



wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 06:48 PM BST

PDB ID : 4V52
Title : Crystal structure of the bacterial ribosome from Escherichia coli in complex with neomycin.
Authors : Borovinskaya, M.A.; Pai, R.D.; Zhang, W.; Schuwirth, B.-S.; Holton, J.M.; Hirokawa, G.; Kaji, H.; Kaji, A.; Cate, J.H.D.
Deposited on : 2007-06-15
Resolution : 3.21 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>

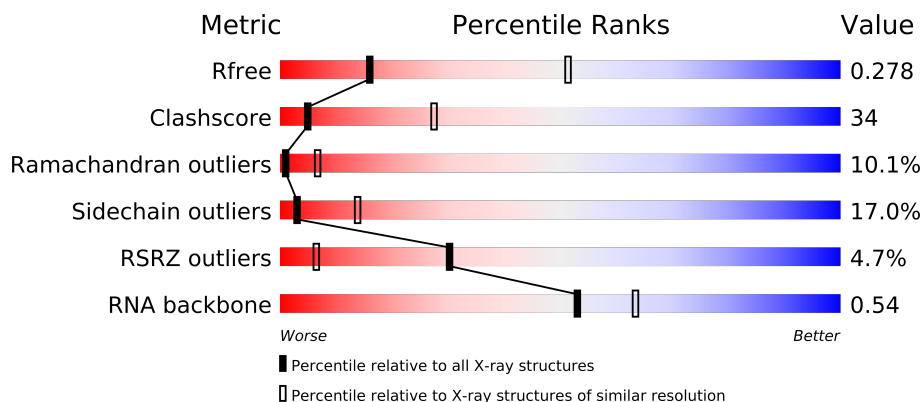
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.21 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	1205 (3.30-3.14)
Clashscore	79885	1072 (3.28-3.16)
Ramachandran outliers	78287	1052 (3.28-3.16)
Sidechain outliers	78261	1051 (3.28-3.16)
RSRZ outliers	66119	1206 (3.30-3.14)
RNA backbone	1838	1004 (3.74-2.70)

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

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

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Mol	Chain	Length	Quality of chain
7	AH	129	
7	CH	129	
8	AI	129	
8	CI	129	
9	AJ	103	
9	CJ	103	
10	AK	128	
10	CK	128	
11	AL	123	
11	CL	123	
12	AM	117	
12	CM	117	
13	AN	100	
13	CN	100	
14	AO	89	
14	CO	89	
15	AP	82	
15	CP	82	
16	AQ	83	
16	CQ	83	
17	AR	74	
17	CR	74	
18	AS	91	
18	CS	91	
19	AT	86	
19	CT	86	
20	AB	240	
20	CB	240	
21	AU	70	
21	CU	70	
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	

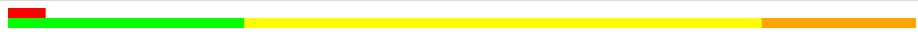
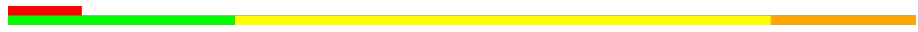
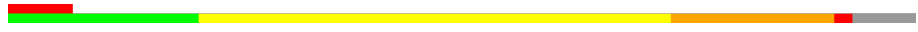

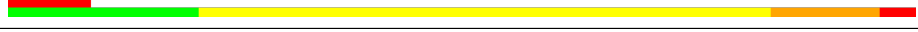
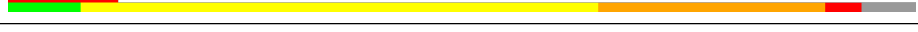

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Mol	Chain	Length	Quality of chain
28	BP	114	
28	DP	114	
29	BE	201	
29	DE	201	
30	BY	58	
30	DY	58	
31	B0	56	
31	D0	56	
32	B4	38	
32	D4	38	
33	B1	54	
33	D1	54	
34	B3	64	
34	D3	64	
35	BV	94	
35	DV	94	
36	B2	46	
36	D2	46	
37	BL	144	
37	DL	144	
38	BM	136	
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	NMY	BB	3001	-	X
53	NMY	CA	1601	-	X
53	NMY	DB	3001	-	X
54	MG	AA	1620	-	X
54	MG	AA	1623	-	X
54	MG	AA	1624	-	X
54	MG	AA	1648	-	X
54	MG	AA	1658	-	X
54	MG	AA	1660	-	X
54	MG	BB	3029	-	X
54	MG	BB	3034	-	X
54	MG	BB	3048	-	X
54	MG	BB	3082	-	X
54	MG	BB	3088	-	X
54	MG	CA	1620	-	X
54	MG	CA	1621	-	X
54	MG	CA	1638	-	X
54	MG	CA	1652	-	X
54	MG	CA	1657	-	X
54	MG	DB	3031	-	X
54	MG	DB	3035	-	X
54	MG	DB	3059	-	X
54	MG	DB	3067	-	X
54	MG	DB	3097	-	X

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 284172 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 S14.

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 20 is a protein called 30S ribosomal protein S2.

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

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

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

- Molecule 22 is a RNA chain called 5S 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			

- 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			

- 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			

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

- Molecule 27 is a protein called 50S ribosomal protein 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			
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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			

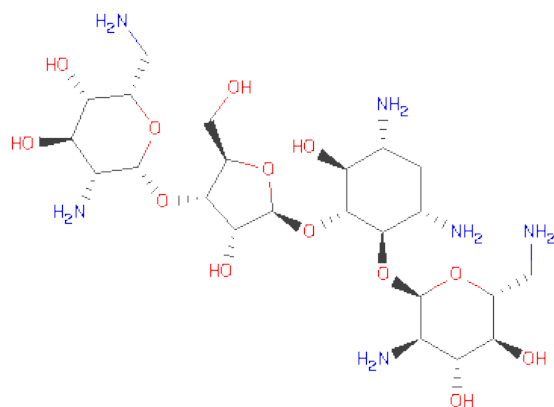
- Molecule 51 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BZ	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			
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 NEOMYCIN (three-letter code: NMY) (formula: C₂₃H₄₆N₆O₁₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
53	AA	1	Total	C	N	O	0	0
			42	23	6	13		
53	BB	1	Total	C	N	O	0	0
			42	23	6	13		
53	CA	1	Total	C	N	O	0	0
			42	23	6	13		
53	DB	1	Total	C	N	O	0	0
			42	23	6	13		

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	BB	110	Total	Mg	0	0
			110	110		
54	CN	1	Total	Mg	0	0
			1	1		
54	CA	60	Total	Mg	0	0
			60	60		
54	AA	60	Total	Mg	0	0
			60	60		
54	CE	1	Total	Mg	0	0
			1	1		
54	DB	111	Total	Mg	0	0
			111	111		

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

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

- Molecule 56 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AA	291	Total 291	O 291	0	0
56	AL	4	Total 4	O 4	0	0
56	AN	4	Total 4	O 4	0	0
56	AT	1	Total 1	O 1	0	0
56	BB	497	Total 497	O 497	0	0
56	BC	5	Total 5	O 5	0	0
56	BE	1	Total 1	O 1	0	0
56	BL	1	Total 1	O 1	0	0
56	BN	1	Total 1	O 1	0	0
56	BR	1	Total 1	O 1	0	0
56	CA	298	Total 298	O 298	0	0
56	CE	3	Total 3	O 3	0	0
56	CL	2	Total 2	O 2	0	0
56	CN	4	Total 4	O 4	0	0
56	CP	1	Total 1	O 1	0	0
56	CT	1	Total 1	O 1	0	0
56	DB	502	Total 502	O 502	0	0
56	DC	6	Total 6	O 6	0	0

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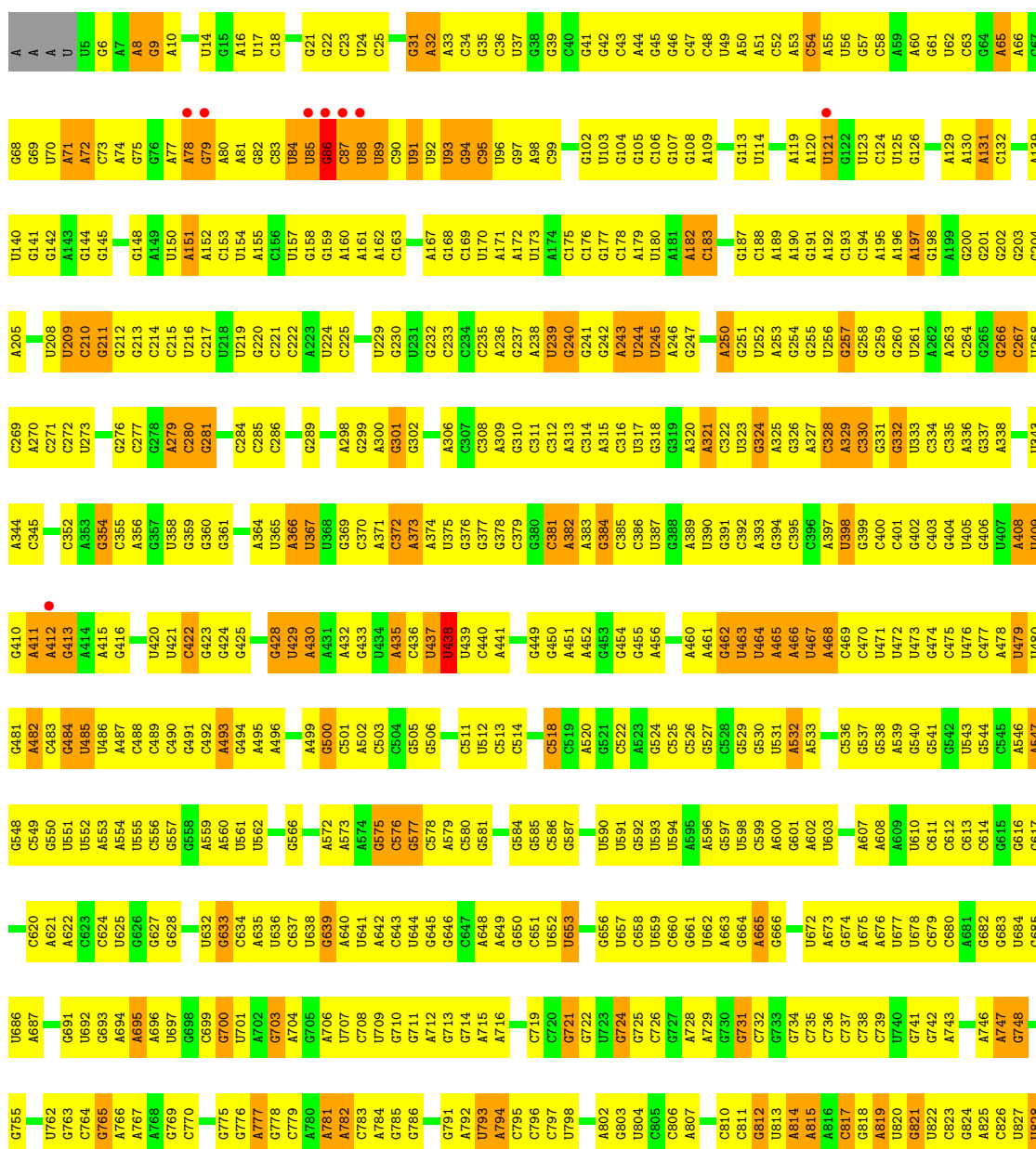
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	DE	1	Total	O	0	0
			1	1		
56	DL	2	Total	O	0	0
			2	2		
56	DR	1	Total	O	0	0
			1	1		

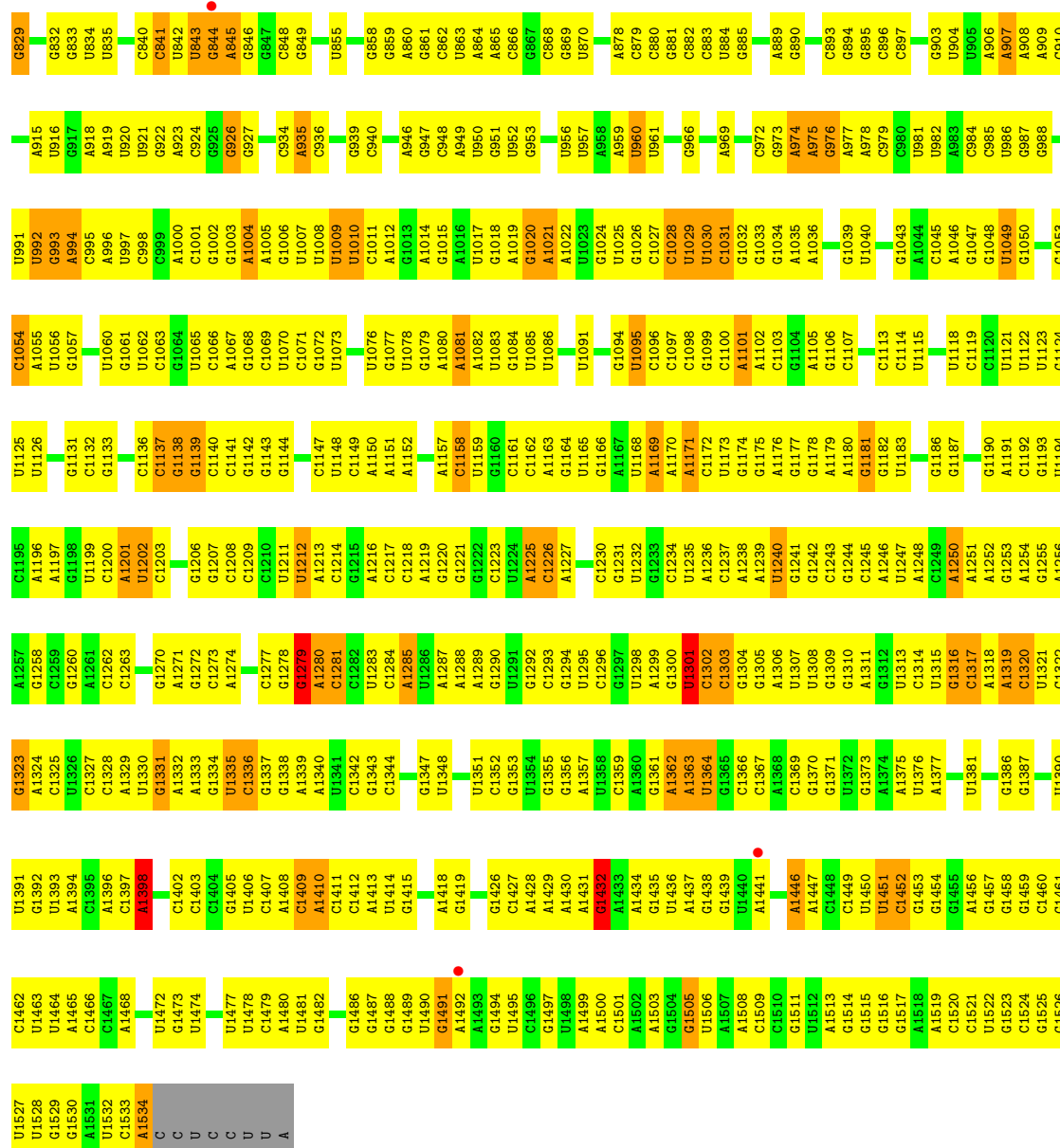
3 Residue-property plots

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.

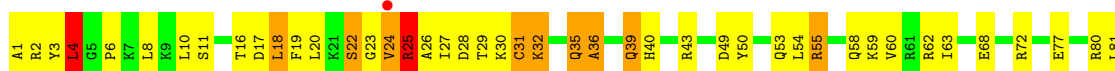
• Molecule 1: 16S rRNA

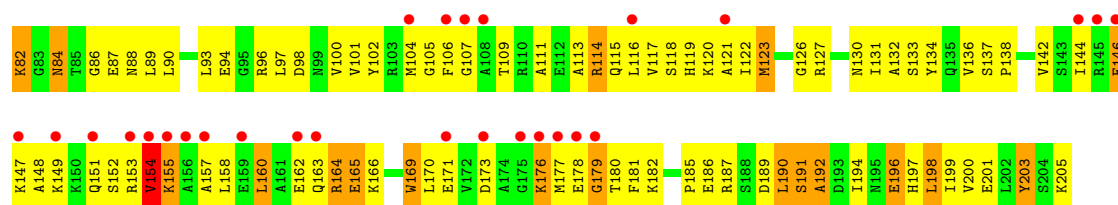
Chain AA: 





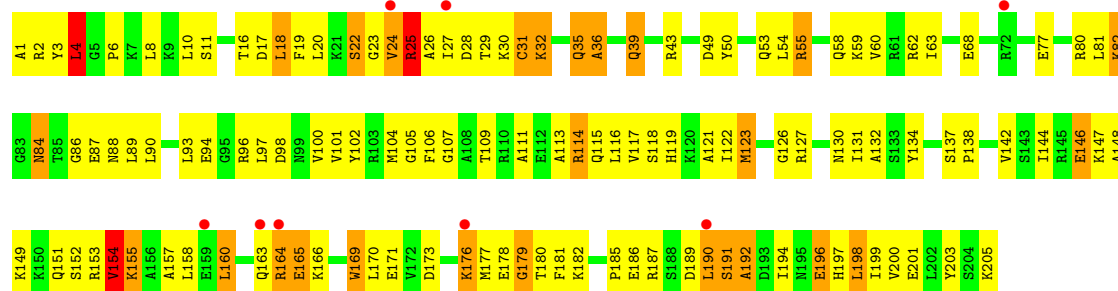
A1319	A1261	G1190	U1118	U1049	C985	A915	G832	G755	A687	G618	G548	G484	G413	C352	U273
C1320	A1262	A1191	C1119	G1050	U986	U916	G833	U762	G691	U619	C549	U485	A414	C352	A274
U1321	G1253	A1192	C1120	G1053	G987	G917	U834	U763	U692	C620	U550	U486	A415	A353	G275
C1322	A1254	U1121	U1121	G1054	G988	A918	U835	G764	G693	A621	U551	U487	G416	G354	G276
G1323	G1255	U1122	U1122	C1054	A918	A919	C840	G765	G694	C622	U552	C488	U420	C355	G277
A1324	A1256	U1123	U1123	U1055	U991	U920	C841	A766	A695	C624	A553	C489	U421	G356	G278
C1325	G1195	U1124	U1124	U1056	G992	U921	U842	A767	A696	U625	A554	C490	U422	G357	A279
U1326	A1196	U1125	U1125	G1057	G993	U922	U843	A768	U697	G626	U555	C491	C423	U358	C280
C1327	A1261	U1126	U1126	U1060	A994	A923	G844	G769	G698	U627	C556	C492	G424	U359	G281
C1328	G1198	U1127	U1127	U1061	C995	A924	G845	C770	G699	G628	G557	G493	G425	G361	C284
A1329	C1263	U1128	U1128	U1062	A996	C924	G846	C771	G699	G628	G558	G494	G425	G361	C285
U1330	C1200	U1129	U1129	U1063	U997	G925	G847	C772	G700	U632	A559	A495	G426	C362	C286
G1331	A1201	U1130	U1130	C1063	C998	G926	G848	C773	U701	U633	A560	A496	G427	A364	
A1332	U1202	U1131	U1131	G1064	C999	G927	C848	C774	A702	G633	A561		U428	U365	
C1333	C1203	U1132	U1132	U1065	A1000	G928	G849	C775	A703	C634	U562	A499	U429	U366	G289
G1334	C1273	U1133	U1133	U1066	C1001	G929	U855	C776	G704	A635	U566	G500	A431	U367	
U1335	A1274	U1134	U1134	U1067	G1002	G930	U856	C777	A705	U636	U567	C501	A432	C370	A298
C1336	G1206	U1135	U1135	G1068	G1003	C932	G858	C778	A706	C637	U568	A502	A433	A371	G299
G1337	G1207	U1136	U1136	U1069	A1004	G933	G859	C779	A707	U638	A572	C503	U434	A372	A300
U1338	C1208	U1137	U1137	U1070	A1005	C934	G860	A782	C708	G639	A573	G504	A435	C373	G301
G1339	C1209	U1138	U1138	U1071	A1006	C935	G861	A783	C709	A640	A574	G505	A436	A374	A302
C1340	G1210	U1139	U1139	U1072	G1007	C936	G862	A784	C710	U641	C575	G506	U437	U375	
A1341	U1211	U1140	U1140	U1073	U1008	C937	C863	C785	G711	A642	C576	A509	U438	U376	A306
U1342	C1281	U1141	U1141	U1074	U1009	G939	U864	C786	G712	C643	C577	A510	U439	G377	C307
G1343	U1282	U1142	U1142	U1075	U1010	C940	A864	C787	G713	C644	C578	A511	U440	G378	C308
C1344	C1283	U1143	U1143	U1076	C1011	G941	A865	C788	G714	A645	C579	C512	U441	C379	A309
U1345	A1284	U1144	U1144	U1077	C1012	G942	C866	C789	A715	G650	C581	C513	G449	G380	C310
G1346	C1285	U1145	U1145	U1078	A1012	G943	G867	C790	A716	U651	C582	C514	G450	C381	C311
C1347	U1286	U1146	U1146	U1079	G1013	A946	G868	C791	C717	C652	C583	C515	G451	A392	C312
U1348	A1287	U1147	U1147	U1080	A1014	G947	G869	C792	C718	U653	C584	U516	A452	A393	C313
A1349	C1288	U1148	U1148	U1081	G1015	G948	C870	C793	C719	C654	C585	U517	A453	A394	C314
U1350	U1289	U1149	U1149	U1082	U1016	A949	C871	C794	C720	G655	C586	C518	G454	C395	A315
G1352	C1290	U1150	U1150	U1083	U1017	U950	A872	C795	G721	G656	C587	C519	G455	C396	C316
C1353	U1291	U1151	U1151	U1084	G1018	G951	A873	C796	G722	U657	C588	C520	A456	U387	C317
U1354	G1292	U1152	U1152	U1085	A1019	U952	G874	C797	U723	C658	C589	C521	A457	G388	C318
G1355	C1293	U1153	U1153	U1086	G1020	G953	C875	C798	G724	U659	C590	C522	A458	A389	G319
C1356	U1294	U1154	U1154	U1087	A1021	U954	C876	C799	C725	U660	C591	C523	A459	U390	A320
U1357	G1295	U1155	U1155	U1088	A1022	U955	C877	C800	C726	G661	C592	A524	A460	U391	A321
G1358	C1296	U1156	U1156	U1089	U1025	U956	C878	C801	G727	U662	C593	G525	A461	G392	C322
C1359	U1297	U1157	U1157	U1090	G1026	U957	C879	C802	A728	U663	C594	C526	A462	C393	C323
A1360	U1298	U1158	U1158	U1091	U1027	U958	C880	C803	C729	U664	C595	C527	A463	A394	G324
G1361	C1300	U1159	U1159	U1092	C1028	U959	C881	C804	G730	G665	C596	G528	A464	G395	A325
U1362	U1301	U1160	U1160	U1093	U1029	G960	C882	C805	G731	U666	C597	G529	A465	C396	G326
C1363	G1302	U1161	U1161	U1094	U1030	U961	C883	C806	C732	G667	C598	G530	A466	C397	A327
U1364	U1303	U1162	U1162	U1095	U1031	U962	C884	C807	G733	U668	C599	G531	A467	C398	C328
G1365	C1304	U1163	U1163	U1096	C1032	U963	C885	C808	G734	U669	C600	G532	A468	A397	C329
C1366	U1305	U1164	U1164	U1097	G1033	U964	C886	C809	C735	U670	C601	U531	C469	U398	A329
A1368	A1306	U1165	U1165	U1098	G1034	U965	C887	C810	C736	A672	C602	U532	C470	G399	C330
G1369	C1307	U1166	U1166	U1099	C1035	U966	C888	C811	C737	G674	U603	C536	U471	C401	G331
U1370	U1308	U1167	U1167	U1100	A1036	U967	C889	C812	C738	A675	A607	C537	U472	C402	G332
G1371	C1309	U1168	U1168	U1101	U1037	U968	C890	C813	C739	U676	A608	C538	U473	C403	C333
U1372	U1310	U1169	U1169	U1102	G1038	U969	C891	C814	U740	U677	A609	C539	G474	C404	C334
C1373	A1311	U1170	U1170	U1103	U1039	U970	C892	C815	G741	U678	C610	A539	C475	G405	C335
G1374	G1312	U1171	U1171	U1104	U1040	U971	C893	C816	C742	C679	U611	G540	C476	U405	A336
A1375	C1313	U1172	U1172	U1105	U1041	U972	C894	C817	C743	C680	C612	G541	C477	G406	G337
U1376	U1314	U1173	U1173	U1106	G1042	U973	C895	C818	C744	A681	C613	G542	U478	U407	A338
G1379	C1315	U1174	U1174	U1107	C1043	U974	C896	C819	C745	G682	C614	U543	U479	A408	
U1380	U1316	U1175	U1175	U1108	C1044	U975	C897	C820	G746	G683	C615	G544	U480	U409	C345
C1381	C1317	U1176	U1176	U1109	C1045	U976	C898	C821	A747	U684	C616	C545	U481	G410	C348
U1382	U1318	U1177	U1177	U1110	U1046	U977	C899	C822	C748	G685	C617	A546	A482	A411	
		U1178	U1178	U1111	G1047	U978	C900	C823	G749	U686	C618	A547	C483	A412	A349
		U1179	U1179	U1112	U1048	U979	C901	C824	U750	U687	C619				
		U1180	U1180	U1113	U1049	U980	C902	C825	U751	U688	C620				
		U1181	U1181	U1114	U1050	U981	C903	C826	U752	U689	C621				
		U1182	U1182	U1115	U1051	U982	C904	C827	U753	U690	C622				
		U1183	U1183	U1116	U1052	U983	C905	C828	U754	U691	C623				
		U1184	U1184	U1117	U1053	U984	C906	C829	U755	U692	C624				
		U1185	U1185	U1118	U1054	U985	C907	C830	U756	U693	C625				
		U1186	U1186	U1119	U1055	U986	C908	C831	U757	U694	C626				
		U1187	U1187	U1120	U1056	U987	C909	C832	U758	U695	C627				
		U1188	U1188	U1121	U1057	U988	C910	C833	U759	U696	C628				





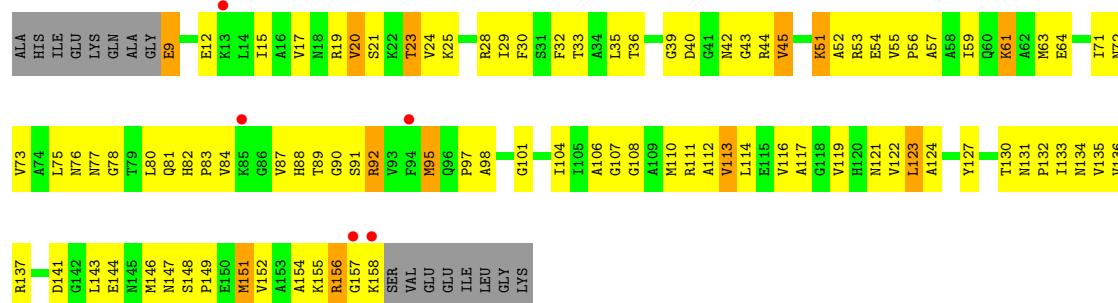
• Molecule 3: 30S ribosomal protein S4

Chain CD:



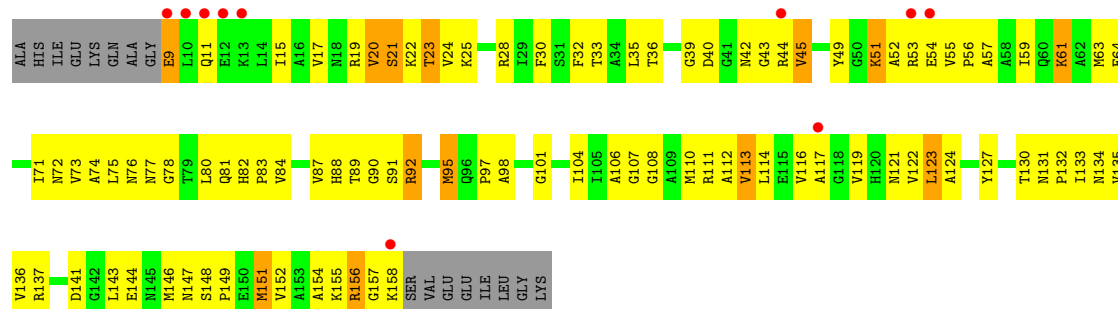
• Molecule 4: 30S ribosomal protein S5

Chain AE:



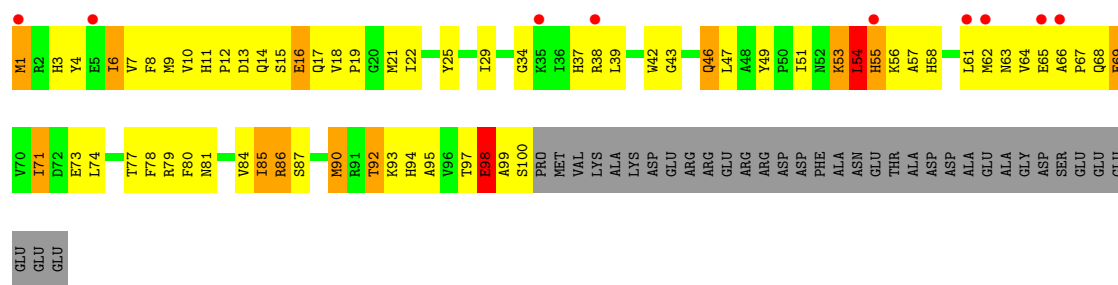
• Molecule 4: 30S ribosomal protein S5

Chain CE:



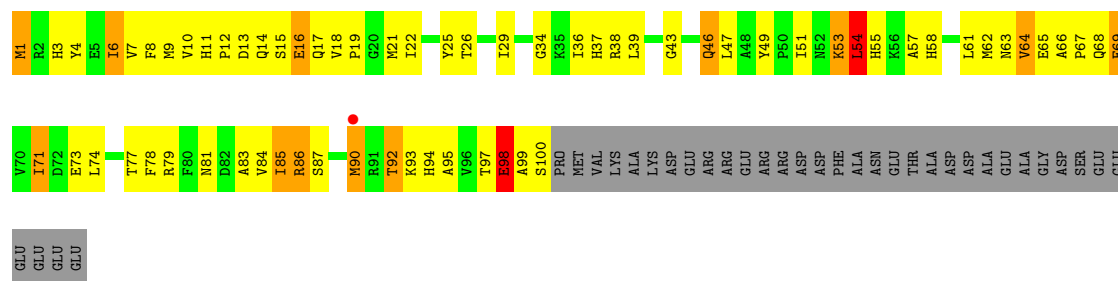
• Molecule 5: 30S ribosomal protein S6

Chain AF:



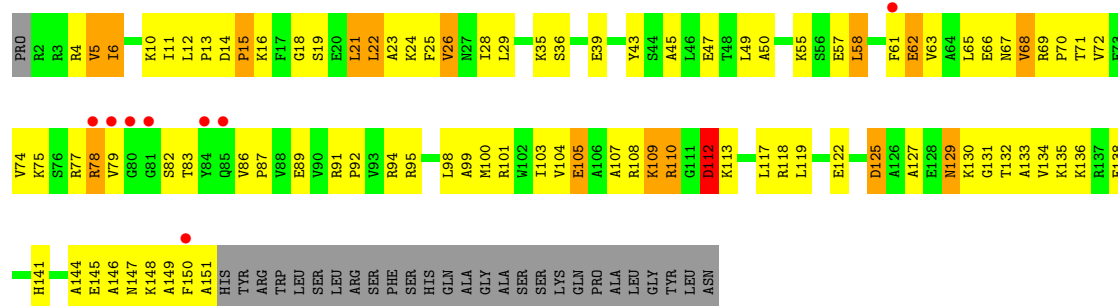
• Molecule 5: 30S ribosomal protein S6

Chain CF:



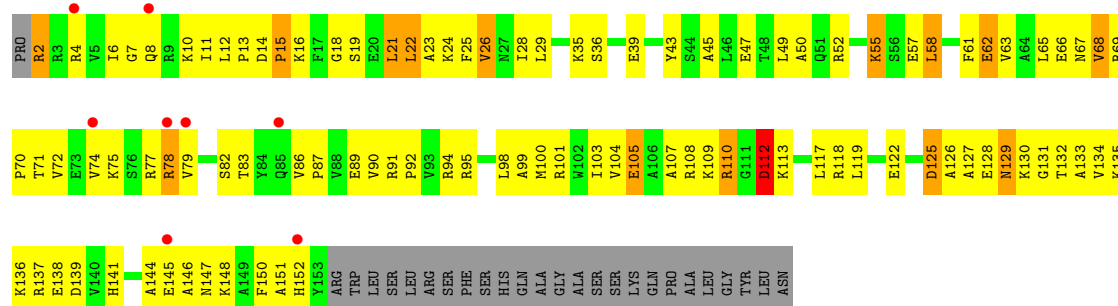
• Molecule 6: 30S ribosomal protein S7

Chain AG:



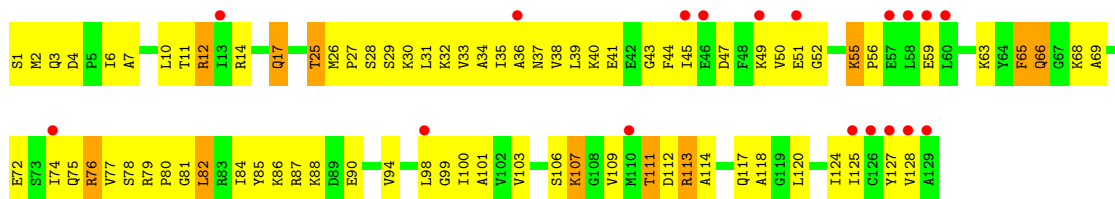
• Molecule 6: 30S ribosomal protein S7

Chain CG:



• Molecule 7: 30S ribosomal protein S8

Chain AH:



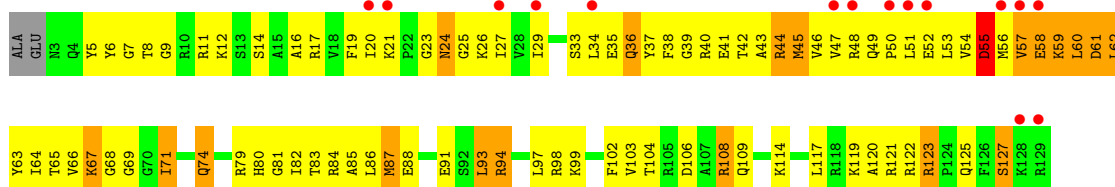
• Molecule 7: 30S ribosomal protein S8

Chain CH:



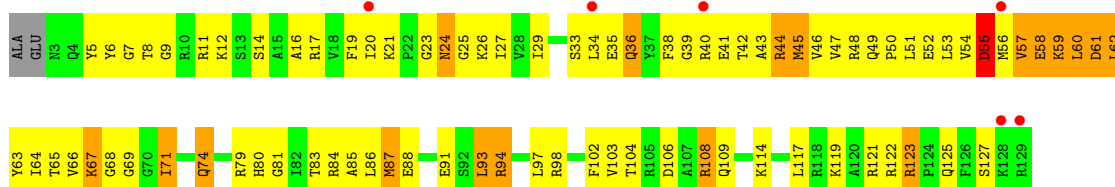
• Molecule 8: 30S ribosomal protein S9

Chain AI:



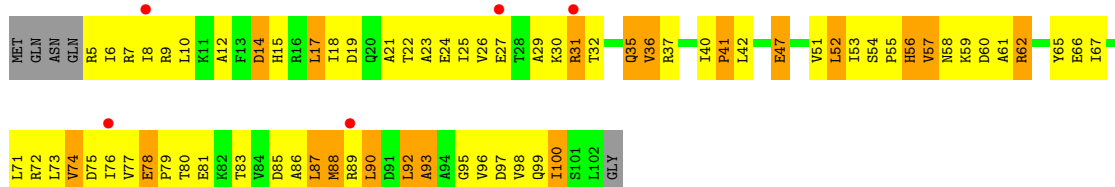
• Molecule 8: 30S ribosomal protein S9

Chain CI:



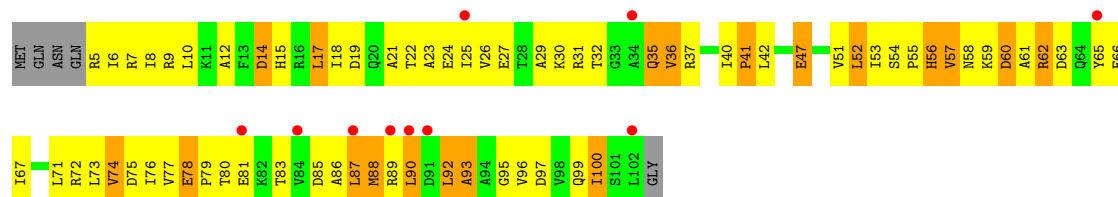
• Molecule 9: 30S ribosomal protein S10

Chain AJ:



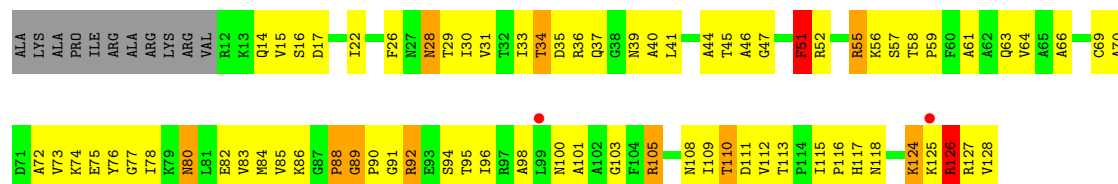
• Molecule 9: 30S ribosomal protein S10

Chain CJ:



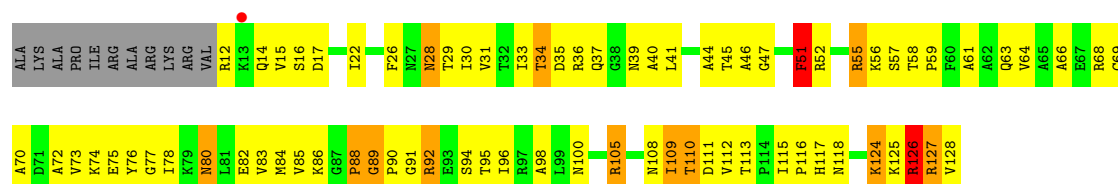
• Molecule 10: 30S ribosomal protein S11

Chain AK:



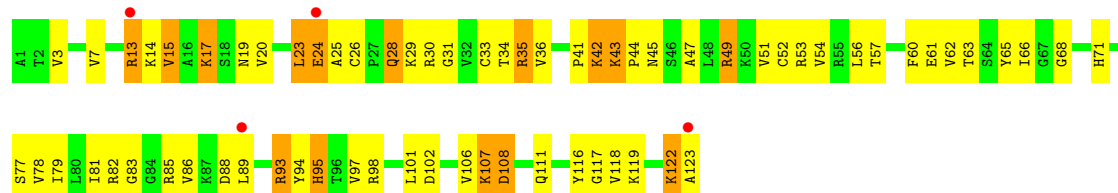
• Molecule 10: 30S ribosomal protein S11

Chain CK:



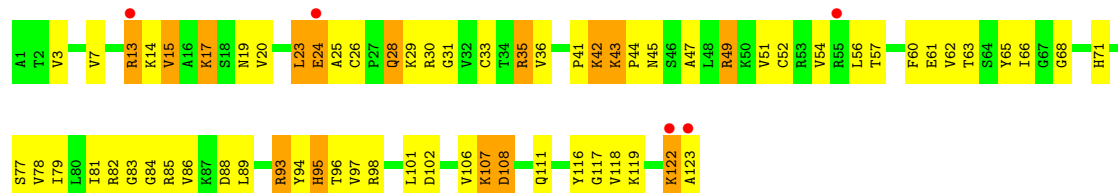
• Molecule 11: 30S ribosomal protein S12

Chain AL:



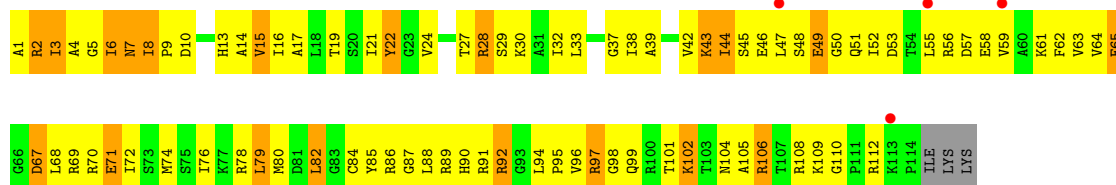
• Molecule 11: 30S ribosomal protein S12

Chain CL:



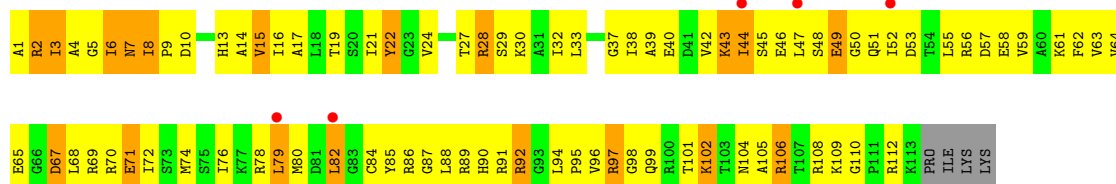
• Molecule 12: 30S ribosomal protein S13

Chain AM:



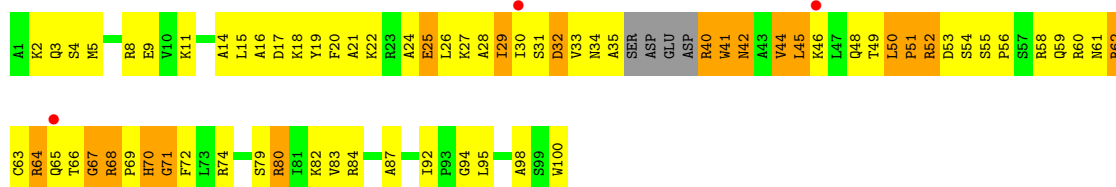
• Molecule 12: 30S ribosomal protein S13

Chain CM:



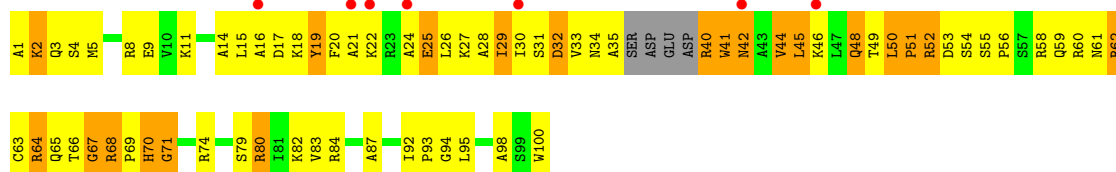
• Molecule 13: 30S ribosomal protein S14

Chain AN:



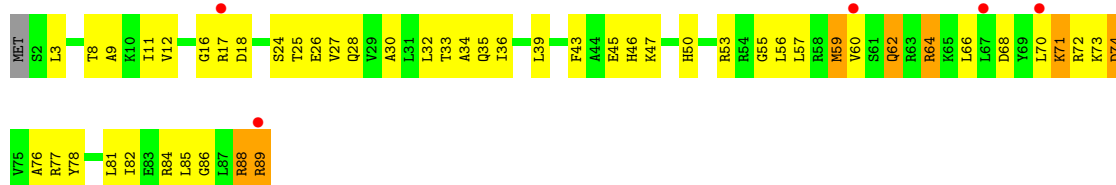
• Molecule 13: 30S ribosomal protein S14

Chain CN:



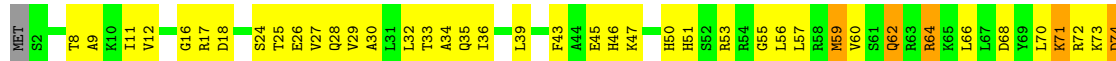
• Molecule 14: 30S ribosomal protein S15

Chain AO:



• Molecule 14: 30S ribosomal protein S15

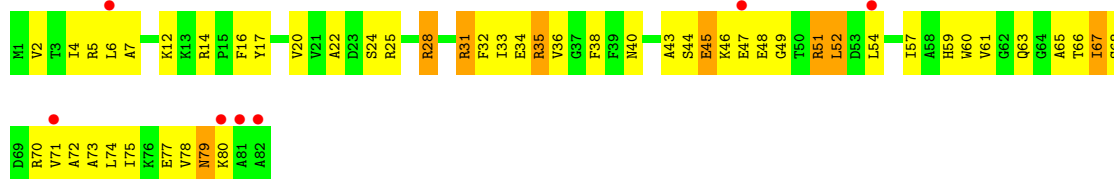
Chain CO:





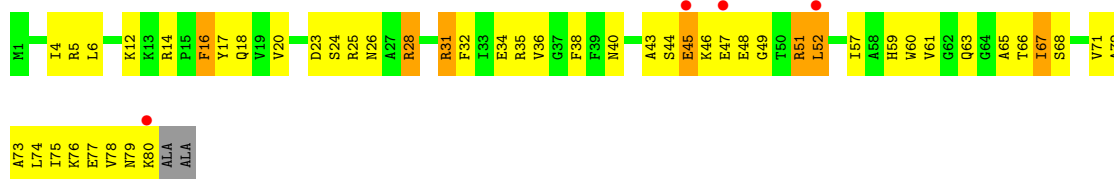
- Molecule 15: 30S ribosomal protein S16

Chain AP:



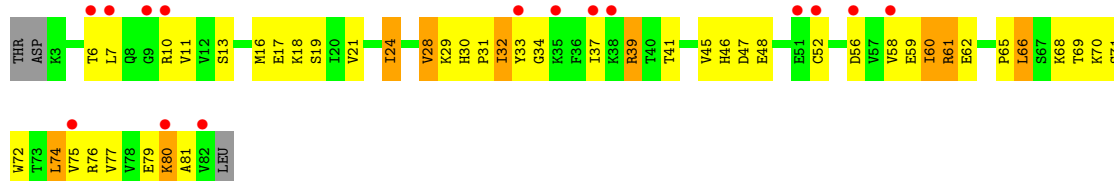
- Molecule 15: 30S ribosomal protein S16

Chain CP:



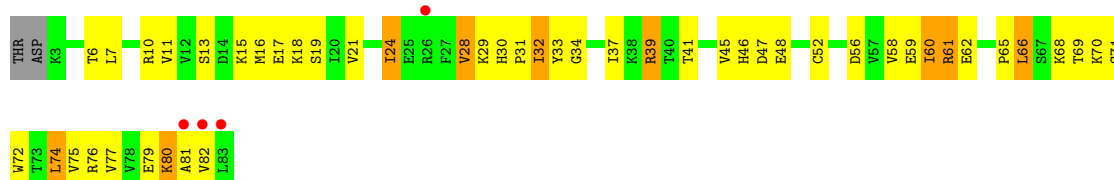
- Molecule 16: 30S ribosomal protein S17

Chain AQ:



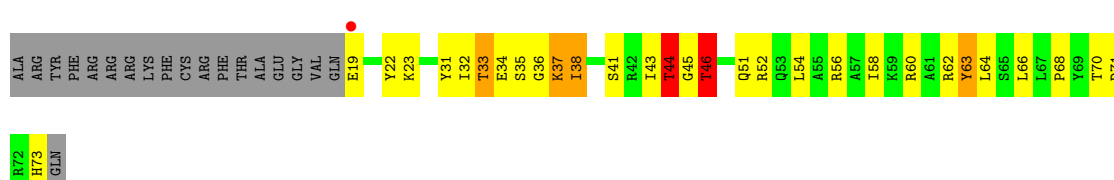
- Molecule 16: 30S ribosomal protein S17

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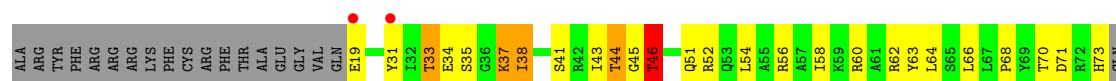
- Molecule 17: 30S ribosomal protein S18

Chain AR:



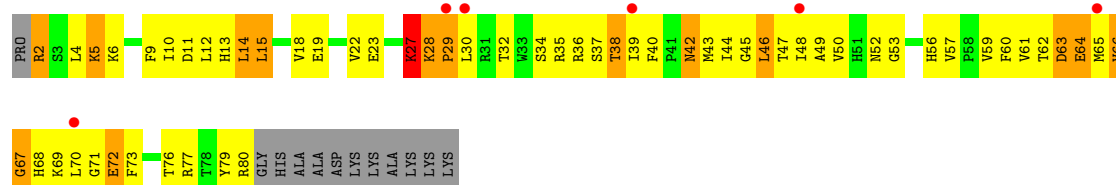
- Molecule 17: 30S ribosomal protein S18

Chain CR:



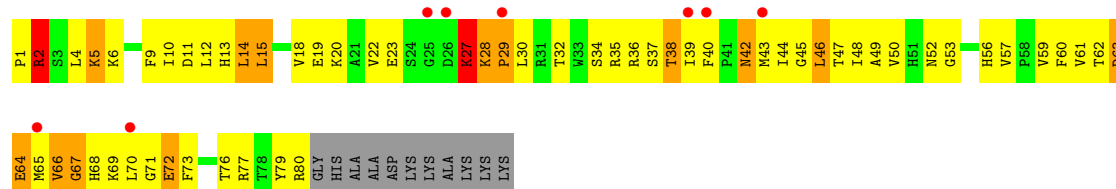
- Molecule 18: 30S ribosomal protein S19

Chain AS:



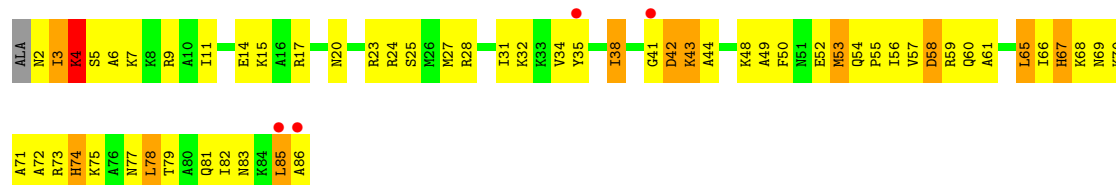
- Molecule 18: 30S ribosomal protein S19

Chain CS:



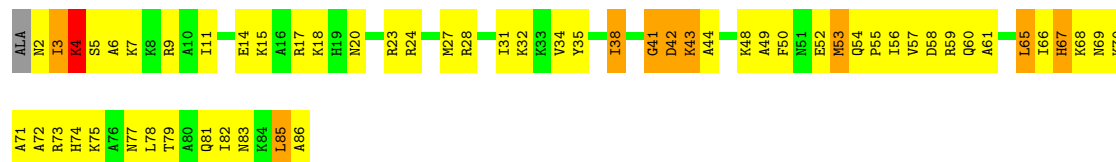
- Molecule 19: 30S ribosomal protein S20

Chain AT:



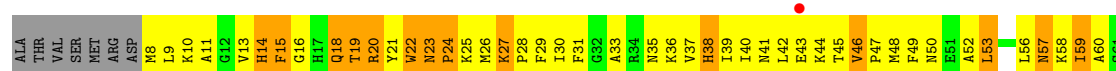
- Molecule 19: 30S ribosomal protein S20

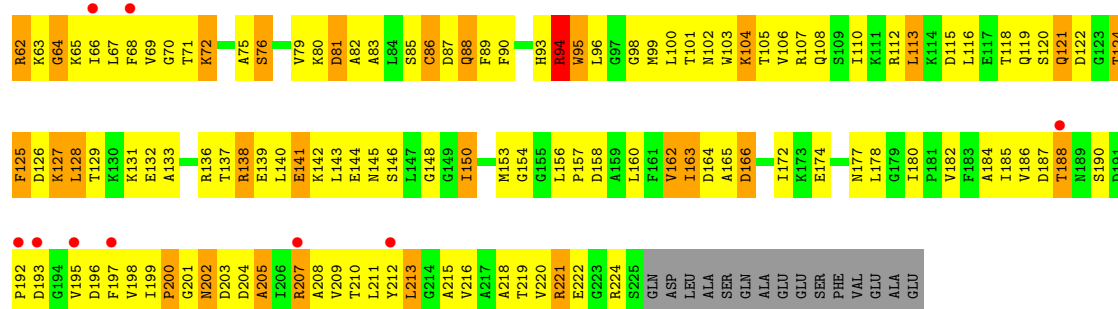
Chain CT:



- Molecule 20: 30S ribosomal protein S2

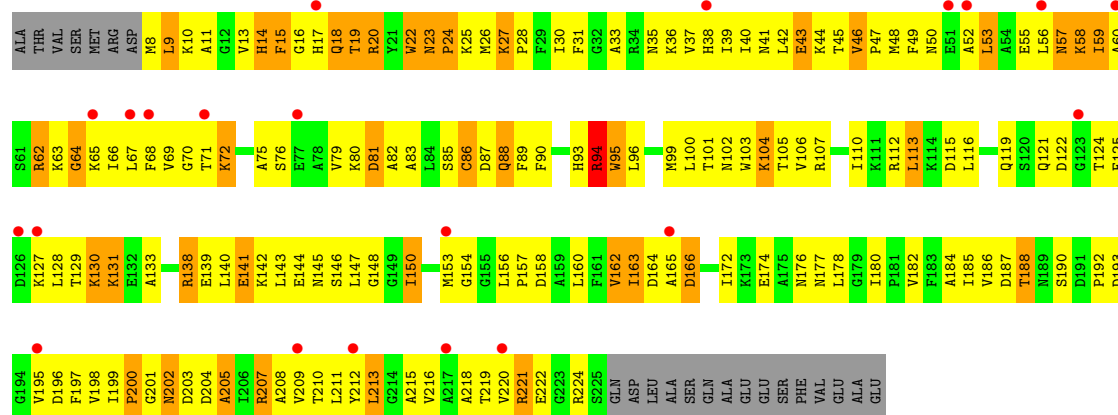
Chain AB:





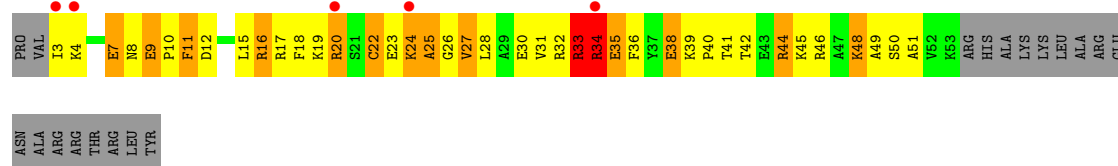
• Molecule 20: 30S ribosomal protein S2

Chain CB:



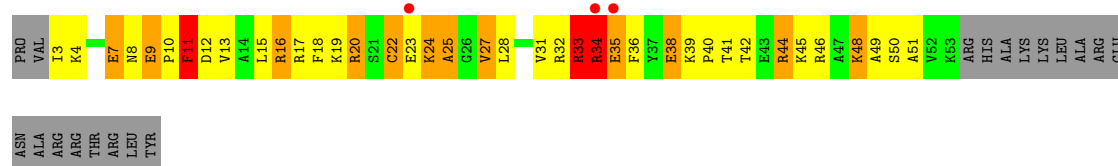
• Molecule 21: 30S ribosomal protein S21

Chain AU:



• Molecule 21: 30S ribosomal protein S21

Chain CU:



• Molecule 22: 5S rRNA

Chain BA:



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A1773	G1629	U1553	U1485	G1343	A1269	G1187	U1119	C1053	A988	A920	C851	G776
U1775	G1633	U1554	U1486	G1418	C1270	G1192	G1124	A1054	A989	C921	U852	G777
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A1800	G1661	U1578	U1513	U1444	G1300	C1229	C1153	U1083	U1015	A947	G	C815
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• Molecule 23: 23S rRNA

Chain DB:

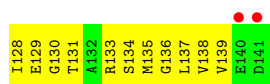
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A		C758		G620	U552	A482	G412	C337	C275	A197	U136	A5
C		G759			G553	A483	C413	G338	U276	C198	U137	A6
C896		G760			U554	A484	C414	G339	C277	A199	U138	G7
A899	C835	A761			G555	C485	C415	A340	A278	U200	U139	C8
A900	G836	G824	C692	G625	A556		U416	C341	A279	G205	C140	G9
C901	C937	A626	A693	A627	C557	G491	U415	A342	U280	G206	G141	A10
C902	C838	G765	G695	G628	U558	A492	C417	A342	C281	U207	A142	G11
C903	U839	U766	G696	G629	G559	A493	C418	A343	A282	A207	C143	U12
C904	C940	G768	G697	G630	C560	G494	U419	A346	G283	C208	U144	
		U769	G698	G631	C561	G495	C420	A347	U284	C209	C79	
G907	U841	G770	A699	A632	U562	G496		A348	G285		G80	G15
U942	G942	G771	C699	A633	C563	A497	G424	U349	U286	G215	C145	C16
G843	G843	C772	G700	A634	A563	G498	G425	U349	G287	A216	U148	U18
A909	A844	U773		C634	C564	G498	C426	G350	U288	A217	A149	A19
A910	U845	G774	G704	C635	C565	U499	U427	C351	U288	A218	A84	
A911	U846	G775	A705	G636	U566	G500	A428	C352	G289	C218	G85	
C912	U847	G776	A706	A637	U567			C353		U219	U150	A21
U913	C948	G777	U709	G638	G570	A503	U431	A354	G295	U224	U90	
A949	U850	G777	U710	U639	U571	A504	A432	C355	G296	G230	U151	A91
U919	C951		G711	C640	A572	A505	C433	G356	U297	A232	U152	U92
A920	U852	G780	U713	A643	U573	A508	U434	U358	G298	U233	A155	
C921	C853	A782	G713	A644	A574		C435	G359	U296	G230	C157	
C922	C854	A783	U714	C645	A575	C510	G438	G361	G297	A231	A160	G26
G923	G855	G784	A716	U646	U576	C511	A439	A362	G298	G232	A161	G27
G924	G856	G785	A716	G647	G577	G512	C440	G363	A300	A233	U162	U34
A925	G857	C786	C717	G648	G578	A513	U441	C364	G301	U234	A101	G35
G926	G858	C787	A718	G649	U579	A514	U442	U365	C302	G235	U102	
			C719	C650	C581	A515	C443	C366	A309	U236	C163	
U929	A863	C795	U720	G651	C581		C444	G367	U304	C236	A103	C37
U931	G864	C796	A722	U652	A582	G518	C445	A368	C305	A244	U166	A38
U932	C865	G797	C723	A654	G583	U519	C446	U369	U306	G245	A167	G39
A933	G866		U724	A655	C587	G520		G370	G307	C246	G168	U40
U934	U870	A804	G725	G656	U588	U521	U451	A371	G308	G247	G169	C41
C935	G805	G805	G726	U657	U589	C522	G452	G372	A309	G248	U170	C42
A936	U871	C906	A727	G658	A590		A453	U373	A310	C249	U171	G43
U872	C872	U807	G728	G659	U591	A526	A454	A374	A311	G250	A172	A44
C937	U873	G808	G729	C660	A592	C527	C455		G312	A251	U173	G45
C938	C873	G809	A730	A661	U593		C456			G252	U174	G46
	G874	U810			U594	A528	C457	G379	G313	G253	U175	C47
A941	G875	G810			U594	A529	A457		C314	C254	U176	G48
A942	C876	U811	C736	G664	C595	G530	G458	G386	G315	G254	C116	C49
G943	A877	C812	C737	U665	U596	C531	U459	C387	G316	A255	G177	U50
C944	U878	U813	G738	A666	G597	A532	A460	U387		G256	G178	G51
A945		C814	A739	U667	U598	G533	C461	G388	G319	C257	G180	C51
		C815	C740	A668	A599		C462	G389	A320	G258	A119	A52
C946	G	C816	U741	G669	G600	G536	G463	U390	U321	C259	U120	A53
A947	G	C817	A742	A670		G537	U464		A322	G260	G121	G54
C948	U	C818	A743	C671		A538	G465	U395	U323	G261	G122	C55
U	G	C819	A743	C672		G539	A466	U395	C323	G262	G123	A56
G950	U	A818	U744	C673		C540	G467	G396	G324	G263	G124	C57
C		A820	G745	C673		C541	G467	G396	G325	C264	A125	G58
C951		C821	U746	G674	A609	A541	G468		G326	A265	G186	
G952	U	G822	U747	A675	C610	C542	G469		G327	G266	G187	A126
	A	C823	U747	A676	C611	C543	G469		U328	C267	G188	A127
U955	C	U824	A751	A677	G612	C544	A472		G329	C268	A190	A63
C956	C	A825	C678	C678	U545	C545	A472		A330	C269	A191	U65
C957	C	A826	A752	C679	A613	U546	A473		A331	C270	C72	C56

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G2018	A1938	G1873	A1805	G1738	G1521	G1448	A1383	G1309	U1242	G1168	U1101	A960
A2019	U1939	C1874	C1585	A1739	C1586	C1451	A1384	G1310	C1243	A1029	C1002	C962
A2020	U1940	G1875	A1810	G1740	A1586	C1452	A1385	G1311	A1244	C1170	C1104	G1031
C2021	U1943	A1876	G1811	C1741	G1524	G1453	A1386	C1315	G1245	U1173	U1105	U967
C2023	U1944	G1878	U1812	U1742	C1526	A1453	A1387	U1316	A1246	A1083	G1106	C968
G2024	G1945	C1879	G1813	G1743	G1527	C1454	G1388	G1317	A1247	U1174	U1033	C969
C2025	U1946	U1880	A1815	A1744	A1529	G1455	G1389	U1318	U1248	A1175	G1034	G970
U2026	C1947	C1881	G1816	A1746	G1530	U1458	U1390	G1319	G1250	G1177	U1035	G971
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C2036	C1958	A1889	G1826	A1757	U1540	A1470	U1405	G1332	U1262	G1187	C1052	A981
A2037	U1959	U1758	U1827	U1758	C1541	A1471	U1406	G1333	U1263	G1190	C1053	A982
U2038	G1962	G1896	G1828	A1759	U1542	U1476	U1407	G1334	G1266	G1191	A1054	A983
G2039	U1963	C1897	A1829	C1760	A1545	A1477	G1408	A1335	U1267	G1192	G1056	A984
G2040	G1964	U1998	C1830	C1761	G1546	G1478	U1409	A1336	A1268	G1193	A1057	C987
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C2043	C1967	A1700	A1833	C1764	U1549	A1483	U1412	G1341	C1271	U1197	U1061	A990
G2048	G1968	A1701	C1834	U1765	A1550	U1484	A1413	A1342	A1272	U1198	G1062	C991
U2049	A1969	C1905	G1845	G1766	U1551	U1485	A1414	A1343	U1273	U1199	G1063	C992
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G1972	C1972	C1908	C1842	C1771	U1554	C1488	U1418	G1346	A1276	A1204	G1068	C995
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A2055	G1983	A1912	U1845	C1774	U1559	G1492	G1422	C1350	A1285	G1210	C1070	U999
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C2062	G1988	U1918	U1851	A1784	C1564	A1501	A1427	G1355	C1290	G1215	U1148	A1009
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C2064	G1992	C1920	A1854	A1787	A1566	A1503	G1429	C1360	G1292	C1219	C1150	A1011
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C2068	A1998	U1923	G1857	C1790	A1569	A1506	G1432	C1366	C1295	C1221	A1085	U1014
G2069	G2002	C1924	U1858	A1791	A1570	C1507	A1433	G1368	G1296	U1222	G1087	A1015
A2070	G2002	C1925	G1859	G1792	A1571	A1508	A1434	C1369	C1297	G1223	A1088	U1016
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U2075	A1931	G1931	A1866	G1797	G1576	G1515	G1441	A1302	G1302	U1231	G1161	A1020
U2076	U1932	U1932	G1867	G1799	U1577	A1516	U1442	C1303	G1303	G1236	G1162	A1021
G2077	G1933	G1933	C1868	C1800	A1579	G1516	U1443	C1304	A1304	A1237	G1163	G1022
C2078	A2013	A2014	G1869	A1901	U1580	G1517	G1444	U1379	A1305	G1238	C1164	U1023
A2015	G1934	G1935	C1870	A1735	G1581	C1518	G1445	G1380	C1306	U1097	A1098	G1024
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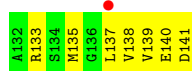
Chain BI:





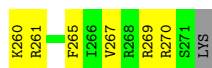
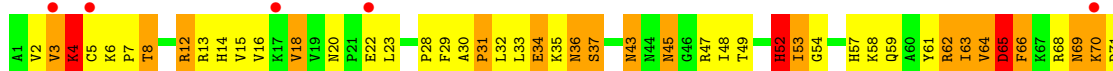
• Molecule 24: 50S ribosomal protein L11

Chain DI:



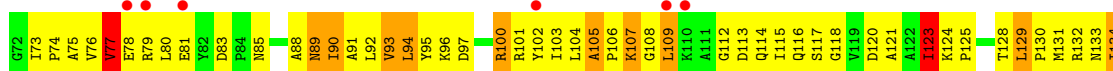
• Molecule 25: 50S ribosomal protein L2

Chain BC:



• Molecule 25: 50S ribosomal protein L2

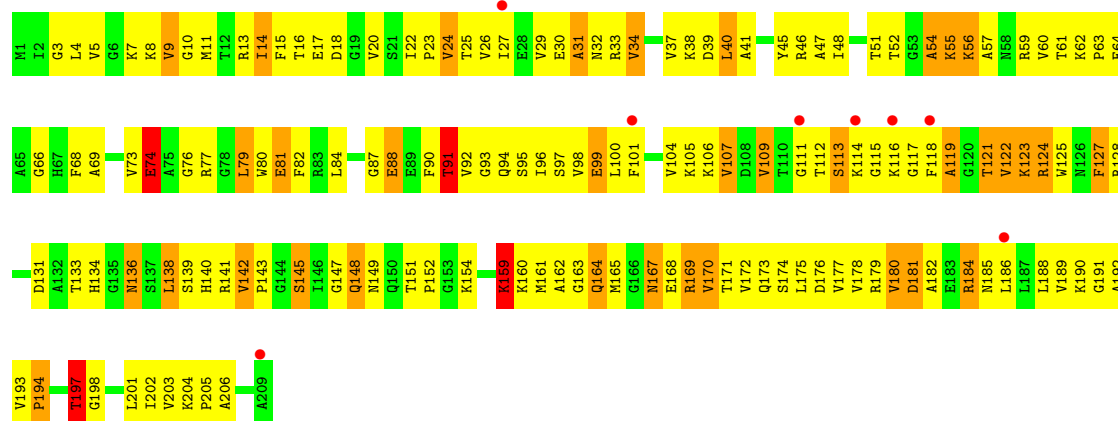
Chain DC:





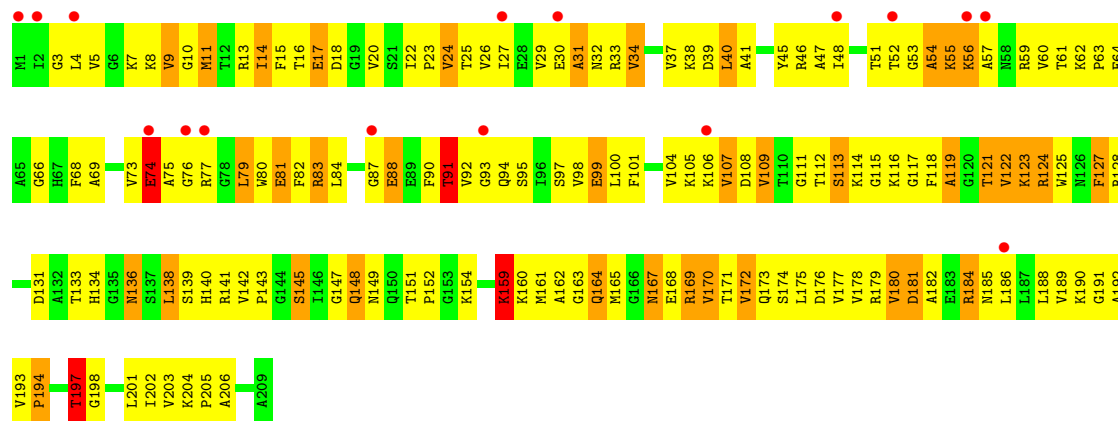
• Molecule 26: 50S ribosomal protein L3

Chain BD:



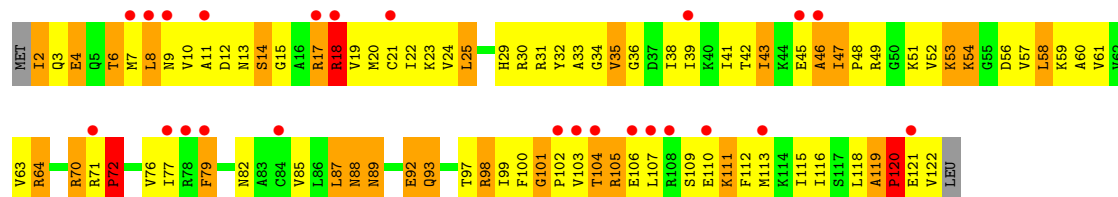
• Molecule 26: 50S ribosomal protein L3

Chain DD:



• Molecule 27: 50S ribosomal protein L14

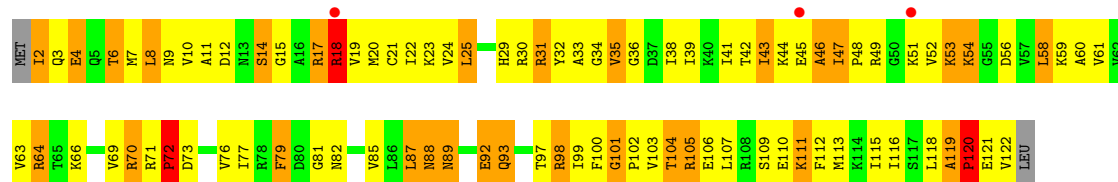
Chain BK:



• Molecule 27: 50S ribosomal protein L14

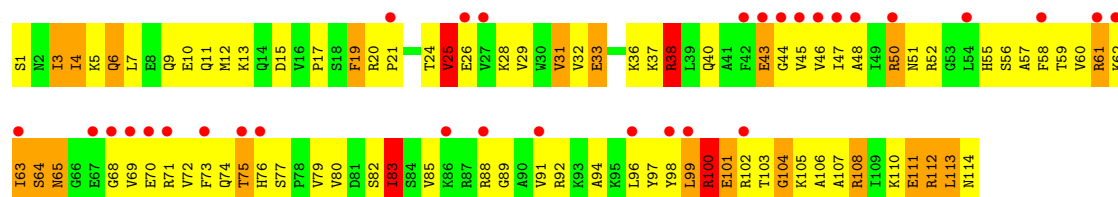
Chain DK:





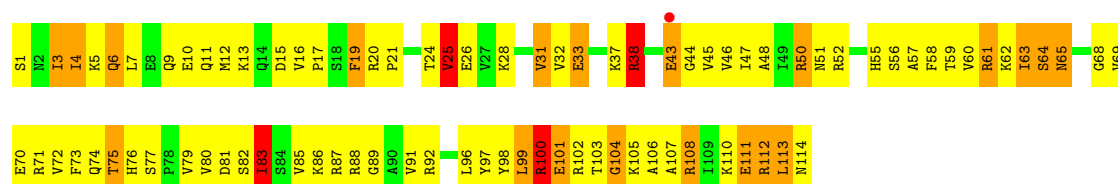
• Molecule 28: 50S ribosomal protein L19

Chain BP:



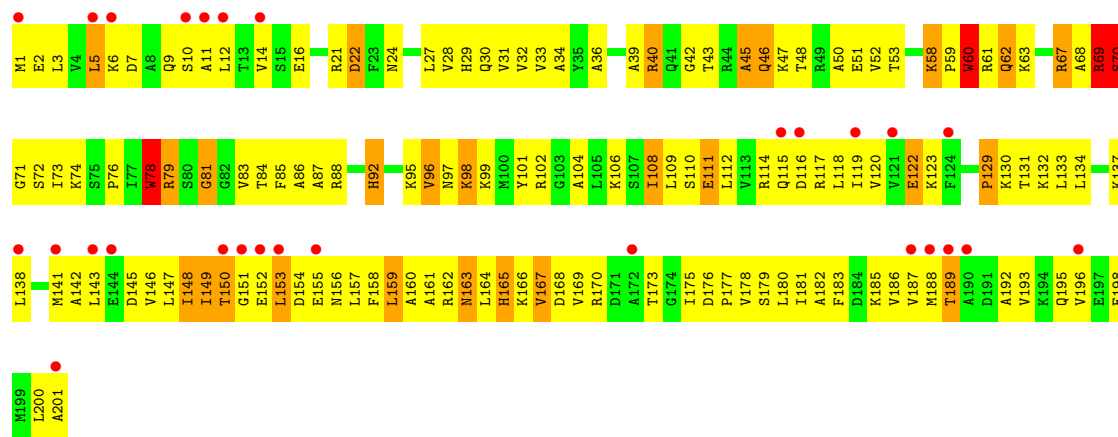
• Molecule 28: 50S ribosomal protein L19

Chain DP:



• Molecule 29: 50S ribosomal protein L4

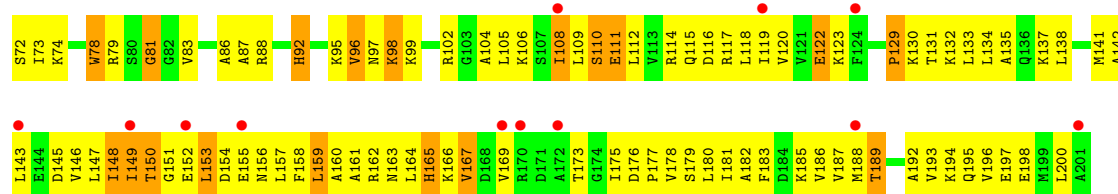
Chain BE:



• Molecule 29: 50S ribosomal protein L4

Chain DE:





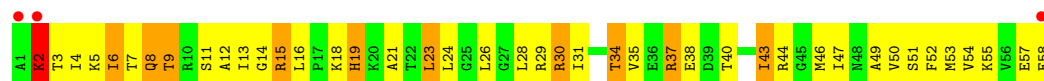
- Molecule 30: 50S ribosomal protein L30

Chain BY:



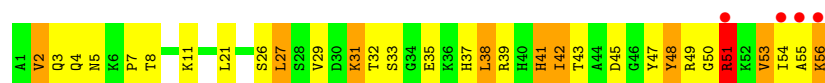
- Molecule 30: 50S ribosomal protein L30

Chain DY:



- Molecule 31: 50S ribosomal protein L32

Chain B0:



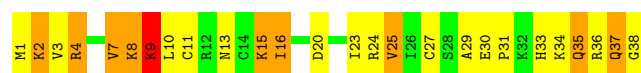
- Molecule 31: 50S ribosomal protein L32

Chain D0:



- Molecule 32: 50S ribosomal protein L36

Chain B4:



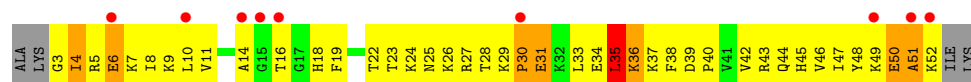
- Molecule 32: 50S ribosomal protein L36

Chain D4:



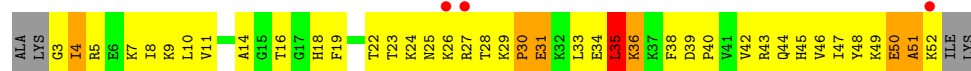
- Molecule 33: 50S ribosomal protein L33

Chain B1:



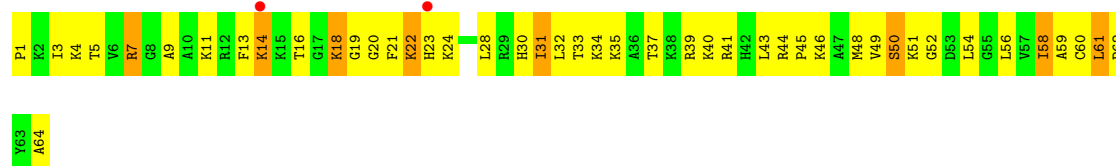
- Molecule 33: 50S ribosomal protein L33

Chain D1: 



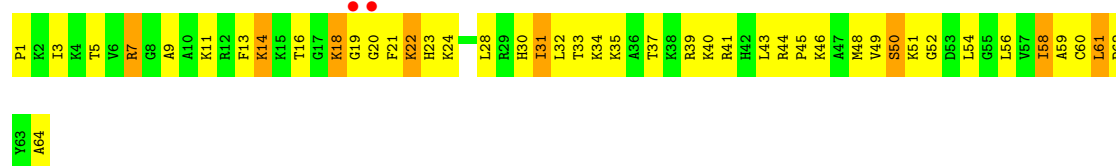
- Molecule 34: 50S ribosomal protein L35

Chain B3: 



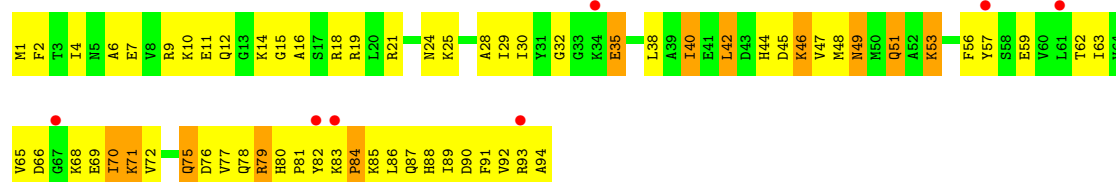
- Molecule 34: 50S ribosomal protein L35

Chain D3: 



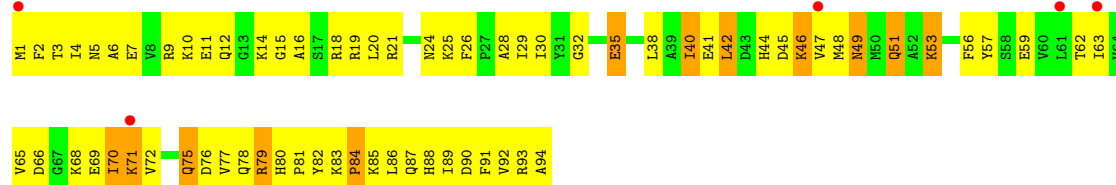
- Molecule 35: 50S ribosomal protein L25

Chain BV: 



- Molecule 35: 50S ribosomal protein L25

Chain DV: 

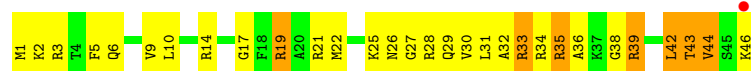


- Molecule 36: 50S ribosomal protein L34

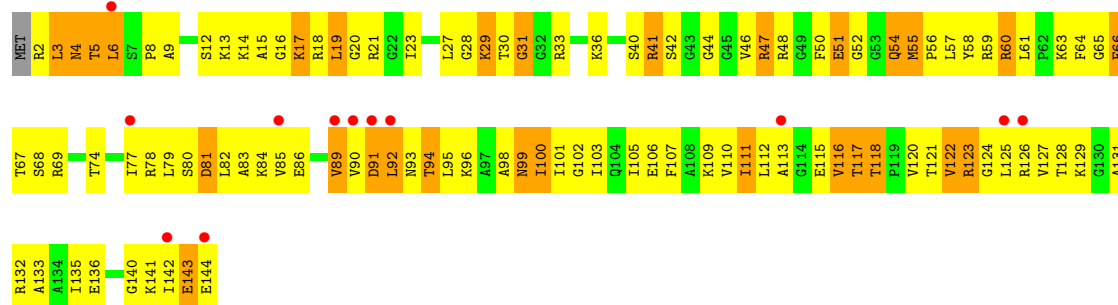
Chain B2: 



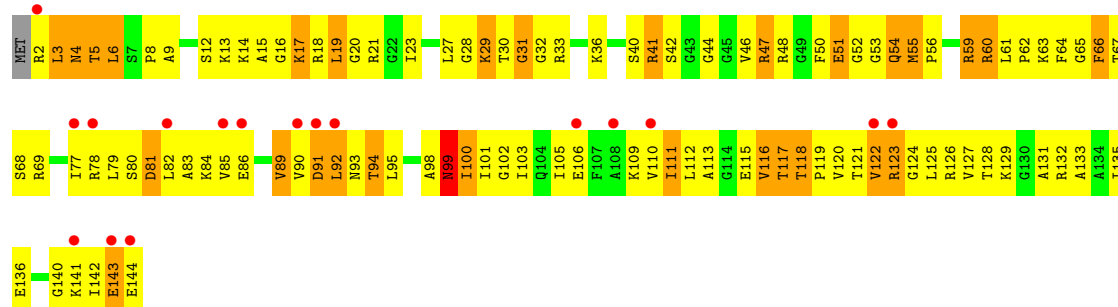
- Chain D2:



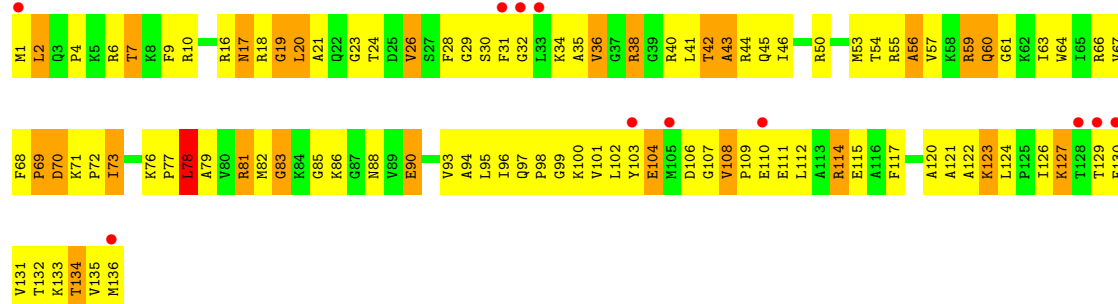
- Chain BL:



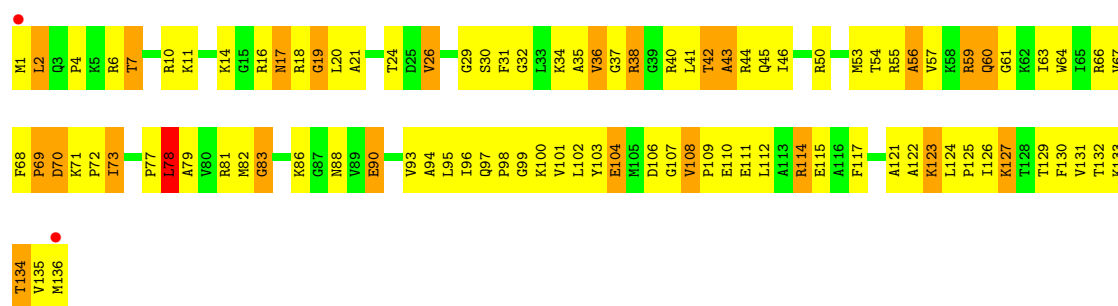
- Chain DL:



- Chain BM:

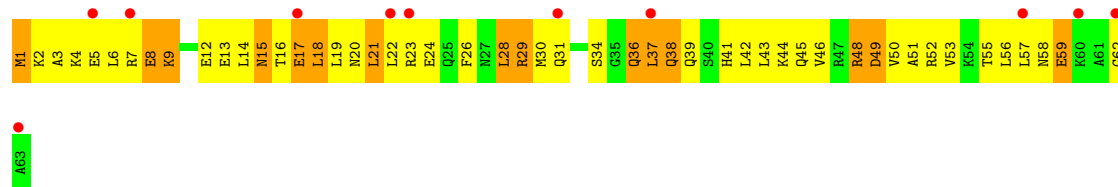


- Chain DM:



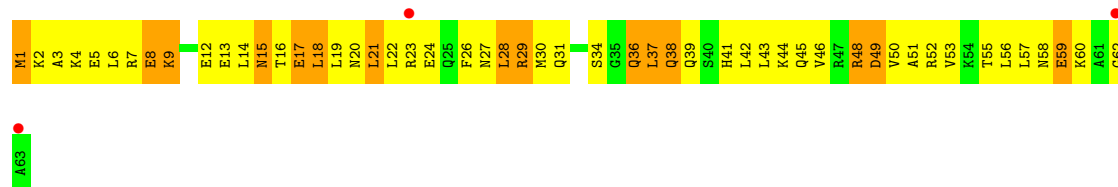
- Molecule 39: 50S ribosomal protein L29

Chain BX:



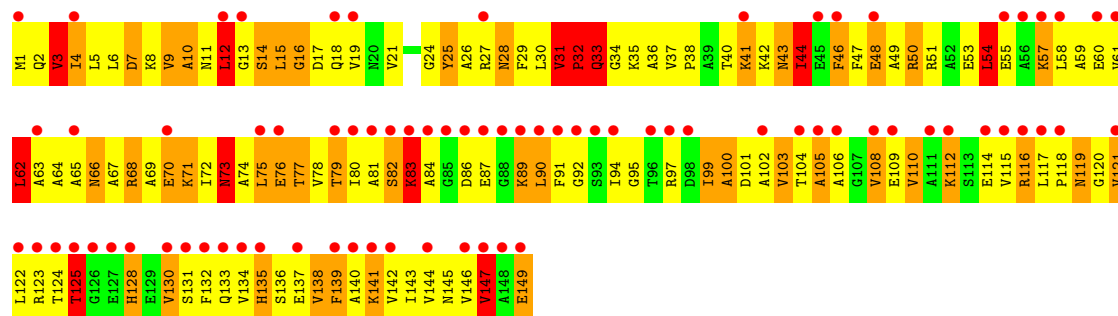
- Molecule 39: 50S ribosomal protein L29

Chain DX:



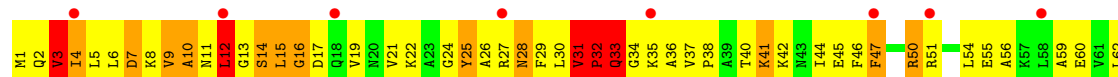
- Molecule 40: 50S ribosomal protein L9

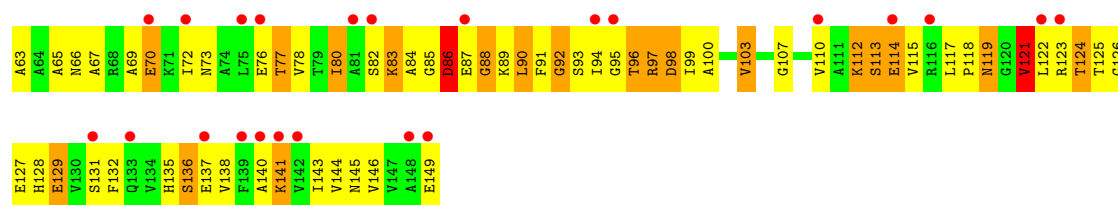
Chain BH:



- Molecule 40: 50S ribosomal protein L9

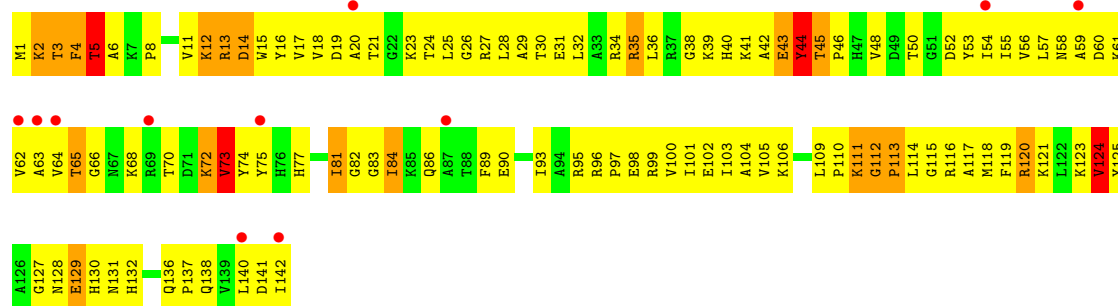
Chain DH:





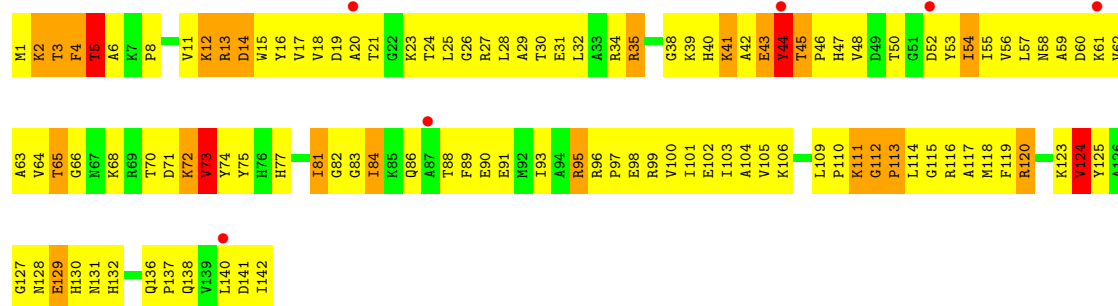
• Molecule 41: 50S ribosomal protein L13

Chain BJ:



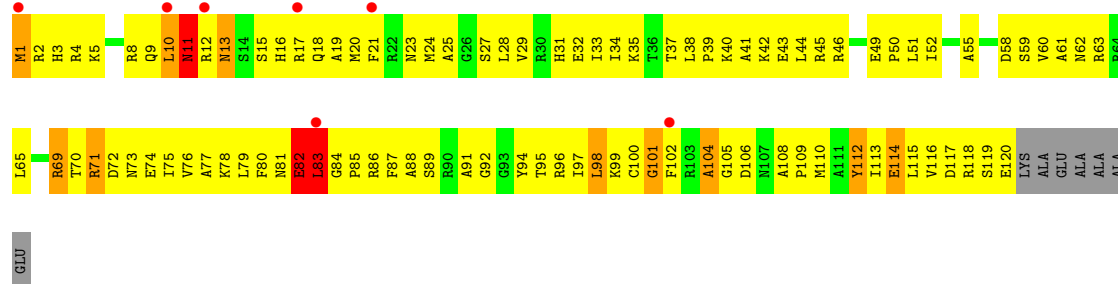
• Molecule 41: 50S ribosomal protein L13

Chain DJ:



• Molecule 42: 50S ribosomal protein L17

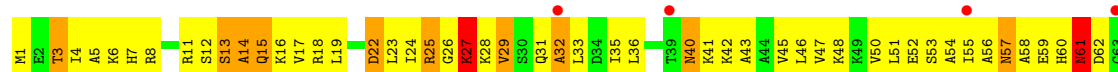
Chain BN:



• Molecule 42: 50S ribosomal protein L17

Chain DN:







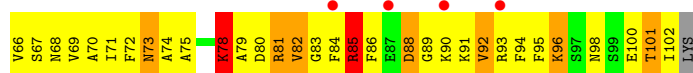
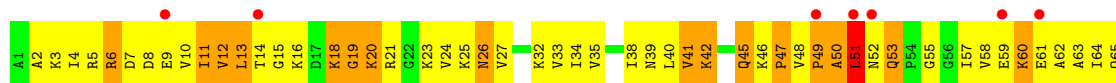
• Molecule 45: 50S ribosomal protein L22

Chain DS:



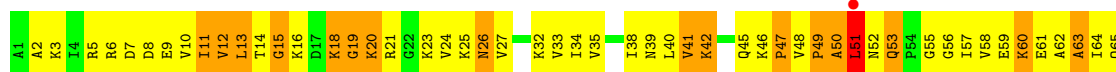
• Molecule 46: 50S ribosomal protein L24

Chain BU:



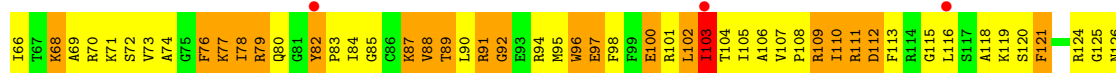
• Molecule 46: 50S ribosomal protein L24

Chain DU:



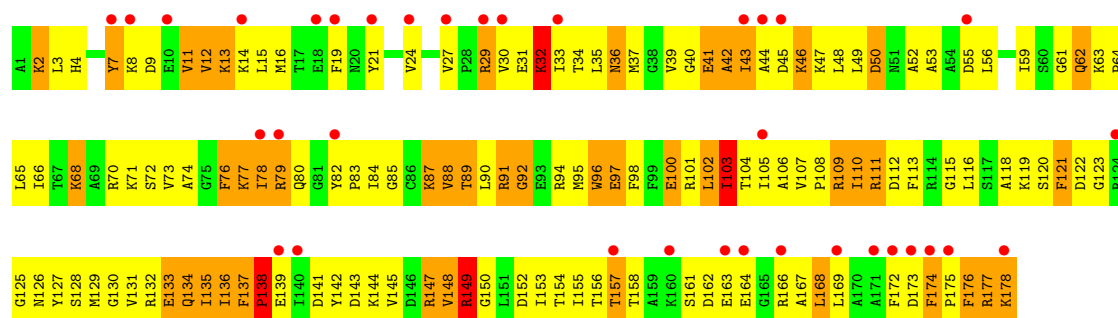
• Molecule 47: 50S ribosomal protein L5

Chain BF:



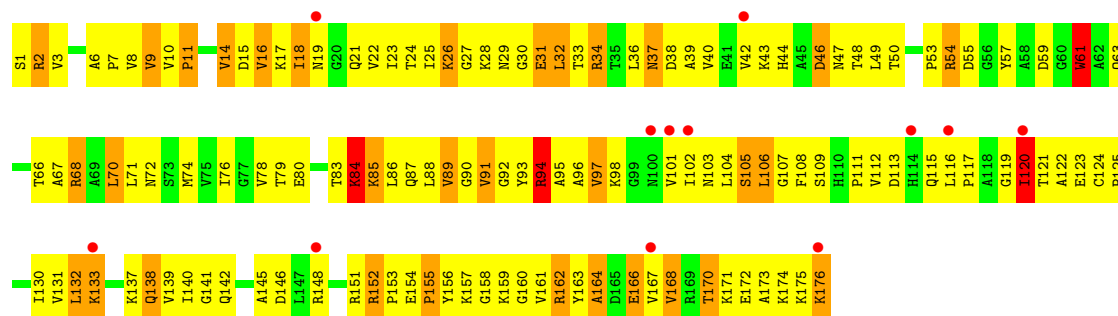
• Molecule 47: 50S ribosomal protein L5

Chain DF:



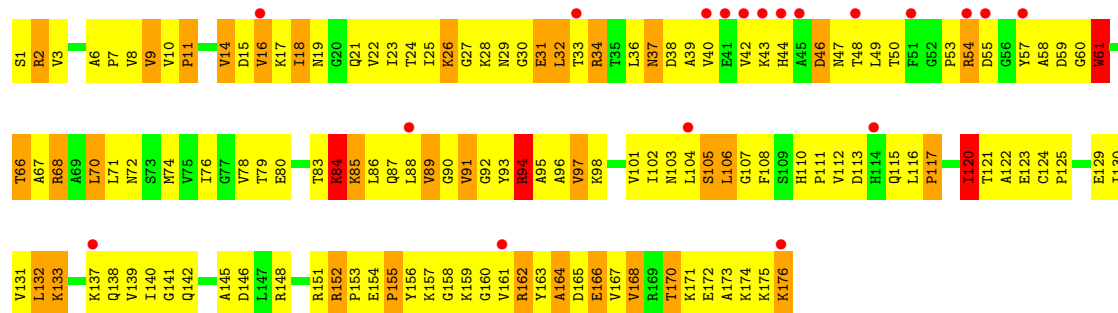
- Molecule 48: 50S ribosomal protein L6

Chain BG:



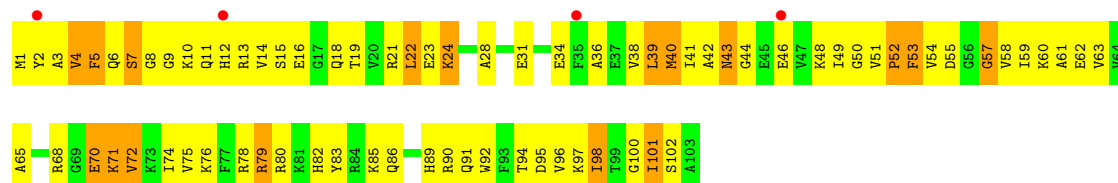
- Molecule 48: 50S ribosomal protein L6

Chain DG:



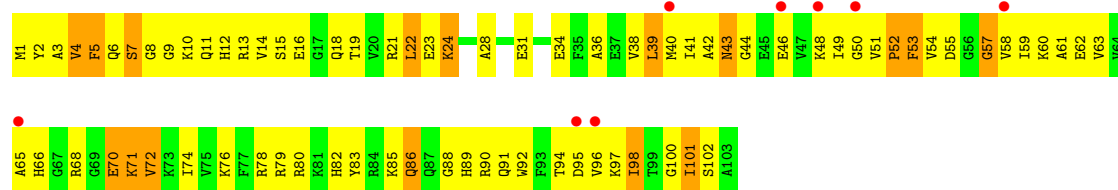
- Molecule 49: 50S ribosomal protein L21

Chain BR:



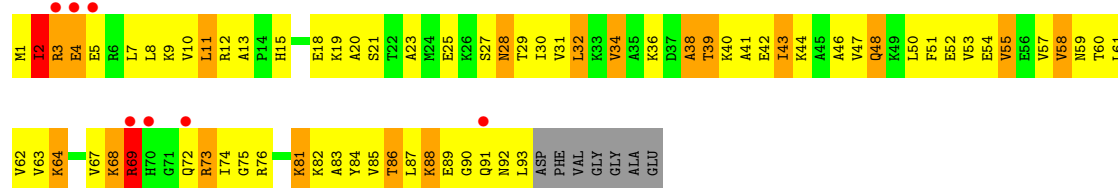
- Molecule 49: 50S ribosomal protein L21

Chain DR:



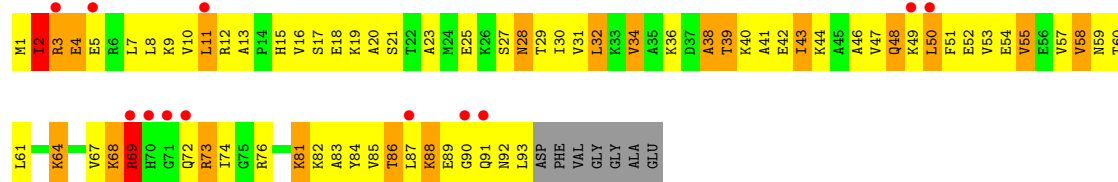
• Molecule 50: 50S ribosomal protein L23

Chain BT:



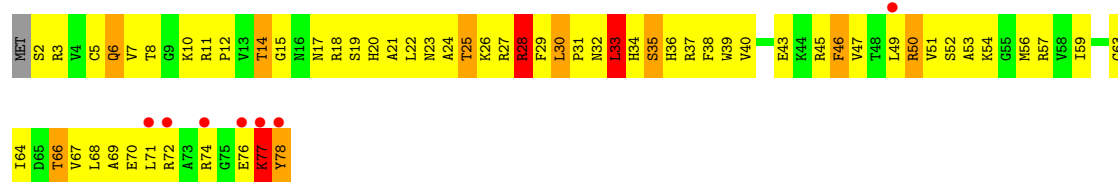
• Molecule 50: 50S ribosomal protein L23

Chain DT:



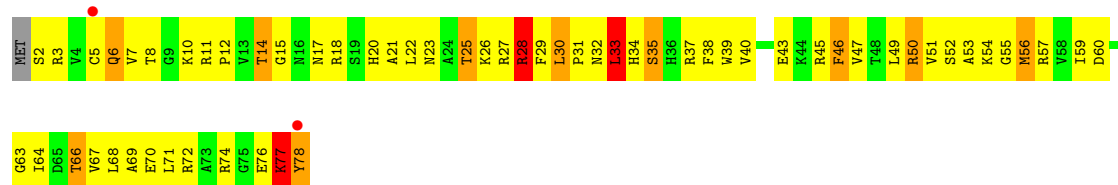
• Molecule 51: 50S ribosomal protein L28

Chain BZ:



• Molecule 51: 50S ribosomal protein L28

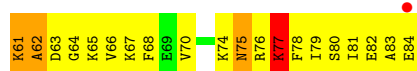
Chain DZ:



• Molecule 52: 50S ribosomal protein L27

Chain BW:





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 – 3.21 138.41 – 3.22	Depositor EDS
% Data completeness (in resolution range)	(Not available) (70.00-3.21) 66.6 (138.41-3.22)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 3.19Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.274 , 0.309 0.250 , 0.278	Depositor DCC
R_{free} test set	30053 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	93.7	Xtriage
Anisotropy	0.398	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 25.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 626512 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	284172	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.25	1/36762 (0.0%)	0.75	12/57350 (0.0%)
1	CA	0.26	1/36762 (0.0%)	0.75	16/57350 (0.0%)
2	AC	0.23	0/1651	0.44	0/2225
2	CC	0.23	0/1651	0.44	0/2225
3	AD	0.23	0/1665	0.44	0/2227
3	CD	0.23	0/1665	0.44	0/2227
4	AE	0.24	0/1118	0.46	0/1504
4	CE	0.23	0/1118	0.46	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	0.45	0/1326
7	CH	0.23	0/989	0.45	0/1326
8	AI	0.24	0/1034	0.45	0/1375
8	CI	0.24	0/1034	0.45	0/1375
9	AJ	0.22	0/796	0.49	0/1077
9	CJ	0.22	0/796	0.49	0/1077
10	AK	0.24	0/893	0.47	0/1205
10	CK	0.24	0/893	0.47	0/1205
11	AL	0.22	0/969	0.49	0/1300
11	CL	0.22	0/969	0.49	0/1300
12	AM	0.21	0/892	0.46	0/1193
12	CM	0.21	0/884	0.45	0/1181
13	AN	0.24	0/785	0.48	0/1043
13	CN	0.24	0/785	0.48	0/1043
14	AO	0.23	0/722	0.47	0/964
14	CO	0.23	0/722	0.47	0/964
15	AP	0.25	0/659	0.46	0/884
15	CP	0.25	0/648	0.46	0/870
16	AQ	0.23	0/657	0.47	0/881
16	CQ	0.23	0/666	0.48	0/892

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AR	0.23	0/462	0.45	0/621
17	CR	0.23	0/462	0.45	0/621
18	AS	0.25	0/652	0.46	0/877
18	CS	0.25	0/660	0.48	0/888
19	AT	0.24	0/671	0.40	0/888
19	CT	0.24	0/671	0.40	0/888
20	AB	0.25	0/1735	0.45	0/2338
20	CB	0.25	0/1735	0.45	0/2338
21	AU	0.26	0/430	0.48	0/570
21	CU	0.26	0/430	0.48	0/570
22	BA	0.24	0/2803	0.75	1/4371 (0.0%)
22	DA	0.24	0/2803	0.75	1/4371 (0.0%)
23	BB	0.28	8/68314 (0.0%)	0.77	42/106569 (0.0%)
23	DB	0.28	9/68314 (0.0%)	0.77	48/106569 (0.0%)
24	BI	0.24	0/1046	0.47	0/1410
24	DI	0.25	0/1046	0.49	0/1410
25	BC	0.22	0/2121	0.48	0/2852
25	DC	0.22	0/2121	0.48	0/2852
26	BD	0.24	0/1586	0.49	0/2134
26	DD	0.24	0/1586	0.49	0/2134
27	BK	0.24	0/939	0.56	0/1258
27	DK	0.24	0/939	0.56	0/1258
28	BP	0.24	0/929	0.51	0/1242
28	DP	0.24	0/929	0.51	0/1242
29	BE	0.24	0/1571	0.51	0/2113
29	DE	0.24	0/1571	0.51	0/2113
30	BY	0.23	0/453	0.50	0/605
30	DY	0.23	0/453	0.50	0/605
31	B0	0.22	0/450	0.56	0/599
31	D0	0.22	0/450	0.56	0/599
32	B4	0.23	0/303	0.48	0/397
32	D4	0.23	0/303	0.47	0/397
33	B1	0.27	0/416	0.49	0/554
33	D1	0.27	0/416	0.49	0/554
34	B3	0.24	0/513	0.48	0/676
34	D3	0.24	0/513	0.48	0/676
35	BV	0.25	0/766	0.42	0/1025
35	DV	0.25	0/766	0.42	0/1025
36	B2	0.26	0/380	0.47	0/498
36	D2	0.26	0/380	0.47	0/498
37	BL	0.23	0/1054	0.48	0/1403
37	DL	0.24	0/1054	0.49	0/1403
38	BM	0.25	0/1093	0.49	0/1460

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DM	0.25	0/1093	0.48	0/1460
39	BX	0.24	0/510	0.53	0/677
39	DX	0.24	0/510	0.53	0/677
40	BH	0.25	0/1122	0.48	0/1515
40	DH	0.25	0/1122	0.49	0/1515
41	BJ	0.23	0/1152	0.48	0/1551
41	DJ	0.23	0/1152	0.48	0/1551
42	BN	0.24	0/973	0.52	0/1301
42	DN	0.24	0/973	0.52	0/1301
43	BO	0.23	0/902	0.49	0/1209
43	DO	0.23	0/902	0.49	0/1209
44	BQ	0.26	0/960	0.50	0/1278
44	DQ	0.26	0/960	0.50	0/1278
45	BS	0.22	0/864	0.52	0/1156
45	DS	0.22	0/864	0.52	0/1156
46	BU	0.25	0/787	0.47	0/1051
46	DU	0.25	0/787	0.48	0/1051
47	BF	0.26	0/1444	0.52	0/1937
47	DF	0.26	0/1444	0.52	0/1937
48	BG	0.23	0/1343	0.47	0/1816
48	DG	0.23	0/1343	0.47	0/1816
49	BR	0.25	0/829	0.49	0/1107
49	DR	0.25	0/829	0.49	0/1107
50	BT	0.23	0/744	0.57	0/994
50	DT	0.23	0/744	0.57	0/994
51	BZ	0.25	0/635	0.52	0/848
51	DZ	0.25	0/635	0.52	0/848
52	BW	0.28	0/603	0.53	0/797
52	DW	0.28	0/603	0.53	0/797
All	All	0.26	19/306360 (0.0%)	0.70	120/457969 (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	13
1	CA	0	11
23	BB	0	43
23	DB	0	42
All	All	0	109

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	DB	1086	A	C5-C6	-16.27	1.26	1.41
23	BB	1086	A	C5-C6	-16.18	1.26	1.41
23	BB	1088	A	C6-N1	-10.58	1.28	1.35
23	DB	1088	A	C6-N1	-10.47	1.28	1.35
23	DB	2323	G	O3'-P	9.74	1.72	1.61

The worst 5 of 120 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	DB	2204	G	O5'-P-OP1	-29.64	75.14	110.70
23	BB	2204	G	O5'-P-OP2	-28.20	76.86	110.70
23	BB	2791	G	O5'-P-OP1	-27.64	77.53	110.70
23	DB	2791	G	O5'-P-OP2	-26.90	78.42	110.70
23	BB	2791	G	O5'-P-OP2	18.64	133.06	110.70

There are no chirality outliers.

5 of 109 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	187	G	Sidechain
1	AA	281	G	Sidechain
1	AA	324	G	Sidechain
1	AA	78	A	Sidechain
1	AA	86	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	1156	0
1	CA	32831	0	16521	1152	0
2	AC	1624	0	1699	127	0
2	CC	1624	0	1699	127	0
3	AD	1643	0	1710	158	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	CD	1643	0	1710	151	0
4	AE	1105	0	1148	92	0
4	CE	1105	0	1148	95	0
5	AF	817	0	808	83	0
5	CF	817	0	808	79	0
6	AG	1174	0	1230	89	0
6	CG	1196	0	1246	88	0
7	AH	979	0	1034	83	0
7	CH	979	0	1034	82	0
8	AI	1022	0	1070	128	0
8	CI	1022	0	1070	118	0
9	AJ	786	0	828	85	0
9	CJ	786	0	828	89	0
10	AK	877	0	887	94	0
10	CK	877	0	887	93	0
11	AL	955	0	1019	75	0
11	CL	955	0	1019	73	0
12	AM	883	0	944	116	0
12	CM	876	0	937	115	0
13	AN	774	0	827	101	0
13	CN	774	0	827	105	0
14	AO	714	0	734	57	0
14	CO	714	0	734	52	0
15	AP	649	0	666	54	0
15	CP	638	0	656	51	0
16	AQ	648	0	691	42	0
16	CQ	657	0	702	45	0
17	AR	455	0	478	28	0
17	CR	455	0	478	26	0
18	AS	637	0	665	86	0
18	CS	644	0	675	89	0
19	AT	665	0	714	55	0
19	CT	665	0	714	52	0
20	AB	1704	0	1732	199	0
20	CB	1704	0	1732	199	0
21	AU	425	0	449	61	0
21	CU	425	0	449	59	0
22	BA	2507	0	1270	96	0
22	DA	2507	0	1270	89	0
23	BB	60995	0	30678	2146	0
23	DB	60995	0	30677	2248	0
24	BI	1032	0	1088	111	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	DI	1032	0	1088	196	0
25	BC	2082	0	2157	259	0
25	DC	2082	0	2157	244	0
26	BD	1565	0	1616	204	0
26	DD	1565	0	1616	214	0
27	BK	930	0	1000	117	0
27	DK	930	0	1000	121	0
28	BP	917	0	965	119	0
28	DP	917	0	965	117	0
29	BE	1552	0	1619	185	0
29	DE	1552	0	1619	165	0
30	BY	449	0	491	52	0
30	DY	449	0	491	47	0
31	B0	444	0	461	45	0
31	D0	444	0	461	46	0
32	B4	302	0	340	30	0
32	D4	302	0	341	28	0
33	B1	409	0	440	51	0
33	D1	409	0	440	42	0
34	B3	504	0	574	56	0
34	D3	504	0	574	51	0
35	BV	753	0	780	80	0
35	DV	753	0	780	83	0
36	B2	377	0	418	44	0
36	D2	377	0	418	47	0
37	BL	1045	0	1117	142	0
37	DL	1045	0	1117	152	0
38	BM	1074	0	1157	115	0
38	DM	1074	0	1157	114	0
39	BX	509	0	543	62	0
39	DX	509	0	543	58	0
40	BH	1111	0	1148	196	0
40	DH	1111	0	1148	153	0
41	BJ	1129	0	1162	146	0
41	DJ	1129	0	1162	148	0
42	BN	960	0	1000	116	0
42	DN	960	0	1000	116	0
43	BO	892	0	923	79	0
43	DO	892	0	923	91	0
44	BQ	947	0	1022	142	0
44	DQ	947	0	1022	147	0
45	BS	857	0	922	103	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	DS	857	0	922	100	0
46	BU	779	0	834	125	0
46	DU	779	0	834	118	0
47	BF	1420	0	1460	231	0
47	DF	1420	0	1460	237	0
48	BG	1323	0	1374	187	0
48	DG	1323	0	1374	189	0
49	BR	816	0	839	97	0
49	DR	816	0	839	102	0
50	BT	738	0	807	129	0
50	DT	738	0	807	122	0
51	BZ	625	0	652	82	0
51	DZ	625	0	652	83	0
52	BW	596	0	610	136	0
52	DW	596	0	610	143	0
53	AA	42	0	46	2	0
53	BB	42	0	46	0	0
53	CA	42	0	46	0	0
53	DB	42	0	46	1	0
54	AA	60	0	0	0	0
54	BB	110	0	0	0	0
54	CA	60	0	0	0	0
54	CE	1	0	0	0	0
54	CN	1	0	0	0	0
54	DB	111	0	0	0	0
55	B4	1	0	0	0	0
55	D4	1	0	0	0	0
56	AA	291	0	0	2	0
56	AL	4	0	0	0	0
56	AN	4	0	0	0	0
56	AT	1	0	0	0	0
56	BB	497	0	0	8	0
56	BC	5	0	0	0	0
56	BE	1	0	0	0	0
56	BL	1	0	0	0	0
56	BN	1	0	0	0	0
56	BR	1	0	0	0	0
56	CA	298	0	0	1	0
56	CE	3	0	0	0	0
56	CL	2	0	0	0	0
56	CN	4	0	0	0	0
56	CP	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	CT	1	0	0	0	0
56	DB	502	0	0	10	0
56	DC	6	0	0	0	0
56	DE	1	0	0	0	0
56	DL	2	0	0	0	0
56	DR	1	0	0	0	0
All	All	284172	0	190846	16001	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 34.

The worst 5 of 16001 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	1.38	1.21
40:DH:31:VAL:HB	40:DH:32:PRO:HD2	1.30	1.11
21:CU:36:PHE:HB3	21:CU:40:PRO:HD3	1.32	1.11
6:CG:2:ARG:HH11	6:CG:2:ARG:HB3	1.10	1.11
40:BH:31:VAL:HB	40:BH:32:PRO:HD2	1.29	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%)	155 (76%)	35 (17%)	14 (7%)	2	14
2	CC	204/232 (88%)	155 (76%)	36 (18%)	13 (6%)	2	17
3	AD	203/205 (99%)	154 (76%)	34 (17%)	15 (7%)	2	12
3	CD	203/205 (99%)	151 (74%)	37 (18%)	15 (7%)	2	12
4	AE	148/166 (89%)	120 (81%)	25 (17%)	3 (2%)	11	56
4	CE	148/166 (89%)	120 (81%)	24 (16%)	4 (3%)	8	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	AF	98/135 (73%)	67 (68%)	26 (26%)	5 (5%)	3	25
5	CF	98/135 (73%)	65 (66%)	28 (29%)	5 (5%)	3	25
6	AG	148/178 (83%)	124 (84%)	18 (12%)	6 (4%)	4	32
6	CG	150/178 (84%)	127 (85%)	18 (12%)	5 (3%)	6	38
7	AH	127/129 (98%)	98 (77%)	25 (20%)	4 (3%)	7	41
7	CH	127/129 (98%)	97 (76%)	27 (21%)	3 (2%)	9	50
8	AI	125/129 (97%)	95 (76%)	20 (16%)	10 (8%)	1	11
8	CI	125/129 (97%)	97 (78%)	19 (15%)	9 (7%)	2	13
9	AJ	96/103 (93%)	73 (76%)	15 (16%)	8 (8%)	1	10
9	CJ	96/103 (93%)	74 (77%)	13 (14%)	9 (9%)	1	8
10	AK	115/128 (90%)	88 (76%)	22 (19%)	5 (4%)	4	31
10	CK	115/128 (90%)	85 (74%)	25 (22%)	5 (4%)	4	31
11	AL	121/123 (98%)	79 (65%)	33 (27%)	9 (7%)	2	12
11	CL	121/123 (98%)	80 (66%)	32 (26%)	9 (7%)	2	12
12	AM	112/117 (96%)	76 (68%)	27 (24%)	9 (8%)	1	11
12	CM	111/117 (95%)	77 (69%)	26 (23%)	8 (7%)	2	13
13	AN	92/100 (92%)	58 (63%)	24 (26%)	10 (11%)	1	5
13	CN	92/100 (92%)	58 (63%)	23 (25%)	11 (12%)	1	4
14	AO	86/89 (97%)	71 (83%)	12 (14%)	3 (4%)	6	37
14	CO	86/89 (97%)	71 (83%)	12 (14%)	3 (4%)	6	37
15	AP	80/82 (98%)	60 (75%)	14 (18%)	6 (8%)	2	12
15	CP	78/82 (95%)	58 (74%)	14 (18%)	6 (8%)	1	11
16	AQ	78/83 (94%)	58 (74%)	16 (20%)	4 (5%)	3	25
16	CQ	79/83 (95%)	59 (75%)	16 (20%)	4 (5%)	3	25
17	AR	53/74 (72%)	43 (81%)	8 (15%)	2 (4%)	5	34
17	CR	53/74 (72%)	43 (81%)	9 (17%)	1 (2%)	12	58
18	AS	77/91 (85%)	54 (70%)	17 (22%)	6 (8%)	1	11
18	CS	78/91 (86%)	54 (69%)	17 (22%)	7 (9%)	1	8
19	AT	83/86 (96%)	65 (78%)	12 (14%)	6 (7%)	2	13
19	CT	83/86 (96%)	66 (80%)	11 (13%)	6 (7%)	2	13
20	AB	216/240 (90%)	150 (69%)	44 (20%)	22 (10%)	1	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	CB	216/240 (90%)	147 (68%)	48 (22%)	21 (10%)	1	7
21	AU	49/70 (70%)	28 (57%)	11 (22%)	10 (20%)	0	0
21	CU	49/70 (70%)	28 (57%)	10 (20%)	11 (22%)	0	0
24	BI	139/141 (99%)	119 (86%)	15 (11%)	5 (4%)	5	36
24	DI	139/141 (99%)	114 (82%)	20 (14%)	5 (4%)	5	36
25	BC	269/272 (99%)	174 (65%)	49 (18%)	46 (17%)	0	1
25	DC	269/272 (99%)	174 (65%)	47 (18%)	48 (18%)	0	1
26	BD	207/209 (99%)	112 (54%)	63 (30%)	32 (16%)	0	1
26	DD	207/209 (99%)	114 (55%)	58 (28%)	35 (17%)	0	1
27	BK	119/123 (97%)	75 (63%)	28 (24%)	16 (13%)	0	2
27	DK	119/123 (97%)	75 (63%)	27 (23%)	17 (14%)	0	2
28	BP	112/114 (98%)	62 (55%)	35 (31%)	15 (13%)	0	2
28	DP	112/114 (98%)	63 (56%)	34 (30%)	15 (13%)	0	2
29	BE	199/201 (99%)	131 (66%)	51 (26%)	17 (8%)	1	9
29	DE	199/201 (99%)	130 (65%)	53 (27%)	16 (8%)	1	11
30	BY	56/58 (97%)	36 (64%)	14 (25%)	6 (11%)	1	5
30	DY	56/58 (97%)	37 (66%)	13 (23%)	6 (11%)	1	5
31	B0	54/56 (96%)	39 (72%)	10 (18%)	5 (9%)	1	8
31	D0	54/56 (96%)	39 (72%)	10 (18%)	5 (9%)	1	8
32	B4	36/38 (95%)	21 (58%)	7 (19%)	8 (22%)	0	0
32	D4	36/38 (95%)	20 (56%)	7 (19%)	9 (25%)	0	0
33	B1	48/54 (89%)	37 (77%)	5 (10%)	6 (12%)	1	3
33	D1	48/54 (89%)	37 (77%)	5 (10%)	6 (12%)	1	3
34	B3	62/64 (97%)	44 (71%)	13 (21%)	5 (8%)	1	10
34	D3	62/64 (97%)	44 (71%)	13 (21%)	5 (8%)	1	10
35	BV	92/94 (98%)	65 (71%)	23 (25%)	4 (4%)	4	31
35	DV	92/94 (98%)	65 (71%)	23 (25%)	4 (4%)	4	31
36	B2	44/46 (96%)	29 (66%)	14 (32%)	1 (2%)	10	52
36	D2	44/46 (96%)	28 (64%)	15 (34%)	1 (2%)	10	52
37	BL	141/144 (98%)	88 (62%)	30 (21%)	23 (16%)	0	1
37	DL	141/144 (98%)	88 (62%)	29 (21%)	24 (17%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	BM	134/136 (98%)	86 (64%)	31 (23%)	17 (13%)	0	3
38	DM	134/136 (98%)	86 (64%)	32 (24%)	16 (12%)	1	4
39	BX	61/63 (97%)	38 (62%)	18 (30%)	5 (8%)	1	10
39	DX	61/63 (97%)	38 (62%)	18 (30%)	5 (8%)	1	10
40	BH	147/149 (99%)	77 (52%)	41 (28%)	29 (20%)	0	0
40	DH	147/149 (99%)	85 (58%)	39 (26%)	23 (16%)	0	1
41	BJ	140/142 (99%)	88 (63%)	36 (26%)	16 (11%)	1	4
41	DJ	140/142 (99%)	89 (64%)	33 (24%)	18 (13%)	0	3
42	BN	118/127 (93%)	72 (61%)	34 (29%)	12 (10%)	1	6
42	DN	118/127 (93%)	71 (60%)	35 (30%)	12 (10%)	1	6
43	BO	114/117 (97%)	84 (74%)	25 (22%)	5 (4%)	4	29
43	DO	114/117 (97%)	83 (73%)	25 (22%)	6 (5%)	3	24
44	BQ	115/117 (98%)	73 (64%)	34 (30%)	8 (7%)	2	14
44	DQ	115/117 (98%)	70 (61%)	38 (33%)	7 (6%)	2	19
45	BS	108/110 (98%)	69 (64%)	28 (26%)	11 (10%)	1	6
45	DS	108/110 (98%)	69 (64%)	29 (27%)	10 (9%)	1	8
46	BU	100/103 (97%)	53 (53%)	25 (25%)	22 (22%)	0	0
46	DU	100/103 (97%)	54 (54%)	23 (23%)	23 (23%)	0	0
47	BF	176/178 (99%)	107 (61%)	44 (25%)	25 (14%)	0	2
47	DF	176/178 (99%)	107 (61%)	44 (25%)	25 (14%)	0	2
48	BG	174/176 (99%)	100 (58%)	48 (28%)	26 (15%)	0	1
48	DG	174/176 (99%)	101 (58%)	48 (28%)	25 (14%)	0	2
49	BR	101/103 (98%)	65 (64%)	25 (25%)	11 (11%)	1	5
49	DR	101/103 (98%)	64 (63%)	28 (28%)	9 (9%)	1	9
50	BT	91/100 (91%)	50 (55%)	31 (34%)	10 (11%)	1	5
50	DT	91/100 (91%)	51 (56%)	30 (33%)	10 (11%)	1	5
51	BZ	75/78 (96%)	53 (71%)	18 (24%)	4 (5%)	3	24
51	DZ	75/78 (96%)	50 (67%)	21 (28%)	4 (5%)	3	24
52	BW	77/84 (92%)	29 (38%)	27 (35%)	21 (27%)	0	0
52	DW	77/84 (92%)	29 (38%)	26 (34%)	22 (29%)	0	0
All	All	11241/11914 (94%)	7579 (67%)	2528 (22%)	1134 (10%)	1	7

5 of 1134 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AC	14	VAL
2	AC	54	ILE
2	AC	153	SER
2	AC	205	GLU
5	AF	92	THR

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%)	137 (81%)	33 (19%)	2	10
2	CC	170/189 (90%)	137 (81%)	33 (19%)	2	10
3	AD	172/172 (100%)	148 (86%)	24 (14%)	5	24
3	CD	172/172 (100%)	148 (86%)	24 (14%)	5	24
4	AE	113/125 (90%)	95 (84%)	18 (16%)	4	16
4	CE	113/125 (90%)	95 (84%)	18 (16%)	4	16
5	AF	87/116 (75%)	71 (82%)	16 (18%)	2	11
5	CF	87/116 (75%)	70 (80%)	17 (20%)	2	10
6	AG	123/146 (84%)	104 (85%)	19 (15%)	4	18
6	CG	125/146 (86%)	103 (82%)	22 (18%)	3	13
7	AH	104/104 (100%)	95 (91%)	9 (9%)	15	51
7	CH	104/104 (100%)	94 (90%)	10 (10%)	12	44
8	AI	105/106 (99%)	88 (84%)	17 (16%)	3	15
8	CI	105/106 (99%)	87 (83%)	18 (17%)	3	14
9	AJ	86/90 (96%)	71 (83%)	15 (17%)	3	13
9	CJ	86/90 (96%)	71 (83%)	15 (17%)	3	13
10	AK	90/98 (92%)	76 (84%)	14 (16%)	4	17
10	CK	90/98 (92%)	74 (82%)	16 (18%)	2	12
11	AL	103/103 (100%)	88 (85%)	15 (15%)	5	21
11	CL	103/103 (100%)	88 (85%)	15 (15%)	5	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	AM	92/95 (97%)	76 (83%)	16 (17%)	3	13
12	CM	91/95 (96%)	75 (82%)	16 (18%)	3	13
13	AN	79/83 (95%)	65 (82%)	14 (18%)	3	13
13	CN	79/83 (95%)	65 (82%)	14 (18%)	3	13
14	AO	76/77 (99%)	70 (92%)	6 (8%)	18	58
14	CO	76/77 (99%)	70 (92%)	6 (8%)	18	58
15	AP	65/65 (100%)	58 (89%)	7 (11%)	9	37
15	CP	65/65 (100%)	59 (91%)	6 (9%)	13	46
16	AQ	74/77 (96%)	65 (88%)	9 (12%)	7	32
16	CQ	75/77 (97%)	66 (88%)	9 (12%)	7	33
17	AR	48/64 (75%)	40 (83%)	8 (17%)	3	14
17	CR	48/64 (75%)	41 (85%)	7 (15%)	5	21
18	AS	70/78 (90%)	56 (80%)	14 (20%)	2	9
18	CS	71/78 (91%)	57 (80%)	14 (20%)	2	9
19	AT	65/65 (100%)	54 (83%)	11 (17%)	3	14
19	CT	65/65 (100%)	54 (83%)	11 (17%)	3	14
20	AB	180/198 (91%)	148 (82%)	32 (18%)	2	12
20	CB	180/198 (91%)	150 (83%)	30 (17%)	3	14
21	AU	44/60 (73%)	30 (68%)	14 (32%)	0	1
21	CU	44/60 (73%)	30 (68%)	14 (32%)	0	1
24	BI	109/109 (100%)	107 (98%)	2 (2%)	71	93
24	DI	109/109 (100%)	104 (95%)	5 (5%)	37	80
25	BC	216/217 (100%)	176 (82%)	40 (18%)	2	11
25	DC	216/217 (100%)	176 (82%)	40 (18%)	2	11
26	BD	164/164 (100%)	142 (87%)	22 (13%)	6	26
26	DD	164/164 (100%)	141 (86%)	23 (14%)	5	24
27	BK	102/104 (98%)	79 (78%)	23 (22%)	1	6
27	DK	102/104 (98%)	79 (78%)	23 (22%)	1	6
28	BP	99/99 (100%)	81 (82%)	18 (18%)	2	12
28	DP	99/99 (100%)	81 (82%)	18 (18%)	2	12
29	BE	165/165 (100%)	136 (82%)	29 (18%)	3	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	DE	165/165 (100%)	137 (83%)	28 (17%)	3	14
30	BY	48/48 (100%)	38 (79%)	10 (21%)	2	8
30	DY	48/48 (100%)	38 (79%)	10 (21%)	2	8
31	B0	47/47 (100%)	36 (77%)	11 (23%)	1	4
31	D0	47/47 (100%)	35 (74%)	12 (26%)	1	2
32	B4	34/34 (100%)	28 (82%)	6 (18%)	3	13
32	D4	34/34 (100%)	28 (82%)	6 (18%)	3	13
33	B1	45/48 (94%)	40 (89%)	5 (11%)	9	36
33	D1	45/48 (94%)	41 (91%)	4 (9%)	14	49
34	B3	51/51 (100%)	47 (92%)	4 (8%)	18	58
34	D3	51/51 (100%)	47 (92%)	4 (8%)	18	58
35	BV	78/78 (100%)	62 (80%)	16 (20%)	2	8
35	DV	78/78 (100%)	62 (80%)	16 (20%)	2	8
36	B2	38/38 (100%)	32 (84%)	6 (16%)	4	16
36	D2	38/38 (100%)	32 (84%)	6 (16%)	4	16
37	BL	102/103 (99%)	89 (87%)	13 (13%)	6	29
37	DL	102/103 (99%)	88 (86%)	14 (14%)	5	25
38	BM	109/109 (100%)	91 (84%)	18 (16%)	3	14
38	DM	109/109 (100%)	91 (84%)	18 (16%)	3	14
39	BX	55/55 (100%)	40 (73%)	15 (27%)	0	2
39	DX	55/55 (100%)	40 (73%)	15 (27%)	0	2
40	BH	114/114 (100%)	64 (56%)	50 (44%)	0	0
40	DH	114/114 (100%)	86 (75%)	28 (25%)	1	3
41	BJ	116/116 (100%)	101 (87%)	15 (13%)	6	28
41	DJ	116/116 (100%)	100 (86%)	16 (14%)	5	24
42	BN	100/103 (97%)	87 (87%)	13 (13%)	6	28
42	DN	100/103 (97%)	87 (87%)	13 (13%)	6	28
43	BO	86/87 (99%)	70 (81%)	16 (19%)	2	11
43	DO	86/87 (99%)	70 (81%)	16 (19%)	2	11
44	BQ	89/89 (100%)	74 (83%)	15 (17%)	3	14
44	DQ	89/89 (100%)	74 (83%)	15 (17%)	3	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	BS	93/93 (100%)	79 (85%)	14 (15%)	4	19
45	DS	93/93 (100%)	79 (85%)	14 (15%)	4	19
46	BU	83/84 (99%)	68 (82%)	15 (18%)	2	12
46	DU	83/84 (99%)	68 (82%)	15 (18%)	2	12
47	BF	149/149 (100%)	114 (76%)	35 (24%)	1	4
47	DF	149/149 (100%)	115 (77%)	34 (23%)	1	5
48	BG	137/137 (100%)	113 (82%)	24 (18%)	3	13
48	DG	137/137 (100%)	113 (82%)	24 (18%)	3	13
49	BR	84/84 (100%)	73 (87%)	11 (13%)	6	28
49	DR	84/84 (100%)	73 (87%)	11 (13%)	6	28
50	BT	80/84 (95%)	66 (82%)	14 (18%)	3	13
50	DT	80/84 (95%)	65 (81%)	15 (19%)	2	11
51	BZ	67/68 (98%)	52 (78%)	15 (22%)	1	6
51	DZ	67/68 (98%)	52 (78%)	15 (22%)	1	6
52	BW	59/62 (95%)	45 (76%)	14 (24%)	1	4
52	DW	59/62 (95%)	45 (76%)	14 (24%)	1	4
All	All	9333/9700 (96%)	7746 (83%)	1587 (17%)	3	14

5 of 1587 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	BF	168	LEU
5	CF	86	ARG
46	DU	51	LEU
48	BG	120	ILE
2	CC	27	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 343 such sidechains are listed below:

Mol	Chain	Res	Type
48	BG	63	GLN
4	CE	81	GLN
46	DU	45	GLN
48	BG	114	HIS
52	BW	75	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1529/1542 (99%)	239 (15%)	16 (1%)
1	CA	1529/1542 (99%)	229 (14%)	17 (1%)
22	BA	116/120 (96%)	17 (14%)	1 (0%)
22	DA	116/120 (96%)	17 (14%)	1 (0%)
23	BB	2837/2904 (97%)	435 (15%)	18 (0%)
23	DB	2837/2904 (97%)	433 (15%)	20 (0%)
All	All	8964/9132 (98%)	1370 (15%)	73 (0%)

5 of 1370 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	8	A
1	AA	9	G
1	AA	14	U
1	AA	31	G
1	AA	32	A

5 of 73 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	BB	2894	G
1	CA	366	A
23	DB	2336	A
1	CA	243	A
1	CA	428	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 349 ligands modelled in this entry, 345 are monoatomic - leaving 4 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$
53	NMY	AA	1601	-	45,45,45	1.84	13 (28%)	67,67,67	1.17	6 (8%)
53	NMY	BB	3001	-	45,45,45	1.84	12 (26%)	67,67,67	1.19	7 (10%)
53	NMY	CA	1601	-	45,45,45	1.84	11 (24%)	67,67,67	1.27	8 (11%)
53	NMY	DB	3001	-	45,45,45	1.90	14 (31%)	67,67,67	1.29	7 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	NMY	AA	1601	-	-	0/18/94/94	0/4/4/4
53	NMY	BB	3001	-	-	0/18/94/94	0/4/4/4
53	NMY	CA	1601	-	-	0/18/94/94	0/4/4/4
53	NMY	DB	3001	-	-	0/18/94/94	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	CA	1601	NMY	O22-C18	4.77	1.54	1.41
53	AA	1601	NMY	O22-C18	4.70	1.53	1.41
53	BB	3001	NMY	O22-C18	4.57	1.53	1.41
53	DB	3001	NMY	O22-C18	4.53	1.53	1.41
53	BB	3001	NMY	C3-C2	4.37	1.59	1.53

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	DB	3001	NMY	O11-C13-O16	5.00	116.41	111.57
53	DB	3001	NMY	O18-C18-C19	3.56	115.12	108.08
53	BB	3001	NMY	O11-C13-O16	3.47	114.93	111.57
53	CA	1601	NMY	O18-C18-C19	3.34	114.67	108.08
53	BB	3001	NMY	O18-C18-C19	3.23	114.46	108.08

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%)	-0.59	11 (0%) 84 40	22, 76, 152, 180	0
1	CA	1530/1542 (99%)	-0.60	4 (0%) 91 60	12, 57, 136, 180	0
2	AC	206/232 (88%)	0.54	8 (3%) 37 8	16, 66, 135, 180	0
2	CC	206/232 (88%)	0.50	7 (3%) 43 9	14, 74, 124, 180	0
3	AD	205/205 (100%)	0.86	28 (13%) 4 1	8, 84, 155, 180	0
3	CD	205/205 (100%)	0.51	8 (3%) 37 8	15, 62, 135, 180	0
4	AE	150/166 (90%)	0.46	5 (3%) 44 10	7, 67, 122, 158	0
4	CE	150/166 (90%)	0.76	10 (6%) 17 4	10, 59, 122, 180	0
5	AF	100/135 (74%)	0.87	9 (9%) 10 2	32, 80, 148, 180	0
5	CF	100/135 (74%)	0.54	1 (1%) 79 31	23, 69, 138, 180	0
6	AG	150/178 (84%)	0.32	8 (5%) 25 5	39, 105, 151, 180	0
6	CG	152/178 (85%)	0.22	8 (5%) 25 5	32, 89, 152, 180	0
7	AH	129/129 (100%)	0.81	18 (13%) 3 1	29, 79, 133, 180	0
7	CH	129/129 (100%)	0.30	3 (2%) 57 15	7, 55, 120, 148	0
8	AI	127/129 (98%)	0.51	15 (11%) 5 2	37, 90, 164, 180	0
8	CI	127/129 (98%)	0.44	6 (4%) 30 6	32, 95, 162, 180	0
9	AJ	98/103 (95%)	0.71	5 (5%) 27 5	17, 85, 158, 180	0
9	CJ	98/103 (95%)	0.62	10 (10%) 7 2	22, 89, 150, 180	0
10	AK	117/128 (91%)	0.23	2 (1%) 67 20	17, 63, 128, 162	0
10	CK	117/128 (91%)	0.06	1 (0%) 81 35	10, 51, 116, 164	0
11	AL	123/123 (100%)	0.50	4 (3%) 44 10	19, 74, 135, 180	0
11	CL	123/123 (100%)	0.34	5 (4%) 35 7	6, 50, 127, 180	0
12	AM	114/117 (97%)	0.29	4 (3%) 42 9	52, 119, 180, 180	0
12	CM	113/117 (96%)	0.35	5 (4%) 33 7	53, 105, 167, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AN	96/100 (96%)	0.46	3 (3%) 47 10	24, 79, 118, 152	0
13	CN	96/100 (96%)	0.49	7 (7%) 15 4	26, 82, 119, 139	0
14	AO	88/89 (98%)	0.77	5 (5%) 23 5	39, 76, 123, 180	0
14	CO	88/89 (98%)	0.17	0 100 100	15, 55, 123, 154	0
15	AP	82/82 (100%)	1.03	7 (8%) 11 3	30, 87, 150, 180	0
15	CP	80/82 (97%)	0.48	4 (5%) 28 6	8, 56, 135, 180	0
16	AQ	80/83 (96%)	0.92	15 (18%) 2 1	49, 96, 155, 180	0
16	CQ	81/83 (97%)	0.38	4 (4%) 28 6	25, 66, 128, 180	0
17	AR	55/74 (74%)	0.51	1 (1%) 65 20	15, 74, 125, 165	0
17	CR	55/74 (74%)	0.37	2 (3%) 41 8	19, 63, 119, 170	0
18	AS	79/91 (86%)	0.61	6 (7%) 14 4	73, 121, 176, 180	0
18	CS	80/91 (87%)	0.54	8 (10%) 8 2	58, 109, 168, 180	0
19	AT	85/86 (98%)	0.42	4 (4%) 30 6	52, 104, 164, 180	0
19	CT	85/86 (98%)	0.09	0 100 100	22, 62, 125, 179	0
20	AB	218/240 (90%)	0.39	10 (4%) 31 6	29, 99, 155, 180	0
20	CB	218/240 (90%)	0.75	21 (9%) 8 2	31, 102, 160, 180	0
21	AU	51/70 (72%)	0.71	5 (9%) 8 2	43, 92, 146, 180	0
21	CU	51/70 (72%)	0.55	3 (5%) 22 5	40, 85, 133, 166	0
22	BA	117/120 (97%)	-0.63	1 (0%) 81 35	49, 83, 138, 174	0
22	DA	117/120 (97%)	-0.52	1 (0%) 81 35	36, 75, 124, 180	0
23	BB	2841/2904 (97%)	-0.37	29 (1%) 79 31	16, 60, 154, 180	0
23	DB	2841/2904 (97%)	-0.40	10 (0%) 90 54	6, 47, 151, 180	0
24	BI	141/141 (100%)	1.93	60 (42%) 1 0	93, 176, 180, 180	0
24	DI	141/141 (100%)	1.00	15 (10%) 7 2	101, 177, 180, 180	0
25	BC	271/272 (99%)	0.59	11 (4%) 35 7	9, 50, 104, 180	0
25	DC	271/272 (99%)	0.53	12 (4%) 33 7	5, 35, 87, 135	0
26	BD	209/209 (100%)	0.49	8 (3%) 38 8	20, 76, 135, 180	0
26	DD	209/209 (100%)	0.68	16 (7%) 13 4	5, 50, 126, 180	0
27	BK	121/123 (98%)	1.32	24 (19%) 2 1	14, 72, 133, 180	0
27	DK	121/123 (98%)	0.83	3 (2%) 54 13	6, 43, 104, 164	0
28	BP	114/114 (100%)	1.40	31 (27%) 1 1	35, 86, 151, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DP	114/114 (100%)	0.41	1 (0%) 81 35	6, 49, 113, 160	0
29	BE	201/201 (100%)	0.88	28 (13%) 4 1	10, 67, 144, 180	0
29	DE	201/201 (100%)	0.63	14 (6%) 16 4	5, 72, 137, 180	0
30	BY	58/58 (100%)	0.55	3 (5%) 26 5	34, 74, 139, 180	0
30	DY	58/58 (100%)	0.41	3 (5%) 26 5	21, 60, 141, 177	0
31	B0	56/56 (100%)	0.55	4 (7%) 16 4	15, 74, 151, 180	0
31	D0	56/56 (100%)	0.24	1 (1%) 65 20	9, 49, 124, 180	0
32	B4	38/38 (100%)	0.42	0 100 100	35, 91, 145, 151	0
32	D4	38/38 (100%)	-0.12	0 100 100	18, 68, 129, 150	0
33	B1	50/54 (92%)	1.40	9 (18%) 2 1	52, 90, 134, 174	0
33	D1	50/54 (92%)	0.78	3 (6%) 21 5	14, 76, 127, 175	0
34	B3	64/64 (100%)	0.66	2 (3%) 47 10	26, 59, 87, 158	0
34	D3	64/64 (100%)	0.44	2 (3%) 47 10	9, 49, 112, 156	0
35	BV	94/94 (100%)	0.56	7 (7%) 14 4	29, 97, 155, 178	0
35	DV	94/94 (100%)	0.65	5 (5%) 25 5	21, 89, 153, 167	0
36	B2	46/46 (100%)	0.36	1 (2%) 59 15	14, 50, 83, 144	0
36	D2	46/46 (100%)	0.43	1 (2%) 59 15	5, 38, 76, 180	0
37	BL	143/144 (99%)	0.58	12 (8%) 11 3	25, 70, 133, 180	0
37	DL	143/144 (99%)	0.72	17 (11%) 5 2	9, 59, 117, 147	0
38	BM	136/136 (100%)	0.64	11 (8%) 12 3	21, 68, 136, 180	0
38	DM	136/136 (100%)	0.31	2 (1%) 70 23	13, 54, 118, 167	0
39	BX	63/63 (100%)	1.16	11 (17%) 2 1	21, 81, 149, 175	0
39	DX	63/63 (100%)	0.42	3 (4%) 29 6	38, 97, 156, 180	0
40	BH	149/149 (100%)	2.57	78 (52%) 0 0	31, 134, 180, 180	0
40	DH	149/149 (100%)	1.28	31 (20%) 1 1	32, 110, 160, 180	0
41	BJ	142/142 (100%)	0.80	11 (7%) 13 4	23, 82, 140, 169	0
41	DJ	142/142 (100%)	0.61	6 (4%) 35 7	17, 61, 126, 180	0
42	BN	120/127 (94%)	0.52	7 (5%) 22 5	24, 71, 139, 180	0
42	DN	120/127 (94%)	0.19	1 (0%) 83 37	7, 43, 91, 172	0
43	BO	116/117 (99%)	0.66	9 (7%) 13 3	35, 83, 145, 180	0
43	DO	116/117 (99%)	0.35	2 (1%) 67 20	19, 73, 135, 172	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BQ	117/117 (100%)	0.18	3 (2%) 53 12	10, 66, 129, 167	0
44	DQ	117/117 (100%)	0.43	4 (3%) 43 9	8, 50, 104, 180	0
45	BS	110/110 (100%)	0.92	10 (9%) 9 2	6, 62, 123, 152	0
45	DS	110/110 (100%)	1.06	15 (13%) 4 1	12, 48, 129, 180	0
46	BU	102/103 (99%)	0.94	11 (10%) 6 2	21, 77, 140, 180	0
46	DU	102/103 (99%)	0.16	1 (0%) 79 31	22, 94, 154, 180	0
47	BF	178/178 (100%)	0.65	8 (4%) 32 7	56, 128, 177, 180	0
47	DF	178/178 (100%)	1.19	35 (19%) 2 1	30, 107, 168, 180	0
48	BG	176/176 (100%)	0.71	12 (6%) 17 4	49, 112, 163, 180	0
48	DG	176/176 (100%)	0.73	19 (10%) 6 2	35, 97, 161, 180	0
49	BR	103/103 (100%)	0.44	4 (3%) 37 8	25, 87, 151, 176	0
49	DR	103/103 (100%)	0.65	8 (7%) 13 3	23, 76, 139, 161	0
50	BT	93/100 (93%)	0.76	7 (7%) 14 4	22, 77, 159, 180	0
50	DT	93/100 (93%)	0.79	12 (12%) 4 1	24, 64, 156, 179	0
51	BZ	77/78 (98%)	0.71	7 (9%) 9 2	12, 51, 112, 143	0
51	DZ	77/78 (98%)	0.44	2 (2%) 53 12	9, 48, 94, 128	0
52	BW	79/84 (94%)	0.96	10 (12%) 4 1	18, 85, 141, 159	0
52	DW	79/84 (94%)	0.63	5 (6%) 19 4	20, 71, 134, 180	0
All	All	20417/21046 (97%)	0.16	969 (4%) 30 6	5, 69, 156, 180	0

The worst 5 of 969 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
40	BH	84	ALA	15.0
40	BH	85	GLY	12.3
23	BB	140	C	9.9
8	CI	129	ARG	9.8
15	AP	81	ALA	9.6

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
54	MG	DB	3059	1/1	1.35	171.71	180,180,180,180	0
54	MG	AA	1660	1/1	0.33	45.75	163,163,163,163	0
54	MG	AA	1623	1/1	0.31	31.00	129,129,129,129	0
53	NMY	DB	3001	42/42	0.56	16.59	88,88,88,88	42
54	MG	AA	1648	1/1	0.48	14.87	94,94,94,94	0
54	MG	CA	1621	1/1	0.31	13.12	118,118,118,118	0
54	MG	AA	1624	1/1	0.33	12.53	32,32,32,32	1
53	NMY	BB	3001	42/42	0.66	11.59	100,100,100,100	42
54	MG	AA	1658	1/1	0.28	8.56	115,115,115,115	0
54	MG	BB	3082	1/1	0.32	7.89	59,59,59,59	0
54	MG	CA	1652	1/1	0.20	6.23	77,77,77,77	0
54	MG	BB	3029	1/1	0.23	5.59	32,32,32,32	0
54	MG	CA	1638	1/1	0.20	5.58	142,142,142,142	0
54	MG	BB	3034	1/1	0.21	5.04	136,136,136,136	0
54	MG	CA	1620	1/1	0.19	4.77	70,70,70,70	0
53	NMY	CA	1601	42/42	0.26	4.31	71,71,71,71	0
54	MG	CA	1657	1/1	0.15	4.27	91,91,91,91	0
54	MG	BB	3088	1/1	0.21	3.39	57,57,57,57	0
54	MG	AA	1620	1/1	0.14	3.32	130,130,130,130	0
54	MG	DB	3035	1/1	0.21	3.20	81,81,81,81	0
54	MG	DB	3031	1/1	0.23	2.49	32,32,32,32	0
54	MG	BB	3048	1/1	0.15	2.40	128,128,128,128	0
54	MG	DB	3067	1/1	0.14	2.12	178,178,178,178	0
54	MG	DB	3097	1/1	0.20	2.04	33,33,33,33	0
54	MG	AA	1636	1/1	0.13	1.73	88,88,88,88	0
54	MG	CA	1641	1/1	0.12	1.65	63,63,63,63	0
54	MG	DB	3012	1/1	0.19	1.65	37,37,37,37	0
54	MG	BB	3081	1/1	0.20	1.62	52,52,52,52	0
54	MG	BB	3094	1/1	0.19	1.46	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	NMY	AA	1601	42/42	0.29	1.18	71,71,71,71	0
54	MG	CA	1632	1/1	0.16	1.11	47,47,47,47	0
54	MG	BB	3087	1/1	0.22	0.87	41,41,41,41	0
54	MG	DB	3084	1/1	0.19	0.73	92,92,92,92	0
54	MG	AA	1656	1/1	0.14	0.62	60,60,60,60	0
54	MG	BB	3023	1/1	0.23	0.57	41,41,41,41	0
54	MG	DB	3098	1/1	0.16	0.52	36,36,36,36	0
54	MG	CA	1645	1/1	0.16	0.51	45,45,45,45	0
54	MG	CA	1629	1/1	0.10	0.50	46,46,46,46	1
54	MG	DB	3005	1/1	0.19	0.44	30,30,30,30	0
54	MG	CA	1626	1/1	0.17	0.41	8,8,8,8	1
54	MG	AA	1625	1/1	0.11	0.39	72,72,72,72	0
54	MG	CA	1633	1/1	0.15	0.31	73,73,73,73	0
54	MG	DB	3046	1/1	0.14	0.25	55,55,55,55	0
54	MG	DB	3052	1/1	0.18	0.22	32,32,32,32	0
54	MG	CA	1609	1/1	0.13	0.12	121,121,121,121	0
54	MG	AA	1640	1/1	0.25	0.12	104,104,104,104	0
54	MG	AA	1635	1/1	0.13	0.07	45,45,45,45	0
54	MG	AA	1641	1/1	0.13	-0.07	56,56,56,56	0
54	MG	DB	3013	1/1	0.17	-0.25	21,21,21,21	0
54	MG	AA	1609	1/1	0.14	-0.26	127,127,127,127	0
54	MG	DB	3050	1/1	0.15	-0.26	32,32,32,32	0
54	MG	BB	3111	1/1	0.13	-0.30	81,81,81,81	0
54	MG	BB	3099	1/1	0.17	-0.31	41,41,41,41	0
54	MG	BB	3100	1/1	0.21	-0.31	68,68,68,68	0
54	MG	BB	3011	1/1	0.13	-0.33	66,66,66,66	0
54	MG	DB	3087	1/1	0.18	-0.34	25,25,25,25	0
54	MG	DB	3112	1/1	0.16	-0.39	37,37,37,37	0
54	MG	DB	3090	1/1	0.17	-0.41	34,34,34,34	0
54	MG	BB	3012	1/1	0.18	-0.42	25,25,25,25	0
54	MG	AA	1637	1/1	0.12	-0.44	89,89,89,89	0
54	MG	AA	1619	1/1	0.13	-0.49	85,85,85,85	0
54	MG	CA	1653	1/1	0.10	-0.55	33,33,33,33	0
54	MG	DB	3111	1/1	0.13	-0.58	28,28,28,28	0
54	MG	AA	1647	1/1	0.15	-0.61	87,87,87,87	0
54	MG	BB	3058	1/1	0.15	-0.63	76,76,76,76	0
54	MG	AA	1605	1/1	0.14	-0.72	48,48,48,48	0
54	MG	DB	3048	1/1	0.18	-0.78	23,23,23,23	0
54	MG	DB	3100	1/1	0.15	-0.78	9,9,9,9	0
54	MG	AA	1616	1/1	0.09	-0.79	77,77,77,77	0
55	ZN	D4	101	1/1	0.14	-0.84	57,57,57,57	0
54	MG	DB	3060	1/1	0.14	-0.85	124,124,124,124	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	AA	1632	1/1	0.13	-0.86	37,37,37,37	0
54	MG	BB	3106	1/1	0.14	-0.91	33,33,33,33	0
54	MG	DB	3085	1/1	0.17	-0.95	25,25,25,25	0
54	MG	BB	3041	1/1	0.14	-1.00	28,28,28,28	0
54	MG	AA	1621	1/1	0.08	-1.01	85,85,85,85	0
54	MG	DB	3070	1/1	0.18	-1.02	23,23,23,23	0
54	MG	DB	3091	1/1	0.07	-1.05	47,47,47,47	0
54	MG	CA	1660	1/1	0.08	-1.07	69,69,69,69	0
54	MG	AA	1645	1/1	0.12	-1.08	60,60,60,60	0
54	MG	CA	1603	1/1	0.12	-1.11	30,30,30,30	0
54	MG	BB	3010	1/1	0.08	-1.12	82,82,82,82	0
54	MG	CA	1613	1/1	0.10	-1.12	77,77,77,77	0
54	MG	AA	1633	1/1	0.11	-1.16	51,51,51,51	0
54	MG	CA	1607	1/1	0.14	-1.16	100,100,100,100	0
54	MG	BB	3055	1/1	0.06	-1.19	58,58,58,58	0
54	MG	BB	3040	1/1	0.11	-1.20	28,28,28,28	0
54	MG	CA	1636	1/1	0.09	-1.22	56,56,56,56	0
54	MG	DB	3092	1/1	0.14	-1.23	46,46,46,46	0
54	MG	CN	201	1/1	0.07	-1.25	48,48,48,48	0
54	MG	CA	1639	1/1	0.09	-1.26	14,14,14,14	0
54	MG	DB	3008	1/1	0.15	-1.27	16,16,16,16	0
54	MG	CA	1616	1/1	0.09	-1.27	167,167,167,167	0
54	MG	DB	3058	1/1	0.06	-1.31	43,43,43,43	0
54	MG	DB	3061	1/1	0.11	-1.33	115,115,115,115	0
54	MG	AA	1604	1/1	0.16	-1.35	36,36,36,36	0
54	MG	DB	3075	1/1	0.12	-1.38	7,7,7,7	0
54	MG	DB	3099	1/1	0.17	-1.38	29,29,29,29	0
54	MG	AA	1631	1/1	0.10	-1.39	107,107,107,107	0
54	MG	BB	3026	1/1	0.11	-1.39	54,54,54,54	0
54	MG	BB	3007	1/1	0.12	-1.42	5,5,5,5	0
54	MG	DB	3080	1/1	0.16	-1.42	39,39,39,39	0
54	MG	AA	1652	1/1	0.08	-1.43	73,73,73,73	0
54	MG	DB	3015	1/1	0.08	-1.48	22,22,22,22	0
54	MG	BB	3096	1/1	0.12	-1.51	42,42,42,42	0
54	MG	CA	1622	1/1	0.10	-1.53	75,75,75,75	0
54	MG	BB	3109	1/1	0.13	-1.56	32,32,32,32	0
54	MG	CA	1615	1/1	0.07	-1.57	41,41,41,41	0
54	MG	AA	1650	1/1	0.07	-1.59	114,114,114,114	0
54	MG	BB	3108	1/1	0.10	-1.62	25,25,25,25	0
54	MG	BB	3093	1/1	0.04	-1.64	36,36,36,36	0
54	MG	BB	3006	1/1	0.15	-1.65	5,5,5,5	0
54	MG	BB	3022	1/1	0.09	-1.67	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BB	3030	1/1	0.10	-1.67	36,36,36,36	0
54	MG	BB	3076	1/1	0.16	-1.72	60,60,60,60	0
54	MG	BB	3045	1/1	0.10	-1.79	67,67,67,67	0
54	MG	AA	1608	1/1	0.07	-1.79	54,54,54,54	0
54	MG	DB	3110	1/1	0.08	-1.79	19,19,19,19	0
54	MG	CA	1635	1/1	0.08	-1.80	96,96,96,96	0
54	MG	BB	3005	1/1	0.04	-1.81	39,39,39,39	0
54	MG	AA	1611	1/1	0.04	-1.82	28,28,28,28	0
54	MG	DB	3038	1/1	0.14	-1.83	17,17,17,17	0
54	MG	BB	3039	1/1	0.07	-1.86	131,131,131,131	0
55	ZN	B4	101	1/1	0.06	-1.93	72,72,72,72	0
54	MG	DB	3063	1/1	0.05	-1.93	71,71,71,71	0
54	MG	DB	3095	1/1	0.05	-1.98	39,39,39,39	0
54	MG	CA	1640	1/1	0.12	-1.99	57,57,57,57	0
54	MG	AA	1612	1/1	0.04	-2.03	37,37,37,37	0
54	MG	AA	1614	1/1	0.03	-2.04	64,64,64,64	0
54	MG	CA	1619	1/1	0.08	-2.07	59,59,59,59	0
54	MG	AA	1639	1/1	0.09	-2.10	57,57,57,57	0
54	MG	BB	3086	1/1	0.13	-2.11	66,66,66,66	0
54	MG	DB	3033	1/1	0.13	-2.13	62,62,62,62	0
54	MG	DB	3078	1/1	0.13	-2.13	46,46,46,46	0
54	MG	DB	3026	1/1	0.13	-2.13	15,15,15,15	0
54	MG	AA	1653	1/1	0.09	-2.14	79,79,79,79	0
54	MG	BB	3038	1/1	0.07	-2.16	50,50,50,50	0
54	MG	BB	3043	1/1	0.06	-2.18	170,170,170,170	0
54	MG	AA	1654	1/1	0.11	-2.18	51,51,51,51	0
54	MG	BB	3046	1/1	0.08	-2.19	46,46,46,46	0
54	MG	AA	1661	1/1	0.14	-2.23	79,79,79,79	0
54	MG	CA	1614	1/1	0.06	-2.32	58,58,58,58	0
54	MG	DB	3041	1/1	0.14	-2.32	15,15,15,15	0
54	MG	DB	3004	1/1	0.09	-2.33	14,14,14,14	0
54	MG	BB	3079	1/1	0.10	-2.36	75,75,75,75	0
54	MG	DB	3102	1/1	0.13	-2.36	14,14,14,14	0
54	MG	DB	3077	1/1	0.15	-2.37	47,47,47,47	0
54	MG	BB	3013	1/1	0.11	-2.48	41,41,41,41	0
54	MG	BB	3073	1/1	0.12	-2.54	67,67,67,67	0
54	MG	BB	3004	1/1	0.07	-2.54	38,38,38,38	0
54	MG	BB	3035	1/1	0.10	-2.54	32,32,32,32	0
54	MG	CA	1637	1/1	0.06	-2.54	79,79,79,79	0
54	MG	DB	3021	1/1	0.15	-2.56	9,9,9,9	0
54	MG	DB	3014	1/1	0.12	-2.59	48,48,48,48	0
54	MG	BB	3098	1/1	0.10	-2.62	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BB	3025	1/1	0.08	-2.62	14,14,14,14	0
54	MG	BB	3110	1/1	0.07	-2.64	30,30,30,30	0
54	MG	DB	3054	1/1	0.09	-2.71	65,65,65,65	0
54	MG	BB	3071	1/1	0.13	-2.71	29,29,29,29	0
54	MG	BB	3085	1/1	0.14	-2.72	44,44,44,44	0
54	MG	DB	3039	1/1	0.13	-2.73	19,19,19,19	0
54	MG	CA	1649	1/1	0.08	-2.73	73,73,73,73	0
54	MG	CA	1642	1/1	0.10	-2.74	94,94,94,94	0
54	MG	AA	1603	1/1	0.15	-2.75	133,133,133,133	0
54	MG	CA	1650	1/1	0.09	-2.77	12,12,12,12	0
54	MG	BB	3083	1/1	0.12	-2.78	5,5,5,5	0
54	MG	CA	1647	1/1	0.07	-2.80	90,90,90,90	0
54	MG	DB	3064	1/1	0.10	-2.83	33,33,33,33	0
54	MG	DB	3016	1/1	0.10	-2.83	49,49,49,49	0
54	MG	DB	3023	1/1	0.11	-2.84	29,29,29,29	0
54	MG	DB	3106	1/1	0.12	-2.86	39,39,39,39	0
54	MG	CA	1634	1/1	0.11	-2.87	8,8,8,8	0
54	MG	BB	3019	1/1	0.11	-2.87	45,45,45,45	0
54	MG	CA	1606	1/1	0.10	-2.88	19,19,19,19	0
54	MG	AA	1628	1/1	0.15	-2.89	57,57,57,57	0
54	MG	CA	1624	1/1	0.04	-2.89	34,34,34,34	0
54	MG	BB	3102	1/1	0.10	-2.92	28,28,28,28	0
54	MG	DB	3049	1/1	0.12	-2.97	46,46,46,46	0
54	MG	CA	1658	1/1	0.09	-3.03	52,52,52,52	0
54	MG	CA	1643	1/1	0.09	-3.04	43,43,43,43	0
54	MG	DB	3089	1/1	0.13	-3.04	10,10,10,10	0
54	MG	BB	3074	1/1	0.08	-3.10	31,31,31,31	0
54	MG	CA	1627	1/1	0.10	-3.10	29,29,29,29	1
54	MG	BB	3037	1/1	0.08	-3.11	42,42,42,42	0
54	MG	BB	3063	1/1	0.14	-3.13	31,31,31,31	0
54	MG	DB	3024	1/1	0.05	-3.20	55,55,55,55	0
54	MG	BB	3101	1/1	0.12	-3.24	138,138,138,138	0
54	MG	BB	3077	1/1	0.09	-3.24	37,37,37,37	0
54	MG	BB	3050	1/1	0.10	-3.25	18,18,18,18	0
54	MG	BB	3089	1/1	0.07	-3.25	45,45,45,45	0
54	MG	BB	3084	1/1	0.10	-3.28	21,21,21,21	0
54	MG	AA	1630	1/1	0.06	-3.28	35,35,35,35	0
54	MG	BB	3075	1/1	0.10	-3.33	13,13,13,13	0
54	MG	DB	3066	1/1	0.07	-3.35	29,29,29,29	0
54	MG	CE	201	1/1	0.09	-3.39	97,97,97,97	0
54	MG	AA	1634	1/1	0.06	-3.40	52,52,52,52	0
54	MG	DB	3028	1/1	0.10	-3.46	8,8,8,8	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DB	3009	1/1	0.09	-3.46	19,19,19,19	0
54	MG	DB	3074	1/1	0.06	-3.47	28,28,28,28	0
54	MG	BB	3024	1/1	0.13	-3.48	7,7,7,7	0
54	MG	DB	3051	1/1	0.08	-3.49	87,87,87,87	0
54	MG	BB	3003	1/1	0.10	-3.53	24,24,24,24	0
54	MG	BB	3092	1/1	0.10	-3.53	32,32,32,32	0
54	MG	AA	1644	1/1	0.09	-3.53	24,24,24,24	0
54	MG	AA	1643	1/1	0.06	-3.56	53,53,53,53	0
54	MG	AA	1649	1/1	0.11	-3.57	19,19,19,19	0
54	MG	DB	3022	1/1	0.09	-3.59	5,5,5,5	0
54	MG	DB	3101	1/1	0.09	-3.62	5,5,5,5	0
54	MG	BB	3028	1/1	0.12	-3.63	32,32,32,32	0
54	MG	AA	1629	1/1	0.05	-3.66	70,70,70,70	0
54	MG	BB	3032	1/1	0.10	-3.69	45,45,45,45	0
54	MG	AA	1602	1/1	0.06	-3.70	29,29,29,29	0
54	MG	BB	3061	1/1	0.14	-3.70	41,41,41,41	0
54	MG	BB	3009	1/1	0.11	-3.73	64,64,64,64	0
54	MG	BB	3080	1/1	0.10	-3.88	37,37,37,37	0
54	MG	AA	1642	1/1	0.05	-3.89	59,59,59,59	0
54	MG	BB	3066	1/1	0.06	-3.91	44,44,44,44	0
54	MG	DB	3086	1/1	0.10	-3.92	18,18,18,18	0
54	MG	BB	3052	1/1	0.09	-3.95	59,59,59,59	0
54	MG	BB	3095	1/1	0.13	-4.04	46,46,46,46	0
54	MG	BB	3054	1/1	0.07	-4.06	46,46,46,46	0
54	MG	BB	3078	1/1	0.07	-4.10	32,32,32,32	0
54	MG	DB	3006	1/1	0.10	-4.11	20,20,20,20	0
54	MG	DB	3104	1/1	0.09	-4.11	21,21,21,21	0
54	MG	CA	1648	1/1	0.09	-4.13	55,55,55,55	0
54	MG	CA	1612	1/1	0.11	-4.13	84,84,84,84	0
54	MG	BB	3020	1/1	0.11	-4.15	45,45,45,45	0
54	MG	BB	3018	1/1	0.08	-4.17	43,43,43,43	0
54	MG	AA	1659	1/1	0.06	-4.20	112,112,112,112	0
54	MG	DB	3079	1/1	0.09	-4.20	43,43,43,43	0
54	MG	AA	1610	1/1	0.10	-4.26	10,10,10,10	0
54	MG	DB	3040	1/1	0.07	-4.33	58,58,58,58	0
54	MG	AA	1657	1/1	0.08	-4.33	69,69,69,69	0
54	MG	DB	3056	1/1	0.07	-4.34	12,12,12,12	0
54	MG	BB	3091	1/1	0.09	-4.42	75,75,75,75	0
54	MG	DB	3011	1/1	0.07	-4.44	7,7,7,7	0
54	MG	CA	1656	1/1	0.07	-4.45	27,27,27,27	0
54	MG	DB	3025	1/1	0.09	-4.49	44,44,44,44	0
54	MG	AA	1646	1/1	0.02	-4.52	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BB	3049	1/1	0.03	-4.54	14,14,14,14	0
54	MG	CA	1646	1/1	0.05	-4.55	72,72,72,72	0
54	MG	CA	1661	1/1	0.09	-4.59	61,61,61,61	0
54	MG	CA	1631	1/1	0.06	-4.61	34,34,34,34	0
54	MG	BB	3065	1/1	0.07	-4.64	24,24,24,24	0
54	MG	DB	3065	1/1	0.08	-4.66	16,16,16,16	0
54	MG	CA	1651	1/1	0.07	-4.67	40,40,40,40	0
54	MG	BB	3056	1/1	0.13	-4.68	34,34,34,34	0
54	MG	CA	1617	1/1	0.06	-4.70	9,9,9,9	0
54	MG	DB	3094	1/1	0.13	-4.73	21,21,21,21	0
54	MG	BB	3060	1/1	0.07	-4.74	30,30,30,30	0
54	MG	BB	3014	1/1	0.06	-4.75	42,42,42,42	0
54	MG	DB	3047	1/1	0.04	-4.79	24,24,24,24	0
54	MG	DB	3081	1/1	0.11	-4.80	18,18,18,18	0
54	MG	BB	3047	1/1	0.09	-4.80	46,46,46,46	0
54	MG	CA	1659	1/1	0.06	-4.81	62,62,62,62	0
54	MG	DB	3043	1/1	0.09	-4.83	15,15,15,15	0
54	MG	BB	3072	1/1	0.09	-4.86	52,52,52,52	0
54	MG	AA	1617	1/1	0.05	-4.97	45,45,45,45	0
54	MG	DB	3088	1/1	0.09	-5.05	48,48,48,48	0
54	MG	DB	3109	1/1	0.05	-5.05	10,10,10,10	0
54	MG	CA	1654	1/1	0.05	-5.06	78,78,78,78	0
54	MG	DB	3093	1/1	0.08	-5.10	67,67,67,67	0
54	MG	BB	3015	1/1	0.04	-5.15	27,27,27,27	0
54	MG	BB	3057	1/1	0.04	-5.16	20,20,20,20	0
54	MG	DB	3107	1/1	0.10	-5.19	27,27,27,27	0
54	MG	DB	3029	1/1	0.08	-5.19	33,33,33,33	0
54	MG	DB	3053	1/1	0.09	-5.35	102,102,102,102	0
54	MG	BB	3027	1/1	0.08	-5.42	34,34,34,34	0
54	MG	CA	1644	1/1	0.08	-5.45	58,58,58,58	0
54	MG	DB	3018	1/1	0.10	-5.47	8,8,8,8	0
54	MG	BB	3104	1/1	0.04	-5.49	8,8,8,8	0
54	MG	DB	3055	1/1	0.08	-5.49	42,42,42,42	0
54	MG	BB	3070	1/1	0.10	-5.49	15,15,15,15	0
54	MG	BB	3062	1/1	0.05	-5.52	29,29,29,29	0
54	MG	DB	3108	1/1	0.07	-5.52	21,21,21,21	0
54	MG	AA	1618	1/1	0.10	-5.56	79,79,79,79	0
54	MG	AA	1606	1/1	0.05	-5.56	47,47,47,47	0
54	MG	BB	3090	1/1	0.07	-5.59	49,49,49,49	0
54	MG	DB	3003	1/1	0.09	-5.62	9,9,9,9	0
54	MG	DB	3057	1/1	0.07	-5.64	5,5,5,5	0
54	MG	BB	3051	1/1	0.07	-5.66	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
54	MG	BB	3105	1/1	0.11	-5.73	21,21,21,21	0
54	MG	DB	3096	1/1	0.11	-5.76	127,127,127,127	0
54	MG	DB	3037	1/1	0.07	-5.76	15,15,15,15	0
54	MG	DB	3019	1/1	0.14	-5.86	48,48,48,48	0
54	MG	DB	3083	1/1	0.09	-5.87	24,24,24,24	0
54	MG	DB	3068	1/1	0.07	-5.91	19,19,19,19	0
54	MG	BB	3033	1/1	0.09	-6.01	55,55,55,55	0
54	MG	DB	3073	1/1	0.08	-6.13	33,33,33,33	0
54	MG	BB	3017	1/1	0.09	-6.17	28,28,28,28	0
54	MG	CA	1655	1/1	0.06	-6.22	69,69,69,69	0
54	MG	CA	1605	1/1	0.04	-6.23	16,16,16,16	0
54	MG	BB	3067	1/1	0.07	-6.34	34,34,34,34	0
54	MG	CA	1618	1/1	0.04	-6.36	8,8,8,8	0
54	MG	CA	1602	1/1	0.05	-6.40	6,6,6,6	0
54	MG	AA	1655	1/1	0.04	-6.40	38,38,38,38	0
54	MG	BB	3059	1/1	0.08	-6.48	30,30,30,30	0
54	MG	DB	3036	1/1	0.05	-6.61	40,40,40,40	0
54	MG	DB	3017	1/1	0.07	-6.62	6,6,6,6	0
54	MG	CA	1608	1/1	0.06	-6.65	40,40,40,40	0
54	MG	BB	3068	1/1	0.09	-6.65	55,55,55,55	0
54	MG	DB	3076	1/1	0.06	-6.65	26,26,26,26	0
54	MG	DB	3045	1/1	0.04	-6.73	22,22,22,22	0
54	MG	BB	3031	1/1	0.03	-6.74	47,47,47,47	0
54	MG	DB	3044	1/1	0.06	-6.77	12,12,12,12	0
54	MG	BB	3103	1/1	0.08	-6.82	37,37,37,37	0
54	MG	BB	3036	1/1	0.07	-6.83	36,36,36,36	0
54	MG	DB	3034	1/1	0.08	-6.92	43,43,43,43	0
54	MG	DB	3103	1/1	0.09	-6.92	16,16,16,16	0
54	MG	BB	3064	1/1	0.06	-6.97	26,26,26,26	0
54	MG	DB	3071	1/1	0.09	-7.12	61,61,61,61	0
54	MG	DB	3069	1/1	0.10	-7.27	6,6,6,6	0
54	MG	BB	3053	1/1	0.05	-7.64	25,25,25,25	0
54	MG	BB	3008	1/1	0.08	-7.64	64,64,64,64	0
54	MG	DB	3082	1/1	0.08	-7.68	6,6,6,6	0
54	MG	CA	1611	1/1	0.05	-7.72	60,60,60,60	0
54	MG	AA	1613	1/1	0.07	-7.73	65,65,65,65	0
54	MG	DB	3042	1/1	0.07	-7.80	7,7,7,7	0
54	MG	AA	1651	1/1	0.08	-7.80	109,109,109,109	0
54	MG	BB	3002	1/1	0.06	-7.84	24,24,24,24	0
54	MG	BB	3016	1/1	0.08	-7.90	18,18,18,18	0
54	MG	DB	3105	1/1	0.10	-8.08	40,40,40,40	0
54	MG	DB	3072	1/1	0.08	-8.22	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DB	3010	1/1	0.07	-8.27	5,5,5,5	0
54	MG	CA	1625	1/1	0.05	-8.84	34,34,34,34	0
54	MG	AA	1622	1/1	0.06	-9.08	27,27,27,27	0
54	MG	DB	3032	1/1	0.11	-9.26	18,18,18,18	0
54	MG	DB	3027	1/1	0.07	-9.36	36,36,36,36	0
54	MG	BB	3021	1/1	0.06	-9.41	22,22,22,22	0
54	MG	CA	1628	1/1	0.05	-9.45	61,61,61,61	0
54	MG	BB	3042	1/1	0.07	-9.80	8,8,8,8	0
54	MG	CA	1610	1/1	0.03	-10.00	79,79,79,79	0
54	MG	DB	3062	1/1	0.04	-10.18	47,47,47,47	0
54	MG	DB	3007	1/1	0.07	-10.22	12,12,12,12	0
54	MG	DB	3002	1/1	0.11	-10.32	5,5,5,5	0
54	MG	DB	3020	1/1	0.05	-11.59	5,5,5,5	0
54	MG	BB	3069	1/1	0.12	-11.62	32,32,32,32	0
54	MG	BB	3044	1/1	0.10	-12.25	108,108,108,108	0
54	MG	CA	1604	1/1	0.09	-12.30	52,52,52,52	0
54	MG	AA	1607	1/1	0.04	-12.87	64,64,64,64	0
54	MG	BB	3107	1/1	0.07	-17.09	54,54,54,54	0
54	MG	CA	1623	1/1	0.03	-17.75	131,131,131,131	0
54	MG	CA	1630	1/1	0.07	-18.83	40,40,40,40	0
54	MG	BB	3097	1/1	0.06	-18.86	32,32,32,32	0
54	MG	AA	1615	1/1	0.08	-25.39	110,110,110,110	0
54	MG	DB	3030	1/1	0.11	-33.00	74,74,74,74	0
54	MG	AA	1626	1/1	0.16	-	64,64,64,64	1
54	MG	AA	1627	1/1	0.09	-	15,15,15,15	1
54	MG	AA	1638	1/1	0.27	-	147,147,147,147	0

6.5 Other polymers ⓘ

There are no such residues in this entry.