



wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 06:05 PM BST

PDB ID : 4V57
Title : Crystal structure of the bacterial ribosome from Escherichia coli in complex with spectinomycin and neomycin.
Authors : Borovinskaya, M.A.; Shoji, S.; Holton, J.M.; Fredrick, K.; Cate, J.H.D.
Deposited on : 2007-07-21
Resolution : 3.50 Å(reported)

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

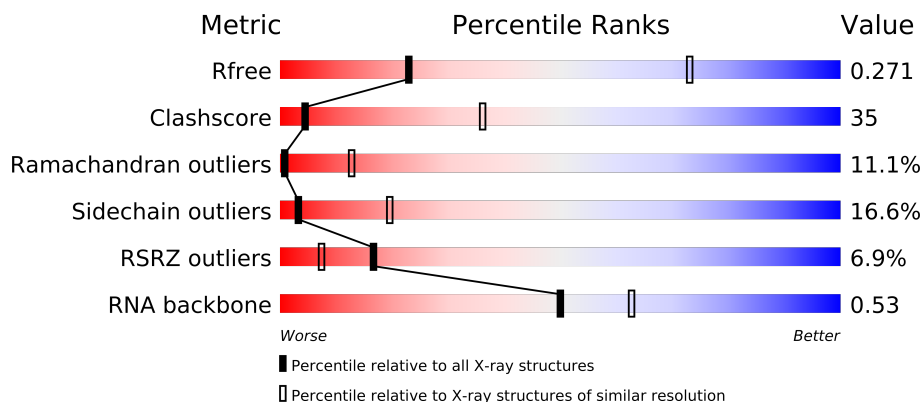
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1243 (3.70-3.30)
Clashscore	79885	1039 (3.66-3.34)
Ramachandran outliers	78287	1000 (3.66-3.34)
Sidechain outliers	78261	1000 (3.66-3.34)
RSRZ outliers	66119	1243 (3.70-3.30)
RNA backbone	1838	1007 (4.22-2.76)

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

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

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Mol	Chain	Length	Quality of chain
7	AH	129	
7	CH	129	
8	AI	129	
8	CI	129	
9	AJ	103	
9	CJ	103	
10	AK	128	
10	CK	128	
11	AL	123	
11	CL	123	
12	AM	117	
12	CM	117	
13	AP	82	
13	CP	82	
14	AQ	83	
14	CQ	83	
15	AR	74	
15	CR	74	
16	AS	91	
16	CS	91	
17	AT	86	
17	CT	86	
18	AB	240	
18	CB	240	
19	AU	70	
19	CU	70	
20	AO	89	
20	CO	89	
21	AN	100	
21	CN	100	
22	BA	120	
22	DA	120	
23	BB	2904	
23	DB	2904	
24	BI	141	
24	DI	141	
25	BC	272	
25	DC	272	
26	BD	209	
26	DD	209	
27	BK	123	
27	DK	123	

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

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

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

Mol	Type	Chain	Res	Geometry	Electron density
53	NMY	BB	3001	-	X
53	NMY	CA	1601	-	X
53	NMY	DB	3001	-	X
54	MG	AA	1606	-	X
54	MG	AA	1607	-	X
54	MG	AA	1624	-	X
54	MG	AA	1625	-	X
54	MG	AA	1626	-	X
54	MG	AA	1633	-	X
54	MG	AA	1638	-	X
54	MG	AA	1648	-	X
54	MG	AA	1657	-	X
54	MG	AA	1658	-	X
54	MG	AA	1660	-	X
54	MG	BB	3018	-	X
54	MG	BB	3023	-	X
54	MG	BB	3029	-	X
54	MG	BB	3034	-	X
54	MG	BB	3040	-	X
54	MG	BB	3087	-	X
54	MG	BB	3088	-	X
54	MG	BB	3106	-	X
54	MG	CA	1613	-	X
54	MG	CA	1614	-	X
54	MG	CA	1618	-	X
54	MG	CA	1650	-	X
54	MG	CA	1651	-	X
54	MG	CA	1658	-	X
54	MG	DB	3038	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
54	MG	DB	3059	-	X
54	MG	DB	3090	-	X
54	MG	DB	3112	-	X

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 284201 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AG	150	Total	C	N	O	S	0	0	0
			1174	730	226	214	4			
6	CG	152	Total	C	N	O	S	0	0	0
			1196	745	230	217	4			

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 13 is a protein called 30S ribosomal protein S16.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

- Molecule 27 is a protein called 50S ribosomal protein L14.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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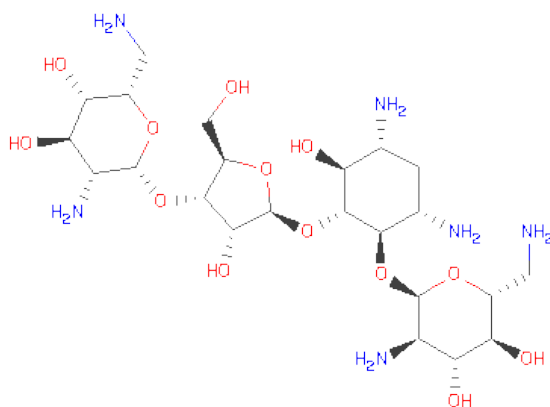
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	DZ	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			

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

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

- Molecule 53 is NEOMYCIN (three-letter code: NMY) (formula: $C_{23}H_{46}N_6O_{13}$).

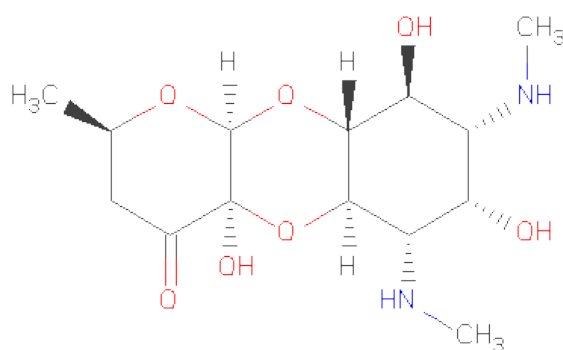


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
53	AA	1	Total	C	N	O	0	0
			42	23	6	13		
53	BB	1	Total	C	N	O	0	0
			42	23	6	13		
53	CA	1	Total	C	N	O	0	0
			42	23	6	13		
53	DB	1	Total	C	N	O	0	0
			42	23	6	13		

- 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	AA	60	Total	Mg	0	0
			60	60		
54	CA	59	Total	Mg	0	0
			59	59		
54	DB	111	Total	Mg	0	0
			111	111		

- Molecule 55 is SPECTINOMYCIN (three-letter code: SCM) (formula: $C_{14}H_{24}N_2O_7$).



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

- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 57 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	AA	290	Total O 290 290	0	0
57	AE	1	Total O 1 1	0	0
57	AK	1	Total O 1 1	0	0
57	AL	4	Total O 4 4	0	0
57	AP	1	Total O 1 1	0	0
57	AT	2	Total O 2 2	0	0
57	AN	1	Total O 1 1	0	0
57	BB	492	Total O 492 492	0	0
57	BC	7	Total O 7 7	0	0
57	BD	1	Total O 1 1	0	0
57	BE	4	Total O 4 4	0	0
57	BL	2	Total O 2 2	0	0
57	BH	1	Total O 1 1	0	0
57	CA	282	Total O 282 282	0	0
57	CE	2	Total O 2 2	0	0
57	CL	4	Total O 4 4	0	0
57	CP	1	Total O 1 1	0	0
57	CT	1	Total O 1 1	0	0
57	CI	1	Total O 1 1	0	0
57	CN	3	Total O 3 3	0	0
57	DB	501	Total O 501 501	0	0
57	DC	4	Total O 4 4	0	0

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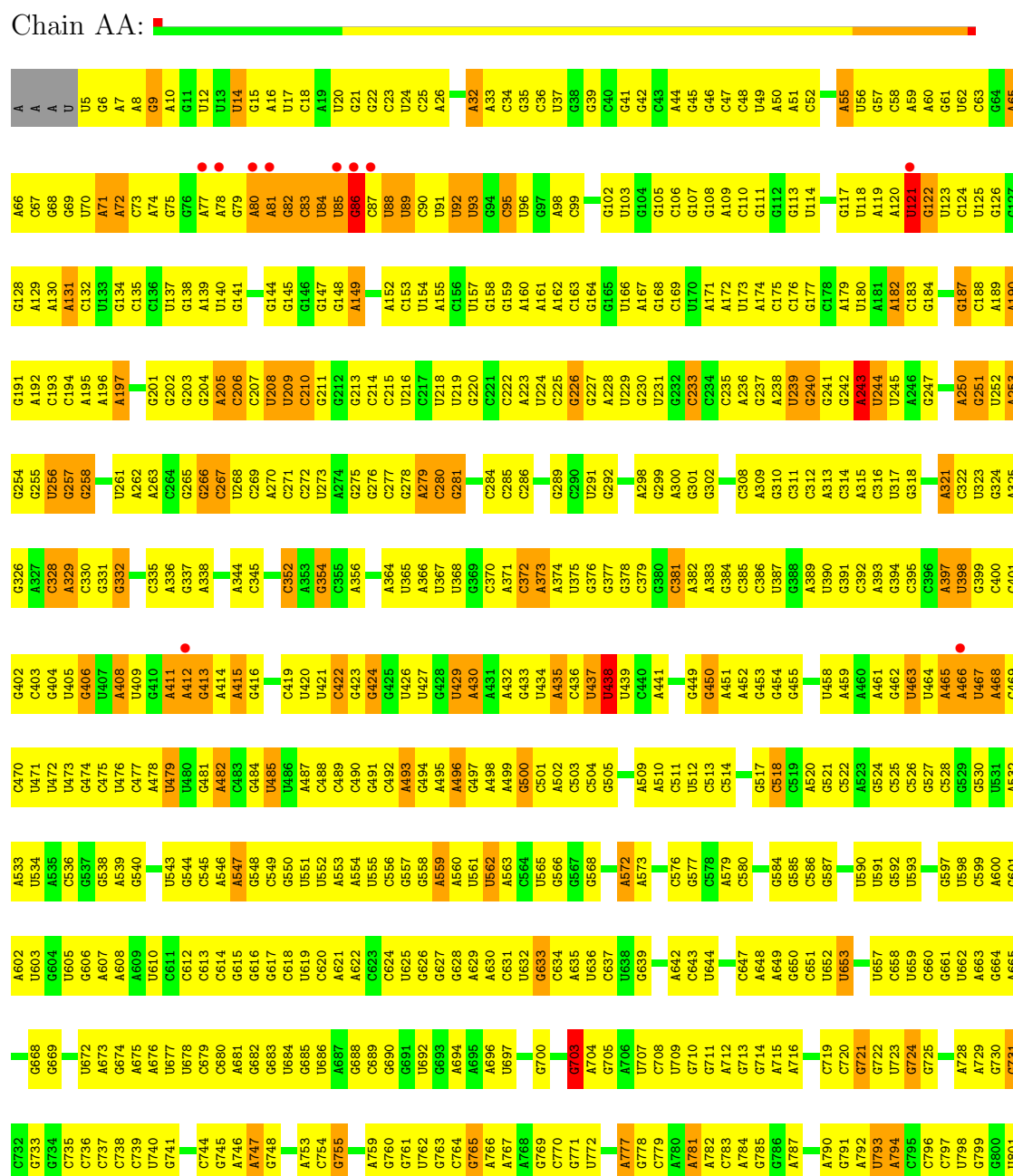
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	DD	1	Total 1	O 1	0	0
57	DE	2	Total 2	O 2	0	0
57	DL	1	Total 1	O 1	0	0
57	DN	2	Total 2	O 2	0	0
57	DR	1	Total 1	O 1	0	0

3 Residue-property plots

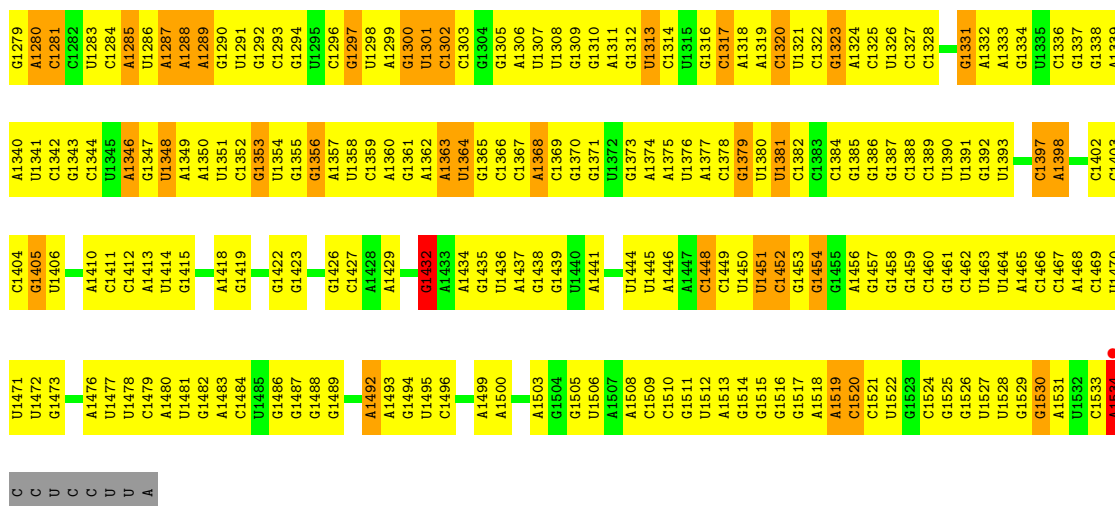
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: 16S rRNA



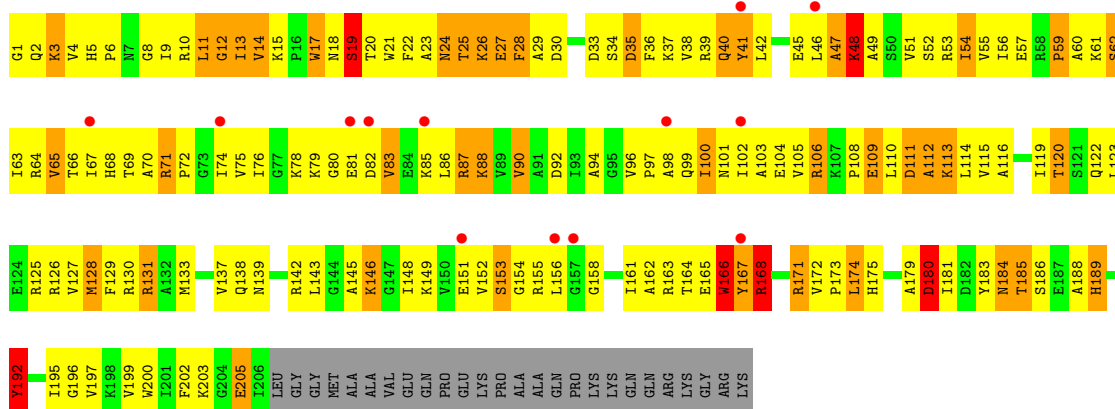


A1216	C1149	U1086	A1022	A959	A889	A816	A746	U678	U610	G544	U479	G410	A262	G200
C1217	A1150	U1090	U1023	U960	G890	C817	A747	C679	C611	C545	U480	A411	A263	G201
C1218	A1151	U1091	G1024	U961	U891	A818	G748	C680	C612	A546	G482	A412	C264	G202
A1219	A1152	U1092	G1025	A964	A892	A819	A749	A681	C613	A547	G483	A413	G265	G203
G1220	G1153	A1093	G1026	U965	C893	G821	C750	G682	C614	G548	C483	A414	G266	G204
G1221	G1094	C1027	C1027	G966	G894	G821	C751	G683	G615	C549	G484	A415	C267	G205
G1222	A1157	U1095	U1028	C967	G895	G824	G755	U684	G616	G550	U485	A416	U268	A205
C1223	C1158	U1096	C1029	A968	C896	A825	G756	G685	G617	U551	U486	A344	C269	C206
U1224	U1159	C1096	U1030	A969	C897	A826	G757	U686	C618	U552	A487	U420	A270	C207
A1225	C1160	C1097	U1031	A970	A900	C826	G758	A687	G619	A553	C488	U421	C271	U208
C1226	C1161	C1098	C1031	C970	C970	U827	G759	G688	C620	A554	C489	C422	C272	U209
A1227	A1162	G1099	G1032	G971	A901	U828	G761	C689	A621	U555	C490	G423	U273	C210
C1228	C1163	C1100	G1033	C972	G902	G830	G762	C690	A622	C556	G491	G424	G211	G211
A1229	G1164	A1101	A1036	G973	G903	G833	G763	G691	C623	G557	C492	G425	G212	G212
C1230	U1165	C1102	C1037	A974	U904	U834	C764	U692	C624	A558	G493	U426	C213	G213
G1231	G1166	C1103	C1037	A975	U905	U835	G765	G693	G626	A559	G494	U427	G214	C214
C1232	A1167	G1104	U1040	G976	A906	G836	A766	A694	G627	A560	A495	U428	A279	C215
G1233	U1168	U1049	U1049	A977	A907	U837	G767	G700	G628	U561	A496	G429	C280	U216
C1234	A1169	G1041	A1041	A978	A908	C840	G769	G701	A629	U562	G497	A430	G281	C217
U1235	A1170	G1042	A1042	C979	A909	C841	C770	A702	A630	A563	A498	A431	C284	U218
A1236	A1171	G1043	G1043	C980	C910	C842	C771	A703	A631	G564	A499	A432	C285	C222
C1237	C1172	A1110	U981	U981	U911	U843	C772	G703	C631	U565	G500	G433	C286	A228
U1238	U1173	A1111	U982	U982	C912	U843	C773	A704	G632	U566	C501	U434	G292	U229
A1239	G1174	C1112	A983	A983	A913	C844	A777	G711	G633	G567	A502	A435	U287	A223
C1240	G1175	C1113	C984	C984	A914	A845	C778	G712	C634	G568	C503	C436	U288	U224
G1241	A1176	C1114	G1050	C985	A914	G846	C779	G713	A635	A572	C504	U437	C289	C225
C1242	G1177	U1115	C1051	U986	G917	C847	A780	U707	G636	A573	G505	U438	C290	G226
C1243	U1178	U1116	U1052	G987	A918	C848	C781	G710	C637	A573	A509	U439	U291	G227
G1244	A1179	C1117	G1053	U988	A919	C849	C782	G711	G638	C576	A510	A441	G292	A228
C1245	U1180	U1118	C1054	U989	U920	U854	C783	A712	U642	G577	C511	G449	C299	G230
G1246	G1181	C1119	A1055	C990	U921	U854	C784	G713	C643	A579	C512	G450	A300	U231
U1247	U1182	C1120	U1056	U991	G922	G856	C785	G714	U644	C580	G517	G451	A301	G232
U1248	U1183	U1121	G1057	U992	A923	C859	C786	A715	C643	A584	C518	G452	A382	G233
C1249	G1184	U1122	G1058	G993	C924	A860	C787	A716	U644	C580	C519	A451	A383	C234
A1251	G1185	U1123	C1059	A994	G925	C861	C788	G717	C647	G584	C518	G453	A384	G302
C1252	U1186	G1124	U1060	C995	G926	C862	C789	C719	A648	G585	C519	G454	C385	C235
A1253	G1187	U1125	G1061	A996	G927	U864	C790	C720	A649	C586	C520	G455	C386	A236
G1254	A1188	U1126	U1062	U997	G927	A865	C791	G722	G650	G587	G521	G456	U387	G237
C1255	U1189	G1127	C1063	C998	G933	C866	C792	U723	C651	U590	C522	U458	G310	A238
A1256	U1190	C1128	U1064	C999	C934	C867	C793	U724	G652	U591	A523	A459	C311	U239
C1257	A1196	A1130	C1065	A1000	A935	C868	C794	G725	U653	U592	C525	A460	A313	G240
G1258	U1197	G1131	U1066	C1001	C1001	C869	C795	G726	C653	G593	C526	A461	A314	G241
C1259	G1198	C1132	G1068	G1002	G939	C870	C796	G727	G656	G594	G527	G462	A315	U244
U1260	U1199	G1133	C1069	G1003	A938	U870	C797	U728	U657	U595	G528	G463	U317	U245
C1261	C1200	U1134	U1070	A1004	C940	U871	C798	A729	C658	A596	C529	U464	U318	G246
G1262	A1201	U1135	C1071	A1005	G941	U872	C799	G730	U659	A596	G530	U465	A321	A250
U1264	U1202	C1136	G1072	G1006	A946	U873	C800	G731	C660	G597	G531	U466	C322	G251
C1265	C1203	C1137	U1073	U1007	G947	C876	G803	C732	G661	U598	U531	U467	U323	U252
G1266	U1204	G1138	G1074	U1008	C948	C877	U804	G733	U662	C599	A532	A468	G324	A253
C1267	U1205	U1139	U1075	U1010	A949	C878	C805	G734	A663	C600	A533	C469	A325	G254
G1268	G1207	C1140	U1076	C1011	U950	C879	C806	C735	G664	A601	U534	C470	G326	G255
A1269	C1208	C1141	G1077	A1012	G951	C880	C807	C736	A665	G602	A535	U471	A327	G256
C1270	C1209	G1142	U1078	G1013	U952	C881	C808	C737	G665	A603	C536	U472	G404	U257
A1271	C1210	G1143	C1078	G1014	G953	C882	G809	C738	U672	U604	G538	U473	C328	G258
G1272	U1211	G1144	A1015	G1015	G954	U884	C810	C739	A673	G605	A539	G474	A329	G259
C1273	U1212	A1145	A1016	U955	U955	C885	G812	U740	G674	G606	G540	G475	G330	G260
A1274	C1213	U1146	U1083	U956	U956	C886	U813	G741	A675	A607	G541	U476	G331	G261
G1275	U1214	C1147	G1084	U957	U957	C887	A814	C744	A676	A608	G542	U477	G332	G262
C1276	G1215	U1148	U1085	A958	A958	G888	A815	G745	U677	A609	U543	A478	G333	G263



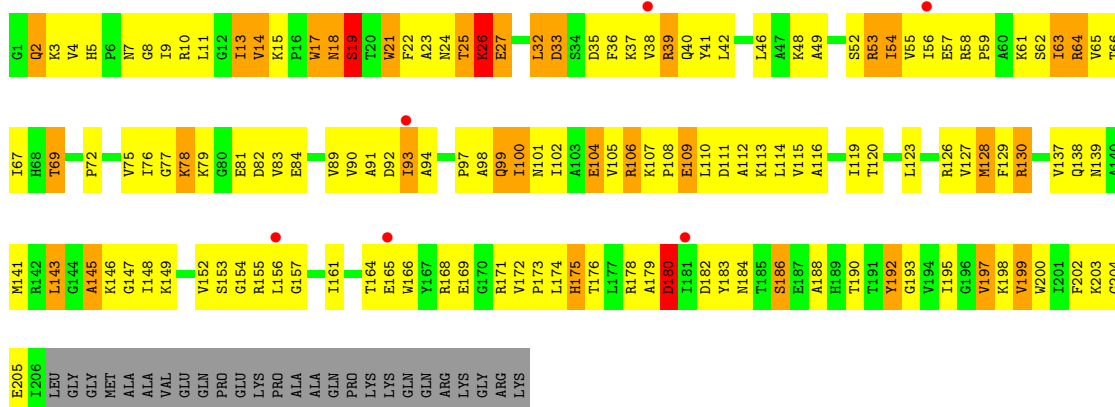
• Molecule 2: 30S ribosomal protein S3

Chain AC:



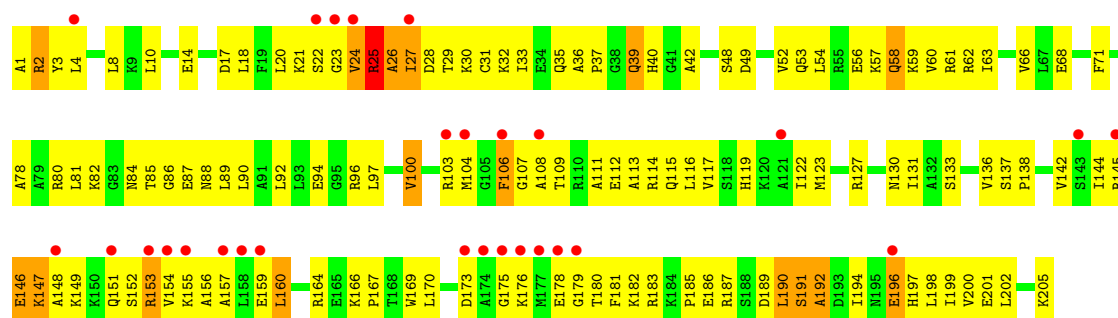
• Molecule 2: 30S ribosomal protein S3

Chain CC:



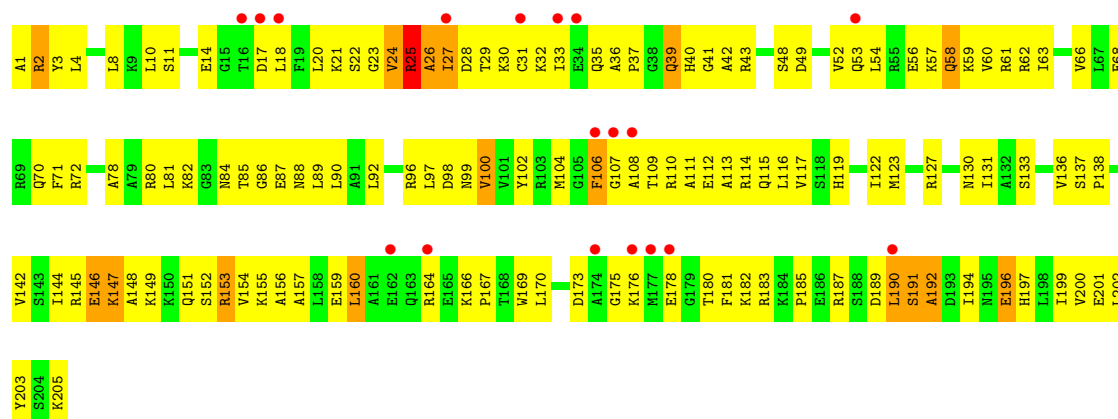
• Molecule 3: 30S ribosomal protein S4

Chain AD:



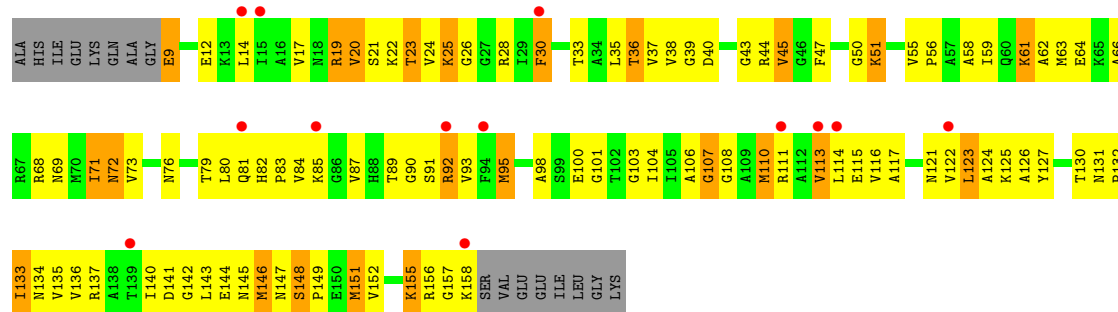
• Molecule 3: 30S ribosomal protein S4

Chain CD:



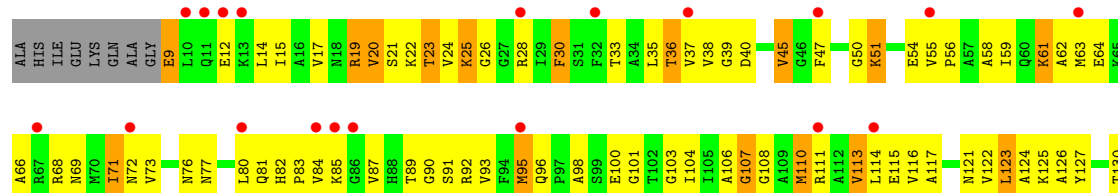
• Molecule 4: 30S ribosomal protein S5

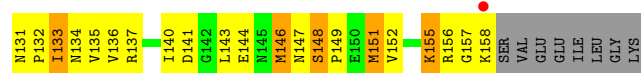
Chain AE:



• Molecule 4: 30S ribosomal protein S5

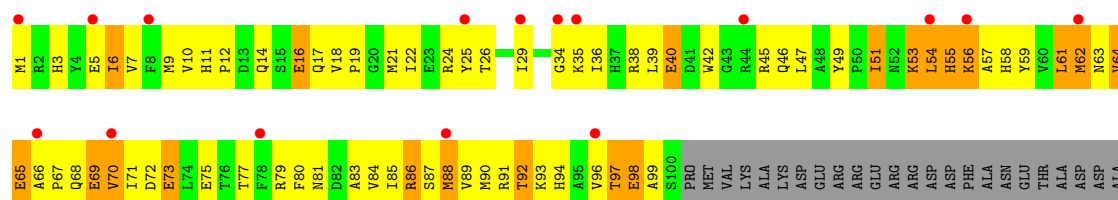
Chain CE:





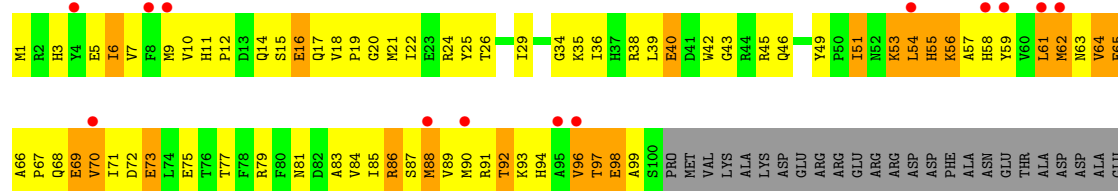
• Molecule 5: 30S ribosomal protein S6

Chain AF:



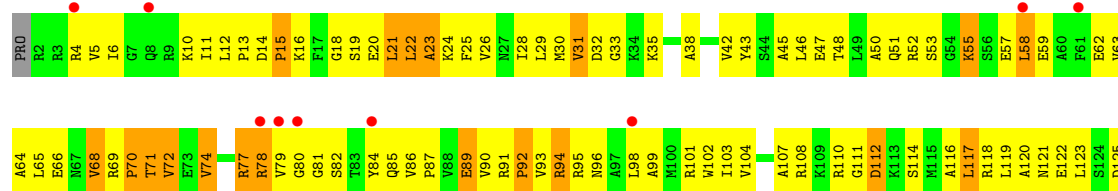
• Molecule 5: 30S ribosomal protein S6

Chain CF:



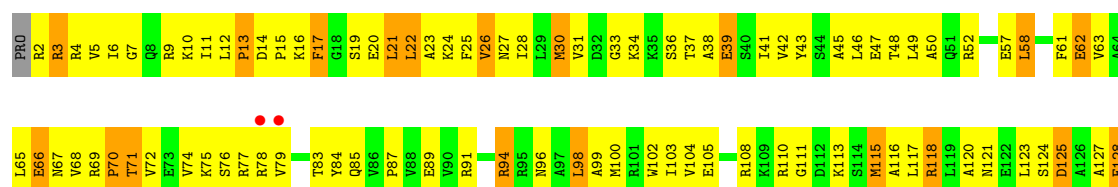
• Molecule 6: 30S ribosomal protein S7

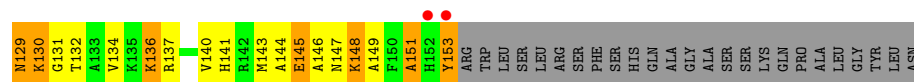
Chain AG:



• Molecule 6: 30S ribosomal protein S7

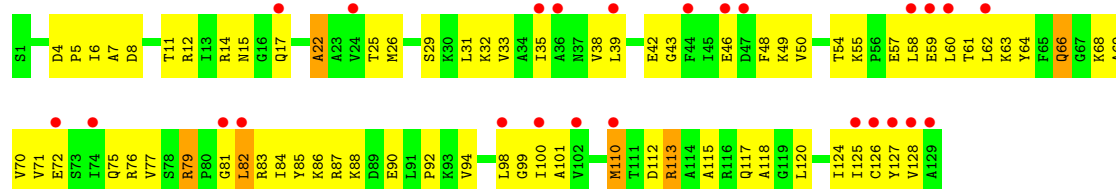
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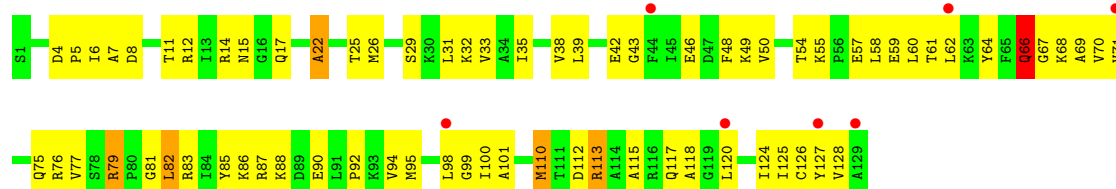
• Molecule 7: 30S ribosomal protein S8

Chain AH:



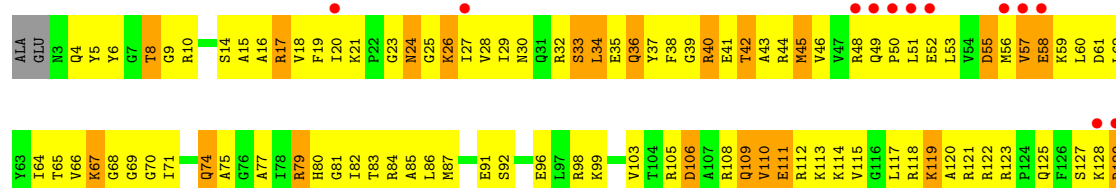
• Molecule 7: 30S ribosomal protein S8

Chain CH:



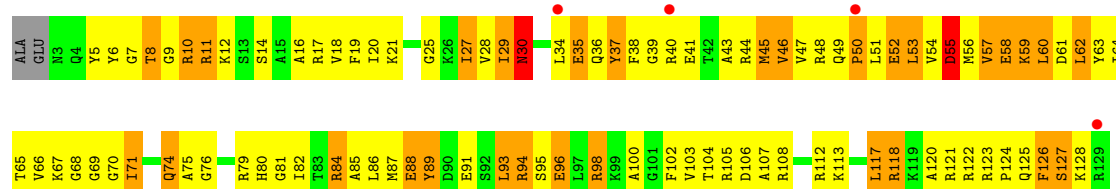
• Molecule 8: 30S ribosomal protein S9

Chain AI:



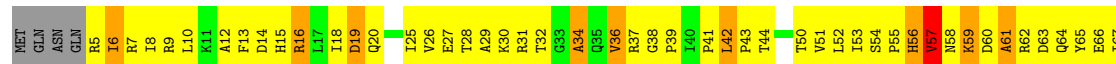
• Molecule 8: 30S ribosomal protein S9

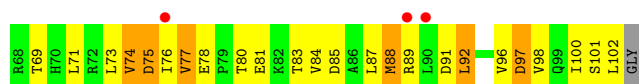
Chain CI:



• Molecule 9: 30S ribosomal protein S10

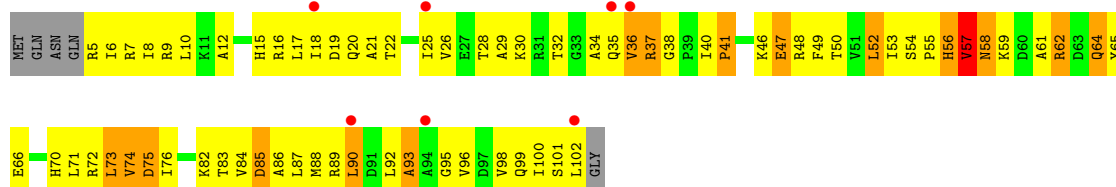
Chain AJ:





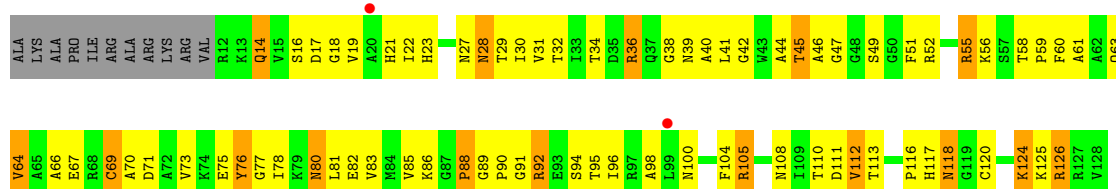
• Molecule 9: 30S ribosomal protein S10

Chain CJ:



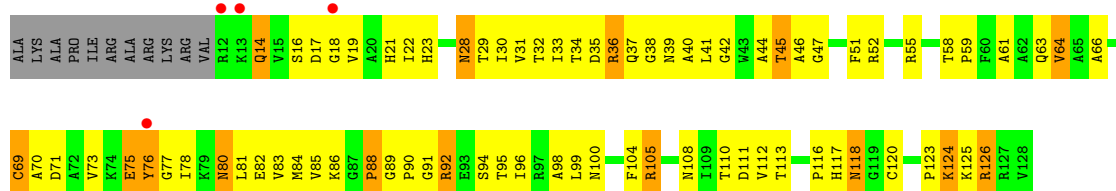
• Molecule 10: 30S ribosomal protein S11

Chain AK:



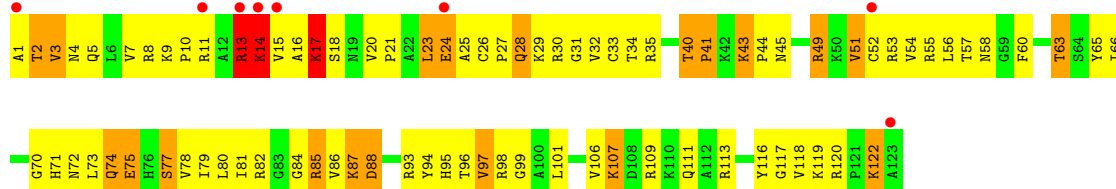
• Molecule 10: 30S ribosomal protein S11

Chain CK:



• Molecule 11: 30S ribosomal protein S12

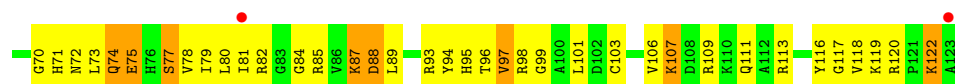
Chain AL:



• Molecule 11: 30S ribosomal protein S12

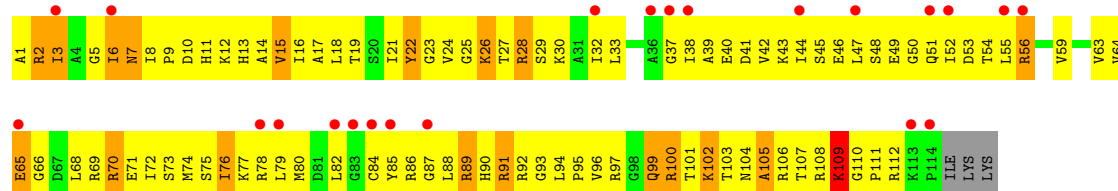
Chain CL:





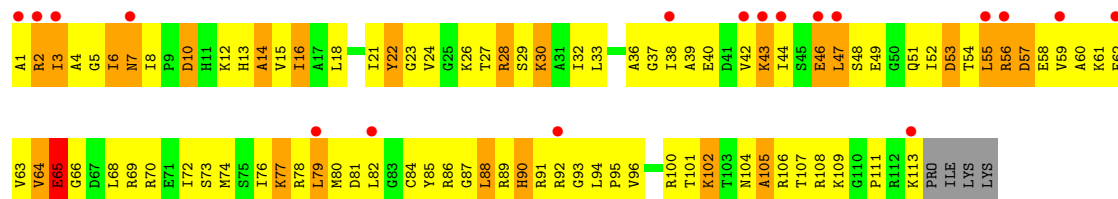
• Molecule 12: 30S ribosomal protein S13

Chain AM:



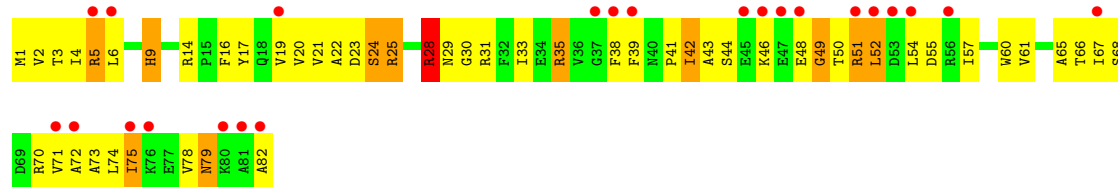
• Molecule 12: 30S ribosomal protein S13

Chain CM:



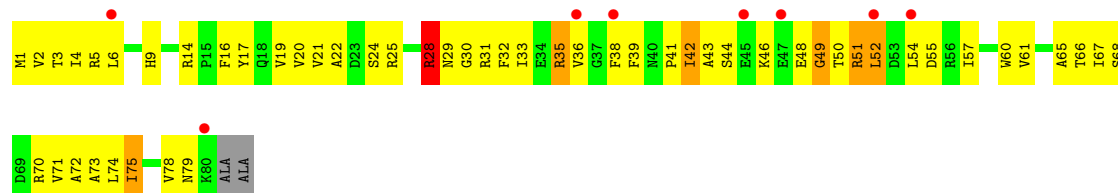
• Molecule 13: 30S ribosomal protein S16

Chain AP:



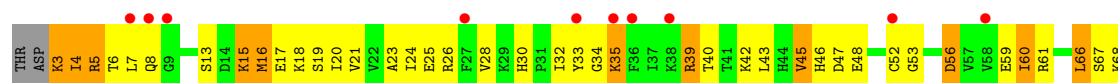
• Molecule 13: 30S ribosomal protein S16

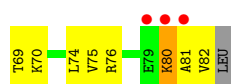
Chain CP:



• Molecule 14: 30S ribosomal protein S17

Chain AQ:





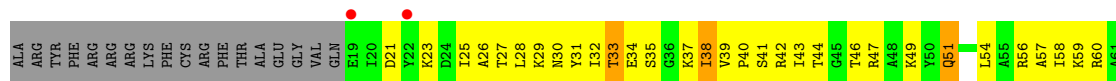
- Molecule 14: 30S ribosomal protein S17

Chain CQ:



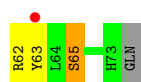
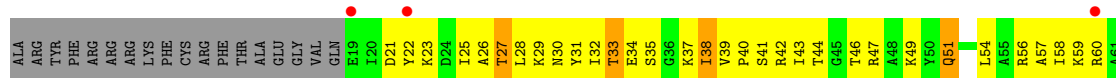
- Molecule 15: 30S ribosomal protein S18

Chain AR:



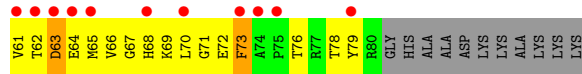
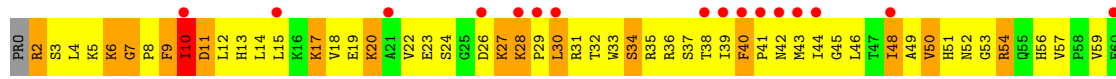
- Molecule 15: 30S ribosomal protein S18

Chain CR:



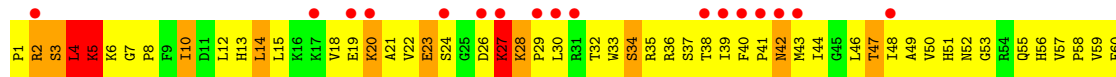
- Molecule 16: 30S ribosomal protein S19

Chain AS:



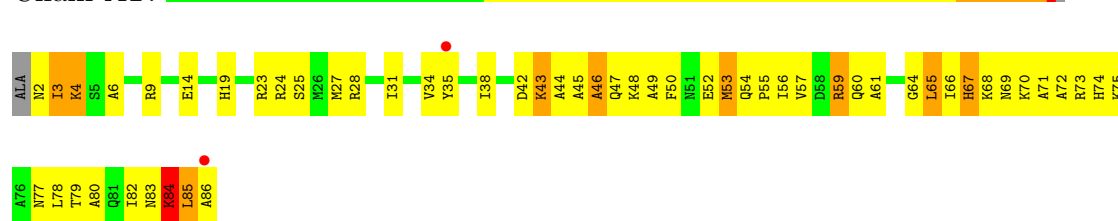
- Molecule 16: 30S ribosomal protein S19

Chain CS:



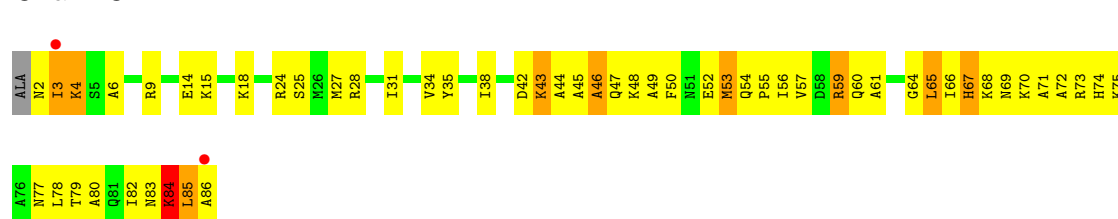
- Molecule 17: 30S ribosomal protein S20

Chain AT:



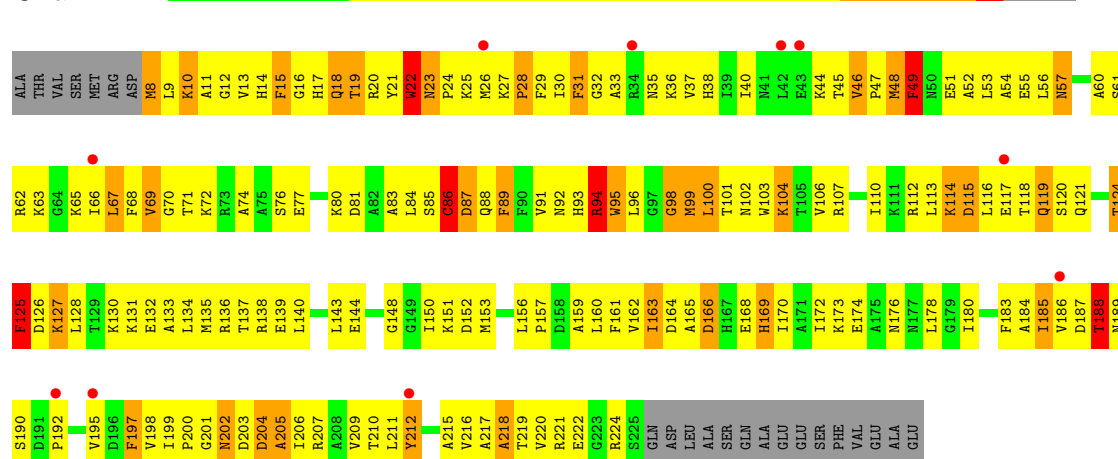
- Molecule 17: 30S ribosomal protein S20

Chain CT:



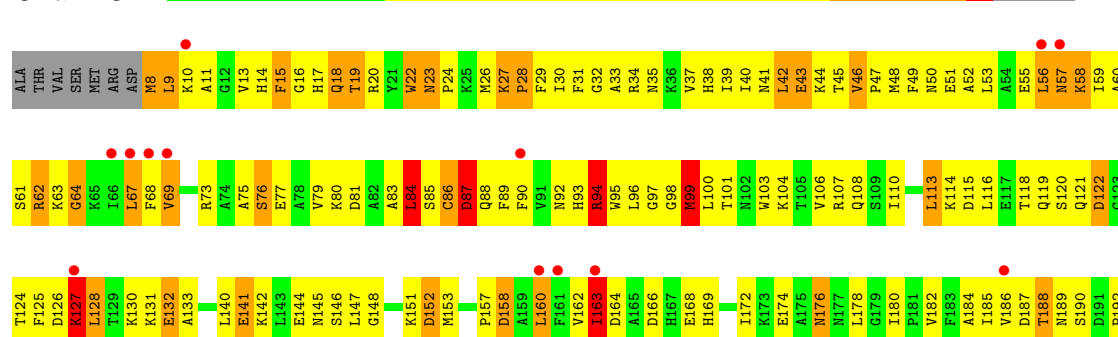
- Molecule 18: 30S ribosomal protein S2

Chain AB:



- Molecule 18: 30S ribosomal protein S2

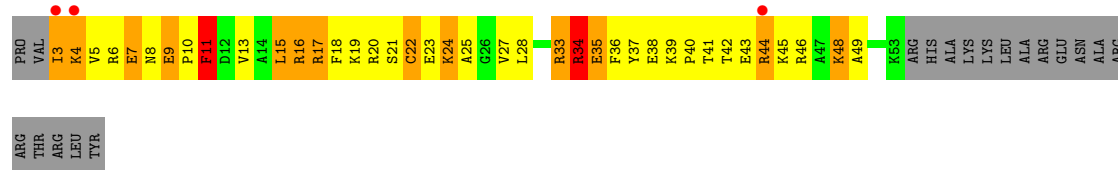
Chain CB:





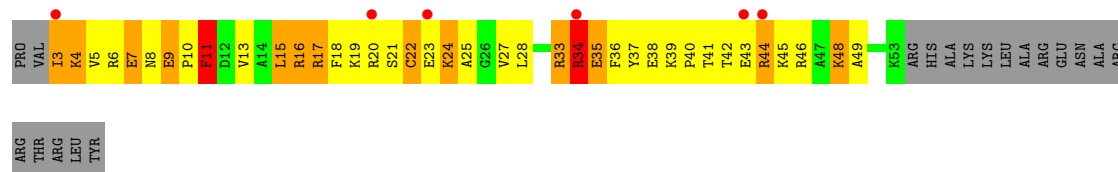
- Molecule 19: 30S ribosomal protein S21

Chain AU:



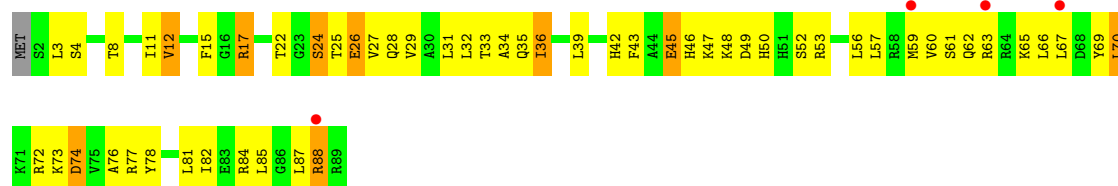
- Molecule 19: 30S ribosomal protein S21

Chain CU:



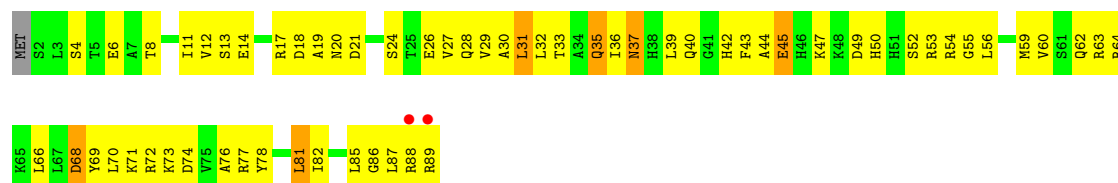
- Molecule 20: 30S ribosomal protein S15

Chain AO:



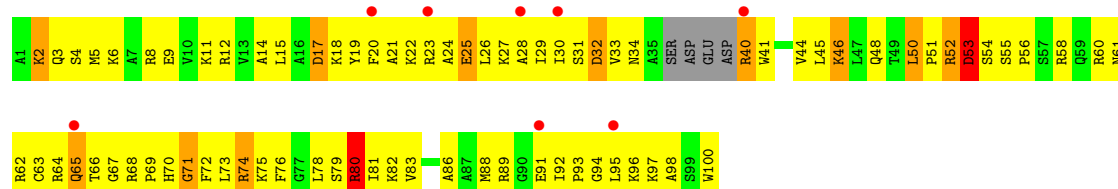
- Molecule 20: 30S ribosomal protein S15

Chain CO:



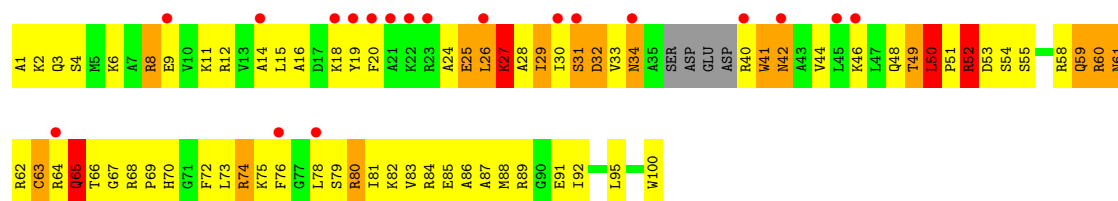
- Molecule 21: 30S ribosomal protein S14

Chain AN:



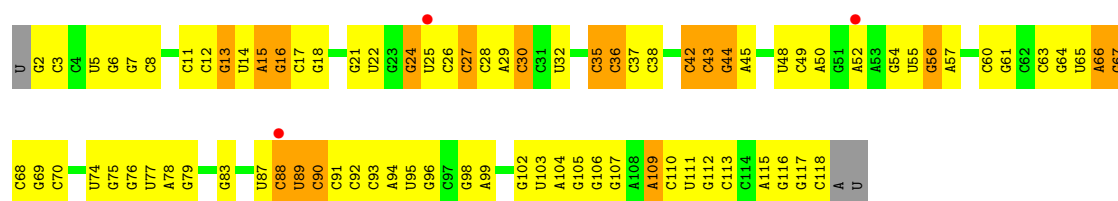
- Molecule 21: 30S ribosomal protein S14

Chain CN:



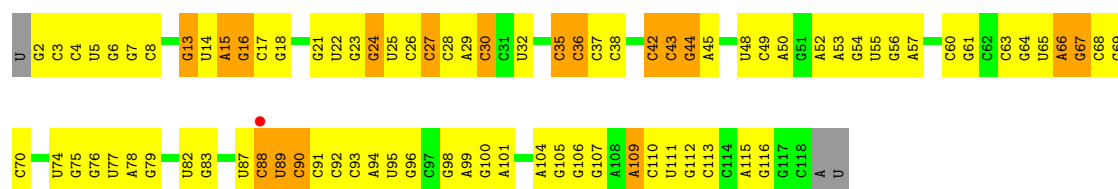
- Molecule 22: 5S rRNA

Chain BA:



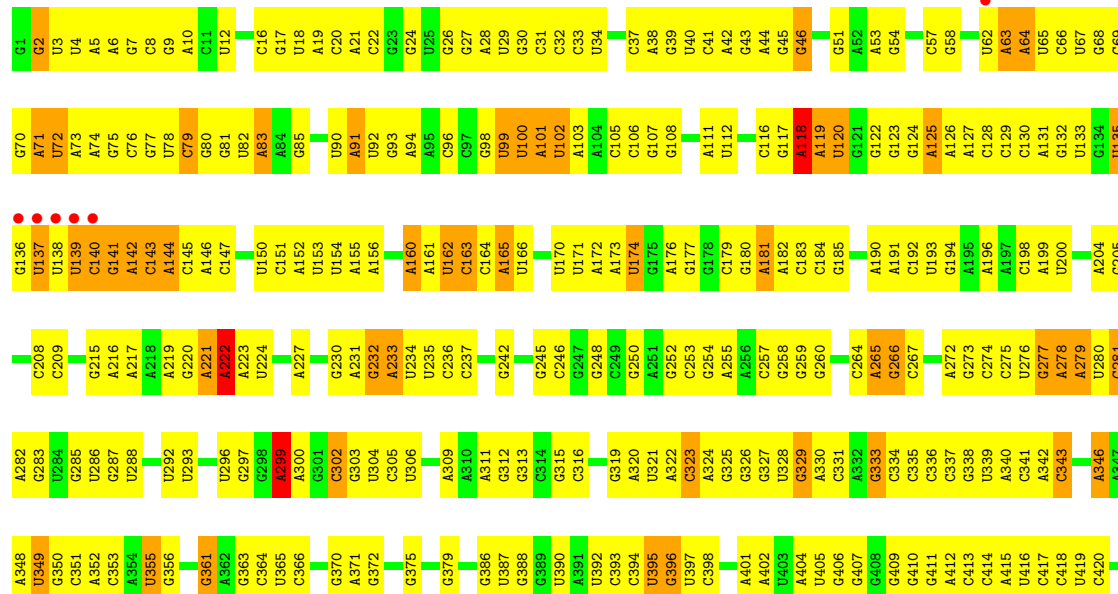
- Molecule 22: 5S rRNA

Chain DA:



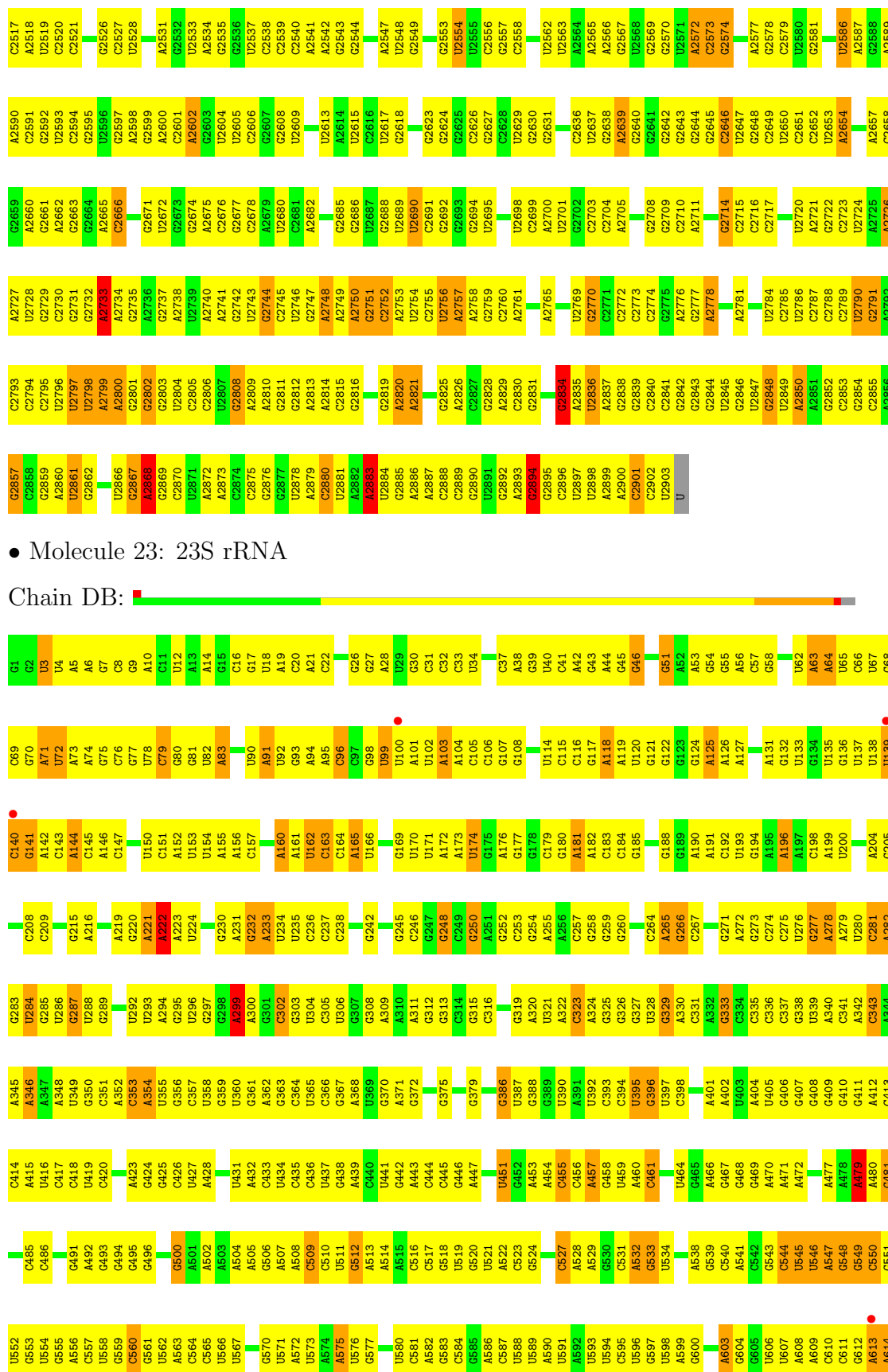
- Molecule 23: 23S rRNA

Chain BB:



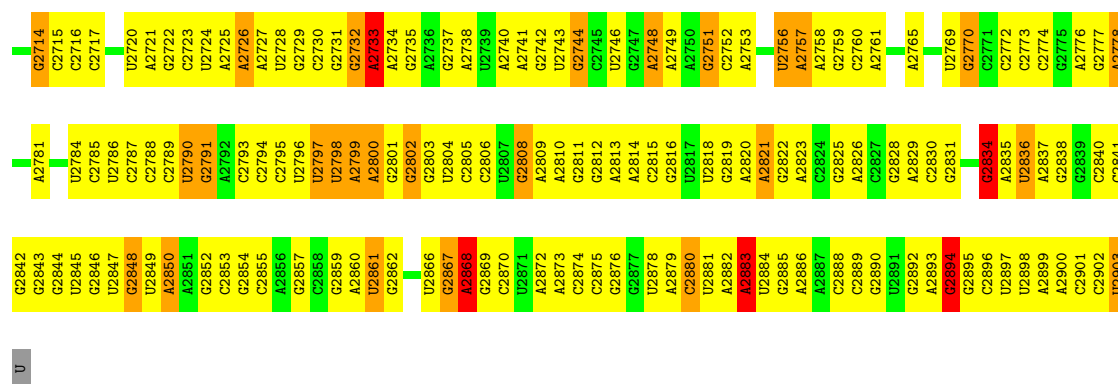
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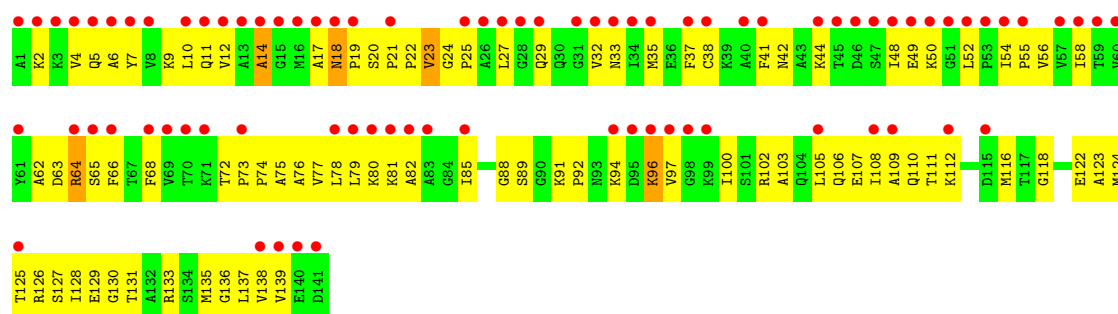
A1640	A1641	G1642	U1647	G1643	A1650	G1651	G1652	G1653	A1654	A1655	G1656	A1657	A1658	A1659	A1660	A1661	U1662	G1663	A1664	G1665	A1666	A1667	A1668	A1669	U1670	A1671	A1672	G1673	G1674	A1675	A1676	A1677	A1678	A1679	A1680	G1681	G1682	U1683	G1684	G1685	G1686	G1687	U1688	A1689	A1690	G1691	A1692	A1693	A1694	A1695	A1696	A1697	A1698	A1699	A1700	A1701	G1704	A1705	G1706	G1707	C1708
A1569	A1570	A1571	A1572	U1576	C1577	U1578	A1579	A1580	G1581	C1582	A1583	U1584	C1585	A1586	G1587	G1588	U1589	A1590	G1591	A1592	A1593	U1594	C1595	A1596	A1597	U1598	A1599	C1600	A1603	G1606	C1607	A1608	A1609	A1610	G1613	A1616	C1617	A1618	G1619	G1622	G1623	U1624	C1625	A1626	U1629	A1634	U1636	A1637	G1638	C1639											
U1438	A1439	U1440	G1441	A1442	U1443	G1444	C1447	U1448	G1449	G1450	A1453	A1454	G1455	U1456	U1457	U1458	U1459	U1460	C1461	C1462	C1463	G1464	G1465	U1466	U1467	U1468	A1469	A1470	C1471	C1472	U1473	U1474	G1475	U1476	G1478	U1479	C1480	U1481	G1482	U1483	U1484	U1485	G1486	U1487	U1488	C1489	U1490	U1491	G1492	C1493	A1494	A1495	A1496	C1499	G1500						
G1374	U1375	C1376	G1377	U1378	G1380	G1381	G1382	A1383	A1384	A1385	A1386	A1387	G1388	U1389	U1390	U1391	A1395	U1396	U1397	C1398	C1399	U1400	G1401	U1402	U1403	C1404	U1405	U1406	G1407	G1408	U1409	U1410	U1411	U1412	U1413	G1416	C1417	U1418	A1419	A1420	G1421	G1422	U1423	U1424	G1425	G1426	A1427	U1428	U1429	G1430	A1431	A1432	A1433	A1434	C1437						
G1310	G1311	U1312	U1313	C1314	C1315	U1316	U1317	C1318	C1319	C1320	A1321	A1322	C1323	G1324	U1325	U1326	A1327	A1328	U1329	C1330	G1331	G1334	C1335	A1336	U1337	C1338	U1339	U1340	G1341	A1342	G1343	U1344	C1345	G1346	A1347	C1348	C1349	C1350	C1351	U1352	A1353	A1354	G1355	G1356	C1357	G1358	A1359	G1360	G1361	C1362	U1363	A1365	G1368	G1371	U1372	A1373					
G1239	U1240	U1241	U1242	C1243	A1244	G1245	G1248	U1249	G1250	G1251	C1252	A1253	G1256	C1257	U1258	G1259	A1260	C1261	G1266	U1267	A1268	A1269	C1270	G1271	A1272	U1273	A1274	A1275	A1276	C1277	C1278	G1281	U1282	G1283	A1286	A1287	C1288	C1289	C1290	C1291	G1292	C1293	G1297	C1298	G1299	A1300	A1301	A1302	C1306	A1307	G1309										
G1166	C1167	A1168	U1169	C1170	G1171	U1172	U1173	U1174	U1175	U1176	G1177	C1178	G1179	U1180	U1181	U1182	U1183	U1184	U1185	U1186	U1187	U1188	U1189	G1190	G1191	U1192	U1193	U1194	C1195	U1196	U1197	U1199	C1200	U1201	G1202	U1203	A1204	A1205	G1206	G1210	C1211	G1212	U1219	G1220	C1221	U1222	G1223	G1228	C1229	A1230	U1231	G1236	A1237	G1238							
U1097	A1098	G1099	C1100	U1101	C1102	A1103	C1104	U1105	G1106	G1107	U1108	C1109	G1110	A1111	U1112	U1113	C1114	G1115	G1116	C1117	U1118	U1119	G1125	A1126	A1129	U1132	A1133	A1134	C1135	U1136	G1137	G1138	U1139	C1140	U1141	A1142	A1143	A1144	C1145	C1146	G1149	C1150	A1151	C1152	C1153	G1154	A1155	A1156	U1159	G1160	G1163	C1164	A1165								
U1033	G1034	G1035	U1036	A1037	U1038	C1039	G1040	U1041	A1042	C1043	C1044	U1045	A1046	G1047	A1048	C1049	A1050	G1051	C1052	A1057	U1058	U1059	U1060	U1061	G1062	G1063	C1064	U1065	A1070	G1076	A1077	U1078	A1080	U1081	U1082	U1083	A1084	A1085	U1086	G1087	A1088	C1089	U1090	U1091	A1092	U1093	U1094	G1099	G1102												
A960	C961	G962	U963	C964	U967	C968	G969	U970	G971	A972	A973	C974	A975	G978	A979	A980	A981	C982	A983	A984	C985	C986	C987	A988	A989	A990	A991	C992	G993	C994	C995	A996	G997	C998	U999	A1000	A1001	C937	G938	A941	G942	A943	C944	A945	C946	A947	C948	G949	A1014	U1015	G1016	G1017	U1018	U1019	A1020	C957	U958	A959			
A832	A833	G834	C835	U836	C837	C838	U839	G840	U841	U842	A845	U846	U847	G848	A849	U850	C851	U852	C853	A854	C855	U856	G857	G858	G859	G862	A863	A864	U865	C866	U870	U871	U872	C873	G874	C875	C876	A877	G805	A878	G	G	G	G	C	A	U	C	C	C	A	U	C	U	G831						
U683	G684	U685	U686	C687	U688	A689	C690	C691	C692	A693	U694	G695	G696	G697	C698	G700	G701	U702	U703	U704	A705	U706	G708	U709	U710	G711	G712	G713	U714	A715	A716	C717	A718	C719	U720	A721	U722	C723	G724	G725	A726	A727	G728	G729	A730	C731	G738	A739	G740	U741	G742	A743	U744	G745	U746	G747					
U615	A616	G617	G620	A621	C622	C623	C624	A627	G630	A631	A632	A633	C634	A635	G636	A637	U642	A643	A644	C645	U646	G647	U648	A715	A716	C717	U653	A654	A655	G656	U657	U658	G725	A726	A661	G664	U665	A666	G669	A670	C671	C672	C673	G674	A675	C679	C680	U681	G682												





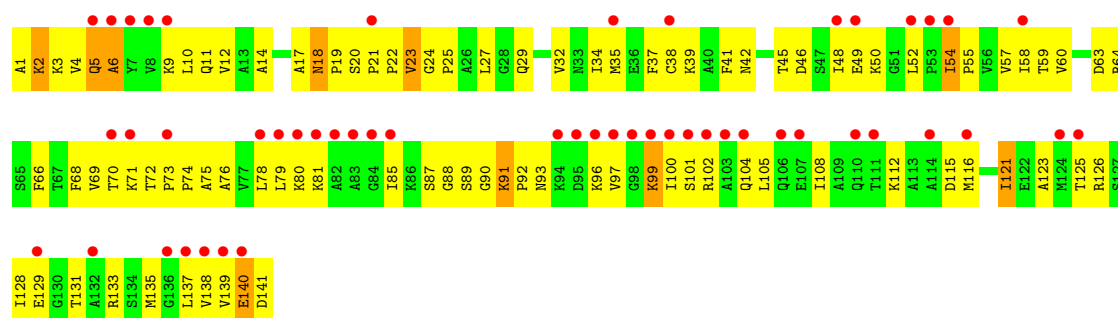
• Molecule 24: 50S ribosomal protein L11

Chain BI:



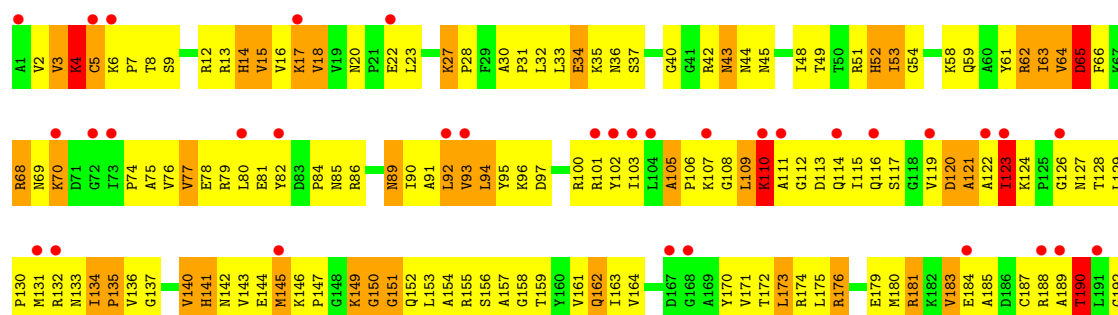
• Molecule 24: 50S ribosomal protein L11

Chain DI:



• Molecule 25: 50S ribosomal protein L2

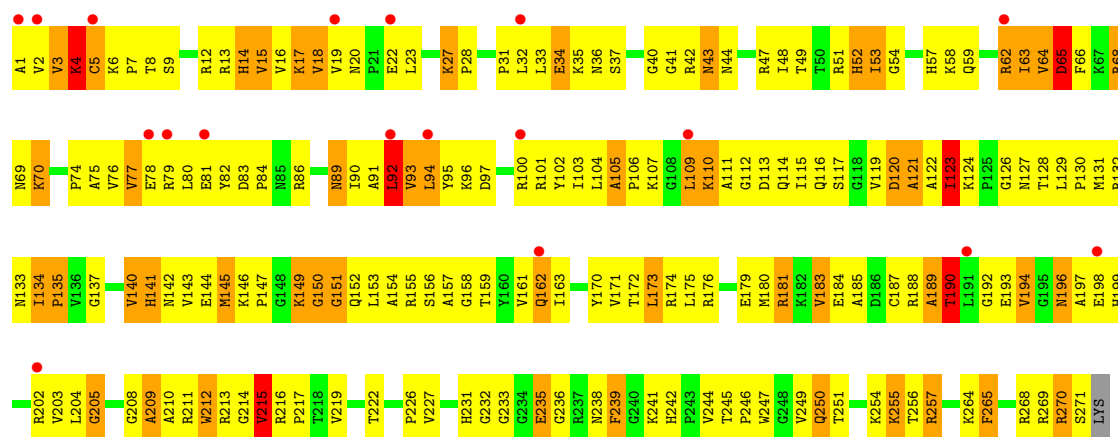
Chain BC:





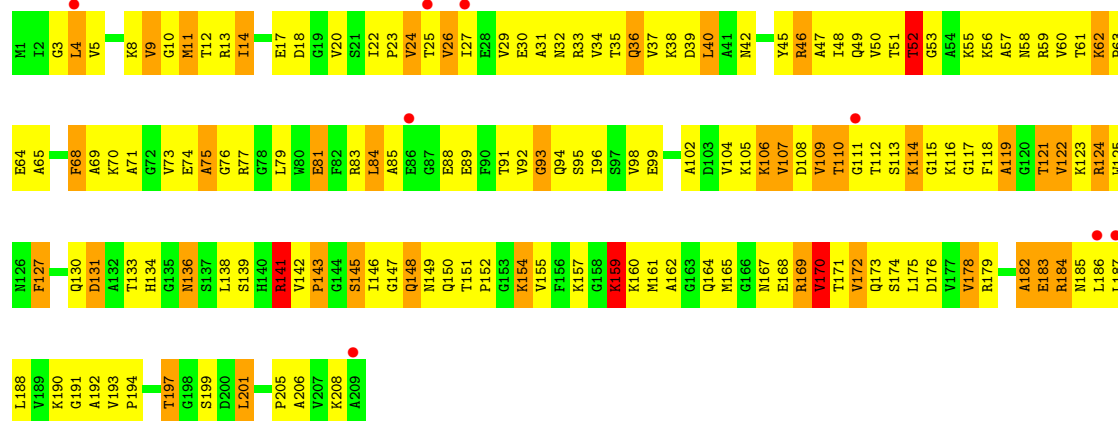
• Molecule 25: 50S ribosomal protein L2

Chain DC:



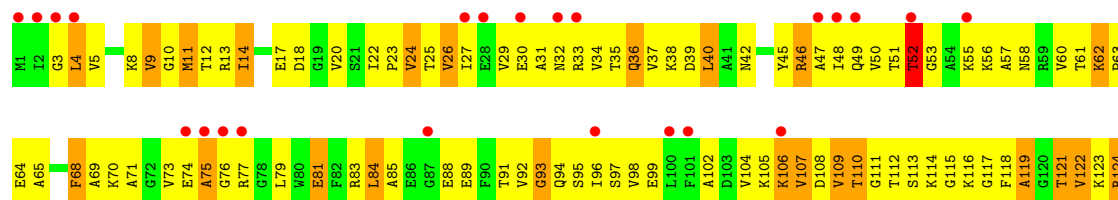
• Molecule 26: 50S ribosomal protein L3

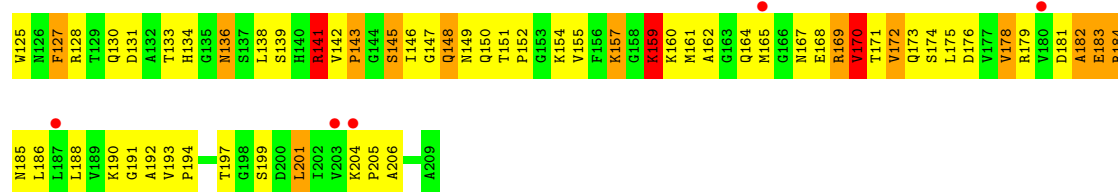
Chain BD:



• Molecule 26: 50S ribosomal protein L3

Chain DD:





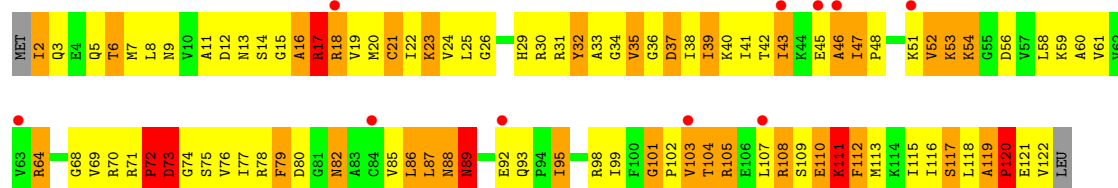
• Molecule 27: 50S ribosomal protein L14

Chain BK:



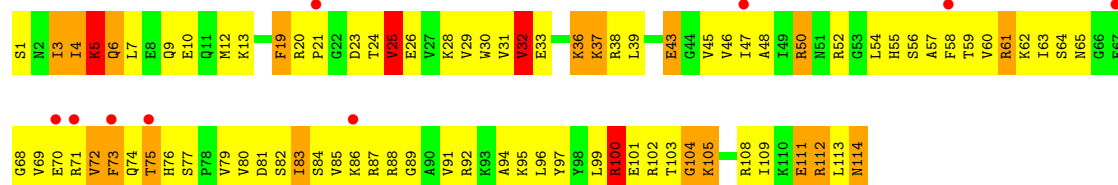
• Molecule 27: 50S ribosomal protein L14

Chain DK:



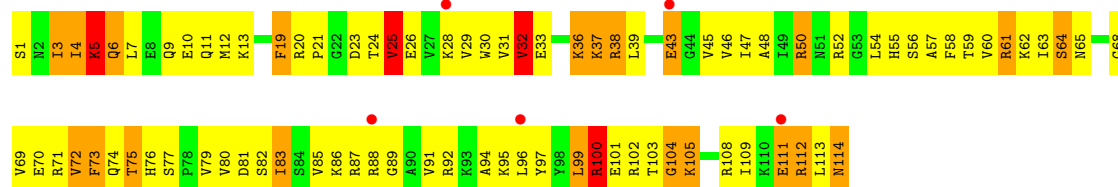
• Molecule 28: 50S ribosomal protein L19

Chain BP:



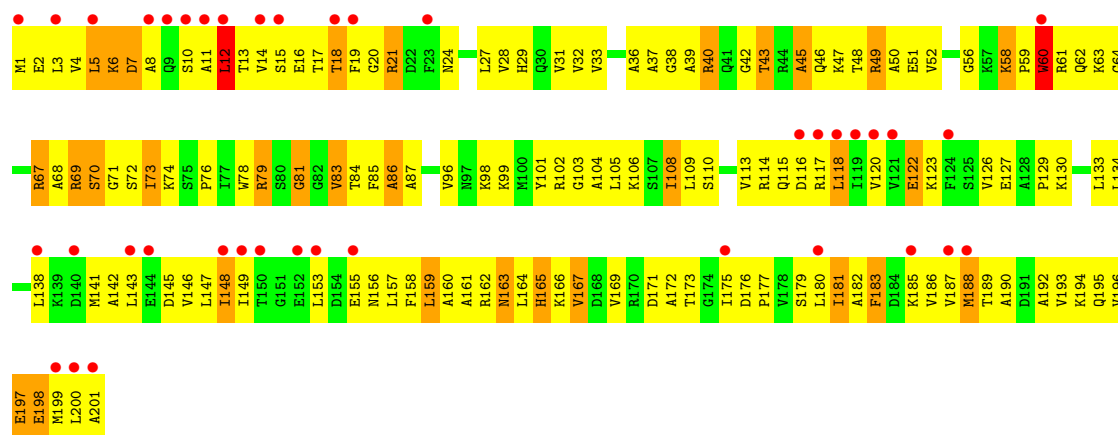
• Molecule 28: 50S ribosomal protein L19

Chain DP:



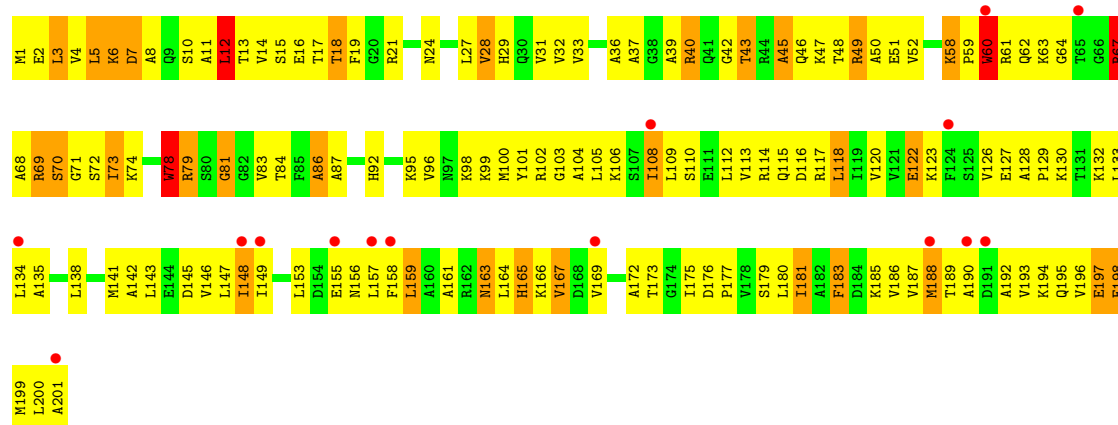
• Molecule 29: 50S ribosomal protein L4

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:



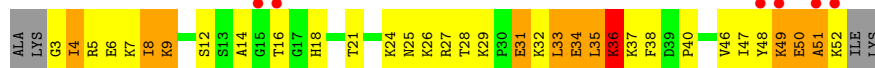
- Molecule 32: 50S ribosomal protein L36

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:



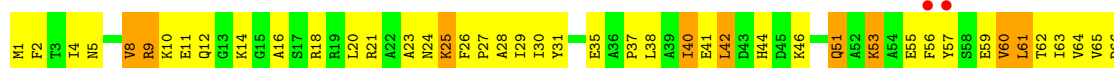
- Molecule 34: 50S ribosomal protein L35

Chain D3:



- Molecule 35: 50S ribosomal protein L25

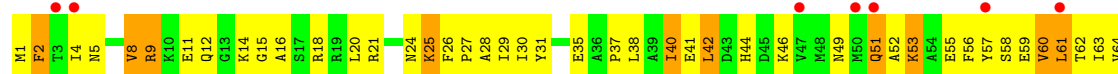
Chain BV:





- Molecule 35: 50S ribosomal protein L25

Chain DV:



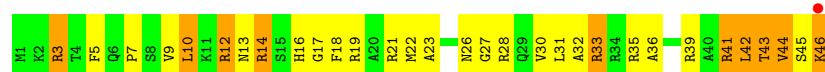
- Molecule 36: 50S ribosomal protein L34

Chain B2:



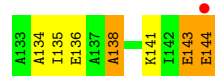
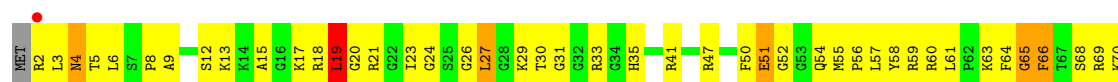
- Molecule 36: 50S ribosomal protein L34

Chain D2:



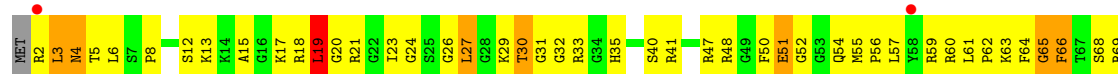
- Molecule 37: 50S ribosomal protein L15

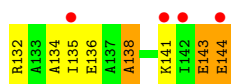
Chain BL:



- Molecule 37: 50S ribosomal protein L15

Chain DL:





• Molecule 38: 50S ribosomal protein L16

Chain BM:



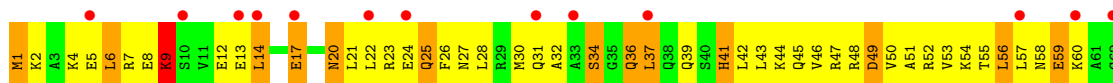
• Molecule 38: 50S ribosomal protein L16

Chain DM:



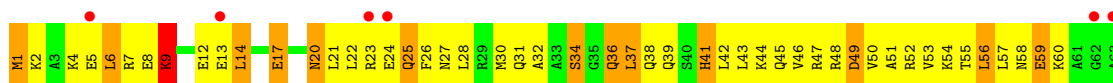
• Molecule 39: 50S ribosomal protein L29

Chain BX:



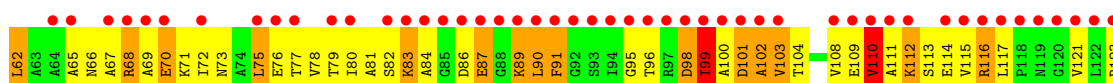
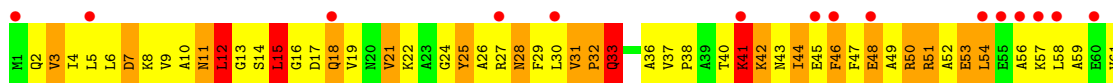
• Molecule 39: 50S ribosomal protein L29

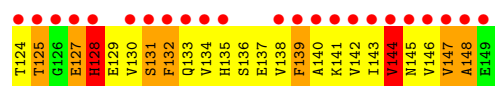
Chain DX:



• Molecule 40: 50S ribosomal protein L9

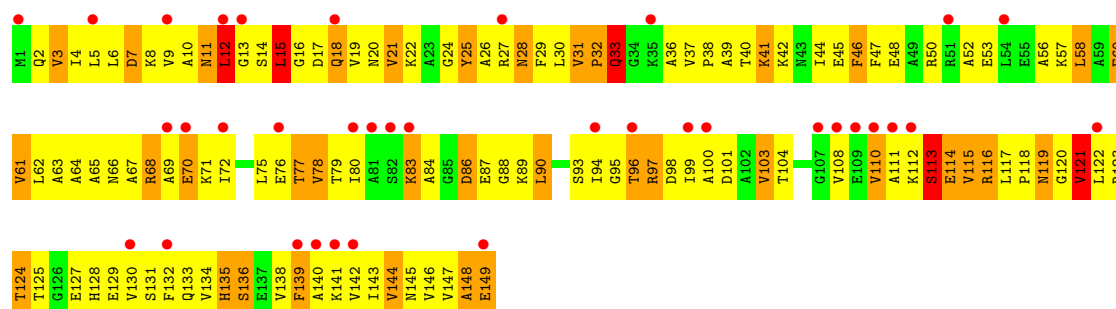
Chain BH:





• Molecule 40: 50S ribosomal protein L9

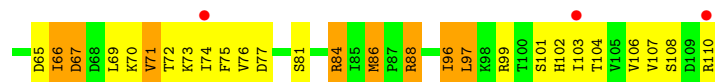
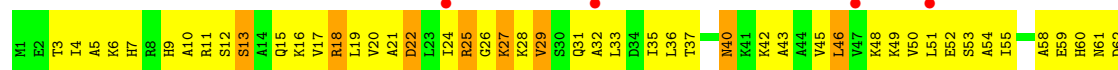
Chain DH:



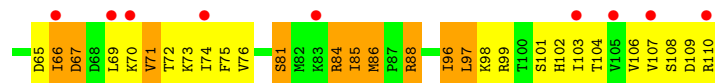
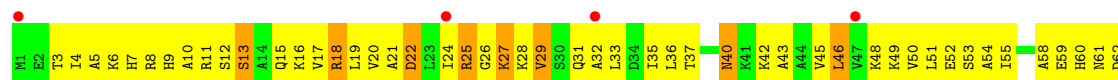




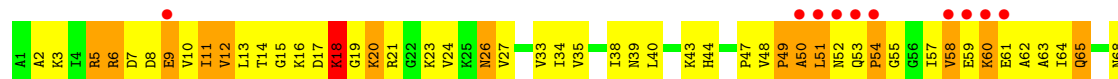
Chain BS:



Chain DS:



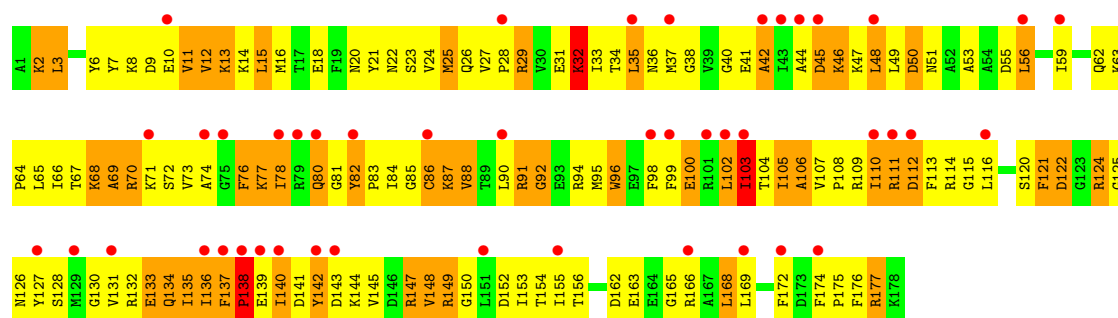
Chain BU:



Chain DU:

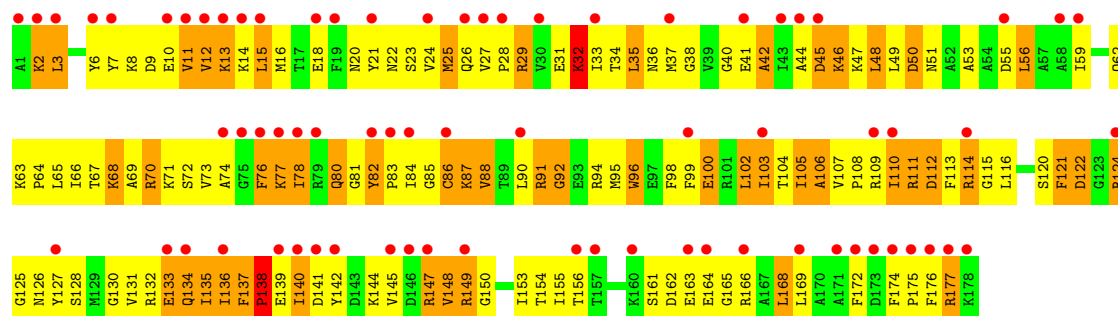


Chain BF:



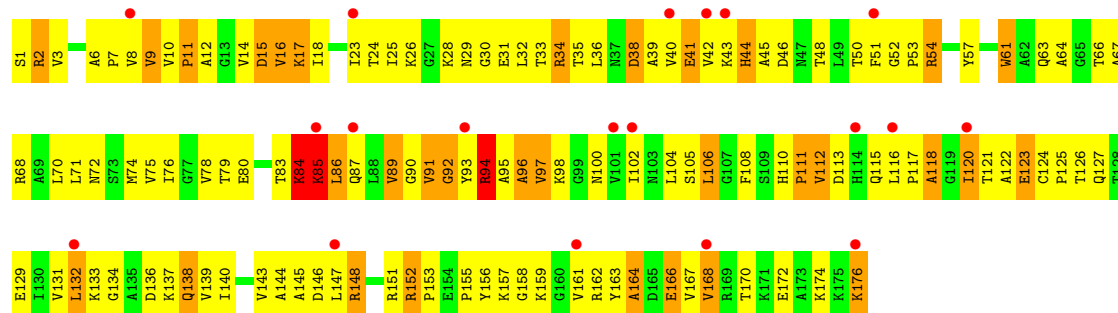
• Molecule 47: 50S ribosomal protein L5

Chain DF:



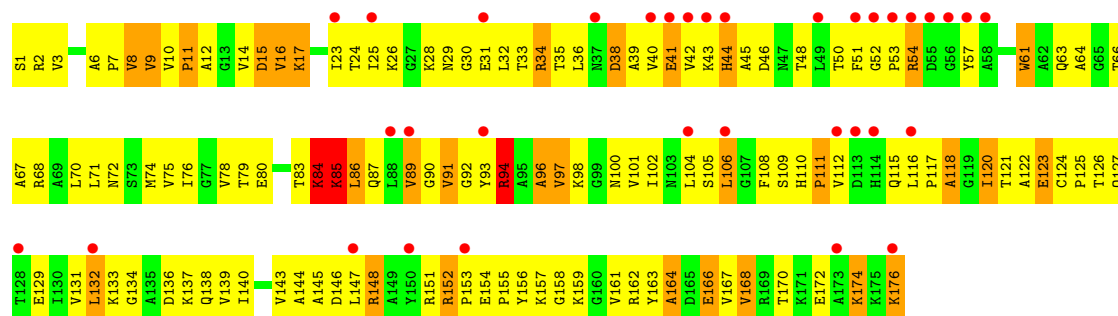
• Molecule 48: 50S ribosomal protein L6

Chain BG:



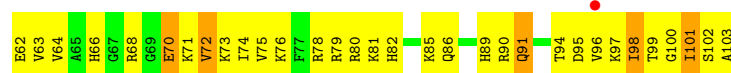
• Molecule 48: 50S ribosomal protein L6

Chain DG:



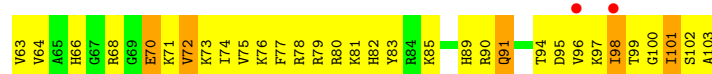
• Molecule 49: 50S ribosomal protein L21

Chain BR: 



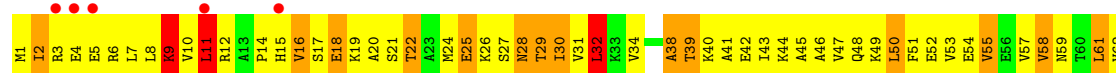
- Molecule 49: 50S ribosomal protein L21

Chain DR: 



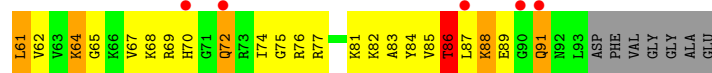
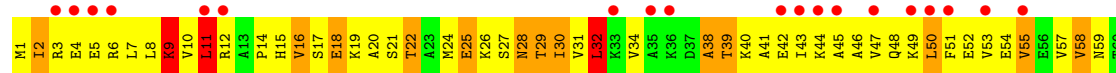
- Molecule 50: 50S ribosomal protein L23

Chain BT: 



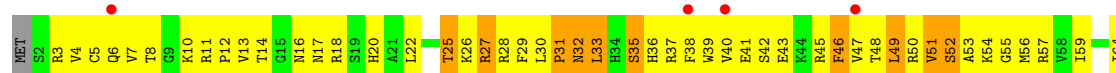
- Molecule 50: 50S ribosomal protein L23

Chain DT: 



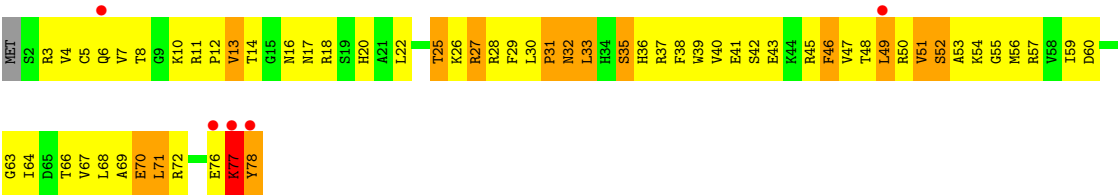
- Molecule 51: 50S ribosomal protein L28

Chain BZ: 

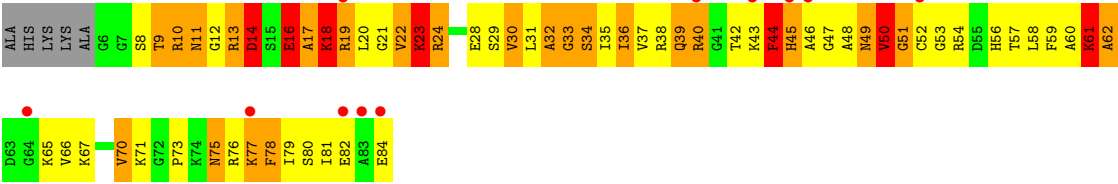


- Molecule 51: 50S ribosomal protein L28

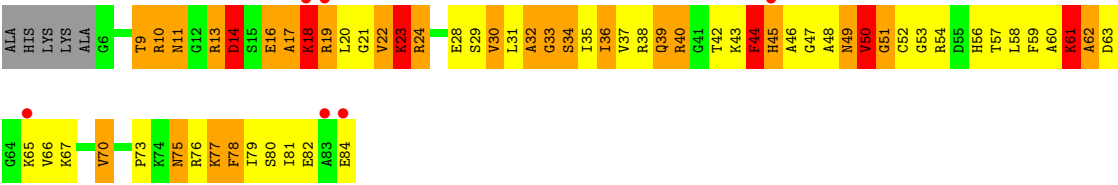
Chain DZ: 



● Molecule 52: 50S ribosomal protein L27



● Molecule 52: 50S ribosomal protein L27



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 – 3.50 182.94 – 3.53	Depositor EDS
% Data completeness (in resolution range)	(Not available) (70.00-3.50) 73.0 (182.94-3.53)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 3.49Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.264 , 0.306 0.241 , 0.271	Depositor DCC
R_{free} test set	25277 reflections (5.10%)	DCC
Wilson B-factor (Å ²)	132.6	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 38.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 521228 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	284201	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SCM, ZN, MG, 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	0.26	1/36762 (0.0%)	0.75	9/57350 (0.0%)
1	CA	0.32	2/36762 (0.0%)	0.77	8/57350 (0.0%)
2	AC	0.23	0/1651	0.45	0/2225
2	CC	0.23	0/1651	0.46	0/2225
3	AD	0.23	0/1665	0.43	0/2227
3	CD	0.23	0/1665	0.43	0/2227
4	AE	0.23	0/1118	0.46	0/1504
4	CE	0.23	0/1118	0.46	0/1504
5	AF	0.24	0/835	0.44	0/1128
5	CF	0.24	0/835	0.44	0/1128
6	AG	0.23	0/1187	0.44	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	0.44	0/1326
8	AI	0.24	0/1034	0.44	0/1375
8	CI	0.24	0/1034	0.45	0/1375
9	AJ	0.22	0/796	0.48	0/1077
9	CJ	0.23	0/796	0.47	0/1077
10	AK	0.24	0/893	0.45	0/1205
10	CK	0.24	0/893	0.45	0/1205
11	AL	0.22	0/969	0.48	0/1300
11	CL	0.22	0/969	0.48	0/1300
12	AM	0.21	0/892	0.46	0/1193
12	CM	0.21	0/884	0.45	0/1181
13	AP	0.25	0/659	0.46	0/884
13	CP	0.25	0/648	0.46	0/870
14	AQ	0.24	0/657	0.46	0/881
14	CQ	0.24	0/666	0.46	0/892
15	AR	0.23	0/462	0.44	0/621
15	CR	0.23	0/462	0.45	0/621
16	AS	0.25	0/652	0.45	0/877
16	CS	0.25	0/660	0.49	0/888

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AT	0.24	0/671	0.40	0/888
17	CT	0.23	0/671	0.40	0/888
18	AB	0.25	0/1735	0.44	0/2338
18	CB	0.25	0/1735	0.45	0/2338
19	AU	0.26	0/430	0.46	0/570
19	CU	0.26	0/430	0.46	0/570
20	AO	0.23	0/722	0.44	0/964
20	CO	0.23	0/722	0.43	0/964
21	AN	0.24	0/785	0.43	0/1043
21	CN	0.24	0/785	0.45	0/1043
22	BA	0.25	0/2803	0.75	0/4371
22	DA	0.25	0/2803	0.74	0/4371
23	BB	0.28	6/68314 (0.0%)	0.77	42/106569 (0.0%)
23	DB	0.28	6/68314 (0.0%)	0.77	41/106569 (0.0%)
24	BI	0.24	0/1046	0.46	0/1410
24	DI	0.25	0/1046	0.47	0/1410
25	BC	0.22	0/2121	0.47	0/2852
25	DC	0.22	0/2121	0.47	0/2852
26	BD	0.24	0/1586	0.47	0/2134
26	DD	0.24	0/1586	0.47	0/2134
27	BK	0.23	0/939	0.52	0/1258
27	DK	0.23	0/939	0.52	0/1258
28	BP	0.24	0/929	0.49	0/1242
28	DP	0.24	0/929	0.49	0/1242
29	BE	0.24	0/1571	0.49	0/2113
29	DE	0.24	0/1571	0.49	0/2113
30	BY	0.24	0/453	0.48	0/605
30	DY	0.24	0/453	0.48	0/605
31	B0	0.22	0/450	0.51	0/599
31	D0	0.22	0/450	0.51	0/599
32	B4	0.23	0/303	0.44	0/397
32	D4	0.23	0/303	0.44	0/397
33	B1	0.27	0/416	0.47	0/554
33	D1	0.27	0/416	0.47	0/554
34	B3	0.24	0/513	0.47	0/676
34	D3	0.24	0/513	0.47	0/676
35	BV	0.25	0/766	0.43	0/1025
35	DV	0.25	0/766	0.43	0/1025
36	B2	0.26	0/380	0.47	0/498
36	D2	0.26	0/380	0.47	0/498
37	BL	0.23	0/1054	0.47	0/1403
37	DL	0.23	0/1054	0.47	0/1403
38	BM	0.25	0/1093	0.47	0/1460

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DM	0.25	0/1093	0.47	0/1460
39	BX	0.24	0/510	0.52	0/677
39	DX	0.24	0/510	0.52	0/677
40	BH	0.25	0/1122	0.45	0/1515
40	DH	0.25	0/1122	0.46	0/1515
41	BJ	0.23	0/1152	0.47	0/1551
41	DJ	0.23	0/1152	0.47	0/1551
42	BN	0.24	0/973	0.49	0/1301
42	DN	0.24	0/973	0.49	0/1301
43	BO	0.23	0/902	0.47	0/1209
43	DO	0.23	0/902	0.47	0/1209
44	BQ	0.25	0/960	0.46	0/1278
44	DQ	0.25	0/960	0.46	0/1278
45	BS	0.21	0/864	0.50	0/1156
45	DS	0.21	0/864	0.50	0/1156
46	BU	0.25	0/787	0.45	0/1051
46	DU	0.25	0/787	0.45	0/1051
47	BF	0.25	0/1444	0.50	0/1937
47	DF	0.25	0/1444	0.50	0/1937
48	BG	0.23	0/1343	0.46	0/1816
48	DG	0.23	0/1343	0.46	0/1816
49	BR	0.25	0/829	0.46	0/1107
49	DR	0.25	0/829	0.46	0/1107
50	BT	0.22	0/744	0.51	0/994
50	DT	0.22	0/744	0.51	0/994
51	BZ	0.25	0/635	0.48	0/848
51	DZ	0.25	0/635	0.48	0/848
52	BW	0.28	0/603	0.48	0/797
52	DW	0.27	0/603	0.48	0/797
All	All	0.27	15/306360 (0.0%)	0.70	100/457969 (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	20
23	BB	0	44
23	DB	0	43
All	All	0	120

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	BB	1086	A	C5-C6	-15.92	1.26	1.41
23	DB	1086	A	C5-C6	-15.80	1.26	1.41
23	BB	1088	A	C6-N1	-10.61	1.28	1.35
23	DB	1088	A	C6-N1	-10.48	1.28	1.35
23	DB	1060	U	C2-N3	7.81	1.43	1.37

The worst 5 of 100 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	DB	2204	G	O5'-P-OP1	-29.68	75.09	110.70
23	BB	2204	G	O5'-P-OP2	-28.72	76.23	110.70
23	DB	2791	G	O5'-P-OP2	-27.53	77.67	110.70
23	BB	2791	G	O5'-P-OP1	-27.53	77.67	110.70
23	DB	2791	G	O5'-P-OP1	17.94	132.23	110.70

There are no chirality outliers.

5 of 120 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	187	G	Sidechain
1	AA	281	G	Sidechain
1	AA	437	U	Sidechain
1	AA	438	U	Sidechain
1	AA	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	1291	0
1	CA	32831	0	16521	1302	0
2	AC	1624	0	1699	189	0
2	CC	1624	0	1699	189	0
3	AD	1643	0	1710	127	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	CD	1643	0	1710	128	0
4	AE	1105	0	1148	94	0
4	CE	1105	0	1148	93	0
5	AF	817	0	808	95	0
5	CF	817	0	808	91	0
6	AG	1174	0	1230	150	0
6	CG	1196	0	1246	114	0
7	AH	979	0	1034	68	0
7	CH	979	0	1034	70	0
8	AI	1022	0	1070	146	0
8	CI	1022	0	1070	136	0
9	AJ	786	0	828	100	0
9	CJ	786	0	828	98	0
10	AK	877	0	887	108	0
10	CK	877	0	887	97	0
11	AL	955	0	1019	96	0
11	CL	955	0	1019	97	0
12	AM	883	0	944	160	0
12	CM	876	0	937	116	0
13	AP	649	0	666	58	0
13	CP	638	0	656	50	0
14	AQ	648	0	691	63	0
14	CQ	657	0	702	59	0
15	AR	455	0	478	40	0
15	CR	455	0	478	43	0
16	AS	637	0	665	107	0
16	CS	644	0	675	106	0
17	AT	665	0	714	60	0
17	CT	665	0	714	64	0
18	AB	1704	0	1732	193	0
18	CB	1704	0	1732	210	0
19	AU	425	0	449	74	0
19	CU	425	0	449	67	0
20	AO	714	0	734	65	0
20	CO	714	0	734	50	0
21	AN	774	0	827	109	0
21	CN	774	0	827	113	0
22	BA	2507	0	1270	104	0
22	DA	2507	0	1270	107	0
23	BB	60995	0	30679	2216	0
23	DB	60995	0	30678	2313	0
24	BI	1032	0	1088	112	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	DI	1032	0	1088	176	0
25	BC	2082	0	2157	217	0
25	DC	2082	0	2157	218	0
26	BD	1565	0	1616	206	0
26	DD	1565	0	1616	207	0
27	BK	930	0	1000	130	0
27	DK	930	0	1000	138	0
28	BP	917	0	965	115	0
28	DP	917	0	965	118	0
29	BE	1552	0	1619	199	0
29	DE	1552	0	1619	183	0
30	BY	449	0	491	58	0
30	DY	449	0	491	57	0
31	B0	444	0	461	35	0
31	D0	444	0	461	40	0
32	B4	302	0	340	42	0
32	D4	302	0	340	39	0
33	B1	409	0	440	34	0
33	D1	409	0	440	38	0
34	B3	504	0	574	50	0
34	D3	504	0	574	44	0
35	BV	753	0	780	102	0
35	DV	753	0	780	100	0
36	B2	377	0	418	48	0
36	D2	377	0	418	45	0
37	BL	1045	0	1117	139	0
37	DL	1045	0	1117	153	0
38	BM	1074	0	1157	116	0
38	DM	1074	0	1157	115	0
39	BX	509	0	543	63	0
39	DX	509	0	543	67	0
40	BH	1111	0	1148	193	0
40	DH	1111	0	1148	179	0
41	BJ	1129	0	1162	130	0
41	DJ	1129	0	1162	127	0
42	BN	960	0	1000	115	0
42	DN	960	0	1000	114	0
43	BO	892	0	923	93	0
43	DO	892	0	923	102	0
44	BQ	947	0	1022	143	0
44	DQ	947	0	1022	143	0
45	BS	857	0	922	86	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	DS	857	0	922	92	0
46	BU	779	0	834	110	0
46	DU	779	0	834	111	0
47	BF	1420	0	1460	223	0
47	DF	1420	0	1460	216	0
48	BG	1323	0	1374	188	0
48	DG	1323	0	1374	178	0
49	BR	816	0	839	110	0
49	DR	816	0	839	105	0
50	BT	738	0	807	107	0
50	DT	738	0	807	116	0
51	BZ	625	0	652	68	0
51	DZ	625	0	652	67	0
52	BW	596	0	610	134	0
52	DW	596	0	610	127	0
53	AA	42	0	46	0	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	59	0	0	0	0
54	DB	111	0	0	0	0
55	AA	23	0	24	5	0
55	CA	23	0	24	1	0
56	B4	1	0	0	0	0
56	D4	1	0	0	0	0
57	AA	290	0	0	2	0
57	AE	1	0	0	0	0
57	AK	1	0	0	0	0
57	AL	4	0	0	0	0
57	AN	1	0	0	0	0
57	AP	1	0	0	0	0
57	AT	2	0	0	0	0
57	BB	492	0	0	4	0
57	BC	7	0	0	0	0
57	BD	1	0	0	0	0
57	BE	4	0	0	0	0
57	BH	1	0	0	0	0
57	BL	2	0	0	0	0
57	CA	282	0	0	2	0
57	CE	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	CI	1	0	0	0	0
57	CL	4	0	0	0	0
57	CN	3	0	0	0	0
57	CP	1	0	0	0	0
57	CT	1	0	0	0	0
57	DB	501	0	0	14	0
57	DC	4	0	0	0	0
57	DD	1	0	0	0	0
57	DE	2	0	0	0	0
57	DL	1	0	0	0	0
57	DN	2	0	0	0	0
57	DR	1	0	0	0	0
All	All	284201	0	190895	16740	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 35.

The worst 5 of 16740 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	1.32	1.27
23:BB:2305:U:H1'	47:BF:132:ARG:HA	1.33	1.10
40:BH:125:THR:HA	40:BH:146:VAL:HB	1.28	1.10
18:CB:69:VAL:HG23	18:CB:162:VAL:HB	1.34	1.09
23:DB:1098:A:H3'	24:DI:3:LYS:HA	1.32	1.08

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%)	130 (64%)	44 (22%)	30 (15%)	0 6
2	CC	204/232 (88%)	137 (67%)	49 (24%)	18 (9%)	1 19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AD	203/205 (99%)	153 (75%)	40 (20%)	10 (5%)	3	37
3	CD	203/205 (99%)	153 (75%)	40 (20%)	10 (5%)	3	37
4	AE	148/166 (89%)	116 (78%)	24 (16%)	8 (5%)	3	35
4	CE	148/166 (89%)	114 (77%)	25 (17%)	9 (6%)	2	30
5	AF	98/135 (73%)	63 (64%)	25 (26%)	10 (10%)	1	14
5	CF	98/135 (73%)	64 (65%)	24 (24%)	10 (10%)	1	14
6	AG	148/178 (83%)	110 (74%)	30 (20%)	8 (5%)	3	35
6	CG	150/178 (84%)	111 (74%)	28 (19%)	11 (7%)	2	25
7	AH	127/129 (98%)	92 (72%)	31 (24%)	4 (3%)	7	53
7	CH	127/129 (98%)	92 (72%)	31 (24%)	4 (3%)	7	53
8	AI	125/129 (97%)	80 (64%)	35 (28%)	10 (8%)	1	21
8	CI	125/129 (97%)	80 (64%)	34 (27%)	11 (9%)	1	19
9	AJ	96/103 (93%)	59 (62%)	25 (26%)	12 (12%)	1	10
9	CJ	96/103 (93%)	64 (67%)	22 (23%)	10 (10%)	1	14
10	AK	115/128 (90%)	87 (76%)	23 (20%)	5 (4%)	4	42
10	CK	115/128 (90%)	86 (75%)	24 (21%)	5 (4%)	4	42
11	AL	121/123 (98%)	69 (57%)	37 (31%)	15 (12%)	1	10
11	CL	121/123 (98%)	72 (60%)	34 (28%)	15 (12%)	1	10
12	AM	112/117 (96%)	74 (66%)	25 (22%)	13 (12%)	1	12
12	CM	111/117 (95%)	78 (70%)	21 (19%)	12 (11%)	1	13
13	AP	80/82 (98%)	53 (66%)	20 (25%)	7 (9%)	1	19
13	CP	78/82 (95%)	52 (67%)	19 (24%)	7 (9%)	1	18
14	AQ	78/83 (94%)	59 (76%)	15 (19%)	4 (5%)	3	36
14	CQ	79/83 (95%)	57 (72%)	18 (23%)	4 (5%)	3	36
15	AR	53/74 (72%)	40 (76%)	13 (24%)	0	100	100
15	CR	53/74 (72%)	41 (77%)	11 (21%)	1 (2%)	12	64
16	AS	77/91 (85%)	49 (64%)	24 (31%)	4 (5%)	3	35
16	CS	78/91 (86%)	57 (73%)	16 (20%)	5 (6%)	2	29
17	AT	83/86 (96%)	62 (75%)	16 (19%)	5 (6%)	2	31
17	CT	83/86 (96%)	63 (76%)	15 (18%)	5 (6%)	2	31
18	AB	216/240 (90%)	135 (62%)	56 (26%)	25 (12%)	1	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	CB	216/240 (90%)	145 (67%)	52 (24%)	19 (9%)	1	19
19	AU	49/70 (70%)	29 (59%)	14 (29%)	6 (12%)	1	11
19	CU	49/70 (70%)	29 (59%)	14 (29%)	6 (12%)	1	11
20	AO	86/89 (97%)	62 (72%)	18 (21%)	6 (7%)	2	26
20	CO	86/89 (97%)	60 (70%)	25 (29%)	1 (1%)	19	75
21	AN	92/100 (92%)	53 (58%)	30 (33%)	9 (10%)	1	16
21	CN	92/100 (92%)	49 (53%)	31 (34%)	12 (13%)	0	10
24	BI	139/141 (99%)	118 (85%)	17 (12%)	4 (3%)	7	54
24	DI	139/141 (99%)	115 (83%)	19 (14%)	5 (4%)	5	49
25	BC	269/272 (99%)	163 (61%)	63 (23%)	43 (16%)	0	5
25	DC	269/272 (99%)	162 (60%)	61 (23%)	46 (17%)	0	4
26	BD	207/209 (99%)	118 (57%)	57 (28%)	32 (16%)	0	5
26	DD	207/209 (99%)	118 (57%)	58 (28%)	31 (15%)	0	6
27	BK	119/123 (97%)	70 (59%)	27 (23%)	22 (18%)	0	3
27	DK	119/123 (97%)	69 (58%)	29 (24%)	21 (18%)	0	4
28	BP	112/114 (98%)	66 (59%)	29 (26%)	17 (15%)	0	6
28	DP	112/114 (98%)	66 (59%)	29 (26%)	17 (15%)	0	6
29	BE	199/201 (99%)	124 (62%)	51 (26%)	24 (12%)	1	11
29	DE	199/201 (99%)	124 (62%)	48 (24%)	27 (14%)	0	8
30	BY	56/58 (97%)	39 (70%)	12 (21%)	5 (9%)	1	18
30	DY	56/58 (97%)	40 (71%)	11 (20%)	5 (9%)	1	18
31	B0	54/56 (96%)	36 (67%)	12 (22%)	6 (11%)	1	13
31	D0	54/56 (96%)	36 (67%)	12 (22%)	6 (11%)	1	13
32	B4	36/38 (95%)	20 (56%)	9 (25%)	7 (19%)	0	3
32	D4	36/38 (95%)	21 (58%)	8 (22%)	7 (19%)	0	3
33	B1	48/54 (89%)	35 (73%)	9 (19%)	4 (8%)	1	20
33	D1	48/54 (89%)	35 (73%)	9 (19%)	4 (8%)	1	20
34	B3	62/64 (97%)	39 (63%)	17 (27%)	6 (10%)	1	16
34	D3	62/64 (97%)	39 (63%)	18 (29%)	5 (8%)	1	21
35	BV	92/94 (98%)	60 (65%)	22 (24%)	10 (11%)	1	13
35	DV	92/94 (98%)	59 (64%)	23 (25%)	10 (11%)	1	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	B2	44/46 (96%)	25 (57%)	16 (36%)	3 (7%)	2	27
36	D2	44/46 (96%)	24 (54%)	16 (36%)	4 (9%)	1	18
37	BL	141/144 (98%)	78 (55%)	44 (31%)	19 (14%)	0	8
37	DL	141/144 (98%)	78 (55%)	42 (30%)	21 (15%)	0	6
38	BM	134/136 (98%)	90 (67%)	28 (21%)	16 (12%)	1	11
38	DM	134/136 (98%)	91 (68%)	26 (19%)	17 (13%)	0	10
39	BX	61/63 (97%)	35 (57%)	22 (36%)	4 (7%)	2	28
39	DX	61/63 (97%)	35 (57%)	22 (36%)	4 (7%)	2	28
40	BH	147/149 (99%)	74 (50%)	42 (29%)	31 (21%)	0	2
40	DH	147/149 (99%)	86 (58%)	38 (26%)	23 (16%)	0	5
41	BJ	140/142 (99%)	88 (63%)	33 (24%)	19 (14%)	0	8
41	DJ	140/142 (99%)	88 (63%)	32 (23%)	20 (14%)	0	7
42	BN	118/127 (93%)	74 (63%)	31 (26%)	13 (11%)	1	13
42	DN	118/127 (93%)	74 (63%)	32 (27%)	12 (10%)	1	14
43	BO	114/117 (97%)	79 (69%)	26 (23%)	9 (8%)	1	22
43	DO	114/117 (97%)	79 (69%)	25 (22%)	10 (9%)	1	19
44	BQ	115/117 (98%)	76 (66%)	32 (28%)	7 (6%)	2	30
44	DQ	115/117 (98%)	75 (65%)	33 (29%)	7 (6%)	2	30
45	BS	108/110 (98%)	67 (62%)	28 (26%)	13 (12%)	1	11
45	DS	108/110 (98%)	67 (62%)	28 (26%)	13 (12%)	1	11
46	BU	100/103 (97%)	50 (50%)	35 (35%)	15 (15%)	0	6
46	DU	100/103 (97%)	54 (54%)	31 (31%)	15 (15%)	0	6
47	BF	176/178 (99%)	102 (58%)	48 (27%)	26 (15%)	0	6
47	DF	176/178 (99%)	102 (58%)	48 (27%)	26 (15%)	0	6
48	BG	174/176 (99%)	111 (64%)	40 (23%)	23 (13%)	0	9
48	DG	174/176 (99%)	110 (63%)	40 (23%)	24 (14%)	0	8
49	BR	101/103 (98%)	59 (58%)	31 (31%)	11 (11%)	1	13
49	DR	101/103 (98%)	59 (58%)	31 (31%)	11 (11%)	1	13
50	BT	91/100 (91%)	49 (54%)	25 (28%)	17 (19%)	0	3
50	DT	91/100 (91%)	47 (52%)	27 (30%)	17 (19%)	0	3
51	BZ	75/78 (96%)	50 (67%)	17 (23%)	8 (11%)	1	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	DZ	75/78 (96%)	48 (64%)	19 (25%)	8 (11%)	1	13
52	BW	77/84 (92%)	26 (34%)	26 (34%)	25 (32%)	0	0
52	DW	77/84 (92%)	26 (34%)	25 (32%)	26 (34%)	0	0
All	All	11241/11914 (94%)	7227 (64%)	2767 (25%)	1247 (11%)	1	13

5 of 1247 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AC	11	LEU
2	AC	14	VAL
2	AC	25	THR
2	AC	54	ILE
2	AC	83	VAL

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	12
2	CC	170/189 (90%)	139 (82%)	31 (18%)	2	14
3	AD	172/172 (100%)	153 (89%)	19 (11%)	9	43
3	CD	172/172 (100%)	154 (90%)	18 (10%)	10	46
4	AE	113/125 (90%)	90 (80%)	23 (20%)	2	10
4	CE	113/125 (90%)	91 (80%)	22 (20%)	2	12
5	AF	87/116 (75%)	75 (86%)	12 (14%)	5	29
5	CF	87/116 (75%)	74 (85%)	13 (15%)	4	26
6	AG	123/146 (84%)	104 (85%)	19 (15%)	4	24
6	CG	125/146 (86%)	102 (82%)	23 (18%)	2	14
7	AH	104/104 (100%)	96 (92%)	8 (8%)	18	64
7	CH	104/104 (100%)	97 (93%)	7 (7%)	23	70
8	AI	105/106 (99%)	88 (84%)	17 (16%)	3	21
8	CI	105/106 (99%)	77 (73%)	28 (27%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	AJ	86/90 (96%)	74 (86%)	12 (14%)	5	28
9	CJ	86/90 (96%)	75 (87%)	11 (13%)	6	33
10	AK	90/98 (92%)	77 (86%)	13 (14%)	5	27
10	CK	90/98 (92%)	76 (84%)	14 (16%)	4	23
11	AL	103/103 (100%)	84 (82%)	19 (18%)	2	14
11	CL	103/103 (100%)	84 (82%)	19 (18%)	2	14
12	AM	92/95 (97%)	79 (86%)	13 (14%)	5	28
12	CM	91/95 (96%)	70 (77%)	21 (23%)	1	7
13	AP	65/65 (100%)	56 (86%)	9 (14%)	5	29
13	CP	65/65 (100%)	56 (86%)	9 (14%)	5	29
14	AQ	74/77 (96%)	65 (88%)	9 (12%)	7	36
14	CQ	75/77 (97%)	66 (88%)	9 (12%)	7	37
15	AR	48/64 (75%)	42 (88%)	6 (12%)	7	35
15	CR	48/64 (75%)	42 (88%)	6 (12%)	7	35
16	AS	70/78 (90%)	48 (69%)	22 (31%)	0	3
16	CS	71/78 (91%)	53 (75%)	18 (25%)	1	5
17	AT	65/65 (100%)	56 (86%)	9 (14%)	5	29
17	CT	65/65 (100%)	56 (86%)	9 (14%)	5	29
18	AB	180/198 (91%)	149 (83%)	31 (17%)	3	18
18	CB	180/198 (91%)	141 (78%)	39 (22%)	1	9
19	AU	44/60 (73%)	33 (75%)	11 (25%)	1	6
19	CU	44/60 (73%)	33 (75%)	11 (25%)	1	6
20	AO	76/77 (99%)	69 (91%)	7 (9%)	13	53
20	CO	76/77 (99%)	64 (84%)	12 (16%)	4	23
21	AN	79/83 (95%)	69 (87%)	10 (13%)	6	33
21	CN	79/83 (95%)	64 (81%)	15 (19%)	2	13
24	BI	109/109 (100%)	108 (99%)	1 (1%)	87	97
24	DI	109/109 (100%)	103 (94%)	6 (6%)	30	77
25	BC	216/217 (100%)	184 (85%)	32 (15%)	4	26
25	DC	216/217 (100%)	184 (85%)	32 (15%)	4	26
26	BD	164/164 (100%)	136 (83%)	28 (17%)	3	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	DD	164/164 (100%)	136 (83%)	28 (17%)	3	18
27	BK	102/104 (98%)	74 (72%)	28 (28%)	0	4
27	DK	102/104 (98%)	73 (72%)	29 (28%)	0	4
28	BP	99/99 (100%)	83 (84%)	16 (16%)	3	21
28	DP	99/99 (100%)	83 (84%)	16 (16%)	3	21
29	BE	165/165 (100%)	146 (88%)	19 (12%)	8	39
29	DE	165/165 (100%)	145 (88%)	20 (12%)	7	36
30	BY	48/48 (100%)	38 (79%)	10 (21%)	2	10
30	DY	48/48 (100%)	37 (77%)	11 (23%)	1	7
31	B0	47/47 (100%)	38 (81%)	9 (19%)	2	13
31	D0	47/47 (100%)	38 (81%)	9 (19%)	2	13
32	B4	34/34 (100%)	31 (91%)	3 (9%)	14	57
32	D4	34/34 (100%)	31 (91%)	3 (9%)	14	57
33	B1	45/48 (94%)	35 (78%)	10 (22%)	1	8
33	D1	45/48 (94%)	35 (78%)	10 (22%)	1	8
34	B3	51/51 (100%)	48 (94%)	3 (6%)	28	75
34	D3	51/51 (100%)	48 (94%)	3 (6%)	28	75
35	BV	78/78 (100%)	65 (83%)	13 (17%)	3	19
35	DV	78/78 (100%)	65 (83%)	13 (17%)	3	19
36	B2	38/38 (100%)	28 (74%)	10 (26%)	1	5
36	D2	38/38 (100%)	28 (74%)	10 (26%)	1	5
37	BL	102/103 (99%)	85 (83%)	17 (17%)	3	19
37	DL	102/103 (99%)	85 (83%)	17 (17%)	3	19
38	BM	109/109 (100%)	93 (85%)	16 (15%)	4	26
38	DM	109/109 (100%)	93 (85%)	16 (15%)	4	26
39	BX	55/55 (100%)	43 (78%)	12 (22%)	1	8
39	DX	55/55 (100%)	43 (78%)	12 (22%)	1	8
40	BH	114/114 (100%)	83 (73%)	31 (27%)	0	4
40	DH	114/114 (100%)	87 (76%)	27 (24%)	1	7
41	BJ	116/116 (100%)	100 (86%)	16 (14%)	5	29
41	DJ	116/116 (100%)	100 (86%)	16 (14%)	5	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	BN	100/103 (97%)	86 (86%)	14 (14%)	5	28
42	DN	100/103 (97%)	85 (85%)	15 (15%)	4	26
43	BO	86/87 (99%)	68 (79%)	18 (21%)	1	10
43	DO	86/87 (99%)	67 (78%)	19 (22%)	1	8
44	BQ	89/89 (100%)	77 (86%)	12 (14%)	6	30
44	DQ	89/89 (100%)	77 (86%)	12 (14%)	6	30
45	BS	93/93 (100%)	85 (91%)	8 (9%)	15	58
45	DS	93/93 (100%)	83 (89%)	10 (11%)	9	44
46	BU	83/84 (99%)	68 (82%)	15 (18%)	2	15
46	DU	83/84 (99%)	68 (82%)	15 (18%)	2	15
47	BF	149/149 (100%)	111 (74%)	38 (26%)	1	5
47	DF	149/149 (100%)	112 (75%)	37 (25%)	1	6
48	BG	137/137 (100%)	114 (83%)	23 (17%)	3	19
48	DG	137/137 (100%)	113 (82%)	24 (18%)	3	17
49	BR	84/84 (100%)	71 (84%)	13 (16%)	4	24
49	DR	84/84 (100%)	72 (86%)	12 (14%)	5	28
50	BT	80/84 (95%)	66 (82%)	14 (18%)	3	17
50	DT	80/84 (95%)	66 (82%)	14 (18%)	3	17
51	BZ	67/68 (98%)	57 (85%)	10 (15%)	4	26
51	DZ	67/68 (98%)	56 (84%)	11 (16%)	3	20
52	BW	59/62 (95%)	44 (75%)	15 (25%)	1	5
52	DW	59/62 (95%)	44 (75%)	15 (25%)	1	5
All	All	9333/9700 (96%)	7780 (83%)	1553 (17%)	3	19

5 of 1553 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
48	BG	174	LYS
15	CR	38	ILE
46	DU	78	LYS
50	BT	25	GLU
4	CE	115	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 349 such sidechains are listed below:

Mol	Chain	Res	Type
48	BG	127	GLN
10	CK	21	HIS
46	DU	26	ASN
49	BR	86	GLN
3	CD	70	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1529/1542 (99%)	285 (18%)	20 (1%)
1	CA	1529/1542 (99%)	255 (16%)	20 (1%)
22	BA	116/120 (96%)	21 (18%)	1 (0%)
22	DA	116/120 (96%)	20 (17%)	1 (0%)
23	BB	2837/2904 (97%)	444 (15%)	16 (0%)
23	DB	2838/2904 (97%)	437 (15%)	20 (0%)
All	All	8965/9132 (98%)	1462 (16%)	78 (0%)

5 of 1462 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	14	U
1	AA	15	G
1	AA	32	A
1	AA	39	G

5 of 78 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	BB	2867	G
1	CA	372	C
23	DB	2336	A
23	BB	2894	G
1	CA	243	A

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 348 ligands modelled in this entry, 342 are monoatomic - leaving 6 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	1.92	13 (28%)	67,67,67	1.16	7 (10%)
55	SCM	AA	1662	-	25,25,25	1.80	9 (36%)	39,39,39	2.28	5 (12%)
53	NMY	BB	3001	-	45,45,45	1.84	13 (28%)	67,67,67	1.21	7 (10%)
53	NMY	CA	1601	-	45,45,45	1.83	13 (28%)	67,67,67	1.17	6 (8%)
55	SCM	CA	1661	-	25,25,25	1.81	9 (36%)	39,39,39	2.31	6 (15%)
53	NMY	DB	3001	-	45,45,45	1.88	13 (28%)	67,67,67	1.23	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
55	SCM	AA	1662	-	-	0/4/57/57	0/3/3/3
53	NMY	BB	3001	-	-	0/18/94/94	0/4/4/4
53	NMY	CA	1601	-	-	0/18/94/94	0/4/4/4
55	SCM	CA	1661	-	-	0/4/57/57	0/3/3/3
53	NMY	DB	3001	-	-	0/18/94/94	0/4/4/4

The worst 5 of 70 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	CA	1601	NMY	O22-C18	4.70	1.53	1.41
53	AA	1601	NMY	O22-C18	4.63	1.53	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	BB	3001	NMY	O22-C18	4.61	1.53	1.41
53	DB	3001	NMY	O22-C18	4.60	1.53	1.41
53	AA	1601	NMY	C3-C2	4.45	1.59	1.53

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	CA	1661	SCM	O5-C5-O1B	-8.92	103.08	111.54
55	AA	1662	SCM	O5-C5-O1B	-8.67	103.32	111.54
55	AA	1662	SCM	C1M-N10-C10	-7.66	107.61	113.65
55	CA	1661	SCM	C1M-N10-C10	-7.61	107.64	113.65
53	DB	3001	NMY	O11-C13-O16	4.38	115.82	111.57

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%)	-0.70	10 (0%) 84 56	16, 81, 159, 180	0
1	CA	1530/1542 (99%)	-0.64	2 (0%) 93 84	9, 57, 133, 180	0
2	AC	206/232 (88%)	0.72	13 (6%) 19 8	9, 76, 136, 180	0
2	CC	206/232 (88%)	0.47	6 (2%) 49 23	7, 75, 127, 180	0
3	AD	205/205 (100%)	0.94	28 (13%) 4 3	24, 92, 157, 180	0
3	CD	205/205 (100%)	0.76	18 (8%) 10 6	10, 64, 139, 180	0
4	AE	150/166 (90%)	0.66	13 (8%) 10 6	11, 74, 139, 176	0
4	CE	150/166 (90%)	0.94	20 (13%) 4 3	5, 61, 132, 180	0
5	AF	100/135 (74%)	1.10	16 (16%) 3 2	11, 86, 144, 172	0
5	CF	100/135 (74%)	0.95	13 (13%) 4 3	7, 83, 173, 180	0
6	AG	150/178 (84%)	0.40	9 (6%) 21 9	23, 104, 153, 180	0
6	CG	152/178 (85%)	0.34	4 (2%) 53 24	27, 90, 147, 180	0
7	AH	129/129 (100%)	1.05	25 (19%) 2 2	13, 88, 155, 180	0
7	CH	129/129 (100%)	0.66	7 (5%) 25 10	5, 61, 127, 180	0
8	AI	127/129 (98%)	0.49	12 (9%) 9 5	36, 91, 150, 180	0
8	CI	127/129 (98%)	0.46	4 (3%) 47 22	20, 92, 148, 180	0
9	AJ	98/103 (95%)	0.61	3 (3%) 47 22	22, 94, 151, 180	0
9	CJ	98/103 (95%)	0.74	7 (7%) 16 7	17, 89, 156, 180	0
10	AK	117/128 (91%)	0.34	2 (1%) 67 34	14, 67, 125, 180	0
10	CK	117/128 (91%)	0.36	4 (3%) 43 19	5, 56, 125, 178	0
11	AL	123/123 (100%)	0.59	8 (6%) 18 8	19, 80, 133, 180	0
11	CL	123/123 (100%)	0.35	4 (3%) 44 20	7, 51, 135, 180	0
12	AM	114/117 (97%)	1.02	22 (19%) 2 2	56, 120, 166, 180	0
12	CM	113/117 (96%)	0.90	18 (15%) 3 2	38, 109, 165, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AP	82/82 (100%)	1.90	23 (28%) 1 1	38, 91, 152, 180	0
13	CP	80/82 (97%)	0.72	8 (10%) 8 5	6, 63, 141, 180	0
14	AQ	80/83 (96%)	0.97	13 (16%) 2 2	37, 99, 151, 180	0
14	CQ	81/83 (97%)	0.70	6 (7%) 14 7	17, 71, 129, 180	0
15	AR	55/74 (74%)	0.62	2 (3%) 41 18	16, 76, 149, 180	0
15	CR	55/74 (74%)	0.56	4 (7%) 15 7	21, 66, 126, 180	0
16	AS	79/91 (86%)	1.54	27 (34%) 1 1	55, 121, 180, 180	0
16	CS	80/91 (87%)	1.39	23 (28%) 1 1	70, 109, 174, 180	0
17	AT	85/86 (98%)	0.23	2 (2%) 56 26	49, 106, 179, 180	0
17	CT	85/86 (98%)	0.21	2 (2%) 56 26	19, 65, 143, 159	0
18	AB	218/240 (90%)	0.43	10 (4%) 31 14	22, 94, 153, 180	0
18	CB	218/240 (90%)	0.66	18 (8%) 11 6	19, 102, 160, 180	0
19	AU	51/70 (72%)	0.58	3 (5%) 22 9	29, 101, 151, 180	0
19	CU	51/70 (72%)	0.77	6 (11%) 5 4	24, 113, 155, 180	0
20	AO	88/89 (98%)	0.62	4 (4%) 32 14	18, 83, 137, 179	0
20	CO	88/89 (98%)	0.31	2 (2%) 57 27	7, 60, 118, 161	0
21	AN	96/100 (96%)	0.78	8 (8%) 11 6	13, 98, 151, 180	0
21	CN	96/100 (96%)	0.99	19 (19%) 2 2	12, 81, 150, 180	0
22	BA	117/120 (97%)	-0.23	3 (2%) 53 24	35, 74, 117, 167	0
22	DA	117/120 (97%)	-0.47	1 (0%) 81 51	36, 86, 127, 180	0
23	BB	2841/2904 (97%)	-0.40	28 (0%) 79 47	6, 54, 148, 180	0
23	DB	2841/2904 (97%)	-0.42	16 (0%) 86 59	5, 48, 146, 180	0
24	BI	141/141 (100%)	2.65	81 (57%) 0 1	95, 172, 180, 180	0
24	DI	141/141 (100%)	1.88	51 (36%) 1 1	91, 179, 180, 180	0
25	BC	271/272 (99%)	0.88	35 (12%) 4 3	5, 50, 103, 180	0
25	DC	271/272 (99%)	0.68	18 (6%) 18 8	5, 40, 100, 146	0
26	BD	209/209 (100%)	0.34	8 (3%) 38 17	7, 68, 146, 180	0
26	DD	209/209 (100%)	0.93	28 (13%) 4 3	5, 49, 129, 180	0
27	BK	121/123 (98%)	0.88	11 (9%) 9 5	7, 69, 139, 180	0
27	DK	121/123 (98%)	0.87	10 (8%) 11 6	5, 41, 118, 180	0
28	BP	114/114 (100%)	0.83	9 (7%) 13 7	26, 85, 142, 175	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
28	DP	114/114 (100%)	0.65	5 (4%)	33 14	5, 49, 103, 145	0
29	BE	201/201 (100%)	1.05	39 (19%)	2 2	5, 63, 143, 180	0
29	DE	201/201 (100%)	0.57	15 (7%)	14 7	5, 70, 144, 180	0
30	BY	58/58 (100%)	0.62	5 (8%)	11 6	20, 62, 140, 180	0
30	DY	58/58 (100%)	0.22	0	100 100	5, 66, 116, 142	0
31	B0	56/56 (100%)	0.34	2 (3%)	41 18	20, 80, 163, 180	0
31	D0	56/56 (100%)	0.32	3 (5%)	25 10	12, 58, 116, 165	0
32	B4	38/38 (100%)	0.48	1 (2%)	53 24	5, 75, 120, 137	0
32	D4	38/38 (100%)	0.13	0	100 100	7, 60, 114, 135	0
33	B1	50/54 (92%)	1.22	6 (12%)	5 4	15, 70, 135, 180	0
33	D1	50/54 (92%)	0.69	4 (8%)	12 7	20, 69, 142, 157	0
34	B3	64/64 (100%)	0.65	4 (6%)	19 8	13, 50, 102, 148	0
34	D3	64/64 (100%)	0.55	2 (3%)	47 22	5, 42, 88, 133	0
35	BV	94/94 (100%)	0.72	6 (6%)	19 8	21, 89, 143, 180	0
35	DV	94/94 (100%)	0.55	9 (9%)	8 5	9, 96, 151, 169	0
36	B2	46/46 (100%)	0.58	3 (6%)	18 8	5, 43, 120, 143	0
36	D2	46/46 (100%)	0.42	1 (2%)	59 28	11, 43, 103, 159	0
37	BL	143/144 (99%)	0.48	7 (4%)	28 12	8, 67, 133, 172	0
37	DL	143/144 (99%)	0.80	21 (14%)	3 3	5, 56, 119, 164	0
38	BM	136/136 (100%)	0.81	15 (11%)	6 4	9, 59, 117, 170	0
38	DM	136/136 (100%)	0.70	13 (9%)	8 5	7, 60, 116, 137	0
39	BX	63/63 (100%)	1.23	14 (22%)	1 2	6, 86, 135, 180	0
39	DX	63/63 (100%)	0.74	6 (9%)	8 5	38, 106, 178, 180	0
40	BH	149/149 (100%)	2.55	87 (58%)	0 1	26, 134, 177, 180	0
40	DH	149/149 (100%)	1.30	36 (24%)	1 2	11, 112, 162, 180	0
41	BJ	142/142 (100%)	0.65	11 (7%)	13 7	5, 74, 127, 180	0
41	DJ	142/142 (100%)	0.87	15 (10%)	7 4	5, 59, 125, 180	0
42	BN	120/127 (94%)	0.51	3 (2%)	54 25	20, 65, 126, 180	0
42	DN	120/127 (94%)	0.49	6 (5%)	28 12	5, 43, 103, 180	0
43	BO	116/117 (99%)	1.10	26 (22%)	1 2	12, 77, 140, 180	0
43	DO	116/117 (99%)	0.60	6 (5%)	26 11	32, 85, 152, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BQ	117/117 (100%)	0.11	4 (3%) 43 19	6, 57, 133, 175	0
44	DQ	117/117 (100%)	0.43	4 (3%) 43 19	5, 52, 112, 161	0
45	BS	110/110 (100%)	0.75	7 (6%) 19 8	5, 50, 125, 180	0
45	DS	110/110 (100%)	0.97	13 (11%) 5 4	5, 52, 131, 180	0
46	BU	102/103 (99%)	0.99	16 (15%) 3 2	5, 70, 146, 180	0
46	DU	102/103 (99%)	0.29	0 100 100	22, 97, 158, 180	0
47	BF	178/178 (100%)	1.43	45 (25%) 1 2	52, 123, 180, 180	0
47	DF	178/178 (100%)	1.87	72 (40%) 1 1	33, 110, 176, 180	0
48	BG	176/176 (100%)	0.84	19 (10%) 6 4	26, 104, 165, 180	0
48	DG	176/176 (100%)	1.05	34 (19%) 2 2	26, 98, 169, 180	0
49	BR	103/103 (100%)	0.70	9 (8%) 10 6	11, 76, 142, 180	0
49	DR	103/103 (100%)	0.75	8 (7%) 13 7	13, 79, 144, 180	0
50	BT	93/100 (93%)	1.04	9 (9%) 8 5	16, 75, 150, 180	0
50	DT	93/100 (93%)	1.18	24 (25%) 1 2	13, 79, 154, 180	0
51	BZ	77/78 (98%)	0.95	10 (12%) 4 3	5, 53, 122, 137	0
51	DZ	77/78 (98%)	0.45	5 (6%) 18 8	5, 47, 124, 144	0
52	BW	79/84 (94%)	1.09	11 (13%) 4 3	8, 74, 121, 180	0
52	DW	79/84 (94%)	0.60	6 (7%) 14 7	9, 77, 144, 164	0
All	All	20417/21046 (97%)	0.24	1414 (6%) 17 7	5, 69, 155, 180	0

The worst 5 of 1414 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	AP	82	ALA	17.2
13	AP	81	ALA	12.0
23	BB	140	C	11.6
24	BI	49	GLU	10.5
13	AP	80	LYS	9.9

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
54	MG	CA	1651	1/1	0.28	36.33	161,161,161,161	0
54	MG	DB	3059	1/1	0.64	26.17	180,180,180,180	0
54	MG	AA	1660	1/1	0.38	25.37	148,148,148,148	0
53	NMY	BB	3001	42/42	0.86	21.80	89,89,89,89	42
54	MG	BB	3034	1/1	0.31	20.26	130,130,130,130	0
54	MG	AA	1624	1/1	0.34	13.53	13,13,13,13	1
53	NMY	DB	3001	42/42	0.51	13.50	68,68,68,68	42
54	MG	AA	1606	1/1	0.19	11.37	56,56,56,56	0
54	MG	CA	1650	1/1	0.37	10.98	180,180,180,180	0
54	MG	DB	3038	1/1	0.20	10.01	10,10,10,10	0
54	MG	BB	3088	1/1	0.25	7.58	87,87,87,87	0
54	MG	DB	3090	1/1	0.26	7.26	99,99,99,99	0
54	MG	AA	1633	1/1	0.13	6.00	65,65,65,65	0
54	MG	AA	1625	1/1	0.16	5.68	102,102,102,102	0
54	MG	BB	3106	1/1	0.22	5.35	11,11,11,11	0
54	MG	CA	1614	1/1	0.25	5.30	139,139,139,139	0
54	MG	AA	1658	1/1	0.22	4.88	120,120,120,120	0
54	MG	AA	1657	1/1	0.19	4.25	95,95,95,95	0
54	MG	BB	3087	1/1	0.22	4.10	23,23,23,23	0
54	MG	CA	1618	1/1	0.16	4.00	104,104,104,104	0
54	MG	AA	1626	1/1	0.15	3.62	87,87,87,87	1
54	MG	AA	1648	1/1	0.32	3.36	110,110,110,110	0
54	MG	DB	3112	1/1	0.23	3.22	87,87,87,87	0
54	MG	BB	3029	1/1	0.22	3.09	21,21,21,21	0
54	MG	AA	1638	1/1	0.22	2.86	126,126,126,126	0
54	MG	BB	3018	1/1	0.18	2.75	31,31,31,31	0
54	MG	AA	1607	1/1	0.14	2.69	93,93,93,93	0
54	MG	BB	3040	1/1	0.22	2.68	44,44,44,44	0
53	NMY	CA	1601	42/42	0.21	2.52	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	CA	1613	1/1	0.21	2.46	108,108,108,108	0
54	MG	CA	1658	1/1	0.15	2.41	50,50,50,50	0
54	MG	BB	3023	1/1	0.22	2.12	12,12,12,12	0
54	MG	BB	3037	1/1	0.21	1.85	35,35,35,35	0
54	MG	AA	1636	1/1	0.16	1.55	121,121,121,121	0
54	MG	AA	1618	1/1	0.17	1.50	160,160,160,160	0
54	MG	AA	1661	1/1	0.14	1.46	62,62,62,62	0
54	MG	CA	1607	1/1	0.15	1.36	129,129,129,129	0
53	NMY	AA	1601	42/42	0.24	1.31	75,75,75,75	0
54	MG	DB	3106	1/1	0.17	1.26	53,53,53,53	0
54	MG	BB	3008	1/1	0.21	1.21	81,81,81,81	0
54	MG	AA	1640	1/1	0.18	1.14	110,110,110,110	0
54	MG	CA	1652	1/1	0.11	1.00	128,128,128,128	0
54	MG	AA	1641	1/1	0.16	0.96	88,88,88,88	0
54	MG	AA	1634	1/1	0.14	0.95	88,88,88,88	0
54	MG	BB	3012	1/1	0.20	0.91	33,33,33,33	0
54	MG	BB	3105	1/1	0.17	0.90	18,18,18,18	0
55	SCM	CA	1661	23/23	0.16	0.84	37,37,37,37	0
54	MG	BB	3078	1/1	0.17	0.70	47,47,47,47	0
54	MG	CA	1631	1/1	0.16	0.62	43,43,43,43	0
54	MG	CA	1639	1/1	0.11	0.54	108,108,108,108	0
54	MG	BB	3084	1/1	0.18	0.52	61,61,61,61	0
55	SCM	AA	1662	23/23	0.15	0.52	23,23,23,23	0
54	MG	BB	3026	1/1	0.18	0.49	68,68,68,68	0
54	MG	AA	1647	1/1	0.13	0.45	133,133,133,133	0
54	MG	DB	3102	1/1	0.18	0.39	6,6,6,6	0
54	MG	BB	3043	1/1	0.25	0.37	145,145,145,145	0
54	MG	DB	3075	1/1	0.18	0.30	58,58,58,58	0
54	MG	DB	3013	1/1	0.17	0.26	12,12,12,12	0
54	MG	CA	1634	1/1	0.14	0.23	75,75,75,75	0
54	MG	CA	1640	1/1	0.15	0.17	43,43,43,43	0
54	MG	BB	3076	1/1	0.18	0.06	33,33,33,33	0
54	MG	BB	3041	1/1	0.17	0.06	34,34,34,34	0
54	MG	DB	3093	1/1	0.14	0.04	98,98,98,98	0
54	MG	DB	3098	1/1	0.15	-0.04	41,41,41,41	0
54	MG	BB	3110	1/1	0.14	-0.06	61,61,61,61	0
54	MG	CA	1623	1/1	0.12	-0.12	21,21,21,21	0
54	MG	BB	3101	1/1	0.14	-0.20	157,157,157,157	0
54	MG	CA	1641	1/1	0.14	-0.25	61,61,61,61	0
54	MG	CA	1643	1/1	0.11	-0.30	75,75,75,75	0
54	MG	BB	3111	1/1	0.11	-0.33	90,90,90,90	0
54	MG	DB	3012	1/1	0.17	-0.35	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	AA	1613	1/1	0.11	-0.35	80,80,80,80	0
54	MG	BB	3024	1/1	0.18	-0.40	12,12,12,12	0
54	MG	AA	1623	1/1	0.16	-0.43	157,157,157,157	0
54	MG	DB	3014	1/1	0.14	-0.46	80,80,80,80	0
54	MG	BB	3027	1/1	0.16	-0.48	42,42,42,42	0
54	MG	BB	3019	1/1	0.13	-0.53	44,44,44,44	0
54	MG	DB	3006	1/1	0.17	-0.53	13,13,13,13	0
54	MG	CA	1603	1/1	0.13	-0.57	25,25,25,25	0
54	MG	DB	3008	1/1	0.17	-0.63	41,41,41,41	0
54	MG	DB	3100	1/1	0.15	-0.82	6,6,6,6	0
54	MG	DB	3111	1/1	0.09	-0.83	36,36,36,36	0
54	MG	AA	1604	1/1	0.14	-0.86	43,43,43,43	0
54	MG	BB	3086	1/1	0.15	-0.87	18,18,18,18	0
54	MG	CA	1622	1/1	0.13	-0.93	44,44,44,44	0
54	MG	DB	3091	1/1	0.06	-0.94	55,55,55,55	0
54	MG	CA	1647	1/1	0.07	-1.00	153,153,153,153	0
54	MG	AA	1616	1/1	0.08	-1.01	113,113,113,113	0
54	MG	BB	3052	1/1	0.14	-1.01	67,67,67,67	0
54	MG	DB	3015	1/1	0.07	-1.03	37,37,37,37	0
54	MG	CA	1654	1/1	0.10	-1.04	82,82,82,82	0
54	MG	AA	1653	1/1	0.09	-1.04	110,110,110,110	0
54	MG	DB	3002	1/1	0.15	-1.06	5,5,5,5	0
54	MG	BB	3100	1/1	0.13	-1.06	34,34,34,34	0
54	MG	DB	3007	1/1	0.16	-1.12	9,9,9,9	0
54	MG	DB	3061	1/1	0.21	-1.13	117,117,117,117	0
54	MG	BB	3054	1/1	0.07	-1.14	46,46,46,46	0
54	MG	DB	3097	1/1	0.15	-1.16	12,12,12,12	0
54	MG	DB	3079	1/1	0.12	-1.17	80,80,80,80	0
54	MG	CA	1642	1/1	0.11	-1.17	49,49,49,49	0
54	MG	BB	3039	1/1	0.09	-1.19	107,107,107,107	0
54	MG	DB	3016	1/1	0.11	-1.20	53,53,53,53	0
54	MG	CA	1630	1/1	0.11	-1.21	81,81,81,81	0
54	MG	DB	3074	1/1	0.14	-1.21	29,29,29,29	0
54	MG	BB	3085	1/1	0.15	-1.22	43,43,43,43	0
54	MG	AA	1612	1/1	0.05	-1.24	70,70,70,70	0
54	MG	CA	1656	1/1	0.10	-1.25	135,135,135,135	0
54	MG	DB	3026	1/1	0.09	-1.30	16,16,16,16	0
54	MG	BB	3108	1/1	0.13	-1.33	36,36,36,36	0
54	MG	DB	3025	1/1	0.12	-1.39	47,47,47,47	0
54	MG	CA	1608	1/1	0.04	-1.40	31,31,31,31	0
54	MG	AA	1614	1/1	0.05	-1.42	66,66,66,66	0
54	MG	CA	1653	1/1	0.09	-1.45	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	CA	1648	1/1	0.06	-1.46	69,69,69,69	0
54	MG	DB	3092	1/1	0.15	-1.46	12,12,12,12	0
54	MG	DB	3101	1/1	0.12	-1.47	20,20,20,20	0
54	MG	CA	1660	1/1	0.09	-1.47	77,77,77,77	0
54	MG	CA	1644	1/1	0.08	-1.53	49,49,49,49	0
54	MG	BB	3006	1/1	0.12	-1.55	9,9,9,9	0
54	MG	AA	1611	1/1	0.04	-1.56	73,73,73,73	0
54	MG	BB	3025	1/1	0.11	-1.56	32,32,32,32	0
54	MG	AA	1619	1/1	0.08	-1.61	48,48,48,48	0
54	MG	AA	1654	1/1	0.08	-1.62	49,49,49,49	0
54	MG	DB	3058	1/1	0.07	-1.62	39,39,39,39	0
54	MG	BB	3099	1/1	0.13	-1.62	23,23,23,23	0
54	MG	AA	1621	1/1	0.08	-1.63	82,82,82,82	0
54	MG	AA	1632	1/1	0.10	-1.63	29,29,29,29	0
54	MG	AA	1629	1/1	0.09	-1.65	55,55,55,55	0
54	MG	AA	1644	1/1	0.10	-1.66	42,42,42,42	0
54	MG	DB	3005	1/1	0.13	-1.68	23,23,23,23	0
54	MG	AA	1620	1/1	0.08	-1.70	132,132,132,132	0
54	MG	DB	3095	1/1	0.05	-1.70	39,39,39,39	0
54	MG	AA	1608	1/1	0.08	-1.71	53,53,53,53	0
54	MG	DB	3018	1/1	0.14	-1.73	5,5,5,5	0
56	ZN	D4	101	1/1	0.06	-1.74	40,40,40,40	0
54	MG	BB	3093	1/1	0.07	-1.74	32,32,32,32	0
54	MG	DB	3096	1/1	0.07	-1.77	115,115,115,115	0
54	MG	AA	1651	1/1	0.08	-1.77	97,97,97,97	0
54	MG	BB	3055	1/1	0.06	-1.80	46,46,46,46	0
54	MG	BB	3002	1/1	0.08	-1.85	19,19,19,19	0
54	MG	DB	3017	1/1	0.12	-1.87	29,29,29,29	0
54	MG	AA	1605	1/1	0.09	-1.92	46,46,46,46	0
54	MG	CA	1646	1/1	0.04	-1.92	52,52,52,52	0
54	MG	CA	1655	1/1	0.07	-1.94	52,52,52,52	0
54	MG	BB	3074	1/1	0.10	-1.94	28,28,28,28	0
54	MG	DB	3110	1/1	0.09	-1.96	17,17,17,17	0
54	MG	DB	3068	1/1	0.12	-1.97	36,36,36,36	0
54	MG	DB	3050	1/1	0.12	-1.98	6,6,6,6	0
54	MG	DB	3051	1/1	0.12	-2.00	67,67,67,67	0
54	MG	BB	3072	1/1	0.08	-2.06	54,54,54,54	0
54	MG	BB	3013	1/1	0.10	-2.06	81,81,81,81	0
54	MG	CA	1611	1/1	0.09	-2.07	5,5,5,5	0
54	MG	BB	3068	1/1	0.11	-2.10	65,65,65,65	0
54	MG	DB	3088	1/1	0.15	-2.13	37,37,37,37	0
56	ZN	B4	101	1/1	0.05	-2.14	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	AA	1635	1/1	0.06	-2.14	86,86,86,86	0
54	MG	BB	3098	1/1	0.09	-2.15	85,85,85,85	0
54	MG	DB	3024	1/1	0.07	-2.16	32,32,32,32	0
54	MG	AA	1646	1/1	0.07	-2.18	89,89,89,89	0
54	MG	BB	3104	1/1	0.12	-2.19	6,6,6,6	0
54	MG	AA	1643	1/1	0.11	-2.19	43,43,43,43	0
54	MG	DB	3031	1/1	0.14	-2.20	21,21,21,21	0
54	MG	BB	3011	1/1	0.10	-2.22	62,62,62,62	0
54	MG	BB	3045	1/1	0.12	-2.31	42,42,42,42	0
54	MG	DB	3099	1/1	0.12	-2.36	9,9,9,9	0
54	MG	DB	3048	1/1	0.15	-2.38	14,14,14,14	0
54	MG	BB	3007	1/1	0.09	-2.40	37,37,37,37	0
54	MG	DB	3046	1/1	0.08	-2.42	104,104,104,104	0
54	MG	DB	3020	1/1	0.11	-2.42	6,6,6,6	0
54	MG	BB	3003	1/1	0.10	-2.43	17,17,17,17	0
54	MG	DB	3023	1/1	0.08	-2.43	7,7,7,7	0
54	MG	BB	3047	1/1	0.11	-2.46	66,66,66,66	0
54	MG	CA	1617	1/1	0.07	-2.48	83,83,83,83	0
54	MG	CA	1649	1/1	0.08	-2.49	92,92,92,92	0
54	MG	AA	1617	1/1	0.10	-2.54	47,47,47,47	0
54	MG	BB	3038	1/1	0.13	-2.56	46,46,46,46	0
54	MG	BB	3021	1/1	0.14	-2.56	30,30,30,30	0
54	MG	AA	1610	1/1	0.11	-2.56	5,5,5,5	0
54	MG	AA	1630	1/1	0.08	-2.57	36,36,36,36	0
54	MG	DB	3004	1/1	0.12	-2.60	41,41,41,41	0
54	MG	DB	3021	1/1	0.12	-2.62	5,5,5,5	0
54	MG	AA	1656	1/1	0.09	-2.65	95,95,95,95	0
54	MG	DB	3034	1/1	0.10	-2.66	5,5,5,5	0
54	MG	DB	3010	1/1	0.11	-2.67	8,8,8,8	0
54	MG	DB	3070	1/1	0.15	-2.67	38,38,38,38	0
54	MG	BB	3083	1/1	0.12	-2.68	5,5,5,5	0
54	MG	BB	3035	1/1	0.06	-2.69	41,41,41,41	0
54	MG	AA	1649	1/1	0.10	-2.69	31,31,31,31	0
54	MG	DB	3084	1/1	0.14	-2.69	109,109,109,109	0
54	MG	DB	3072	1/1	0.09	-2.74	36,36,36,36	0
54	MG	BB	3092	1/1	0.10	-2.77	5,5,5,5	0
54	MG	BB	3066	1/1	0.06	-2.78	10,10,10,10	0
54	MG	BB	3050	1/1	0.07	-2.83	16,16,16,16	0
54	MG	DB	3108	1/1	0.08	-2.86	27,27,27,27	0
54	MG	CA	1610	1/1	0.09	-2.86	103,103,103,103	0
54	MG	AA	1642	1/1	0.05	-2.88	51,51,51,51	0
54	MG	AA	1652	1/1	0.04	-2.90	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DB	3067	1/1	0.09	-2.92	137,137,137,137	0
54	MG	BB	3094	1/1	0.10	-2.93	75,75,75,75	0
54	MG	CA	1645	1/1	0.08	-2.94	70,70,70,70	0
54	MG	CA	1615	1/1	0.04	-2.94	29,29,29,29	0
54	MG	DB	3104	1/1	0.11	-2.96	31,31,31,31	0
54	MG	CA	1626	1/1	0.07	-2.99	117,117,117,117	0
54	MG	DB	3105	1/1	0.09	-3.02	41,41,41,41	0
54	MG	DB	3022	1/1	0.08	-3.07	5,5,5,5	0
54	MG	DB	3073	1/1	0.08	-3.07	62,62,62,62	0
54	MG	CA	1659	1/1	0.06	-3.08	45,45,45,45	0
54	MG	AA	1631	1/1	0.05	-3.08	84,84,84,84	0
54	MG	AA	1645	1/1	0.08	-3.10	67,67,67,67	0
54	MG	CA	1609	1/1	0.07	-3.10	110,110,110,110	0
54	MG	DB	3056	1/1	0.11	-3.11	34,34,34,34	0
54	MG	DB	3009	1/1	0.09	-3.12	49,49,49,49	0
54	MG	BB	3046	1/1	0.10	-3.12	50,50,50,50	0
54	MG	DB	3086	1/1	0.10	-3.20	41,41,41,41	0
54	MG	DB	3087	1/1	0.07	-3.20	11,11,11,11	0
54	MG	BB	3061	1/1	0.12	-3.29	5,5,5,5	0
54	MG	DB	3043	1/1	0.10	-3.38	32,32,32,32	0
54	MG	DB	3065	1/1	0.06	-3.41	20,20,20,20	0
54	MG	CA	1628	1/1	0.09	-3.41	41,41,41,41	0
54	MG	BB	3090	1/1	0.08	-3.42	54,54,54,54	0
54	MG	DB	3030	1/1	0.10	-3.44	81,81,81,81	0
54	MG	BB	3044	1/1	0.11	-3.47	118,118,118,118	0
54	MG	DB	3049	1/1	0.12	-3.49	66,66,66,66	0
54	MG	AA	1650	1/1	0.05	-3.51	105,105,105,105	0
54	MG	BB	3015	1/1	0.03	-3.53	32,32,32,32	0
54	MG	DB	3103	1/1	0.11	-3.55	14,14,14,14	0
54	MG	DB	3036	1/1	0.09	-3.61	85,85,85,85	0
54	MG	DB	3089	1/1	0.09	-3.62	13,13,13,13	0
54	MG	BB	3063	1/1	0.12	-3.63	7,7,7,7	0
54	MG	CA	1627	1/1	0.06	-3.64	40,40,40,40	0
54	MG	AA	1637	1/1	0.04	-3.66	62,62,62,62	0
54	MG	AA	1609	1/1	0.06	-3.68	107,107,107,107	0
54	MG	CA	1629	1/1	0.08	-3.71	57,57,57,57	0
54	MG	CA	1621	1/1	0.11	-3.74	34,34,34,34	0
54	MG	BB	3022	1/1	0.07	-3.77	35,35,35,35	0
54	MG	CA	1636	1/1	0.07	-3.79	37,37,37,37	0
54	MG	BB	3082	1/1	0.11	-3.81	34,34,34,34	0
54	MG	DB	3060	1/1	0.08	-3.83	96,96,96,96	0
54	MG	DB	3033	1/1	0.07	-3.86	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DB	3041	1/1	0.09	-3.86	9,9,9,9	0
54	MG	DB	3019	1/1	0.09	-3.87	25,25,25,25	0
54	MG	DB	3077	1/1	0.13	-3.88	28,28,28,28	0
54	MG	CA	1637	1/1	0.08	-3.90	26,26,26,26	0
54	MG	BB	3014	1/1	0.07	-3.91	11,11,11,11	0
54	MG	DB	3069	1/1	0.07	-3.91	8,8,8,8	0
54	MG	CA	1633	1/1	0.07	-3.96	48,48,48,48	0
54	MG	DB	3057	1/1	0.08	-3.98	11,11,11,11	0
54	MG	BB	3075	1/1	0.09	-3.99	6,6,6,6	0
54	MG	BB	3031	1/1	0.07	-4.08	53,53,53,53	0
54	MG	AA	1639	1/1	0.06	-4.22	65,65,65,65	0
54	MG	DB	3078	1/1	0.09	-4.23	24,24,24,24	0
54	MG	DB	3032	1/1	0.15	-4.25	5,5,5,5	0
54	MG	DB	3082	1/1	0.08	-4.27	9,9,9,9	0
54	MG	AA	1627	1/1	0.11	-4.33	5,5,5,5	1
54	MG	CA	1612	1/1	0.06	-4.35	25,25,25,25	0
54	MG	BB	3062	1/1	0.08	-4.36	38,38,38,38	0
54	MG	BB	3089	1/1	0.07	-4.38	7,7,7,7	0
54	MG	DB	3094	1/1	0.13	-4.40	5,5,5,5	0
54	MG	DB	3109	1/1	0.07	-4.41	33,33,33,33	0
54	MG	CA	1619	1/1	0.09	-4.43	53,53,53,53	0
54	MG	DB	3066	1/1	0.06	-4.47	32,32,32,32	0
54	MG	DB	3071	1/1	0.13	-4.52	93,93,93,93	0
54	MG	BB	3107	1/1	0.08	-4.56	30,30,30,30	0
54	MG	DB	3011	1/1	0.08	-4.64	9,9,9,9	0
54	MG	AA	1655	1/1	0.04	-4.65	73,73,73,73	0
54	MG	CA	1635	1/1	0.07	-4.68	64,64,64,64	0
54	MG	DB	3052	1/1	0.11	-4.75	40,40,40,40	0
54	MG	BB	3091	1/1	0.05	-4.79	105,105,105,105	0
54	MG	BB	3071	1/1	0.10	-4.81	33,33,33,33	0
54	MG	BB	3030	1/1	0.10	-4.84	16,16,16,16	0
54	MG	CA	1625	1/1	0.06	-4.87	36,36,36,36	0
54	MG	DB	3080	1/1	0.09	-4.88	46,46,46,46	0
54	MG	BB	3109	1/1	0.09	-4.94	19,19,19,19	0
54	MG	CA	1657	1/1	0.06	-4.95	14,14,14,14	0
54	MG	BB	3016	1/1	0.08	-4.95	31,31,31,31	0
54	MG	DB	3085	1/1	0.12	-4.98	12,12,12,12	0
54	MG	DB	3039	1/1	0.10	-4.99	19,19,19,19	0
54	MG	DB	3042	1/1	0.08	-5.01	17,17,17,17	0
54	MG	BB	3070	1/1	0.10	-5.08	9,9,9,9	0
54	MG	AA	1603	1/1	0.08	-5.10	100,100,100,100	0
54	MG	CA	1620	1/1	0.07	-5.11	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BB	3102	1/1	0.11	-5.11	10,10,10,10	0
54	MG	BB	3097	1/1	0.08	-5.15	5,5,5,5	0
54	MG	BB	3096	1/1	0.07	-5.23	5,5,5,5	0
54	MG	BB	3080	1/1	0.10	-5.29	44,44,44,44	0
54	MG	DB	3055	1/1	0.10	-5.29	22,22,22,22	0
54	MG	AA	1622	1/1	0.05	-5.45	24,24,24,24	0
54	MG	DB	3037	1/1	0.10	-5.46	23,23,23,23	0
54	MG	CA	1632	1/1	0.04	-5.57	31,31,31,31	0
54	MG	BB	3095	1/1	0.08	-5.64	36,36,36,36	0
54	MG	CA	1616	1/1	0.08	-5.66	15,15,15,15	0
54	MG	DB	3040	1/1	0.07	-5.66	78,78,78,78	0
54	MG	DB	3083	1/1	0.07	-5.68	37,37,37,37	0
54	MG	CA	1638	1/1	0.08	-5.72	123,123,123,123	0
54	MG	BB	3077	1/1	0.10	-5.74	5,5,5,5	0
54	MG	CA	1604	1/1	0.06	-5.78	66,66,66,66	0
54	MG	DB	3027	1/1	0.11	-5.78	72,72,72,72	0
54	MG	DB	3064	1/1	0.04	-5.82	34,34,34,34	0
54	MG	DB	3062	1/1	0.05	-5.93	75,75,75,75	0
54	MG	BB	3079	1/1	0.07	-5.99	68,68,68,68	0
54	MG	CA	1606	1/1	0.07	-6.01	7,7,7,7	0
54	MG	BB	3032	1/1	0.07	-6.05	38,38,38,38	0
54	MG	DB	3003	1/1	0.08	-6.07	21,21,21,21	0
54	MG	BB	3067	1/1	0.08	-6.11	26,26,26,26	0
54	MG	DB	3047	1/1	0.07	-6.19	27,27,27,27	0
54	MG	AA	1602	1/1	0.05	-6.24	28,28,28,28	0
54	MG	BB	3020	1/1	0.11	-6.32	28,28,28,28	0
54	MG	BB	3004	1/1	0.09	-6.34	31,31,31,31	0
54	MG	DB	3044	1/1	0.07	-6.41	11,11,11,11	0
54	MG	DB	3054	1/1	0.11	-6.43	80,80,80,80	0
54	MG	DB	3045	1/1	0.05	-6.43	32,32,32,32	0
54	MG	BB	3056	1/1	0.14	-6.46	23,23,23,23	0
54	MG	DB	3076	1/1	0.05	-6.54	22,22,22,22	0
54	MG	BB	3010	1/1	0.06	-6.58	123,123,123,123	0
54	MG	DB	3063	1/1	0.04	-6.63	50,50,50,50	0
54	MG	BB	3009	1/1	0.08	-6.81	80,80,80,80	0
54	MG	AA	1628	1/1	0.07	-6.82	53,53,53,53	0
54	MG	DB	3107	1/1	0.07	-7.13	20,20,20,20	0
54	MG	BB	3017	1/1	0.09	-7.19	43,43,43,43	0
54	MG	BB	3059	1/1	0.05	-7.29	13,13,13,13	0
54	MG	BB	3073	1/1	0.08	-7.32	35,35,35,35	0
54	MG	CA	1602	1/1	0.05	-7.32	7,7,7,7	0
54	MG	DB	3035	1/1	0.10	-7.35	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	3033	1/1	0.06	-7.76	25,25,25,25	0
54	MG	BB	3036	1/1	0.07	-7.83	26,26,26,26	0
54	MG	BB	3081	1/1	0.09	-7.84	77,77,77,77	0
54	MG	BB	3048	1/1	0.08	-7.90	145,145,145,145	0
54	MG	BB	3065	1/1	0.09	-8.04	24,24,24,24	0
54	MG	BB	3057	1/1	0.05	-8.06	15,15,15,15	0
54	MG	BB	3051	1/1	0.07	-8.10	34,34,34,34	0
54	MG	BB	3069	1/1	0.07	-8.50	41,41,41,41	0
54	MG	BB	3028	1/1	0.07	-8.69	24,24,24,24	0
54	MG	BB	3005	1/1	0.07	-9.15	29,29,29,29	0
54	MG	DB	3028	1/1	0.10	-9.45	17,17,17,17	0
54	MG	BB	3042	1/1	0.11	-10.09	10,10,10,10	0
54	MG	BB	3060	1/1	0.06	-10.16	5,5,5,5	0
54	MG	BB	3103	1/1	0.12	-10.42	25,25,25,25	0
54	MG	DB	3081	1/1	0.08	-11.41	35,35,35,35	0
54	MG	CA	1624	1/1	0.09	-11.69	21,21,21,21	0
54	MG	BB	3064	1/1	0.09	-11.75	10,10,10,10	0
54	MG	CA	1605	1/1	0.06	-12.25	12,12,12,12	0
54	MG	BB	3053	1/1	0.08	-13.57	30,30,30,30	0
54	MG	DB	3053	1/1	0.07	-14.30	90,90,90,90	0
54	MG	AA	1659	1/1	0.06	-14.88	111,111,111,111	0
54	MG	DB	3029	1/1	0.04	-19.39	30,30,30,30	0
54	MG	BB	3058	1/1	0.12	-21.00	63,63,63,63	0
54	MG	BB	3049	1/1	0.05	-30.51	24,24,24,24	0
54	MG	AA	1615	1/1	0.08	-	123,123,123,123	0

6.5 Other polymers ⓘ

There are no such residues in this entry.