (92%)	54 (59%)	29 (32%)	9 (10%)	1	21
21	CN	92/100 (92%)	45 (49%)	31 (34%)	16 (17%)	0	5
24	BI	139/141 (99%)	118 (85%)	16 (12%)	5 (4%)	5	54
24	DI	139/141 (99%)	115 (83%)	19 (14%)	5 (4%)	5	54
25	BC	269/272 (99%)	149 (55%)	68 (25%)	52 (19%)	0	4
25	DC	269/272 (99%)	147 (55%)	70 (26%)	52 (19%)	0	4
26	BD	207/209 (99%)	113 (55%)	58 (28%)	36 (17%)	0	5
26	DD	207/209 (99%)	114 (55%)	58 (28%)	35 (17%)	0	6
27	BK	119/123 (97%)	73 (61%)	24 (20%)	22 (18%)	0	5
27	DK	119/123 (97%)	73 (61%)	25 (21%)	21 (18%)	0	5
28	BP	112/114 (98%)	67 (60%)	28 (25%)	17 (15%)	0	8
28	DP	112/114 (98%)	66 (59%)	31 (28%)	15 (13%)	0	11
29	BE	199/201 (99%)	120 (60%)	49 (25%)	30 (15%)	0	8
29	DE	199/201 (99%)	123 (62%)	47 (24%)	29 (15%)	0	9
30	BY	56/58 (97%)	36 (64%)	16 (29%)	4 (7%)	2	32
30	DY	56/58 (97%)	36 (64%)	14 (25%)	6 (11%)	1	17
31	B0	54/56 (96%)	34 (63%)	10 (18%)	10 (18%)	0	5
31	D0	54/56 (96%)	35 (65%)	9 (17%)	10 (18%)	0	5
32	B4	36/38 (95%)	19 (53%)	13 (36%)	4 (11%)	1	16
32	D4	36/38 (95%)	19 (53%)	13 (36%)	4 (11%)	1	16
33	B1	48/54 (89%)	36 (75%)	8 (17%)	4 (8%)	1	27
33	D1	48/54 (89%)	35 (73%)	9 (19%)	4 (8%)	1	27
34	B3	62/64 (97%)	34 (55%)	20 (32%)	8 (13%)	0	13
34	D3	62/64 (97%)	35 (56%)	19 (31%)	8 (13%)	0	13
35	BV	92/94 (98%)	60 (65%)	25 (27%)	7 (8%)	2	29
35	DV	92/94 (98%)	61 (66%)	24 (26%)	7 (8%)	2	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	B2	44/46 (96%)	23 (52%)	16 (36%)	5 (11%)	1	15
36	D2	44/46 (96%)	23 (52%)	12 (27%)	9 (20%)	0	4
37	BL	141/144 (98%)	76 (54%)	37 (26%)	28 (20%)	0	4
37	DL	141/144 (98%)	76 (54%)	39 (28%)	26 (18%)	0	5
38	BM	134/136 (98%)	79 (59%)	39 (29%)	16 (12%)	1	14
38	DM	134/136 (98%)	82 (61%)	35 (26%)	17 (13%)	0	13
39	BX	61/63 (97%)	35 (57%)	20 (33%)	6 (10%)	1	21
39	DX	61/63 (97%)	35 (57%)	20 (33%)	6 (10%)	1	21
40	BH	147/149 (99%)	78 (53%)	42 (29%)	27 (18%)	0	5
40	DH	147/149 (99%)	91 (62%)	30 (20%)	26 (18%)	0	5
41	BJ	140/142 (99%)	85 (61%)	37 (26%)	18 (13%)	0	13
41	DJ	140/142 (99%)	85 (61%)	36 (26%)	19 (14%)	0	11
42	BN	118/127 (93%)	73 (62%)	33 (28%)	12 (10%)	1	19
42	DN	118/127 (93%)	74 (63%)	33 (28%)	11 (9%)	1	23
43	BO	114/117 (97%)	68 (60%)	28 (25%)	18 (16%)	0	7
43	DO	114/117 (97%)	66 (58%)	30 (26%)	18 (16%)	0	7
44	BQ	115/117 (98%)	76 (66%)	29 (25%)	10 (9%)	1	25
44	DQ	115/117 (98%)	76 (66%)	30 (26%)	9 (8%)	1	29
45	BS	108/110 (98%)	59 (55%)	34 (32%)	15 (14%)	0	10
45	DS	108/110 (98%)	60 (56%)	33 (31%)	15 (14%)	0	10
46	BU	100/103 (97%)	58 (58%)	25 (25%)	17 (17%)	0	6
46	DU	100/103 (97%)	57 (57%)	24 (24%)	19 (19%)	0	4
47	BF	176/178 (99%)	91 (52%)	51 (29%)	34 (19%)	0	4
47	DF	176/178 (99%)	93 (53%)	49 (28%)	34 (19%)	0	4
48	BG	174/176 (99%)	100 (58%)	42 (24%)	32 (18%)	0	5
48	DG	174/176 (99%)	101 (58%)	42 (24%)	31 (18%)	0	5
49	BR	101/103 (98%)	57 (56%)	26 (26%)	18 (18%)	0	5
49	DR	101/103 (98%)	58 (57%)	26 (26%)	17 (17%)	0	6
50	BT	91/100 (91%)	40 (44%)	40 (44%)	11 (12%)	1	14
50	DT	91/100 (91%)	41 (45%)	39 (43%)	11 (12%)	1	14
51	BZ	75/78 (96%)	53 (71%)	16 (21%)	6 (8%)	1	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	DZ	75/78 (96%)	54 (72%)	14 (19%)	7 (9%)	1	23
52	BW	77/84 (92%)	29 (38%)	24 (31%)	24 (31%)	0	0
52	DW	77/84 (92%)	27 (35%)	26 (34%)	24 (31%)	0	0
All	All	11241/11914 (94%)	6932 (62%)	2908 (26%)	1401 (12%)	1	13

5 of 1401 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AC	14	VAL
2	AC	19	SER
2	AC	26	LYS
2	AC	47	ALA
2	AC	54	ILE

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%)	139 (82%)	31 (18%)	2	19
2	CC	170/189 (90%)	134 (79%)	36 (21%)	1	12
3	AD	172/172 (100%)	145 (84%)	27 (16%)	4	28
3	CD	172/172 (100%)	146 (85%)	26 (15%)	4	30
4	AE	113/125 (90%)	93 (82%)	20 (18%)	3	20
4	CE	113/125 (90%)	93 (82%)	20 (18%)	3	20
5	AF	87/116 (75%)	76 (87%)	11 (13%)	7	39
5	CF	87/116 (75%)	75 (86%)	12 (14%)	5	35
6	AG	123/146 (84%)	102 (83%)	21 (17%)	3	23
6	CG	125/146 (86%)	98 (78%)	27 (22%)	1	11
7	AH	104/104 (100%)	95 (91%)	9 (9%)	15	59
7	CH	104/104 (100%)	95 (91%)	9 (9%)	15	59
8	AI	105/106 (99%)	78 (74%)	27 (26%)	1	8
8	CI	105/106 (99%)	79 (75%)	26 (25%)	1	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	AJ	86/90 (96%)	73 (85%)	13 (15%)	4	30
9	CJ	86/90 (96%)	72 (84%)	14 (16%)	3	26
10	AK	90/98 (92%)	73 (81%)	17 (19%)	2	17
10	CK	90/98 (92%)	73 (81%)	17 (19%)	2	17
11	AL	103/103 (100%)	87 (84%)	16 (16%)	4	28
11	CL	103/103 (100%)	87 (84%)	16 (16%)	4	28
12	AM	92/95 (97%)	72 (78%)	20 (22%)	1	11
12	CM	91/95 (96%)	75 (82%)	16 (18%)	3	21
13	AP	65/65 (100%)	61 (94%)	4 (6%)	26	74
13	CP	65/65 (100%)	61 (94%)	4 (6%)	26	74
14	AQ	74/77 (96%)	63 (85%)	11 (15%)	4	31
14	CQ	75/77 (97%)	63 (84%)	12 (16%)	3	27
15	AR	48/64 (75%)	41 (85%)	7 (15%)	5	31
15	CR	48/64 (75%)	40 (83%)	8 (17%)	3	24
16	AS	70/78 (90%)	49 (70%)	21 (30%)	0	5
16	CS	71/78 (91%)	51 (72%)	20 (28%)	0	5
17	AT	65/65 (100%)	51 (78%)	14 (22%)	1	12
17	CT	65/65 (100%)	51 (78%)	14 (22%)	1	12
18	AB	180/198 (91%)	141 (78%)	39 (22%)	1	11
18	CB	180/198 (91%)	133 (74%)	47 (26%)	1	7
19	AU	44/60 (73%)	31 (70%)	13 (30%)	0	5
19	CU	44/60 (73%)	32 (73%)	12 (27%)	0	6
20	AO	76/77 (99%)	65 (86%)	11 (14%)	5	32
20	CO	76/77 (99%)	61 (80%)	15 (20%)	2	15
21	AN	79/83 (95%)	63 (80%)	16 (20%)	2	14
21	CN	79/83 (95%)	64 (81%)	15 (19%)	2	17
24	BI	109/109 (100%)	108 (99%)	1 (1%)	87	97
24	DI	109/109 (100%)	103 (94%)	6 (6%)	30	78
25	BC	216/217 (100%)	180 (83%)	36 (17%)	3	24
25	DC	216/217 (100%)	181 (84%)	35 (16%)	3	26
26	BD	164/164 (100%)	134 (82%)	30 (18%)	2	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	DD	164/164 (100%)	133 (81%)	31 (19%)	2	17
27	BK	102/104 (98%)	76 (74%)	26 (26%)	1	8
27	DK	102/104 (98%)	78 (76%)	24 (24%)	1	9
28	BP	99/99 (100%)	77 (78%)	22 (22%)	1	11
28	DP	99/99 (100%)	77 (78%)	22 (22%)	1	11
29	BE	165/165 (100%)	143 (87%)	22 (13%)	6	37
29	DE	165/165 (100%)	143 (87%)	22 (13%)	6	37
30	BY	48/48 (100%)	39 (81%)	9 (19%)	2	17
30	DY	48/48 (100%)	39 (81%)	9 (19%)	2	17
31	B0	47/47 (100%)	36 (77%)	11 (23%)	1	9
31	D0	47/47 (100%)	37 (79%)	10 (21%)	1	12
32	B4	34/34 (100%)	30 (88%)	4 (12%)	8	43
32	D4	34/34 (100%)	31 (91%)	3 (9%)	14	59
33	B1	45/48 (94%)	39 (87%)	6 (13%)	6	37
33	D1	45/48 (94%)	39 (87%)	6 (13%)	6	37
34	B3	51/51 (100%)	45 (88%)	6 (12%)	8	43
34	D3	51/51 (100%)	45 (88%)	6 (12%)	8	43
35	BV	78/78 (100%)	64 (82%)	14 (18%)	2	20
35	DV	78/78 (100%)	64 (82%)	14 (18%)	2	20
36	B2	38/38 (100%)	32 (84%)	6 (16%)	4	28
36	D2	38/38 (100%)	33 (87%)	5 (13%)	6	37
37	BL	102/103 (99%)	89 (87%)	13 (13%)	6	39
37	DL	102/103 (99%)	90 (88%)	12 (12%)	8	43
38	BM	109/109 (100%)	86 (79%)	23 (21%)	1	12
38	DM	109/109 (100%)	86 (79%)	23 (21%)	1	12
39	BX	55/55 (100%)	43 (78%)	12 (22%)	1	11
39	DX	55/55 (100%)	45 (82%)	10 (18%)	2	19
40	BH	114/114 (100%)	81 (71%)	33 (29%)	0	5
40	DH	114/114 (100%)	89 (78%)	25 (22%)	1	11
41	BJ	116/116 (100%)	95 (82%)	21 (18%)	2	19
41	DJ	116/116 (100%)	96 (83%)	20 (17%)	3	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	BN	100/103 (97%)	87 (87%)	13 (13%)	6	38
42	DN	100/103 (97%)	87 (87%)	13 (13%)	6	38
43	BO	86/87 (99%)	72 (84%)	14 (16%)	3	26
43	DO	86/87 (99%)	72 (84%)	14 (16%)	3	26
44	BQ	89/89 (100%)	74 (83%)	15 (17%)	3	24
44	DQ	89/89 (100%)	74 (83%)	15 (17%)	3	24
45	BS	93/93 (100%)	80 (86%)	13 (14%)	5	34
45	DS	93/93 (100%)	80 (86%)	13 (14%)	5	34
46	BU	83/84 (99%)	69 (83%)	14 (17%)	3	24
46	DU	83/84 (99%)	69 (83%)	14 (17%)	3	24
47	BF	149/149 (100%)	117 (78%)	32 (22%)	1	12
47	DF	149/149 (100%)	116 (78%)	33 (22%)	1	11
48	BG	137/137 (100%)	112 (82%)	25 (18%)	2	19
48	DG	137/137 (100%)	112 (82%)	25 (18%)	2	19
49	BR	84/84 (100%)	71 (84%)	13 (16%)	4	28
49	DR	84/84 (100%)	73 (87%)	11 (13%)	6	37
50	BT	80/84 (95%)	59 (74%)	21 (26%)	1	7
50	DT	80/84 (95%)	60 (75%)	20 (25%)	1	8
51	BZ	67/68 (98%)	53 (79%)	14 (21%)	1	13
51	DZ	67/68 (98%)	53 (79%)	14 (21%)	1	13
52	BW	59/62 (95%)	42 (71%)	17 (29%)	0	5
52	DW	59/62 (95%)	42 (71%)	17 (29%)	0	5
All	All	9333/9700 (96%)	7661 (82%)	1672 (18%)	2	20

5 of 1672 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
48	BG	84	LYS
13	CP	28	ARG
46	DU	51	LEU
49	BR	66	HIS
3	CD	147	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 332 such sidechains are listed below:

Mol	Chain	Res	Type
47	BF	126	ASN
5	CF	17	GLN
46	DU	26	ASN
48	BG	127	GLN
3	CD	35	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1529/1542 (99%)	292 (19%)	25 (1%)
1	CA	1529/1542 (99%)	282 (18%)	21 (1%)
22	BA	116/120 (96%)	21 (18%)	1 (0%)
22	DA	116/120 (96%)	19 (16%)	1 (0%)
23	BB	2837/2904 (97%)	456 (16%)	18 (0%)
23	DB	2837/2904 (97%)	469 (16%)	20 (0%)
All	All	8964/9132 (98%)	1539 (17%)	86 (0%)

5 of 1539 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	7	A
1	AA	9	G
1	AA	14	U
1	AA	32	A
1	AA	39	G

5 of 86 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	BB	2425	A
1	CA	279	A
23	DB	2336	A
23	BB	2430	A
23	BB	2894	G

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 344 ligands modelled in this entry, 342 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	SCM	AA	1661	-	25,25,25	1.78	10 (40%)	39,39,39	2.31	6 (15%)
54	SCM	CA	1659	-	25,25,25	1.74	7 (28%)	39,39,39	2.37	6 (15%)

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	SCM	AA	1661	-	-	0/4/57/57	0/3/3/3
54	SCM	CA	1659	-	-	0/4/57/57	0/3/3/3

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	CA	1659	SCM	O1B-C5	4.08	1.47	1.43
54	AA	1661	SCM	O1B-C5	4.06	1.47	1.43
54	AA	1661	SCM	C3-C2	3.05	1.58	1.51
54	CA	1659	SCM	C3-C2	2.86	1.57	1.51
54	CA	1659	SCM	C9-C8	2.85	1.59	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	CA	1659	SCM	O5-C5-O1B	-9.19	102.82	111.54
54	AA	1661	SCM	O5-C5-O1B	-8.56	103.42	111.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	AA	1661	SCM	C1M-N10-C10	-8.07	107.28	113.65
54	CA	1659	SCM	C1M-N10-C10	-7.47	107.76	113.65
54	CA	1659	SCM	C2M-C2-C3	-4.36	108.11	113.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1530/1542 (99%)	-0.72	9 (0%) 86 74	12, 77, 142, 179	0
1	CA	1530/1542 (99%)	-0.69	2 (0%) 93 90	5, 57, 124, 180	0
2	AC	206/232 (88%)	0.62	14 (6%) 17 16	5, 70, 115, 162	0
2	CC	206/232 (88%)	0.53	7 (3%) 43 33	5, 71, 111, 150	0
3	AD	205/205 (100%)	0.28	11 (5%) 25 21	5, 79, 127, 173	0
3	CD	205/205 (100%)	1.13	43 (20%) 1 3	5, 66, 125, 166	0
4	AE	150/166 (90%)	0.32	4 (2%) 52 39	5, 68, 122, 157	0
4	CE	150/166 (90%)	1.27	34 (22%) 1 3	5, 67, 121, 180	0
5	AF	100/135 (74%)	2.08	50 (50%) 0 2	10, 81, 133, 147	0
5	CF	100/135 (74%)	0.09	3 (3%) 48 36	5, 73, 131, 172	0
6	AG	150/178 (84%)	0.85	23 (15%) 3 5	16, 89, 125, 143	0
6	CG	152/178 (85%)	-0.16	1 (0%) 84 72	6, 79, 125, 172	0
7	AH	129/129 (100%)	0.83	21 (16%) 2 4	19, 77, 130, 158	0
7	CH	129/129 (100%)	0.73	12 (9%) 9 11	5, 62, 116, 158	0
8	AI	127/129 (98%)	0.71	15 (11%) 5 7	6, 83, 117, 155	0
8	CI	127/129 (98%)	0.24	1 (0%) 83 69	5, 80, 122, 157	0
9	AJ	98/103 (95%)	0.60	3 (3%) 47 36	9, 79, 126, 147	0
9	CJ	98/103 (95%)	0.92	15 (15%) 3 5	16, 82, 113, 137	0
10	AK	117/128 (91%)	0.54	8 (6%) 17 16	5, 72, 117, 155	0
10	CK	117/128 (91%)	-0.20	0 100 100	5, 67, 123, 136	0
11	AL	123/123 (100%)	0.97	19 (15%) 3 5	6, 79, 123, 158	0
11	CL	123/123 (100%)	0.45	4 (3%) 44 34	5, 54, 103, 151	0
12	AM	114/117 (97%)	1.47	31 (27%) 1 3	23, 96, 137, 169	0
12	CM	113/117 (96%)	0.57	10 (8%) 10 12	22, 96, 142, 162	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
13	AP	82/82 (100%)	0.81	7 (8%)	11 12	15, 82, 130, 163	0
13	CP	80/82 (97%)	0.73	12 (15%)	3 5	5, 58, 126, 180	0
14	AQ	80/83 (96%)	1.39	26 (32%)	1 2	15, 92, 145, 154	0
14	CQ	81/83 (97%)	0.55	5 (6%)	20 18	5, 72, 119, 149	0
15	AR	55/74 (74%)	1.21	15 (27%)	1 3	5, 73, 129, 164	0
15	CR	55/74 (74%)	0.03	1 (1%)	65 50	5, 66, 127, 143	0
16	AS	79/91 (86%)	2.22	43 (54%)	0 2	52, 98, 142, 167	0
16	CS	80/91 (87%)	1.38	27 (33%)	1 2	41, 95, 133, 159	0
17	AT	85/86 (98%)	0.12	4 (4%)	30 25	19, 88, 126, 156	0
17	CT	85/86 (98%)	0.07	1 (1%)	75 60	5, 66, 113, 154	0
18	AB	218/240 (90%)	0.17	6 (2%)	50 38	12, 81, 120, 160	0
18	CB	218/240 (90%)	0.63	22 (10%)	7 10	5, 87, 133, 163	0
19	AU	51/70 (72%)	1.34	12 (23%)	1 3	20, 94, 139, 153	0
19	CU	51/70 (72%)	0.30	2 (3%)	37 30	57, 96, 137, 171	0
20	AO	88/89 (98%)	1.44	23 (26%)	1 3	5, 73, 118, 177	0
20	CO	88/89 (98%)	-0.03	1 (1%)	77 61	5, 56, 108, 135	0
21	AN	96/100 (96%)	1.28	25 (26%)	1 3	5, 84, 128, 155	0
21	CN	96/100 (96%)	0.92	16 (16%)	2 4	5, 75, 129, 145	0
22	BA	117/120 (97%)	-0.09	3 (2%)	53 40	35, 77, 125, 167	0
22	DA	117/120 (97%)	-0.33	1 (0%)	81 67	31, 87, 133, 176	0
23	BB	2841/2904 (97%)	-0.41	29 (1%)	79 64	5, 60, 136, 180	0
23	DB	2841/2904 (97%)	-0.44	22 (0%)	83 69	5, 51, 136, 180	0
24	BI	141/141 (100%)	3.24	96 (68%)	0 1	60, 135, 178, 180	0
24	DI	141/141 (100%)	1.86	59 (41%)	1 2	66, 135, 180, 180	0
25	BC	271/272 (99%)	1.52	100 (36%)	1 2	5, 61, 109, 132	0
25	DC	271/272 (99%)	0.77	31 (11%)	6 8	5, 45, 99, 144	0
26	BD	209/209 (100%)	0.47	15 (7%)	15 15	5, 71, 118, 148	0
26	DD	209/209 (100%)	1.02	38 (18%)	2 3	5, 60, 110, 168	0
27	BK	121/123 (98%)	1.88	51 (42%)	1 2	5, 75, 125, 159	0
27	DK	121/123 (98%)	1.32	24 (19%)	2 3	5, 45, 112, 150	0
28	BP	114/114 (100%)	1.58	41 (35%)	1 2	7, 82, 125, 155	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DP	114/114 (100%)	1.00	16 (14%) 3 5	5, 64, 118, 139	0
29	BE	201/201 (100%)	1.17	48 (23%) 1 3	5, 65, 128, 164	0
29	DE	201/201 (100%)	1.05	36 (17%) 2 4	5, 73, 123, 160	0
30	BY	58/58 (100%)	0.23	2 (3%) 43 33	5, 75, 129, 160	0
30	DY	58/58 (100%)	0.49	4 (6%) 17 16	5, 72, 116, 147	0
31	B0	56/56 (100%)	0.39	2 (3%) 41 32	5, 78, 118, 147	0
31	D0	56/56 (100%)	0.24	1 (1%) 65 50	5, 62, 129, 153	0
32	B4	38/38 (100%)	1.34	8 (21%) 1 3	27, 81, 131, 145	0
32	D4	38/38 (100%)	0.64	1 (2%) 53 40	5, 67, 106, 117	0
33	B1	50/54 (92%)	0.51	4 (8%) 12 13	17, 70, 120, 134	0
33	D1	50/54 (92%)	0.95	7 (14%) 3 5	17, 73, 116, 137	0
34	B3	64/64 (100%)	0.18	2 (3%) 47 36	5, 68, 103, 129	0
34	D3	64/64 (100%)	1.17	18 (28%) 1 2	5, 55, 86, 122	0
35	BV	94/94 (100%)	1.01	17 (18%) 2 3	5, 81, 126, 152	0
35	DV	94/94 (100%)	1.32	28 (29%) 1 2	5, 88, 120, 160	0
36	B2	46/46 (100%)	0.42	1 (2%) 59 44	5, 53, 104, 141	0
36	D2	46/46 (100%)	1.36	12 (26%) 1 3	9, 48, 110, 141	0
37	BL	143/144 (99%)	0.19	4 (2%) 50 38	5, 67, 121, 145	0
37	DL	143/144 (99%)	1.36	44 (30%) 1 2	5, 63, 111, 145	0
38	BM	136/136 (100%)	1.34	32 (23%) 1 3	7, 68, 121, 179	0
38	DM	136/136 (100%)	1.50	38 (27%) 1 2	5, 65, 117, 144	0
39	BX	63/63 (100%)	0.76	9 (14%) 3 5	16, 79, 128, 159	0
39	DX	63/63 (100%)	1.09	10 (15%) 3 4	16, 91, 144, 169	0
40	BH	149/149 (100%)	2.18	74 (49%) 1 2	7, 104, 149, 180	0
40	DH	149/149 (100%)	0.99	22 (14%) 3 5	5, 91, 131, 162	0
41	BJ	142/142 (100%)	0.86	20 (14%) 3 5	5, 77, 118, 140	0
41	DJ	142/142 (100%)	0.56	8 (5%) 24 20	5, 70, 119, 173	0
42	BN	120/127 (94%)	0.78	11 (9%) 9 11	5, 69, 111, 154	0
42	DN	120/127 (94%)	0.60	12 (10%) 8 10	5, 51, 94, 163	0
43	BO	116/117 (99%)	0.45	7 (6%) 21 19	6, 80, 109, 172	0
43	DO	116/117 (99%)	1.17	26 (22%) 1 3	5, 83, 136, 158	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BQ	117/117 (100%)	0.03	4 (3%) 43 33	5, 62, 115, 144	0
44	DQ	117/117 (100%)	0.37	5 (4%) 34 27	5, 60, 111, 154	0
45	BS	110/110 (100%)	0.74	4 (3%) 41 32	5, 62, 121, 148	0
45	DS	110/110 (100%)	1.36	37 (33%) 1 2	5, 64, 127, 156	0
46	BU	102/103 (99%)	0.95	13 (12%) 4 6	12, 80, 125, 157	0
46	DU	102/103 (99%)	0.42	1 (0%) 79 64	8, 94, 127, 149	0
47	BF	178/178 (100%)	1.10	34 (19%) 2 3	29, 100, 146, 180	0
47	DF	178/178 (100%)	2.14	80 (44%) 1 2	12, 93, 142, 163	0
48	BG	176/176 (100%)	0.88	22 (12%) 5 6	18, 94, 133, 171	0
48	DG	176/176 (100%)	0.92	32 (18%) 2 3	8, 90, 136, 166	0
49	BR	103/103 (100%)	0.83	13 (12%) 4 6	5, 83, 123, 133	0
49	DR	103/103 (100%)	0.46	8 (7%) 13 13	10, 76, 135, 149	0
50	BT	93/100 (93%)	0.77	3 (3%) 45 35	8, 83, 130, 165	0
50	DT	93/100 (93%)	2.34	51 (54%) 0 2	5, 84, 144, 172	0
51	BZ	77/78 (98%)	0.66	10 (12%) 4 6	5, 63, 120, 142	0
51	DZ	77/78 (98%)	0.65	7 (9%) 9 11	5, 56, 106, 120	0
52	BW	79/84 (94%)	0.53	6 (7%) 14 14	5, 75, 124, 180	0
52	DW	79/84 (94%)	1.27	13 (16%) 2 4	5, 71, 121, 166	0
All	All	20417/21046 (97%)	0.28	1965 (9%) 8 10	5, 70, 134, 180	0

The worst 5 of 1965 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	BB	1730	C	11.8
23	BB	140	C	11.4
24	BI	49	GLU	10.4
33	D1	52	LYS	9.5
23	BB	1731	G	8.9

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	1659	1/1	0.39	96.52	108,108,108,108	0
53	MG	DB	3029	1/1	0.32	32.75	87,87,87,87	0
53	MG	AA	1657	1/1	0.40	16.10	91,91,91,91	0
53	MG	CA	1616	1/1	0.40	15.21	58,58,58,58	1
53	MG	BB	3028	1/1	0.27	10.88	9,9,9,9	0
53	MG	AA	1623	1/1	0.37	10.68	33,33,33,33	1
53	MG	BB	3047	1/1	0.15	10.57	104,104,104,104	0
53	MG	DB	3054	1/1	0.17	10.23	21,21,21,21	0
53	MG	BB	3017	1/1	0.20	9.96	50,50,50,50	0
53	MG	AA	1632	1/1	0.27	9.74	96,96,96,96	0
53	MG	AA	1624	1/1	0.21	8.18	83,83,83,83	0
53	MG	CA	1613	1/1	0.20	7.45	126,126,126,126	0
53	MG	CA	1612	1/1	0.30	7.42	93,93,93,93	0
53	MG	BB	3033	1/1	0.19	6.36	102,102,102,102	0
53	MG	CA	1632	1/1	0.16	6.12	76,76,76,76	0
53	MG	CA	1649	1/1	0.14	5.48	123,123,123,123	0
53	MG	CA	1654	1/1	0.21	5.31	105,105,105,105	0
53	MG	BB	3087	1/1	0.25	4.85	80,80,80,80	0
53	MG	DB	3066	1/1	0.36	4.74	65,65,65,65	0
53	MG	DB	3037	1/1	0.16	4.46	8,8,8,8	0
53	MG	AA	1626	1/1	0.13	3.80	36,36,36,36	1
53	MG	AA	1647	1/1	0.49	3.51	113,113,113,113	0
53	MG	BB	3039	1/1	0.19	3.16	41,41,41,41	0
53	MG	CA	1617	1/1	0.15	3.12	88,88,88,88	0
53	MG	CA	1656	1/1	0.17	2.99	38,38,38,38	0
53	MG	AA	1622	1/1	0.34	2.71	130,130,130,130	0
53	MG	DB	3052	1/1	0.26	2.64	105,105,105,105	0
53	MG	BB	3036	1/1	0.22	2.51	51,51,51,51	0
53	MG	AA	1637	1/1	0.22	1.83	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	DB	3026	1/1	0.20	1.81	45,45,45,45	0
53	MG	DB	3005	1/1	0.20	1.77	25,25,25,25	0
53	MG	DB	3017	1/1	0.18	1.75	5,5,5,5	0
53	MG	BB	3105	1/1	0.22	1.72	5,5,5,5	0
53	MG	CA	1606	1/1	0.14	1.52	106,106,106,106	0
53	MG	CA	1622	1/1	0.17	1.50	5,5,5,5	0
53	MG	AA	1631	1/1	0.11	1.48	5,5,5,5	0
53	MG	AA	1628	1/1	0.14	1.40	70,70,70,70	0
53	MG	DN	201	1/1	0.35	1.13	145,145,145,145	0
53	MG	CA	1621	1/1	0.17	1.09	80,80,80,80	0
53	MG	DB	3064	1/1	0.33	1.07	49,49,49,49	0
53	MG	BB	3104	1/1	0.19	1.02	26,26,26,26	0
53	MG	BB	3030	1/1	0.13	1.00	51,51,51,51	0
53	MG	DB	3088	1/1	0.16	0.88	87,87,87,87	0
53	MG	BB	3098	1/1	0.17	0.85	14,14,14,14	0
53	MG	BB	3053	1/1	0.13	0.84	60,60,60,60	0
53	MG	BB	3018	1/1	0.14	0.81	39,39,39,39	0
53	MG	CA	1644	1/1	0.13	0.79	57,57,57,57	0
53	MG	DB	3030	1/1	0.19	0.77	47,47,47,47	0
53	MG	CA	1651	1/1	0.10	0.75	101,101,101,101	0
53	MG	DB	3063	1/1	0.12	0.71	72,72,72,72	0
53	MG	AA	1617	1/1	0.13	0.67	112,112,112,112	0
54	SCM	CA	1659	23/23	0.15	0.67	18,18,18,18	0
53	MG	DB	3071	1/1	0.15	0.66	57,57,57,57	0
53	MG	DB	3110	1/1	0.17	0.60	84,84,84,84	0
53	MG	CA	1629	1/1	0.15	0.58	67,67,67,67	0
53	MG	AA	1640	1/1	0.13	0.49	46,46,46,46	0
53	MG	DB	3097	1/1	0.18	0.45	41,41,41,41	0
53	MG	AA	1642	1/1	0.11	0.38	49,49,49,49	0
53	MG	BB	3001	1/1	0.18	0.38	5,5,5,5	0
53	MG	BB	3107	1/1	0.17	0.33	46,46,46,46	0
53	MG	BB	3050	1/1	0.15	0.30	53,53,53,53	0
53	MG	BB	3110	1/1	0.11	0.25	80,80,80,80	0
53	MG	DB	3095	1/1	0.16	0.25	92,92,92,92	0
53	MG	CA	1610	1/1	0.14	0.22	5,5,5,5	0
53	MG	BB	3054	1/1	0.14	0.16	49,49,49,49	0
53	MG	BB	3026	1/1	0.18	0.16	65,65,65,65	0
53	MG	AA	1656	1/1	0.11	0.11	87,87,87,87	0
53	MG	AA	1635	1/1	0.14	0.09	80,80,80,80	0
53	MG	DB	3007	1/1	0.14	0.03	62,62,62,62	0
53	MG	AA	1615	1/1	0.26	0.00	96,96,96,96	0
53	MG	BB	3042	1/1	0.23	-0.01	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	BB	3060	1/1	0.19	-0.04	30,30,30,30	0
53	MG	BB	3076	1/1	0.15	-0.13	35,35,35,35	0
53	MG	DB	3049	1/1	0.13	-0.14	42,42,42,42	0
53	MG	BB	3011	1/1	0.14	-0.18	5,5,5,5	0
53	MG	AA	1621	1/1	0.12	-0.19	36,36,36,36	0
53	MG	DB	3069	1/1	0.25	-0.20	64,64,64,64	0
53	MG	AA	1643	1/1	0.10	-0.22	40,40,40,40	0
54	SCM	AA	1661	23/23	0.10	-0.25	13,13,13,13	0
53	MG	BB	3038	1/1	0.11	-0.25	92,92,92,92	0
53	MG	DB	3100	1/1	0.17	-0.25	19,19,19,19	0
53	MG	BB	3006	1/1	0.14	-0.28	61,61,61,61	0
53	MG	DB	3028	1/1	0.11	-0.35	70,70,70,70	0
53	MG	BB	3020	1/1	0.22	-0.35	6,6,6,6	0
53	MG	CA	1658	1/1	0.10	-0.35	37,37,37,37	0
53	MG	DB	3010	1/1	0.15	-0.38	5,5,5,5	0
53	MG	BB	3083	1/1	0.18	-0.40	30,30,30,30	0
53	MG	AA	1652	1/1	0.12	-0.42	84,84,84,84	0
53	MG	BB	3046	1/1	0.11	-0.42	89,89,89,89	0
53	MG	DB	3098	1/1	0.14	-0.44	5,5,5,5	0
53	MG	DB	3104	1/1	0.14	-0.46	29,29,29,29	0
53	MG	CA	1602	1/1	0.10	-0.48	5,5,5,5	0
53	MG	AA	1644	1/1	0.09	-0.50	75,75,75,75	0
53	MG	BB	3022	1/1	0.14	-0.51	32,32,32,32	0
53	MG	AA	1612	1/1	0.10	-0.57	61,61,61,61	0
53	MG	BB	3025	1/1	0.15	-0.58	30,30,30,30	0
53	MG	BB	3007	1/1	0.15	-0.59	68,68,68,68	0
53	MG	AA	1608	1/1	0.08	-0.62	123,123,123,123	0
53	MG	AA	1618	1/1	0.08	-0.68	38,38,38,38	0
53	MG	DB	3102	1/1	0.23	-0.69	28,28,28,28	0
53	MG	AA	1605	1/1	0.10	-0.70	50,50,50,50	0
53	MG	BB	3024	1/1	0.14	-0.74	55,55,55,55	0
53	MG	CA	1620	1/1	0.11	-0.75	72,72,72,72	0
53	MG	BB	3043	1/1	0.12	-0.76	107,107,107,107	0
53	MG	BB	3019	1/1	0.14	-0.78	21,21,21,21	0
53	MG	BB	3010	1/1	0.12	-0.79	53,53,53,53	0
53	MG	BB	3049	1/1	0.14	-0.81	67,67,67,67	0
53	MG	AA	1604	1/1	0.09	-0.82	38,38,38,38	0
53	MG	CA	1607	1/1	0.06	-0.84	5,5,5,5	0
53	MG	CA	1623	1/1	0.12	-0.85	11,11,11,11	0
53	MG	DB	3045	1/1	0.07	-0.86	110,110,110,110	0
53	MG	BB	3009	1/1	0.09	-0.86	98,98,98,98	0
53	MG	AA	1606	1/1	0.10	-0.90	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	BB	3109	1/1	0.12	-0.94	11,11,11,11	0
53	MG	BB	3075	1/1	0.13	-0.94	40,40,40,40	0
53	MG	DB	3077	1/1	0.10	-0.96	45,45,45,45	0
53	MG	BB	3023	1/1	0.14	-0.97	5,5,5,5	0
53	MG	DB	3109	1/1	0.05	-1.02	9,9,9,9	0
53	MG	CA	1630	1/1	0.12	-1.02	37,37,37,37	0
53	MG	DB	3099	1/1	0.12	-1.03	58,58,58,58	0
53	MG	AA	1636	1/1	0.03	-1.04	64,64,64,64	0
53	MG	BB	3034	1/1	0.12	-1.04	86,86,86,86	0
53	MG	BB	3080	1/1	0.12	-1.08	53,53,53,53	0
53	MG	CA	1647	1/1	0.07	-1.12	75,75,75,75	0
53	MG	DB	3014	1/1	0.06	-1.13	21,21,21,21	0
53	MG	DB	3032	1/1	0.14	-1.13	73,73,73,73	0
53	MG	DB	3057	1/1	0.06	-1.13	48,48,48,48	0
53	MG	BB	3086	1/1	0.12	-1.15	5,5,5,5	0
53	MG	CA	1634	1/1	0.10	-1.23	74,74,74,74	0
53	MG	BB	3090	1/1	0.09	-1.24	88,88,88,88	0
53	MG	CA	1609	1/1	0.11	-1.28	85,85,85,85	0
53	MG	CA	1642	1/1	0.08	-1.29	79,79,79,79	0
53	MG	BB	3005	1/1	0.11	-1.32	5,5,5,5	0
53	MG	BB	3031	1/1	0.10	-1.36	60,60,60,60	0
53	MG	BB	3099	1/1	0.08	-1.36	41,41,41,41	0
53	MG	DB	3050	1/1	0.10	-1.37	80,80,80,80	0
53	MG	BB	3040	1/1	0.09	-1.38	12,12,12,12	0
53	MG	BB	3077	1/1	0.13	-1.40	53,53,53,53	0
53	MG	AA	1614	1/1	0.07	-1.41	119,119,119,119	0
53	MG	DB	3023	1/1	0.08	-1.41	69,69,69,69	0
53	MG	AA	1645	1/1	0.10	-1.43	70,70,70,70	0
53	MG	DB	3068	1/1	0.14	-1.43	5,5,5,5	0
53	MG	AA	1660	1/1	0.06	-1.43	56,56,56,56	0
53	MG	BB	3071	1/1	0.10	-1.44	68,68,68,68	0
53	MG	AA	1613	1/1	0.04	-1.44	58,58,58,58	0
53	MG	DB	3081	1/1	0.06	-1.46	41,41,41,41	0
53	MG	BB	3045	1/1	0.12	-1.47	72,72,72,72	0
53	MG	AA	1630	1/1	0.08	-1.48	88,88,88,88	0
53	MG	CA	1618	1/1	0.12	-1.50	73,73,73,73	0
53	MG	BB	3068	1/1	0.14	-1.50	13,13,13,13	0
53	MG	AA	1611	1/1	0.05	-1.50	43,43,43,43	0
53	MG	BB	3012	1/1	0.07	-1.54	67,67,67,67	0
53	MG	BB	3067	1/1	0.11	-1.56	63,63,63,63	0
55	ZN	D4	101	1/1	0.07	-1.57	62,62,62,62	0
53	MG	AA	1648	1/1	0.06	-1.57	6,6,6,6	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	BB	3091	1/1	0.10	-1.60	5,5,5,5	0
53	MG	DB	3059	1/1	0.10	-1.61	99,99,99,99	0
53	MG	DB	3003	1/1	0.08	-1.62	30,30,30,30	0
53	MG	BB	3051	1/1	0.10	-1.64	107,107,107,107	0
53	MG	AA	1610	1/1	0.04	-1.65	78,78,78,78	0
53	MG	DB	3011	1/1	0.14	-1.67	5,5,5,5	0
53	MG	CA	1645	1/1	0.06	-1.69	55,55,55,55	0
53	MG	AA	1653	1/1	0.08	-1.70	21,21,21,21	0
53	MG	AA	1634	1/1	0.05	-1.72	72,72,72,72	0
53	MG	DB	3093	1/1	0.04	-1.72	59,59,59,59	0
53	MG	BB	3082	1/1	0.14	-1.72	18,18,18,18	0
53	MG	CA	1605	1/1	0.07	-1.72	12,12,12,12	0
53	MG	BB	3013	1/1	0.12	-1.73	45,45,45,45	0
53	MG	BB	3052	1/1	0.12	-1.74	71,71,71,71	0
53	MG	DB	3106	1/1	0.07	-1.75	61,61,61,61	0
53	MG	BB	3073	1/1	0.10	-1.76	44,44,44,44	0
53	MG	CA	1614	1/1	0.05	-1.78	83,83,83,83	0
53	MG	CA	1650	1/1	0.08	-1.79	105,105,105,105	0
53	MG	DB	3004	1/1	0.08	-1.81	8,8,8,8	0
53	MG	DB	3047	1/1	0.13	-1.82	43,43,43,43	0
53	MG	DB	3094	1/1	0.13	-1.83	100,100,100,100	0
53	MG	DB	3062	1/1	0.12	-1.86	58,58,58,58	0
53	MG	BB	3108	1/1	0.10	-1.87	10,10,10,10	0
53	MG	DB	3021	1/1	0.04	-1.87	16,16,16,16	0
53	MG	DB	3012	1/1	0.12	-1.87	9,9,9,9	0
53	MG	DB	3101	1/1	0.09	-1.87	26,26,26,26	0
53	MG	DB	3038	1/1	0.08	-1.89	5,5,5,5	0
53	MG	DB	3108	1/1	0.08	-1.90	43,43,43,43	0
53	MG	AA	1607	1/1	0.05	-1.90	57,57,57,57	0
53	MG	CA	1641	1/1	0.10	-1.93	42,42,42,42	0
53	MG	BB	3041	1/1	0.11	-1.94	5,5,5,5	0
55	ZN	B4	101	1/1	0.10	-1.95	67,67,67,67	0
53	MG	DB	3027	1/1	0.08	-1.95	13,13,13,13	0
53	MG	BB	3062	1/1	0.10	-1.95	7,7,7,7	0
53	MG	BB	3101	1/1	0.09	-1.96	19,19,19,19	0
53	MG	DB	3091	1/1	0.08	-1.96	90,90,90,90	0
53	MG	CE	201	1/1	0.08	-1.96	109,109,109,109	0
53	MG	BB	3014	1/1	0.05	-1.99	37,37,37,37	0
53	MG	DB	3015	1/1	0.08	-2.01	42,42,42,42	0
53	MG	BB	3002	1/1	0.10	-2.02	23,23,23,23	0
53	MG	DB	3096	1/1	0.09	-2.05	26,26,26,26	0
53	MG	AA	1603	1/1	0.10	-2.07	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	DB	3022	1/1	0.08	-2.09	11,11,11,11	0
53	MG	AA	1651	1/1	0.05	-2.11	35,35,35,35	0
53	MG	BB	3044	1/1	0.10	-2.16	45,45,45,45	0
53	MG	AA	1616	1/1	0.09	-2.17	5,5,5,5	0
53	MG	CA	1657	1/1	0.05	-2.17	73,73,73,73	0
53	MG	CA	1611	1/1	0.07	-2.18	28,28,28,28	0
53	MG	AA	1655	1/1	0.07	-2.20	88,88,88,88	0
53	MG	DB	3084	1/1	0.09	-2.20	29,29,29,29	0
53	MG	DB	3092	1/1	0.11	-2.23	10,10,10,10	0
53	MG	BB	3084	1/1	0.08	-2.24	32,32,32,32	0
53	MG	BB	3079	1/1	0.07	-2.27	38,38,38,38	0
53	MG	BB	3078	1/1	0.10	-2.30	27,27,27,27	0
53	MG	DB	3035	1/1	0.09	-2.30	79,79,79,79	0
53	MG	BB	3092	1/1	0.07	-2.31	46,46,46,46	0
53	MG	BB	3008	1/1	0.08	-2.34	82,82,82,82	0
53	MG	CA	1643	1/1	0.05	-2.35	36,36,36,36	0
53	MG	CA	1637	1/1	0.08	-2.35	98,98,98,98	0
53	MG	DB	3075	1/1	0.10	-2.36	44,44,44,44	0
53	MG	BB	3070	1/1	0.09	-2.39	74,74,74,74	0
53	MG	DB	3085	1/1	0.06	-2.40	38,38,38,38	0
53	MG	CA	1653	1/1	0.07	-2.42	48,48,48,48	0
53	MG	DB	3065	1/1	0.06	-2.45	128,128,128,128	0
53	MG	CA	1633	1/1	0.06	-2.46	23,23,23,23	0
53	MG	BB	3093	1/1	0.11	-2.46	108,108,108,108	0
53	MG	CA	1652	1/1	0.07	-2.46	49,49,49,49	0
53	MG	AA	1627	1/1	0.09	-2.47	63,63,63,63	0
53	MG	CA	1635	1/1	0.07	-2.50	30,30,30,30	0
53	MG	DB	3103	1/1	0.08	-2.51	36,36,36,36	0
53	MG	AA	1609	1/1	0.06	-2.54	40,40,40,40	0
53	MG	BB	3085	1/1	0.08	-2.55	34,34,34,34	0
53	MG	CA	1648	1/1	0.06	-2.55	104,104,104,104	0
53	MG	BB	3081	1/1	0.10	-2.57	30,30,30,30	0
53	MG	BB	3048	1/1	0.06	-2.57	12,12,12,12	0
53	MG	DB	3086	1/1	0.10	-2.65	18,18,18,18	0
53	MG	DB	3008	1/1	0.07	-2.67	13,13,13,13	0
53	MG	DB	3033	1/1	0.05	-2.67	11,11,11,11	0
53	MG	AA	1601	1/1	0.06	-2.70	36,36,36,36	0
53	MG	DB	3107	1/1	0.04	-2.72	5,5,5,5	0
53	MG	DB	3058	1/1	0.08	-2.74	139,139,139,139	0
53	MG	CA	1626	1/1	0.05	-2.75	8,8,8,8	0
53	MG	CA	1624	1/1	0.09	-2.79	38,38,38,38	0
53	MG	DB	3083	1/1	0.08	-2.81	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	DB	3070	1/1	0.05	-2.82	33,33,33,33	0
53	MG	CA	1640	1/1	0.07	-2.88	62,62,62,62	0
53	MG	BB	3069	1/1	0.06	-2.89	5,5,5,5	0
53	MG	DB	3067	1/1	0.07	-2.90	5,5,5,5	0
53	MG	AA	1633	1/1	0.06	-2.91	65,65,65,65	0
53	MG	DB	3024	1/1	0.06	-2.91	40,40,40,40	0
53	MG	AA	1641	1/1	0.04	-2.93	32,32,32,32	0
53	MG	CA	1628	1/1	0.06	-2.93	52,52,52,52	0
53	MG	DB	3040	1/1	0.07	-2.95	5,5,5,5	0
53	MG	AA	1638	1/1	0.06	-2.98	51,51,51,51	0
53	MG	DB	3056	1/1	0.06	-3.02	5,5,5,5	0
53	MG	DB	3051	1/1	0.11	-3.03	75,75,75,75	0
53	MG	DB	3073	1/1	0.07	-3.07	50,50,50,50	0
53	MG	BB	3061	1/1	0.07	-3.09	24,24,24,24	0
53	MG	DB	3078	1/1	0.04	-3.10	25,25,25,25	0
53	MG	BB	3035	1/1	0.05	-3.12	13,13,13,13	0
53	MG	BB	3097	1/1	0.06	-3.13	113,113,113,113	0
53	MG	BB	3106	1/1	0.11	-3.14	10,10,10,10	0
53	MG	BB	3065	1/1	0.06	-3.14	32,32,32,32	0
53	MG	DB	3036	1/1	0.05	-3.20	87,87,87,87	0
53	MG	DB	3053	1/1	0.08	-3.21	65,65,65,65	0
53	MG	CA	1627	1/1	0.06	-3.28	27,27,27,27	0
53	MG	BB	3088	1/1	0.08	-3.30	11,11,11,11	0
53	MG	DB	3080	1/1	0.09	-3.32	62,62,62,62	0
53	MG	DB	3044	1/1	0.07	-3.35	18,18,18,18	0
53	MG	DB	3016	1/1	0.09	-3.39	5,5,5,5	0
53	MG	DB	3082	1/1	0.08	-3.40	83,83,83,83	0
53	MG	AA	1629	1/1	0.05	-3.53	12,12,12,12	0
53	MG	CA	1638	1/1	0.05	-3.57	86,86,86,86	0
53	MG	DB	3076	1/1	0.08	-3.59	33,33,33,33	0
53	MG	BB	3029	1/1	0.07	-3.61	5,5,5,5	0
53	MG	DB	3031	1/1	0.09	-3.69	46,46,46,46	0
53	MG	CA	1619	1/1	0.07	-3.75	36,36,36,36	0
53	MG	CA	1636	1/1	0.04	-3.77	5,5,5,5	0
53	MG	BB	3021	1/1	0.10	-3.86	52,52,52,52	0
53	MG	CA	1646	1/1	0.04	-3.86	139,139,139,139	0
53	MG	BB	3096	1/1	0.07	-3.92	58,58,58,58	0
53	MG	DB	3020	1/1	0.09	-4.07	5,5,5,5	0
53	MG	BB	3037	1/1	0.13	-4.07	45,45,45,45	0
53	MG	BB	3066	1/1	0.06	-4.10	5,5,5,5	0
53	MG	DB	3072	1/1	0.06	-4.13	20,20,20,20	0
53	MG	BB	3094	1/1	0.06	-4.15	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	DB	3042	1/1	0.06	-4.16	37,37,37,37	0
53	MG	BB	3103	1/1	0.06	-4.16	11,11,11,11	0
53	MG	BB	3004	1/1	0.05	-4.18	80,80,80,80	0
53	MG	DB	3089	1/1	0.06	-4.18	79,79,79,79	0
53	MG	CA	1604	1/1	0.05	-4.21	20,20,20,20	0
53	MG	DB	3018	1/1	0.06	-4.36	7,7,7,7	0
53	MG	DB	3041	1/1	0.08	-4.38	40,40,40,40	0
53	MG	BB	3100	1/1	0.08	-4.39	116,116,116,116	0
53	MG	AA	1649	1/1	0.05	-4.45	89,89,89,89	0
53	MG	DB	3025	1/1	0.07	-4.47	44,44,44,44	0
53	MG	DB	3019	1/1	0.04	-4.48	5,5,5,5	0
53	MG	AA	1654	1/1	0.07	-4.48	67,67,67,67	0
53	MG	DB	3061	1/1	0.05	-4.55	66,66,66,66	0
53	MG	DB	3105	1/1	0.05	-4.56	40,40,40,40	0
53	MG	DB	3013	1/1	0.08	-4.56	52,52,52,52	0
53	MG	DB	3034	1/1	0.10	-4.60	57,57,57,57	0
53	MG	BB	3003	1/1	0.10	-4.74	53,53,53,53	0
53	MG	CA	1601	1/1	0.06	-4.76	5,5,5,5	0
53	MG	DB	3046	1/1	0.04	-4.80	23,23,23,23	0
53	MG	DB	3002	1/1	0.07	-4.84	11,11,11,11	0
53	MG	DB	3055	1/1	0.06	-4.88	44,44,44,44	0
53	MG	AA	1620	1/1	0.05	-4.89	60,60,60,60	0
53	MG	DB	3074	1/1	0.06	-4.91	26,26,26,26	0
53	MG	DB	3048	1/1	0.07	-4.93	38,38,38,38	0
53	MG	BB	3064	1/1	0.11	-5.00	78,78,78,78	0
53	MG	BB	3063	1/1	0.06	-5.04	33,33,33,33	0
53	MG	CA	1655	1/1	0.04	-5.10	32,32,32,32	0
53	MG	BB	3072	1/1	0.05	-5.15	35,35,35,35	0
53	MG	CA	1631	1/1	0.04	-5.18	41,41,41,41	0
53	MG	DB	3090	1/1	0.12	-5.28	14,14,14,14	0
53	MG	BB	3016	1/1	0.06	-5.28	55,55,55,55	0
53	MG	AA	1619	1/1	0.04	-5.29	111,111,111,111	0
53	MG	BB	3055	1/1	0.13	-5.31	6,6,6,6	0
53	MG	BB	3058	1/1	0.07	-5.46	15,15,15,15	0
53	MG	DB	3006	1/1	0.10	-5.52	10,10,10,10	0
53	MG	BB	3027	1/1	0.08	-5.61	50,50,50,50	0
53	MG	DB	3087	1/1	0.07	-5.81	5,5,5,5	0
53	MG	BB	3074	1/1	0.08	-5.94	10,10,10,10	0
53	MG	DB	3009	1/1	0.07	-5.97	9,9,9,9	0
53	MG	DB	3079	1/1	0.06	-6.31	7,7,7,7	0
53	MG	CA	1608	1/1	0.06	-6.35	76,76,76,76	0
53	MG	DB	3043	1/1	0.06	-6.44	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	DB	3001	1/1	0.07	-6.50	5,5,5,5	0
53	MG	BB	3056	1/1	0.04	-6.91	5,5,5,5	0
53	MG	AA	1646	1/1	0.06	-6.93	84,84,84,84	0
53	MG	CA	1603	1/1	0.03	-7.02	56,56,56,56	0
53	MG	BB	3059	1/1	0.11	-7.23	10,10,10,10	0
53	MG	BB	3057	1/1	0.06	-7.29	53,53,53,53	0
53	MG	CA	1615	1/1	0.06	-7.51	13,13,13,13	0
53	MG	BB	3089	1/1	0.10	-7.57	72,72,72,72	0
53	MG	AA	1650	1/1	0.05	-7.76	94,94,94,94	0
53	MG	CA	1625	1/1	0.04	-7.78	70,70,70,70	0
53	MG	BB	3102	1/1	0.10	-8.24	43,43,43,43	0
53	MG	BB	3095	1/1	0.08	-9.34	62,62,62,62	0
53	MG	AA	1602	1/1	0.08	-9.67	85,85,85,85	0
53	MG	DB	3039	1/1	0.06	-9.77	62,62,62,62	0
53	MG	DB	3060	1/1	0.04	-10.12	83,83,83,83	0
53	MG	BB	3015	1/1	0.12	-10.31	25,25,25,25	0
53	MG	AA	1658	1/1	0.07	-10.87	120,120,120,120	0
53	MG	BB	3032	1/1	0.09	-11.76	22,22,22,22	0
53	MG	CA	1639	1/1	0.04	-18.59	35,35,35,35	0
53	MG	AA	1639	1/1	0.06	-	93,93,93,93	0
53	MG	AA	1625	1/1	0.14	-	79,79,79,79	1

6.5 Other polymers ⓘ

There are no such residues in this entry.