



wwPDB X-ray Structure Validation Summary Report i

Jun 16, 2014 – 07:09 PM BST

PDB ID : 4V7V
Title : Crystal structure of the E. coli ribosome bound to clindamycin.
Authors : Dunkle, J.A.; Xiong, L.; Mankin, A.S.; Cate, J.H.D.
Deposited on : 2010-08-16
Resolution : 3.29 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>

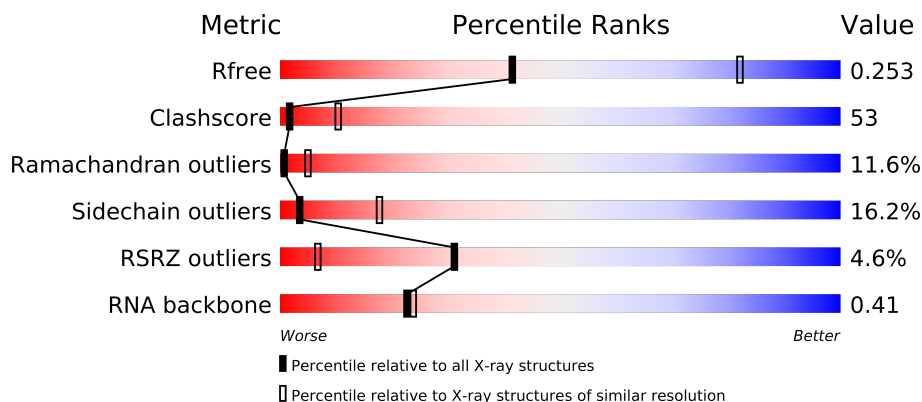
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.29 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	1151 (3.36-3.20)
Clashscore	79885	1464 (3.36-3.20)
Ramachandran outliers	78287	1435 (3.36-3.20)
Sidechain outliers	78261	1433 (3.36-3.20)
RSRZ outliers	66119	1152 (3.36-3.20)
RNA backbone	1838	1033 (3.86-2.70)

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

Mol	Chain	Length	Quality of chain
1	AA	1533	
2	AB	218	
2	CB	218	
3	AC	206	
3	CC	206	
4	AD	205	
4	CD	205	
5	AE	150	
5	CE	150	
6	AF	100	
6	CF	100	
7	AG	151	

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Mol	Chain	Length	Quality of chain
8	AH	129	
8	CH	129	
9	AI	127	
9	CI	127	
10	AJ	98	
10	CJ	98	
11	AK	117	
11	CK	117	
12	AL	123	
12	CL	123	
13	AM	114	
14	AN	100	
14	CN	100	
15	AO	88	
15	CO	88	
16	AP	82	
17	AQ	80	
17	CQ	80	
18	AR	55	
18	CR	55	
19	AS	79	
19	CS	79	
20	AT	85	
20	CT	85	
21	AU	51	
21	CU	51	
22	BA	2903	
22	DA	2903	
23	BB	118	
24	BC	271	
24	DC	271	
25	BD	209	
25	DD	209	
26	BE	201	
26	DE	201	
27	BF	177	
28	BG	176	
28	DG	176	
29	BH	149	
29	DH	149	
30	BI	141	
30	DI	141	

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Mol	Chain	Length	Quality of chain
31	BJ	142	
31	DJ	142	
32	BK	122	
32	DK	122	
33	BL	143	
33	DL	143	
34	BM	136	
34	DM	136	
35	BN	120	
35	DN	120	
36	BO	116	
36	DO	116	
37	BP	114	
37	DP	114	
38	BQ	117	
38	DQ	117	
39	BR	103	
39	DR	103	
40	BS	110	
40	DS	110	
41	BT	93	
41	DT	93	
42	BU	102	
42	DU	102	
43	BV	94	
43	DV	94	
44	BW	79	
44	DW	79	
45	BX	77	
45	DX	77	
46	BY	63	
46	DY	63	
47	BZ	58	
47	DZ	58	
48	B0	56	
48	D0	56	
49	B1	50	
49	D1	50	
50	B2	46	
50	D2	46	
51	B3	64	
51	D3	64	

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Mol	Chain	Length	Quality of chain
52	B4	38	
52	D4	38	
53	CA	1530	
54	CG	150	
55	CM	113	
56	CP	80	
57	DB	117	
58	DF	178	

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

Mol	Type	Chain	Res	Geometry	Electron density
59	MG	AA	1608	-	X
59	MG	AA	1612	-	X
59	MG	AA	1614	-	X
59	MG	AA	1618	-	X
59	MG	AA	1625	-	X
59	MG	AA	1626	-	X
59	MG	AA	1630	-	X
59	MG	AA	1635	-	X
59	MG	BA	3002	-	X
59	MG	BA	3018	-	X
59	MG	BA	3024	-	X
59	MG	BA	3026	-	X
59	MG	BA	3027	-	X
59	MG	BA	3029	-	X
59	MG	BA	3032	-	X
59	MG	BA	3033	-	X
59	MG	BA	3035	-	X
59	MG	BA	3039	-	X
59	MG	BA	3043	-	X
59	MG	BA	3054	-	X
59	MG	BA	3055	-	X
59	MG	BA	3056	-	X
59	MG	BA	3060	-	X
59	MG	BA	3069	-	X
59	MG	BA	3073	-	X
59	MG	BA	3074	-	X
59	MG	BA	3081	-	X
59	MG	BA	3082	-	X
59	MG	BA	3085	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
59	MG	BA	3096	-	X
59	MG	BA	3100	-	X
59	MG	BA	3102	-	X
59	MG	BA	3107	-	X
59	MG	BA	3110	-	X
59	MG	BA	3111	-	X
59	MG	BA	3117	-	X
59	MG	BA	3129	-	X
59	MG	BA	3131	-	X
59	MG	BB	201	-	X
59	MG	CA	1603	-	X
59	MG	CA	1607	-	X
59	MG	CA	1608	-	X
59	MG	CA	1611	-	X
59	MG	CA	1612	-	X
59	MG	CA	1614	-	X
59	MG	CA	1619	-	X
59	MG	CA	1624	-	X
59	MG	CA	1625	-	X
59	MG	CA	1626	-	X
59	MG	CA	1627	-	X
59	MG	CA	1628	-	X
59	MG	CA	1641	-	X
59	MG	DA	3002	-	X
59	MG	DA	3003	-	X
59	MG	DA	3005	-	X
59	MG	DA	3007	-	X
59	MG	DA	3014	-	X
59	MG	DA	3015	-	X
59	MG	DA	3019	-	X
59	MG	DA	3021	-	X
59	MG	DA	3025	-	X
59	MG	DA	3027	-	X
59	MG	DA	3034	-	X
59	MG	DA	3035	-	X
59	MG	DA	3044	-	X
59	MG	DA	3048	-	X
59	MG	DA	3056	-	X
59	MG	DA	3057	-	X
59	MG	DA	3059	-	X
59	MG	DA	3061	-	X
59	MG	DA	3062	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
59	MG	DA	3063	-	X
59	MG	DA	3068	-	X
59	MG	DA	3073	-	X
59	MG	DA	3074	-	X
59	MG	DA	3075	-	X
59	MG	DA	3077	-	X
59	MG	DA	3078	-	X
59	MG	DA	3084	-	X
59	MG	DA	3087	-	X
59	MG	DA	3090	-	X
59	MG	DA	3107	-	X
59	MG	DA	3108	-	X
59	MG	DA	3114	-	X
59	MG	DA	3122	-	X
59	MG	DA	3124	-	X
59	MG	DA	3126	-	X
59	MG	DA	3128	-	X
59	MG	DA	3129	-	X
59	MG	DA	3131	-	X
59	MG	DC	302	-	X
59	MG	DE	301	-	X
59	MG	DJ	201	-	X
60	CLY	BA	3135	-	X

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 284501 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	1533	Total	C	N	O	P	0	0	0
			32895	14671	6036	10655	1533			

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	218	Total	C	N	O	S	0	0	0
			1705	1081	305	312	7			
2	CB	218	Total	C	N	O	S	0	0	0
			1705	1081	305	312	7			

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0	0
			1625	1028	305	289	3			
3	CC	206	Total	C	N	O	S	0	0	0
			1625	1028	305	289	3			

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	150	Total	C	N	O	S	0	0	0
			1106	687	211	202	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	CE	150	Total	C	N	O	S	0	0	0
			1106	687	211	202	6			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	100	Total	C	N	O	S	0	0	0
			818	515	148	149	6			
6	CF	100	Total	C	N	O	S	0	0	0
			818	515	148	149	6			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	151	Total	C	N	O	S	0	0	0
			1182	735	227	216	4			

- Molecule 8 is a protein called 30S ribosomal protein S8.

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

- Molecule 9 is a protein called 30S ribosomal protein S9.

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

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	98	Total	C	N	O	S	0	0	0
			787	493	150	143	1			
10	CJ	98	Total	C	N	O	S	0	0	0
			787	493	150	143	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

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

- Molecule 12 is a protein called 30S ribosomal protein S12.

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

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	114	Total	C	N	O	S	0	0	0
			884	546	178	157	3			

- Molecule 14 is a protein called 30S ribosomal protein S14.

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

- Molecule 15 is a protein called 30S ribosomal protein S15.

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

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	80	Total	C	N	O	S	0	0	0
			649	411	121	114	3			
17	CQ	80	Total	C	N	O	S	0	0	0
			649	411	121	114	3			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AR	55	Total	C	N	O		0	0	0
			456	288	86	82				
18	CR	55	Total	C	N	O		0	0	0
			456	288	86	82				

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	79	Total	C	N	O	S	0	0	0
			638	408	120	108	2			
19	CS	79	Total	C	N	O	S	0	0	0
			638	408	120	108	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AU	51	Total	C	N	O	S	0	0	0
			426	265	86	74	1			
21	CU	51	Total	C	N	O	S	0	0	0
			426	265	86	74	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	BA	2854	Total	C	N	O	P	0	0	0
			61274	27334	11279	19807	2854			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	DA	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	BC	271	Total	C	N	O	S	0	0	0
			2083	1288	423	365	7			
24	DC	271	Total	C	N	O	S	0	0	0
			2083	1288	423	365	7			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BF	177	Total	C	N	O	S	0	0	0
			1411	899	249	257	6			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BK	122	Total	C	N	O	S	0	0	0
			939	587	180	166	6			
32	DK	122	Total	C	N	O	S	0	0	0
			939	587	180	166	6			

- Molecule 33 is a protein called 50S ribosomal protein L15.

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

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

- Molecule 34 is a protein called 50S ribosomal protein L16.

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

- Molecule 35 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BN	120	Total	C	N	O	S	0	0	0
			961	593	196	167	5			
35	DN	120	Total	C	N	O	S	0	0	0
			961	593	196	167	5			

- Molecule 36 is a protein called 50S ribosomal protein L18.

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

- Molecule 37 is a protein called 50S ribosomal protein L19.

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

- Molecule 38 is a protein called 50S ribosomal protein L20.

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BT	93	Total	C	N	O	S	0	0	0
			739	466	139	132	2			
41	DT	93	Total	C	N	O	S	0	0	0
			739	466	139	132	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
42	BU	102	Total	C	N	O	0	0	0
			780	492	146	142			
42	DU	102	Total	C	N	O	0	0	0
			780	492	146	142			

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 49 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	B1	50	Total	C	N	O	0	0	0
			410	263	75	72			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	D1	50	Total	C	N	O	0	0	0
			410	263	75	72			

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

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

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

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

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

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

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

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

- Molecule 54 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	CG	150	Total	C	N	O	S	0	0	0
			1175	730	226	215	4			

- Molecule 55 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	CM	113	Total	C	N	O	S	0	0	0
			877	541	177	156	3			

- Molecule 56 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	CP	80	Total	C	N	O	S	0	0	0
			639	400	126	112	1			

- Molecule 57 is a RNA chain called 5S rRNA.

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

- Molecule 58 is a protein called 50S ribosomal protein L5.

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

- Molecule 59 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

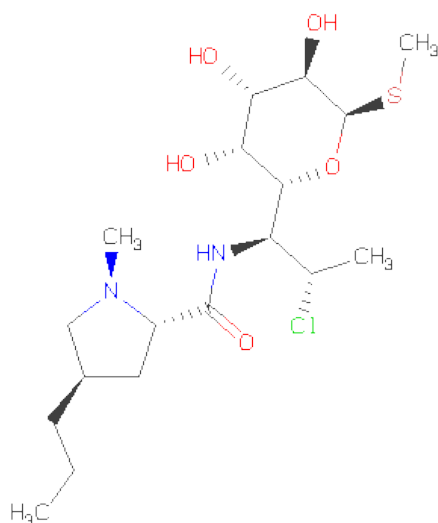
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	BB	4	Total	Mg	0	0
			4	4		
59	DE	1	Total	Mg	0	0
			1	1		
59	BA	134	Total	Mg	0	0
			134	134		
59	CA	42	Total	Mg	0	0
			42	42		
59	DJ	1	Total	Mg	0	0
			1	1		
59	BL	1	Total	Mg	0	0
			1	1		
59	DA	132	Total	Mg	0	0
			132	132		
59	AA	42	Total	Mg	0	0
			42	42		
59	AN	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	DC	2	Total	Mg	0	0
			2	2		
59	DB	1	Total	Mg	0	0
			1	1		

- Molecule 60 is CLINDAMYCIN (three-letter code: CLY) (formula: $C_{18}H_{33}ClN_2O_5S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
60	BA	1	Total	C	Cl	N	O	S	0	0
			27	18	1	2	5	1		

- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 62 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	AA	197	Total	O	0	0
			197	197		
62	AE	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	AL	1	Total 1	O 1	0	0
62	AN	6	Total 6	O 6	0	0
62	AT	2	Total 2	O 2	0	0
62	AU	1	Total 1	O 1	0	0
62	BA	601	Total 601	O 601	0	0
62	BB	20	Total 20	O 20	0	0
62	BC	8	Total 8	O 8	0	0
62	BD	4	Total 4	O 4	0	0
62	BE	1	Total 1	O 1	0	0
62	BL	3	Total 3	O 3	0	0
62	BN	3	Total 3	O 3	0	0
62	BQ	1	Total 1	O 1	0	0
62	BR	1	Total 1	O 1	0	0
62	BT	3	Total 3	O 3	0	0
62	B2	2	Total 2	O 2	0	0
62	B3	2	Total 2	O 2	0	0
62	B4	1	Total 1	O 1	0	0
62	CA	193	Total 193	O 193	0	0
62	CE	4	Total 4	O 4	0	0
62	CI	1	Total 1	O 1	0	0
62	CL	1	Total 1	O 1	0	0

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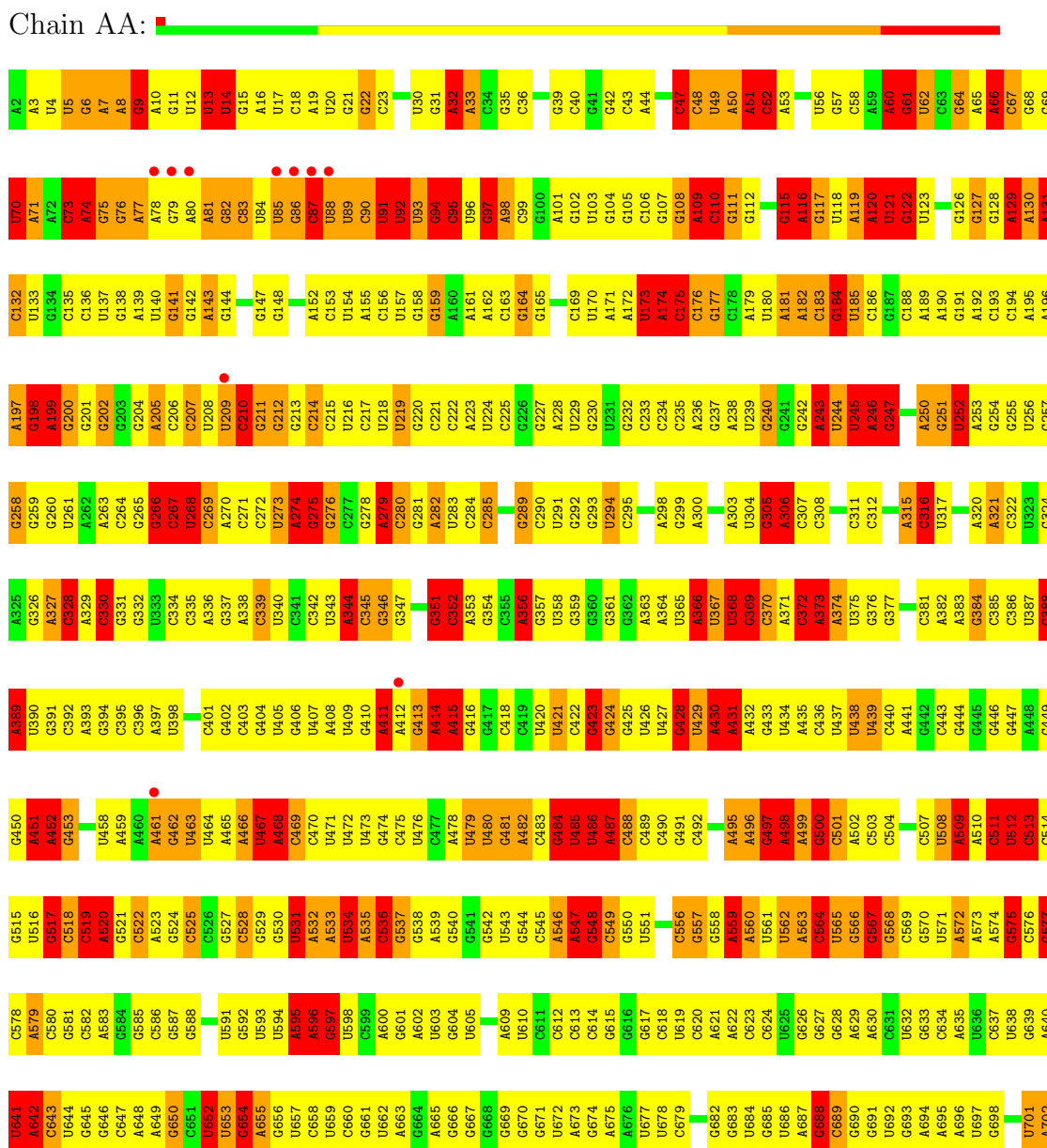
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	CN	3	Total 3	O 3	0	0
62	CT	3	Total 3	O 3	0	0
62	CU	2	Total 2	O 2	0	0
62	DA	599	Total 599	O 599	0	0
62	DB	4	Total 4	O 4	0	0
62	DC	9	Total 9	O 9	0	0
62	DD	2	Total 2	O 2	0	0
62	DE	3	Total 3	O 3	0	0
62	DJ	5	Total 5	O 5	0	0
62	DL	5	Total 5	O 5	0	0
62	DN	3	Total 3	O 3	0	0
62	DT	3	Total 3	O 3	0	0
62	DU	2	Total 2	O 2	0	0
62	DV	1	Total 1	O 1	0	0
62	D2	2	Total 2	O 2	0	0
62	D3	1	Total 1	O 1	0	0
62	D4	4	Total 4	O 4	0	0

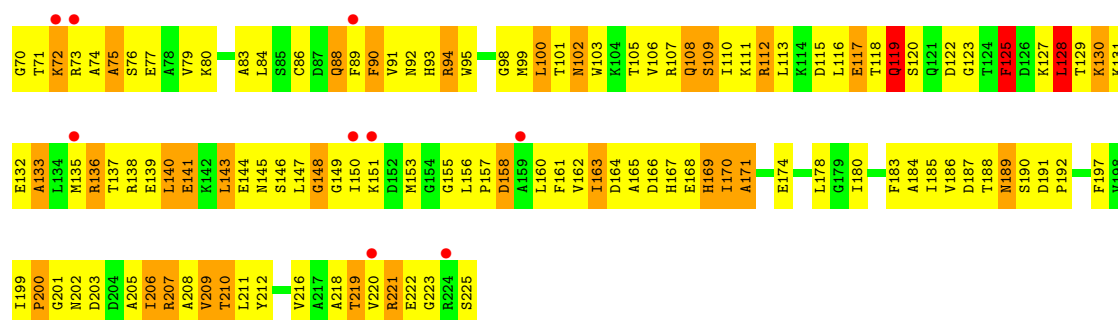
3 Residue-property plots

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

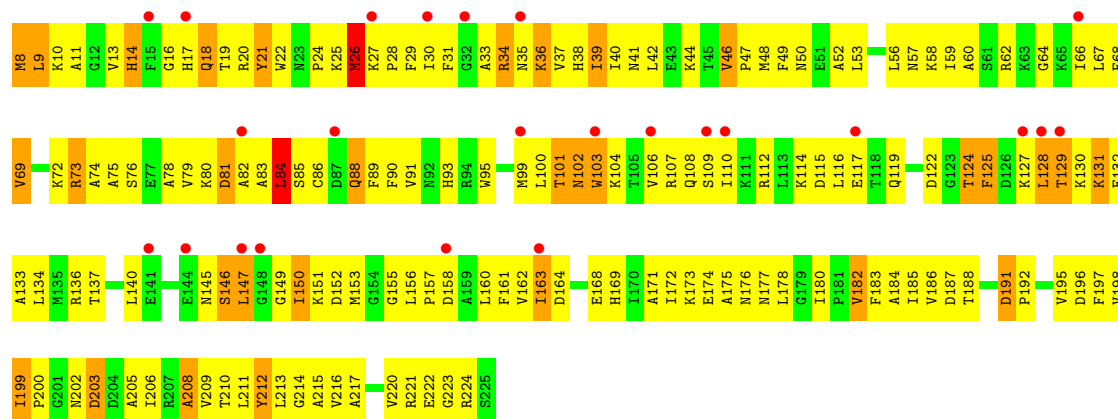






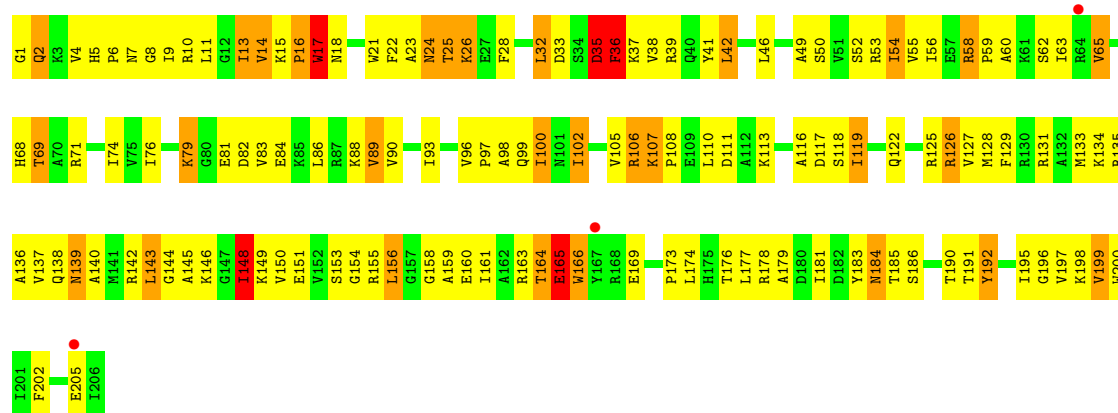
• Molecule 2: 30S ribosomal protein S2

Chain CB:



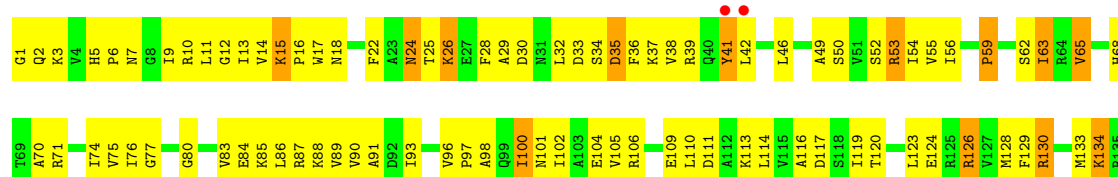
• Molecule 3: 30S ribosomal protein S3

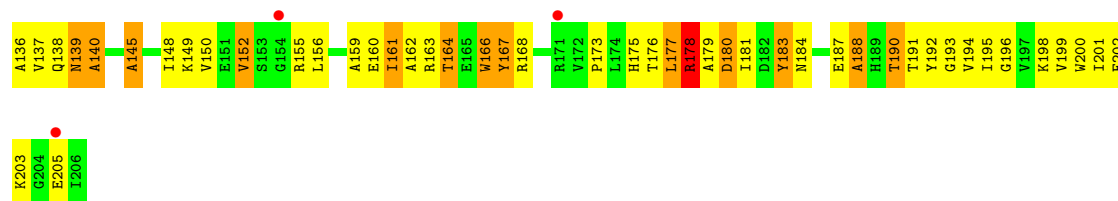
Chain AC:



• Molecule 3: 30S ribosomal protein S3

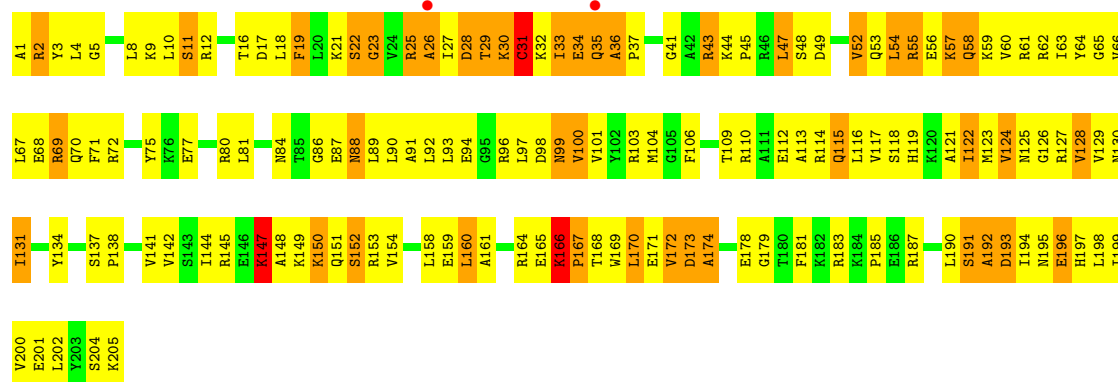
Chain CC:





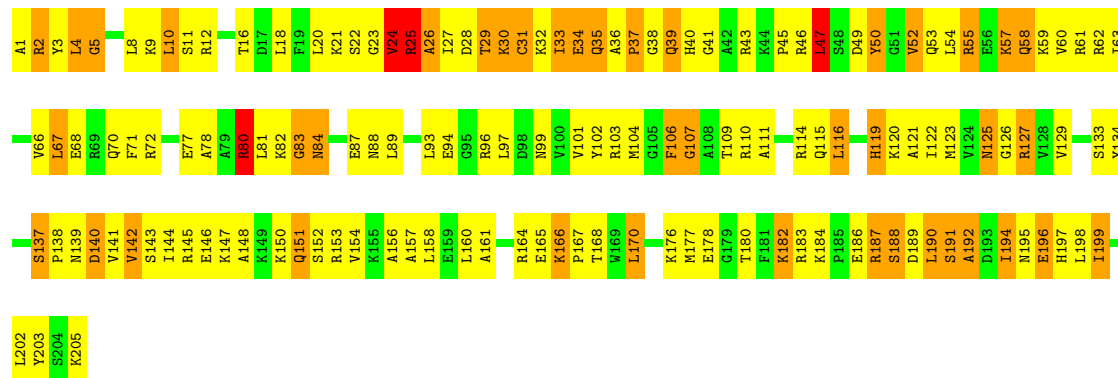
• Molecule 4: 30S ribosomal protein S4

Chain AD:



• Molecule 4: 30S ribosomal protein S4

Chain CD:



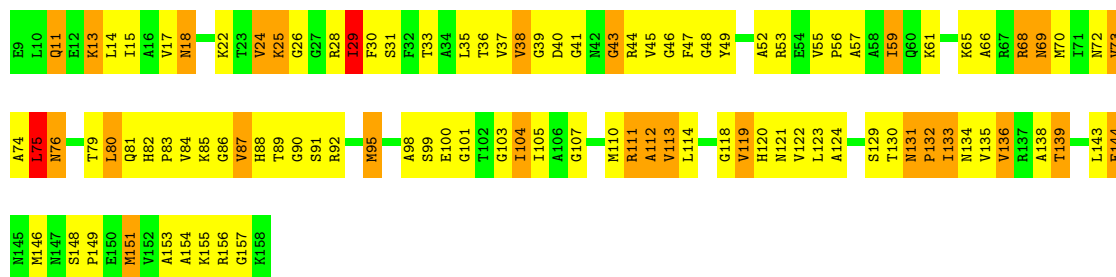
• Molecule 5: 30S ribosomal protein S5

Chain AE:



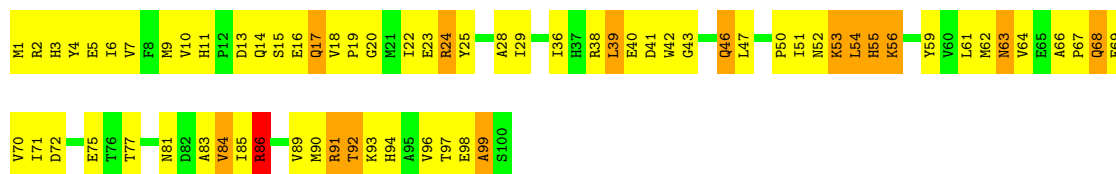
• Molecule 5: 30S ribosomal protein S5

Chain CE:



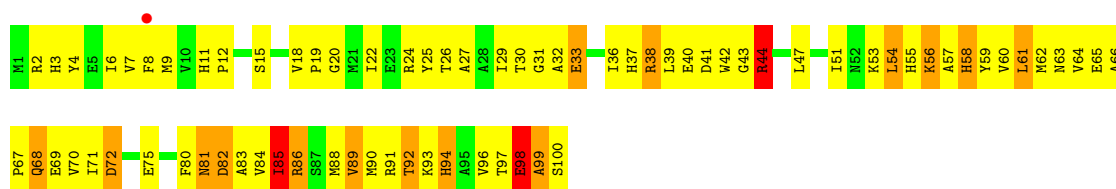
- Molecule 6: 30S ribosomal protein S6

Chain AF:



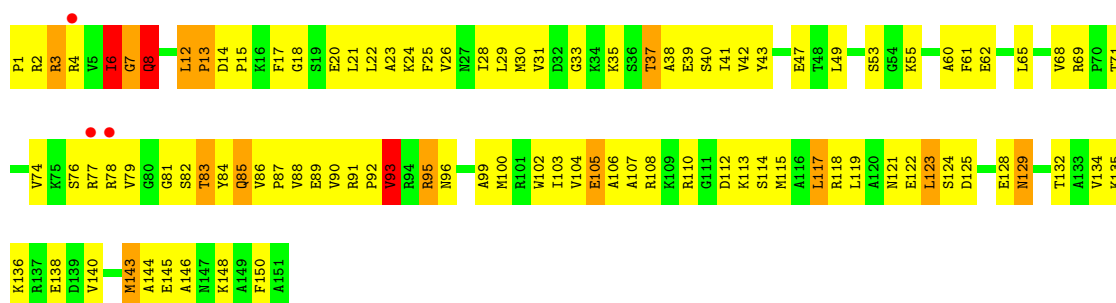
- Molecule 6: 30S ribosomal protein S6

Chain CF:



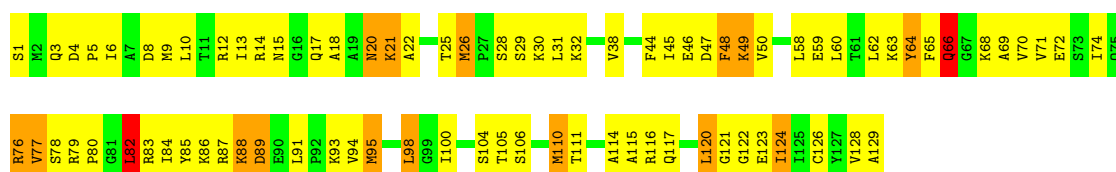
- Molecule 7: 30S ribosomal protein S7

Chain AG:



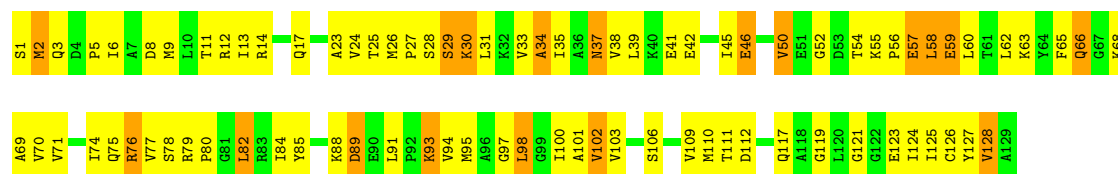
- Molecule 8: 30S ribosomal protein S8

Chain AH:



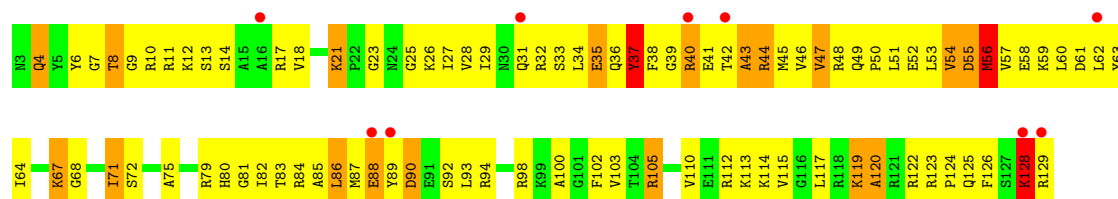
- Molecule 8: 30S ribosomal protein S8

Chain CH:



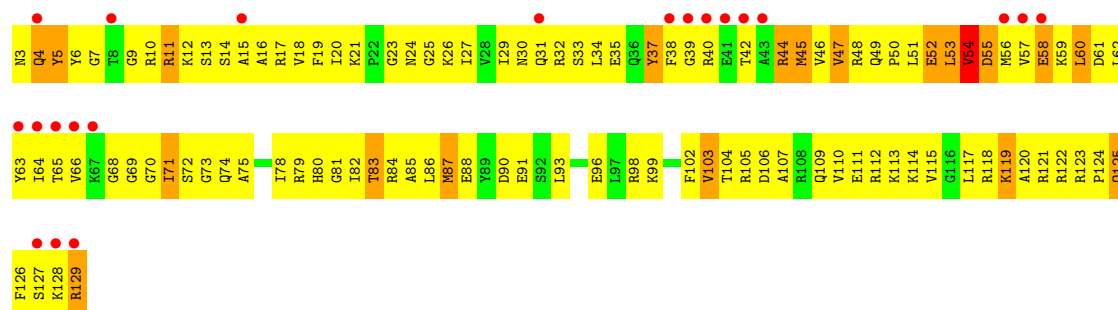
- Molecule 9: 30S ribosomal protein S9

Chain AI:



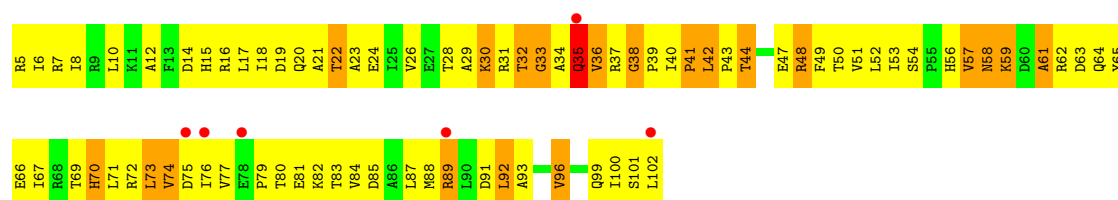
- Molecule 9: 30S ribosomal protein S9

Chain CI:



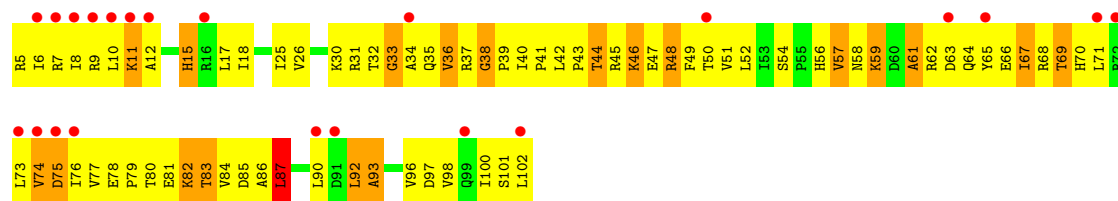
- Molecule 10: 30S ribosomal protein S10

Chain AJ:



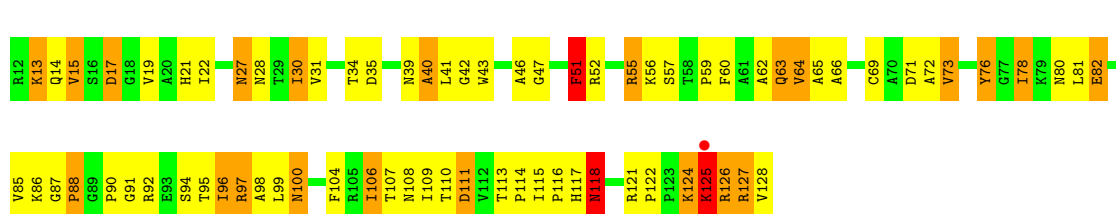
- Molecule 10: 30S ribosomal protein S10

Chain CJ:



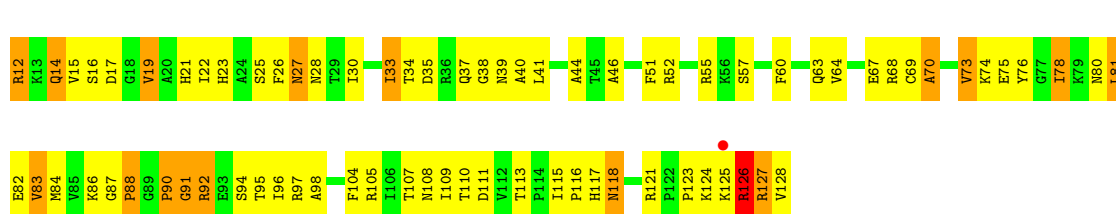
- Molecule 11: 30S ribosomal protein S11

Chain AK:



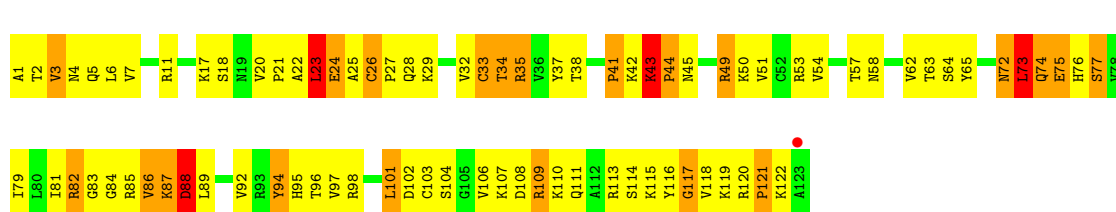
- Molecule 11: 30S ribosomal protein S11

Chain CK:



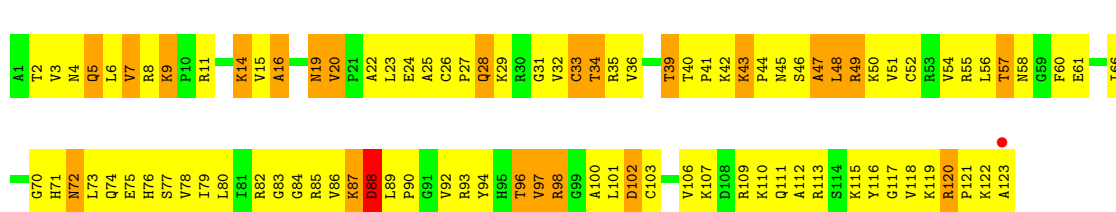
- Molecule 12: 30S ribosomal protein S12

Chain AL:



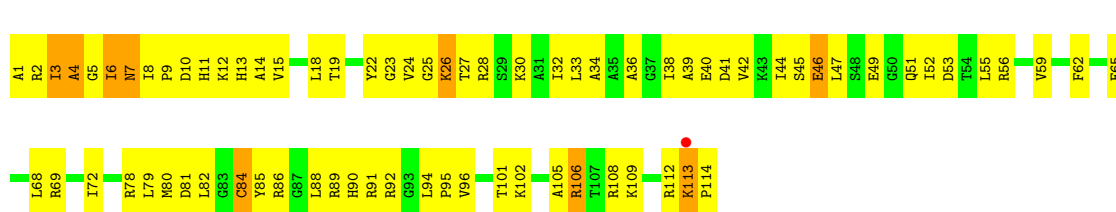
- Molecule 12: 30S ribosomal protein S12

Chain CL:



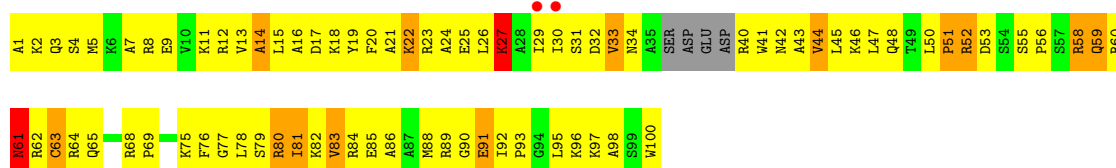
- Molecule 13: 30S ribosomal protein S13

Chain AM:



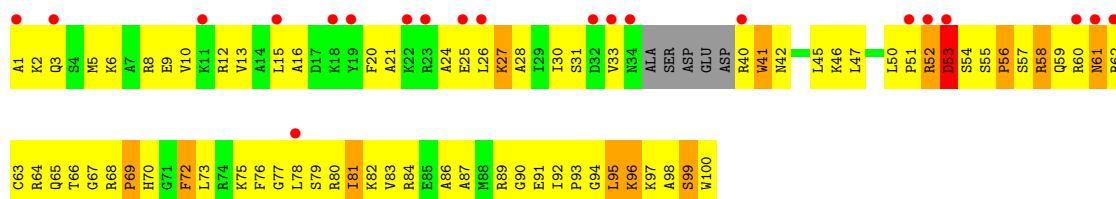
- Molecule 14: 30S ribosomal protein S14

Chain AN:



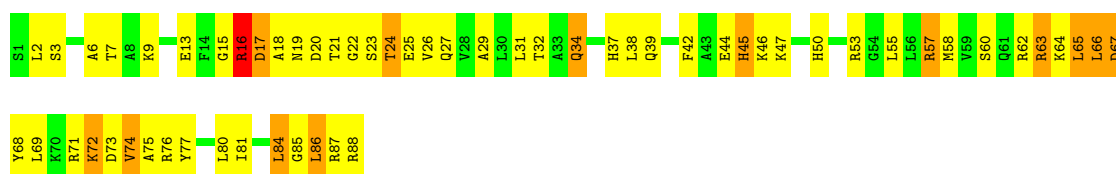
• Molecule 14: 30S ribosomal protein S14

Chain CN:



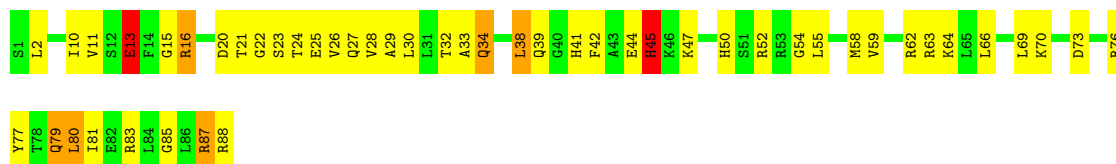
• Molecule 15: 30S ribosomal protein S15

Chain AO:



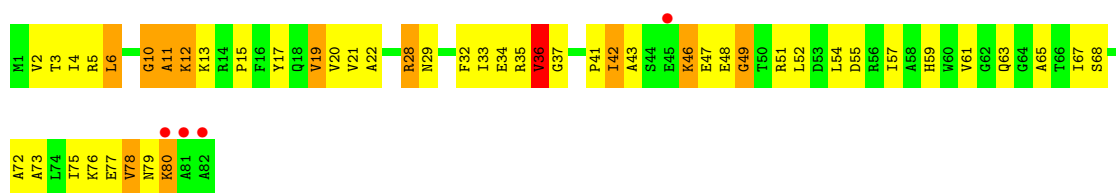
• Molecule 15: 30S ribosomal protein S15

Chain CO:



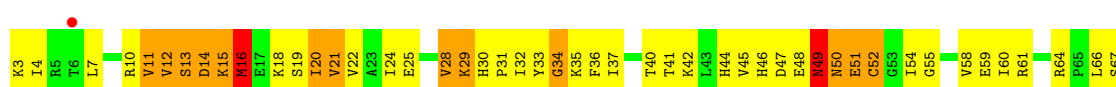
• Molecule 16: 30S ribosomal protein S16

Chain AP:



• Molecule 17: 30S ribosomal protein S17

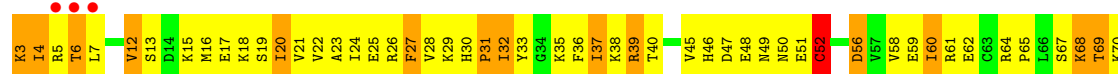
Chain AQ:





- Molecule 17: 30S ribosomal protein S17

Chain CQ:



- Molecule 18: 30S ribosomal protein S18

Chain AR:



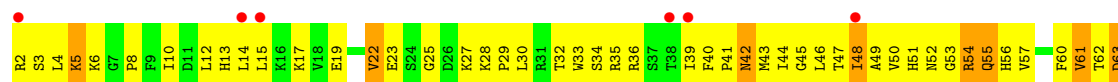
- Molecule 18: 30S ribosomal protein S18

Chain CR:



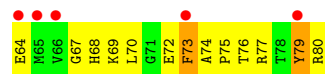
- Molecule 19: 30S ribosomal protein S19

Chain AS:



- Molecule 19: 30S ribosomal protein S19

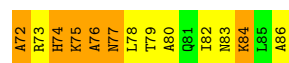
Chain CS:



- Molecule 20: 30S ribosomal protein S20

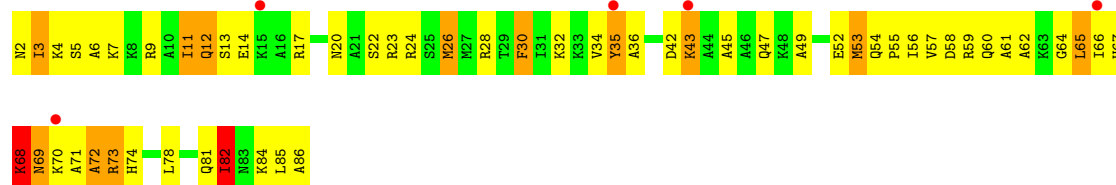
Chain AT:





- Molecule 20: 30S ribosomal protein S20

Chain CT:



- Molecule 21: 30S ribosomal protein S21

Chain AU:



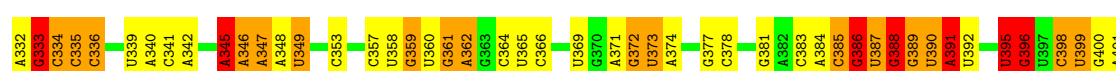
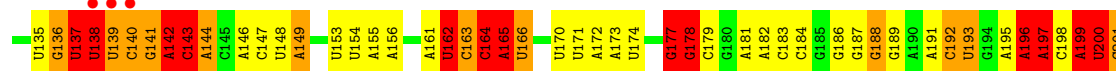
- Molecule 21: 30S ribosomal protein S21

Chain CU:



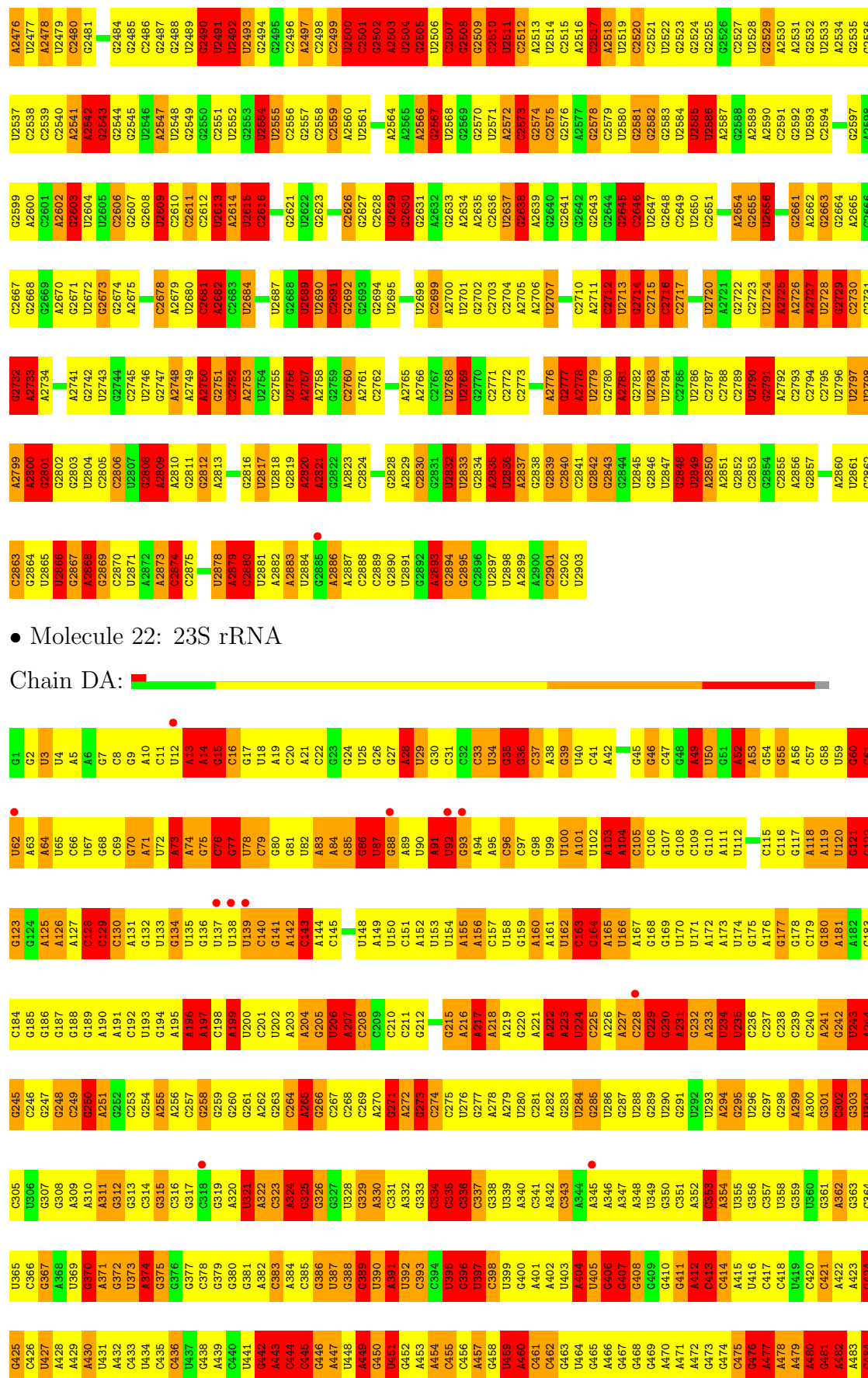
- Molecule 22: 23S rRNA

Chain BA:



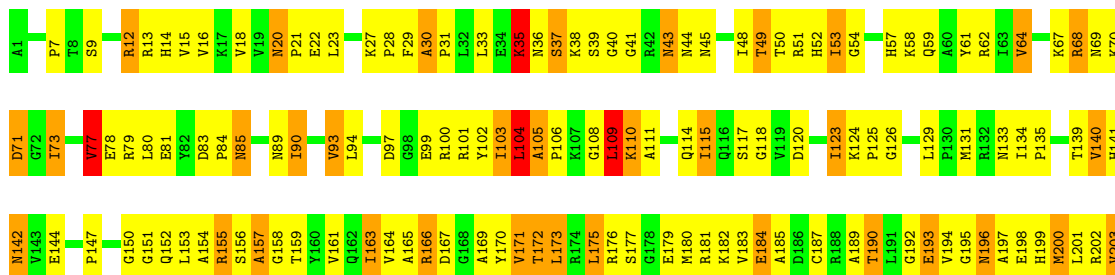
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G1432	G1371	A1304	U1242	U1174	A1111	G1047	A984	A918	C851	A788	U724	A651	A599	G539	A472
A1433	C1305	C1306	C1243	A1175	G1112	A1048	C985	U919	U852	A789	G726	G663	G500	C540	G473
A1434	C1372	C1306	A1244	U1176	U1113	C1049	C986	A920	C853	U790	G725	G662	G500	A541	G474
G1435	A1373	G1245	G1245	G1177	C1114	A1050	C987	C921	C854	C791	G727	G665	A603	C542	C475
G1436	G1374	G1246	A1246	C1178	G1115	A1054	A988	C922	G855	A792	G728	G666	A603	G543	G476
C1437	U1375	A1247	A1247	G1179	G1116	A1054	C989	G923	G856	A793	G729	A666	G604	C544	A477
U1438	C1376	G1248	U1248	U1180	C1117	G1056	A990	G927	G857	A794	A730	U687	G605	U545	A478
A1439	G1377	U1249	U1249	U1181	C1118	G1056	C993	A927	G858	C795	C731	A668	U606	U546	A479
U1440	C1377	U1249	U1249	U1181	C1118	G1056	C993	A928	G859	C796	C732	G669	U607	A547	A480
G1441	C1378	C1313	C1250	U1182	U1119	A1057	G994	U929	U860	C797	G733	G669	A608	C548	G481
G1442	U1379	C1314	C1251	U1183	C994	A1058	G995	U929	U860	C797	G733	G669	A608	C548	G481
G1443	C1380	C1315	G1252	U1184	C995	A1059	C995	G930	A861	C798	A734	C671	A609	C549	A482
G1444	G1381	U1316	A1253	G1185	G1125	U1060	A996	U931	G862	C799	A735	C672	C510	C550	A483
G1445	G1382	U1317	A1254	G1186	A1126	U1061	G997	U932	A863	A800	C736	C673	C511	G551	C484
C1446	C1383	U1318	U1255	U1187	A1127	G1062	C998	U933	G864	A801	C737	G674	G612	U552	C485
C1447	A1384	C1319	G1256	U1188	G1128	A1063	U999	U934	C865	A802	C738	A675	A613	U554	C486
G1450	A1385	A1320	C1257	A1189	U1129	C1064	A1000	C935	A866	U803	A739	A676	A614	U555	G489
C1451	C1386	C1321	U1258	G1190	U1130	U1065	A1001	A936	C867	A804	C740	C679	U615	A556	C490
G1452	A1387	A1322	U1259	G1191	G1131	U1066	G1002	C937	U868	C805	U741	C679	A616	A557	C491
A1453	G1388	C1323	A1260	G1191	U1132	U1067	G1003	G938	C869	C806	A742	C680	G617	C557	G492
C1454	G1389	C1324	C1261	C1196	A1133	G1068	U1004	G939	U870	C807	U744	G682	G620	C560	G495
G1455	A1392	U1325	A1265	U1197	A1134	A1070	C1005	G942	U871	U810	U745	A685	A621	C561	C496
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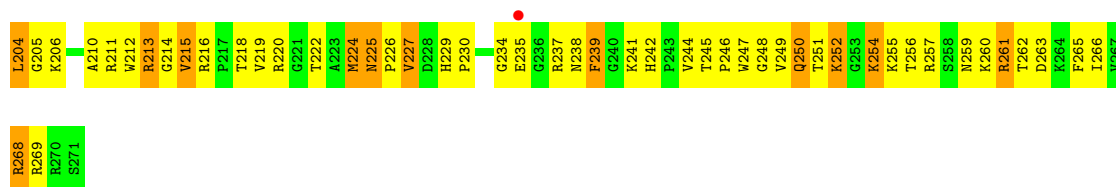




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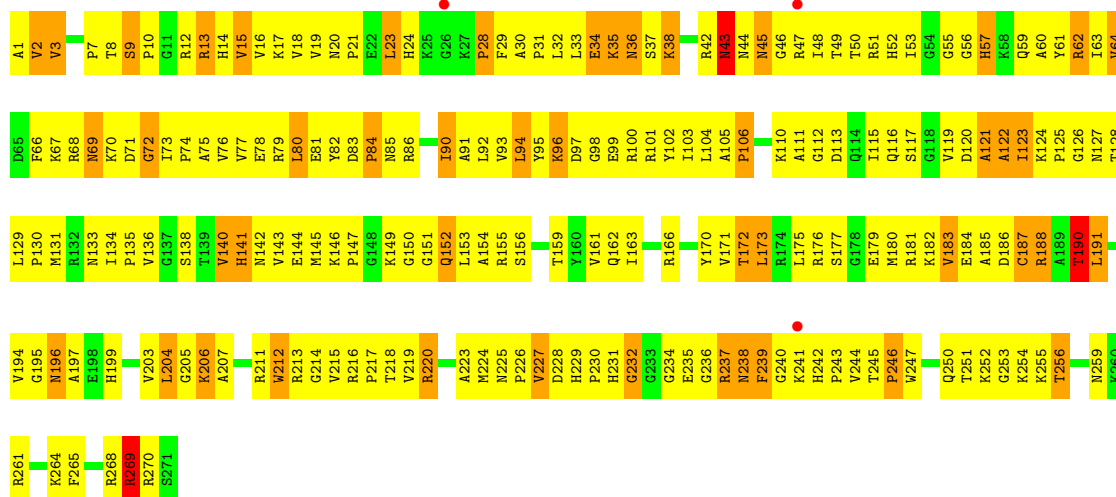
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C2364	U2242	G	G2056	U1991	A1919	A1790	A1790	G1724	U1663	A1532	A1532	A1470
G2365	U2243	U	G2057	U1992	C1920	C1790	C1790	U1729	G1664	A1533	A1533	C1471
A2366	U2244	G	C2058	U1993	G1921	A1791	A1791	C1730	A1664	U1597	U1597	G1472
U2367	U2245	U	A2059	U1994	G1922	G1792	G1792	C1731	G1666	U1599	U1599	A1535
C2368	G2246	G	A2060	C1994	C1924	A1858	C1793	C1732	U1666	U1599	U1599	A1535





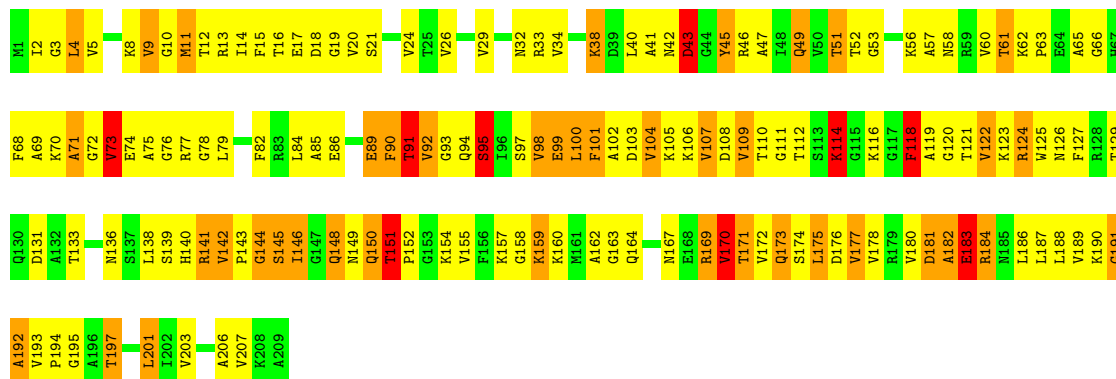
• Molecule 24: 50S ribosomal protein L2

Chain DC:



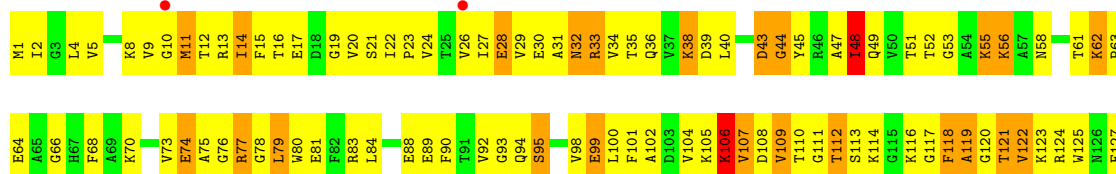
• Molecule 25: 50S ribosomal protein L3

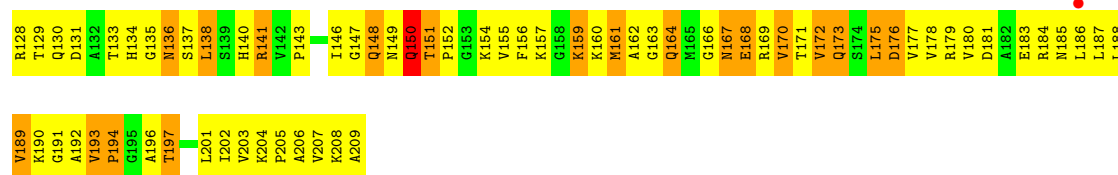
Chain BD:



• Molecule 25: 50S ribosomal protein L3

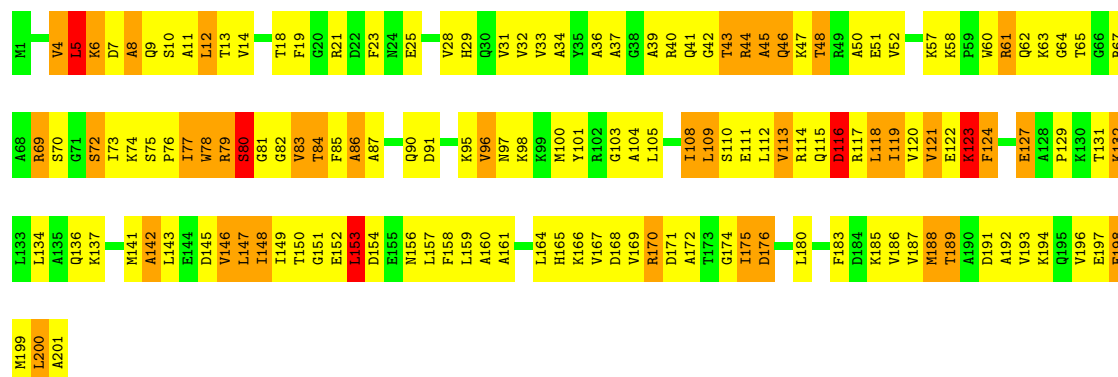
Chain DD:





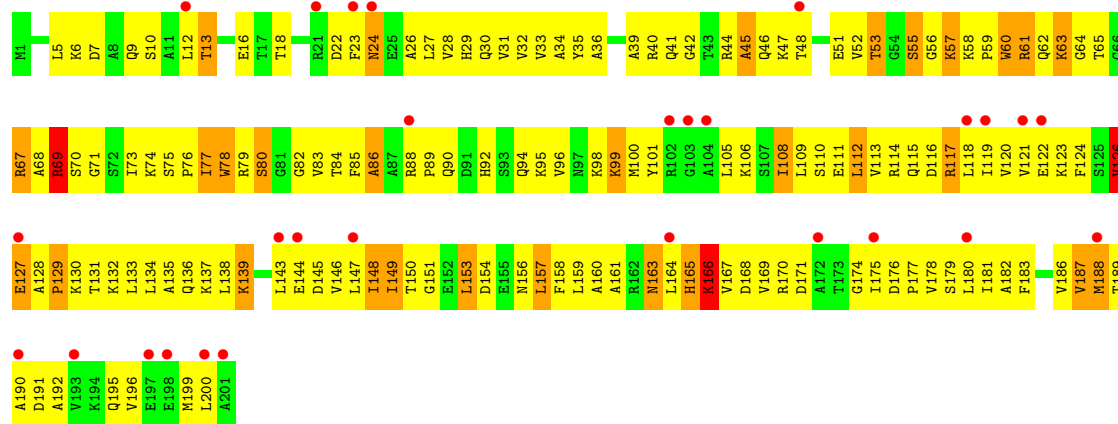
• Molecule 26: 50S ribosomal protein L4

Chain BE:



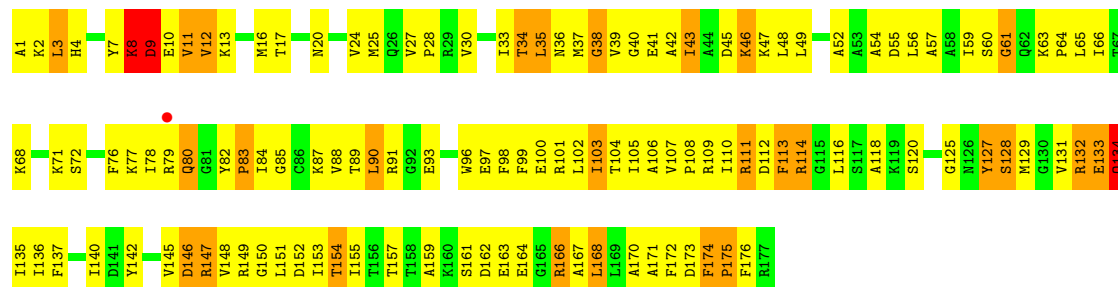
• Molecule 26: 50S ribosomal protein L4

Chain DE:



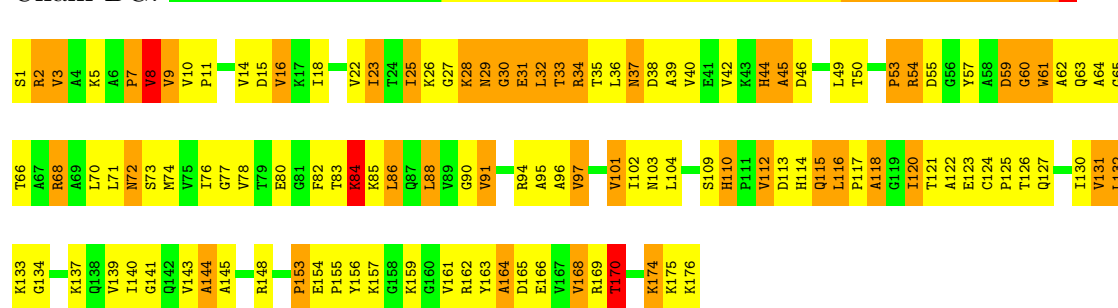
• Molecule 27: 50S ribosomal protein L5

Chain BF:



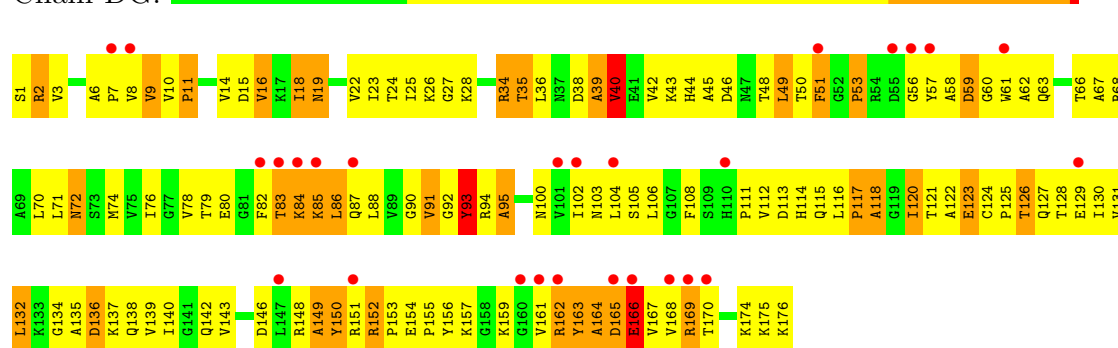
- Molecule 28: 50S ribosomal protein L6

Chain BG:



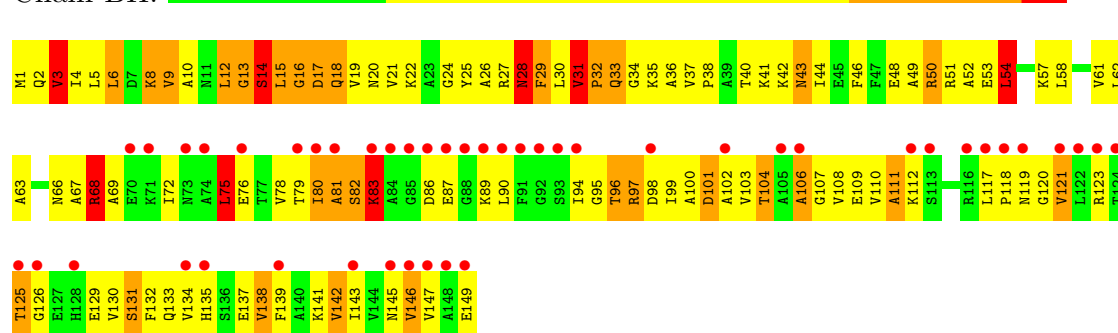
- Molecule 28: 50S ribosomal protein L6

Chain DG:



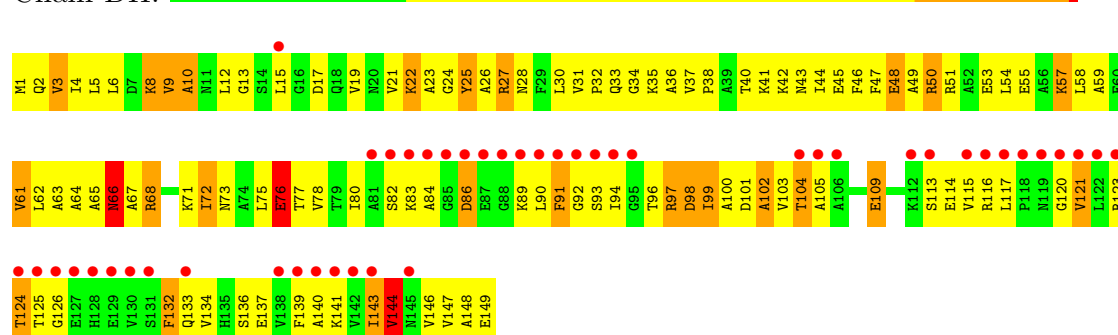
- Molecule 29: 50S ribosomal protein L9

Chain BH:



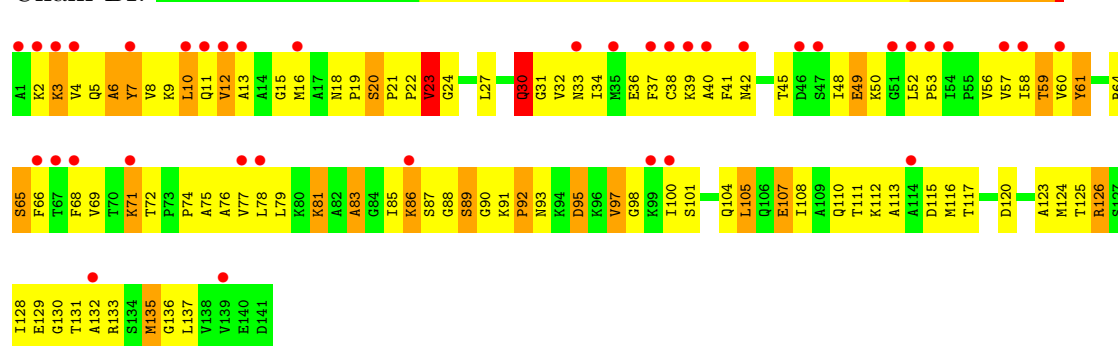
- Molecule 29: 50S ribosomal protein L9

Chain DH:



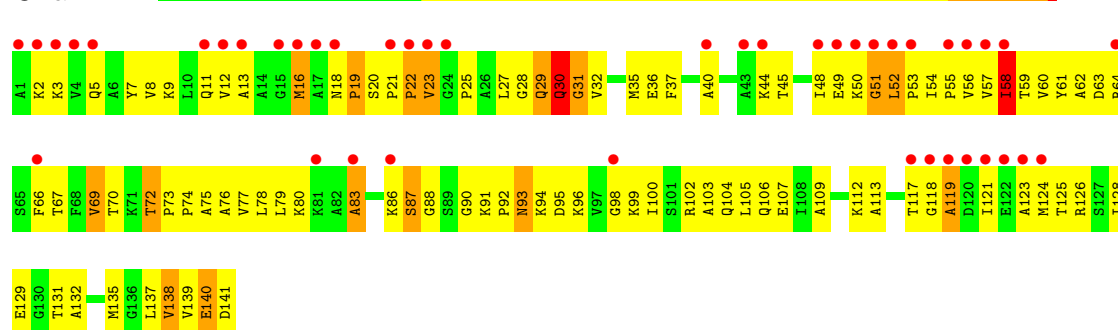
- Molecule 30: 50S ribosomal protein L11

Chain BI:



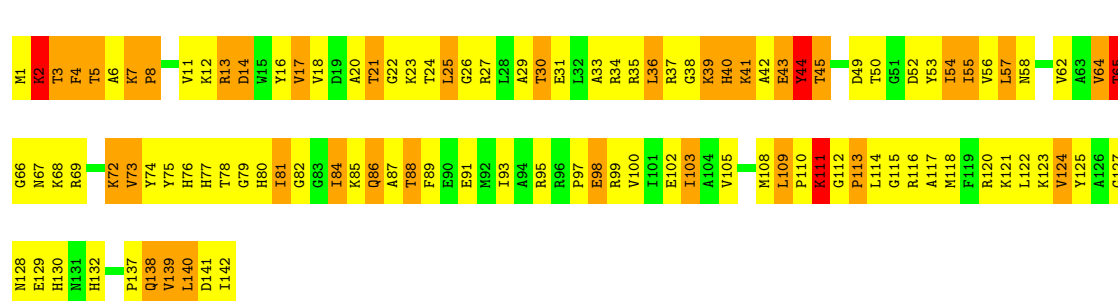
- Molecule 30: 50S ribosomal protein L11

Chain DI:



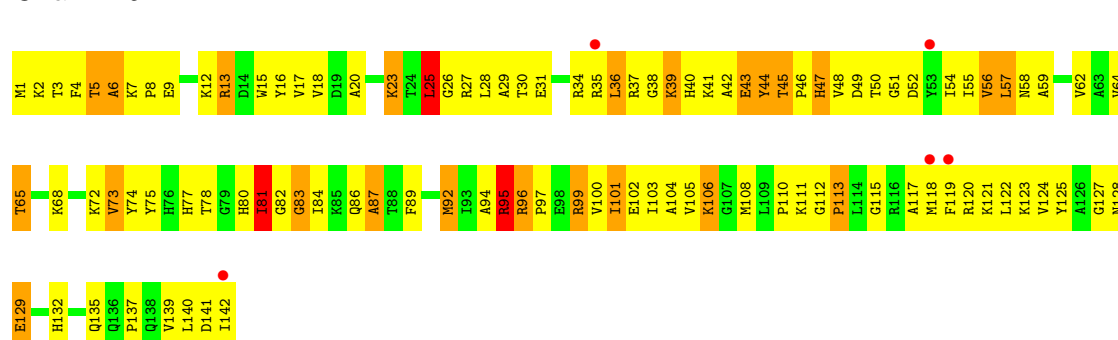
- Molecule 31: 50S ribosomal protein L13

Chain BJ:



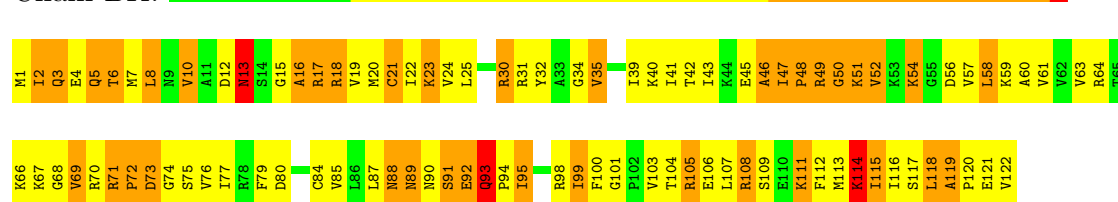
- Molecule 31: 50S ribosomal protein L13

Chain DJ:



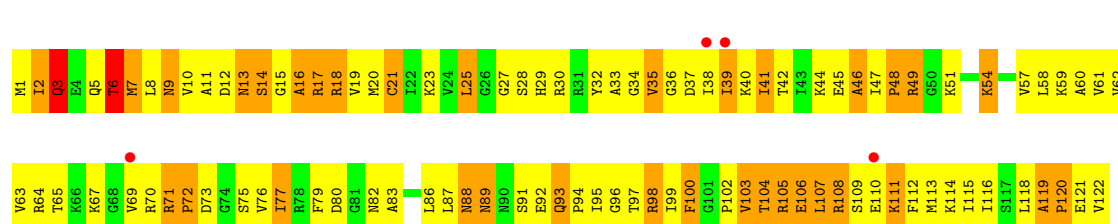
- Molecule 32: 50S ribosomal protein L14

Chain BK:



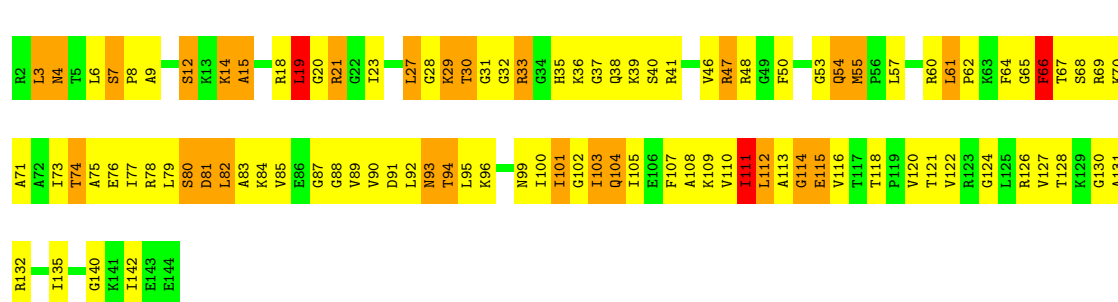
- Molecule 32: 50S ribosomal protein L14

Chain DK:



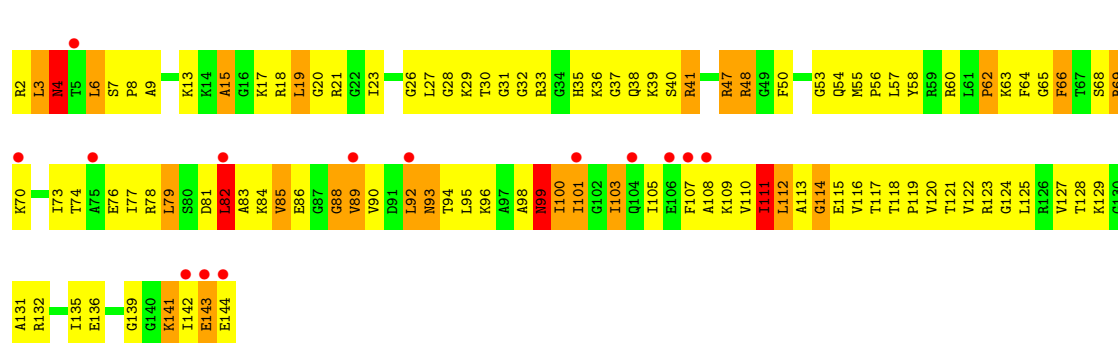
- Molecule 33: 50S ribosomal protein L15

Chain BL:



- Molecule 33: 50S ribosomal protein L15

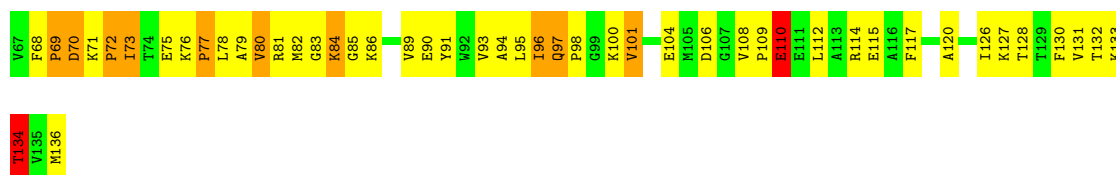
Chain DL:



- Molecule 34: 50S ribosomal protein L16

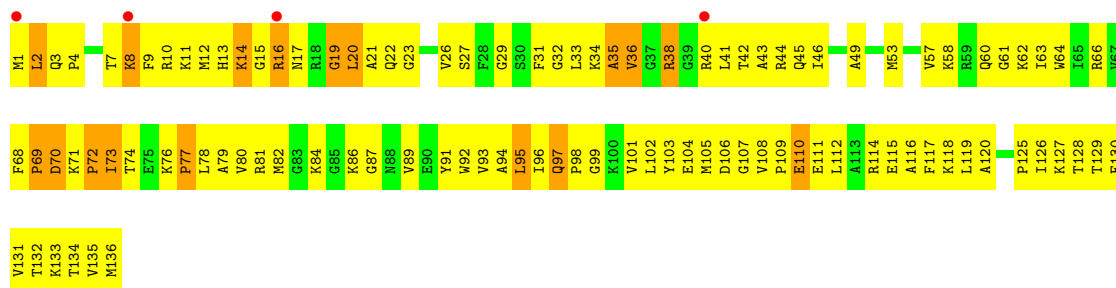
Chain BM:





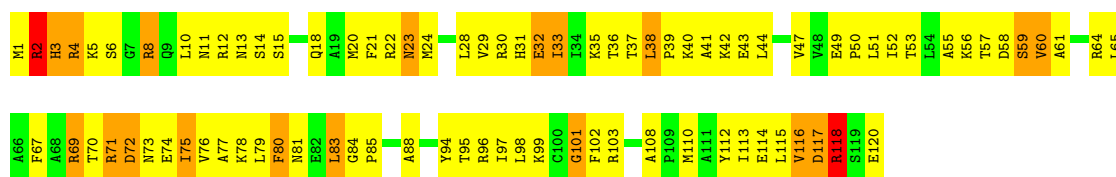
- Molecule 34: 50S ribosomal protein L16

Chain DM:



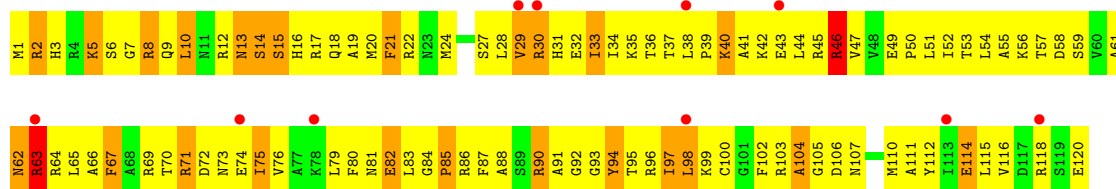
- Molecule 35: 50S ribosomal protein L17

Chain BN:



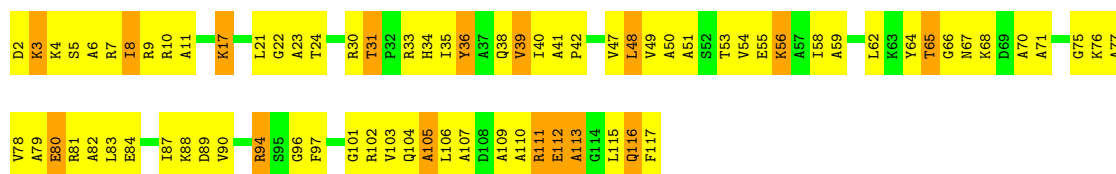
- Molecule 35: 50S ribosomal protein L17

Chain DN:



- Molecule 36: 50S ribosomal protein L18

Chain BO:



- Molecule 36: 50S ribosomal protein L18

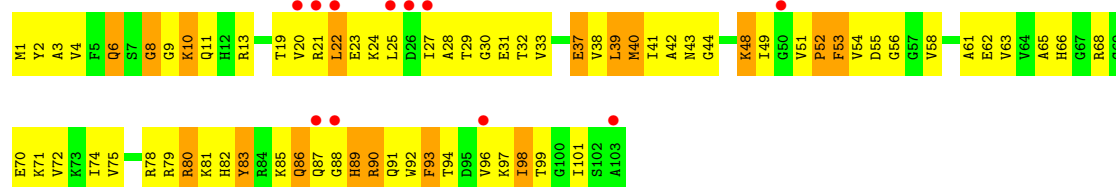
Chain DO:





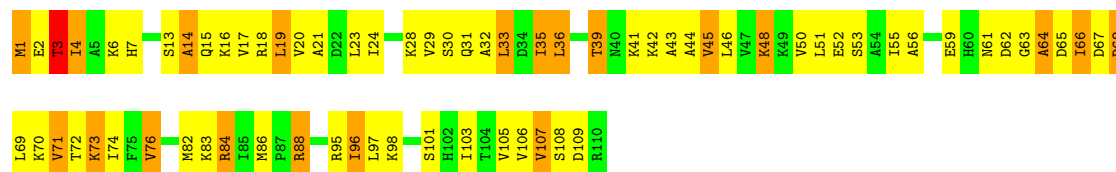
• Molecule 39: 50S ribosomal protein L21

Chain DR:



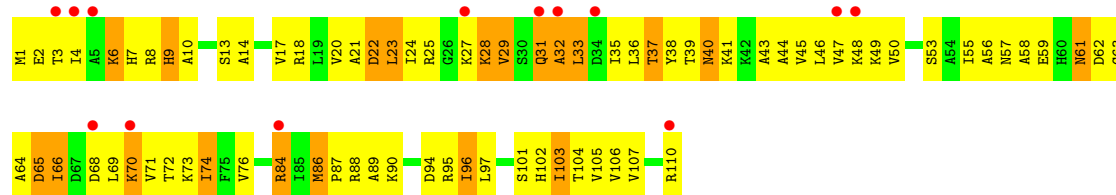
• Molecule 40: 50S ribosomal protein L22

Chain BS:



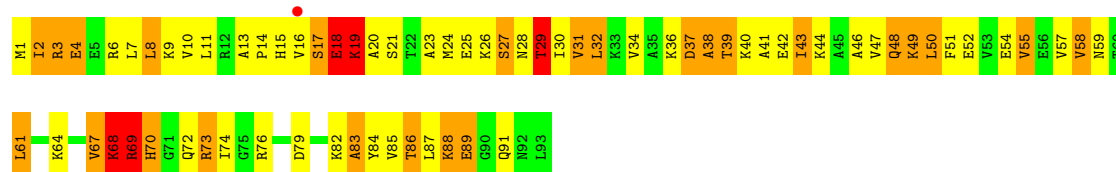
• Molecule 40: 50S ribosomal protein L22

Chain DS:



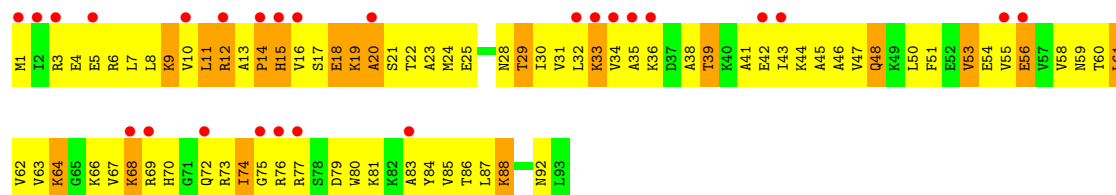
• Molecule 41: 50S ribosomal protein L23

Chain BT:



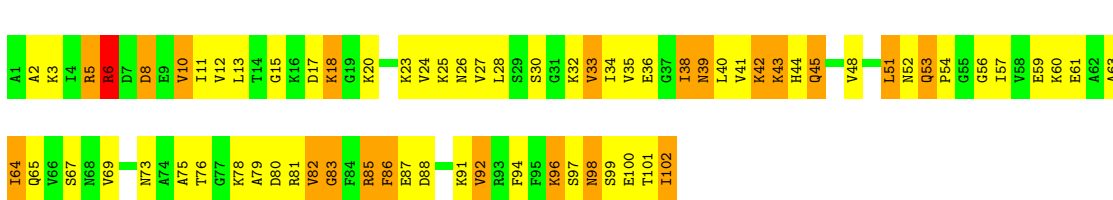
• Molecule 41: 50S ribosomal protein L23

Chain DT:



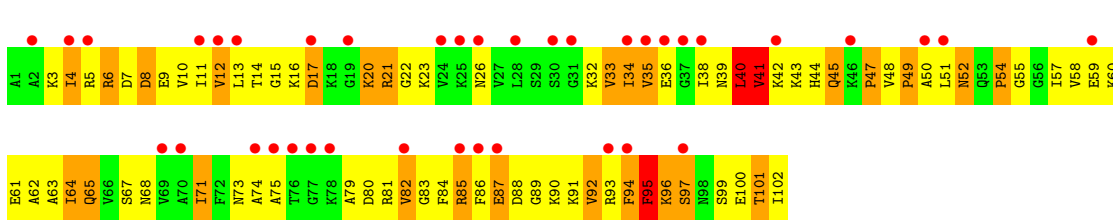
- Molecule 42: 50S ribosomal protein L24

Chain BU:



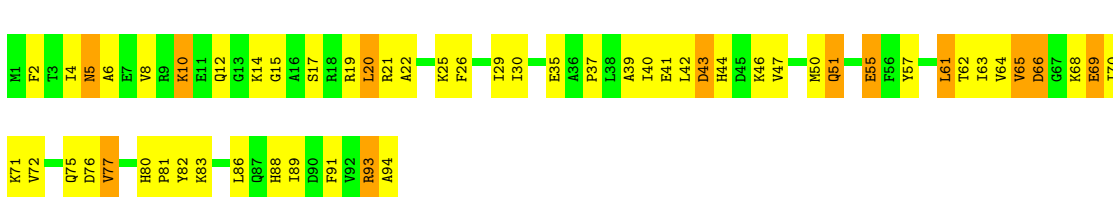
- Molecule 42: 50S ribosomal protein L24

Chain DU:



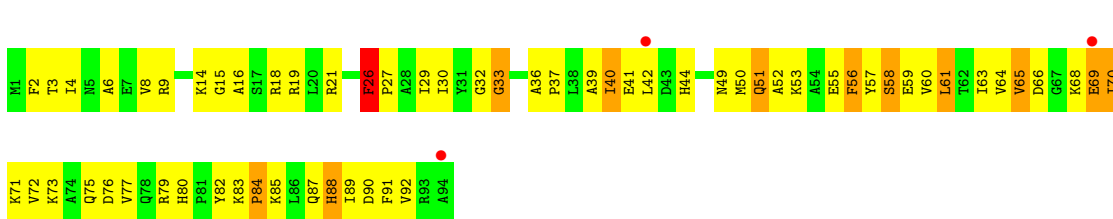
- Molecule 43: 50S ribosomal protein L25

Chain BV:



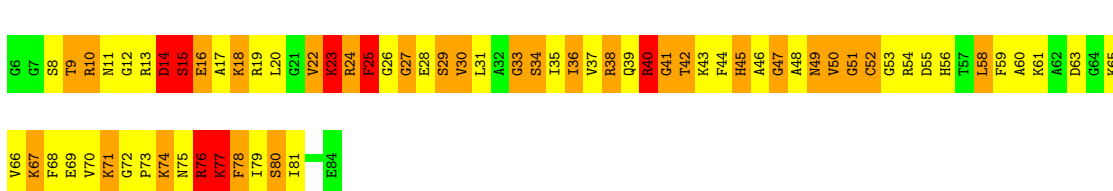
- Molecule 43: 50S ribosomal protein L25

Chain DV:



- Molecule 44: 50S ribosomal protein L27

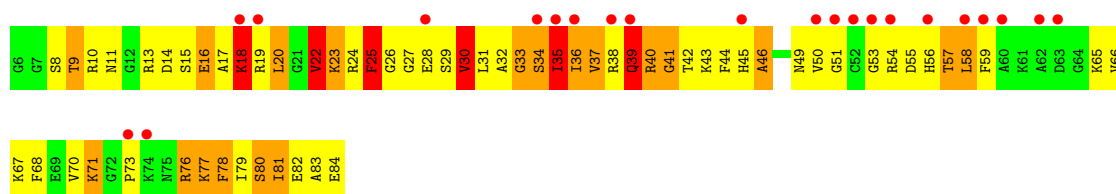
Chain BW:



- Molecule 44: 50S ribosomal protein L27

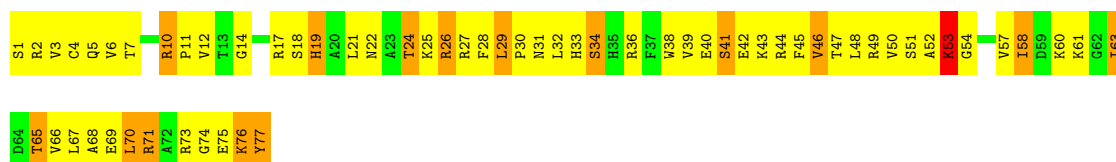
Chain DW:





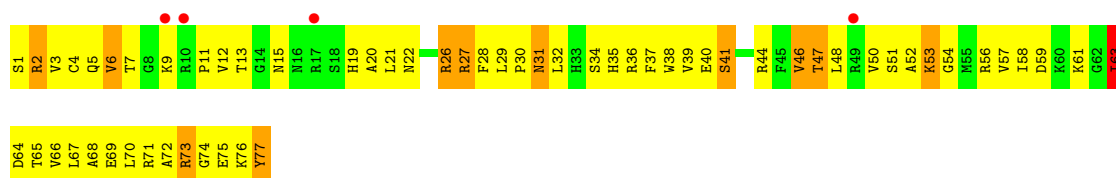
- Molecule 45: 50S ribosomal protein L28

Chain BX:



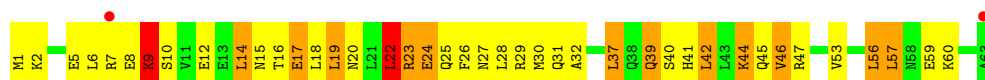
- Molecule 45: 50S ribosomal protein L28

Chain DX:



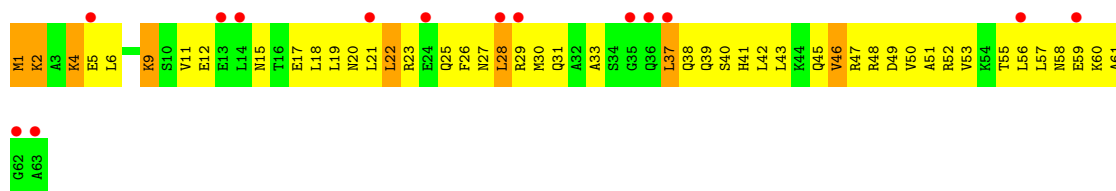
- Molecule 46: 50S ribosomal protein L29

Chain BY:



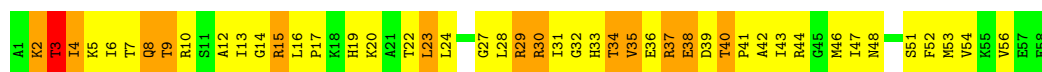
- Molecule 46: 50S ribosomal protein L29

Chain DY:



- Molecule 47: 50S ribosomal protein L30

Chain BZ:



- Molecule 47: 50S ribosomal protein L30

Chain DZ:



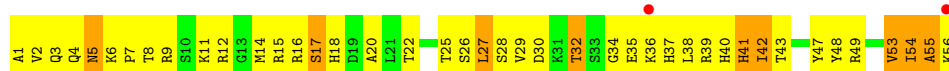
- Molecule 48: 50S ribosomal protein L32

Chain B0:



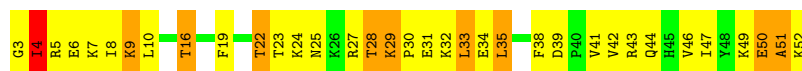
- Molecule 48: 50S ribosomal protein L32

Chain D0:



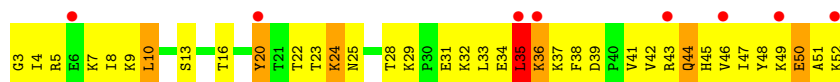
- Molecule 49: 50S ribosomal protein L33

Chain B1:



- Molecule 49: 50S ribosomal protein L33

Chain D1:



- Molecule 50: 50S ribosomal protein L34

Chain B2:



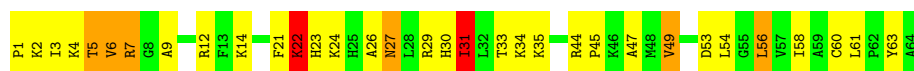
- Molecule 50: 50S ribosomal protein L34

Chain D2:



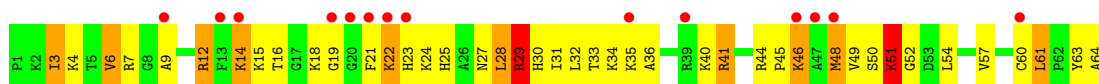
- Molecule 51: 50S ribosomal protein L35

Chain B3:



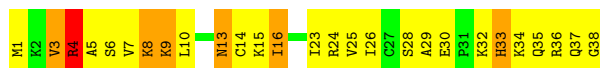
- Molecule 51: 50S ribosomal protein L35

Chain D3:



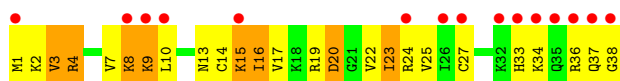
- Molecule 52: 50S ribosomal protein L36

Chain B4:



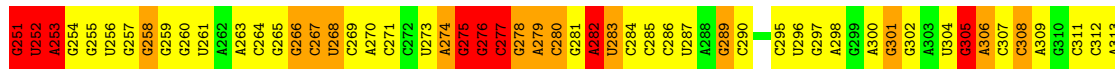
- Molecule 52: 50S ribosomal protein L36

Chain D4:



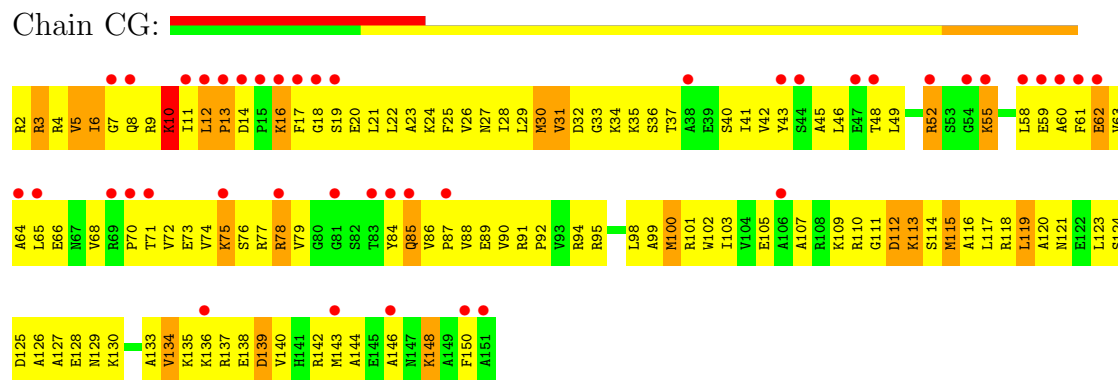
- Molecule 53: 16S rRNA

Chain CA:



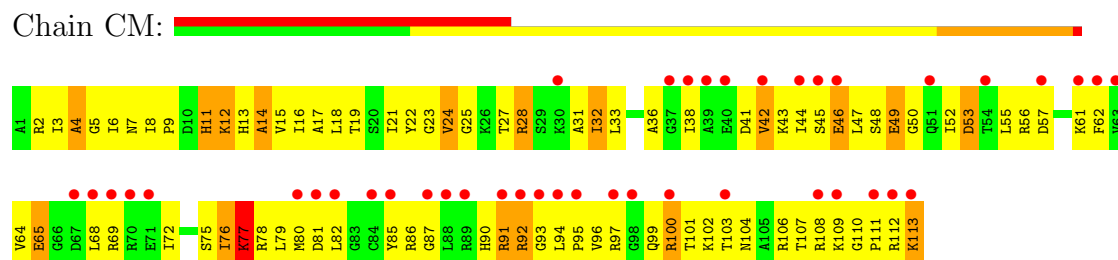
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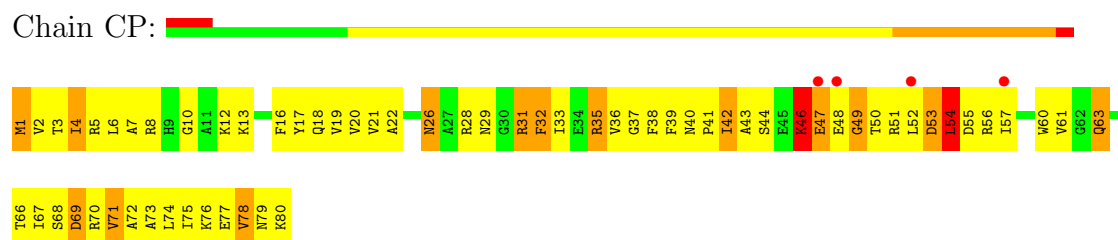
- Molecule 55: 30S ribosomal protein S13

Chain CM:



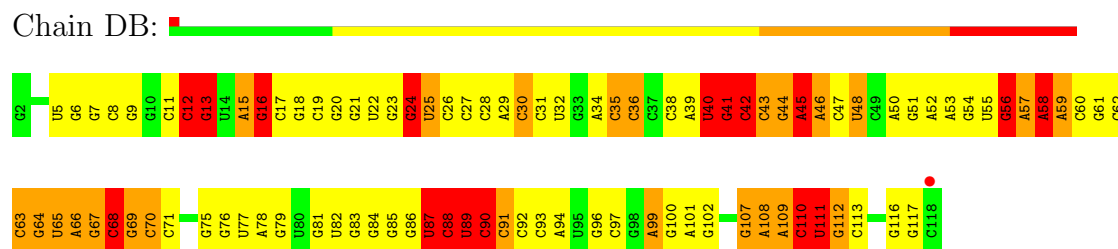
- Molecule 56: 30S ribosomal protein S16

Chain CP:



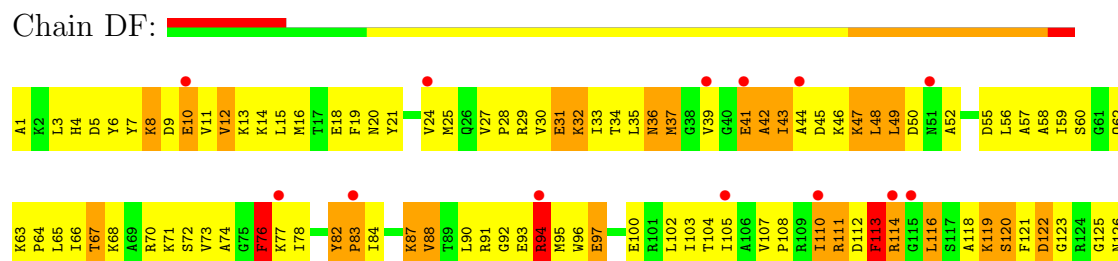
- Molecule 57: 5S rRNA

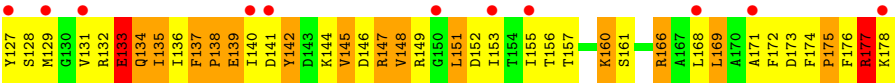
Chain DB:



- Molecule 58: 50S ribosomal protein L5

Chain DF:





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.08Å 434.46Å 618.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	76.35 – 3.29 76.35 – 3.29	Depositor EDS
% Data completeness (in resolution range)	77.5 (76.35-3.29) 77.5 (76.35-3.29)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 3.26Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.189 , 0.241 0.204 , 0.253	Depositor DCC
R_{free} test set	13298 reflections (2.05%)	DCC
Wilson B-factor (Å ²)	66.6	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 36.5	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	1 of 700316 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	284501	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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: MG, ZN, CLY

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	0.50	2/36834 (0.0%)	1.24	439/57462 (0.8%)
2	AB	0.24	0/1736	0.44	0/2338
2	CB	0.23	0/1736	0.44	0/2338
3	AC	0.26	0/1652	0.48	0/2225
3	CC	0.22	0/1652	0.42	0/2225
4	AD	0.29	0/1665	0.50	0/2227
4	CD	0.32	0/1665	0.55	0/2227
5	AE	0.31	0/1119	0.56	0/1504
5	CE	0.35	1/1119 (0.1%)	0.53	0/1504
6	AF	0.28	0/836	0.47	0/1128
6	CF	0.26	0/836	0.48	0/1128
7	AG	0.23	0/1196	0.45	0/1602
8	AH	0.30	0/989	0.52	0/1326
8	CH	0.26	0/989	0.49	0/1326
9	AI	0.24	0/1034	0.45	0/1375
9	CI	0.21	0/1034	0.41	0/1375
10	AJ	0.24	0/797	0.47	0/1077
10	CJ	0.21	0/797	0.45	0/1077
11	AK	0.26	0/893	0.51	0/1205
11	CK	0.26	0/893	0.50	0/1205
12	AL	0.35	0/969	0.66	1/1300 (0.1%)
12	CL	0.29	0/969	0.54	0/1300
13	AM	0.23	0/893	0.47	0/1193
14	AN	0.26	0/785	0.46	0/1043
14	CN	0.21	0/780	0.37	0/1036
15	AO	0.29	0/722	0.45	0/964
15	CO	0.25	0/722	0.42	0/964
16	AP	0.30	0/659	0.48	0/884
17	AQ	0.35	0/658	0.56	0/881
17	CQ	0.27	0/658	0.49	0/881
18	AR	0.28	0/463	0.47	0/621
18	CR	0.26	0/463	0.45	0/621

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	AS	0.24	0/653	0.43	0/877
19	CS	0.20	0/653	0.41	0/877
20	AT	0.31	0/671	0.52	0/888
20	CT	0.25	0/671	0.49	0/888
21	AU	0.27	0/431	0.45	0/570
21	CU	0.32	0/431	0.57	0/570
22	BA	0.73	7/68626 (0.0%)	1.54	1278/107056 (1.2%)
22	DA	0.45	2/68314 (0.0%)	1.23	934/106569 (0.9%)
23	BB	0.68	0/2828	1.42	40/4410 (0.9%)
24	BC	0.40	0/2122	0.67	0/2852
24	DC	0.29	0/2122	0.51	0/2852
25	BD	0.51	0/1586	0.72	1/2134 (0.0%)
25	DD	0.28	0/1586	0.54	0/2134
26	BE	0.42	0/1571	0.63	0/2113
26	DE	0.24	0/1571	0.46	0/2113
27	BF	0.32	0/1435	0.52	0/1926
28	BG	0.36	0/1343	0.59	0/1816
28	DG	0.22	0/1343	0.44	0/1816
29	BH	0.27	0/1122	0.47	0/1515
29	DH	0.25	0/1122	0.51	2/1515 (0.1%)
30	BI	0.23	0/1046	0.47	0/1410
30	DI	0.20	0/1046	0.42	0/1410
31	BJ	0.52	0/1152	0.77	0/1551
31	DJ	0.26	0/1152	0.55	1/1551 (0.1%)
32	BK	0.49	0/948	0.71	0/1268
32	DK	0.29	0/948	0.52	0/1268
33	BL	0.41	0/1054	0.71	1/1403 (0.1%)
33	DL	0.25	0/1054	0.50	0/1403
34	BM	0.46	0/1093	0.68	0/1460
34	DM	0.27	0/1093	0.46	0/1460
35	BN	0.42	0/974	0.68	0/1301
35	DN	0.26	0/974	0.48	0/1301
36	BO	0.39	0/902	0.59	0/1209
36	DO	0.21	0/902	0.40	0/1209
37	BP	0.45	0/929	0.71	0/1242
37	DP	0.27	0/929	0.47	0/1242
38	BQ	0.55	0/960	0.69	0/1278
38	DQ	0.27	0/960	0.44	0/1278
39	BR	0.54	0/829	0.72	0/1107
39	DR	0.26	0/829	0.49	0/1107
40	BS	0.51	0/864	0.73	0/1156
40	DS	0.26	0/864	0.50	0/1156
41	BT	0.43	0/745	0.68	0/994

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
41	DT	0.22	0/745	0.45	0/994
42	BU	0.39	0/788	0.67	0/1051
42	DU	0.22	0/788	0.45	0/1051
43	BV	0.41	0/766	0.60	0/1025
43	DV	0.23	0/766	0.42	0/1025
44	BW	0.49	0/603	0.77	0/797
44	DW	0.25	0/603	0.46	0/797
45	BX	0.39	0/635	0.66	0/848
45	DX	0.26	0/635	0.52	0/848
46	BY	0.36	0/510	0.60	0/677
46	DY	0.21	0/510	0.42	0/677
47	BZ	0.51	0/453	0.73	0/605
47	DZ	0.25	0/453	0.50	0/605
48	B0	0.44	0/450	0.69	0/599
48	D0	0.26	0/450	0.48	0/599
49	B1	0.36	0/417	0.54	0/554
49	D1	0.24	0/417	0.44	0/554
50	B2	0.45	0/380	0.62	0/498
50	D2	0.25	0/380	0.47	0/498
51	B3	0.44	0/513	0.62	0/676
51	D3	0.25	0/513	0.49	0/676
52	B4	0.47	0/303	0.74	0/397
52	D4	0.32	0/303	0.45	0/397
53	CA	0.46	3/36762 (0.0%)	1.18	421/57350 (0.7%)
54	CG	0.21	0/1188	0.42	0/1591
55	CM	0.19	0/885	0.39	0/1181
56	CP	0.27	0/649	0.49	0/870
57	DB	0.43	1/2803 (0.0%)	1.07	30/4371 (0.7%)
58	DF	0.22	0/1444	0.45	0/1937
All	All	0.51	16/306773 (0.0%)	1.17	3148/458565 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
25	BD	0	1
31	BJ	0	1
35	BN	0	1
58	DF	0	1
All	All	0	4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	CA	1396	A	O3'-P	-16.33	1.41	1.61
1	AA	1047	G	O3'-P	-13.54	1.45	1.61
22	BA	1905	C	O3'-P	-12.21	1.46	1.61
22	BA	2197	U	O3'-P	-9.98	1.49	1.61
22	BA	876	C	O3'-P	-9.54	1.49	1.61

The worst 5 of 3148 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	DA	2586	U	N1-C1'-C2'	-16.52	92.53	114.00
22	BA	627	A	P-O3'-C3'	15.92	138.81	119.70
22	BA	531	C	P-O3'-C3'	15.89	138.77	119.70
1	AA	1047	G	P-O3'-C3'	-15.60	100.98	119.70
22	BA	2068	U	N1-C1'-C2'	-15.16	94.30	114.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
25	BD	9	VAL	Peptide
31	BJ	43	GLU	Peptide
35	BN	101	GLY	Peptide
58	DF	177	ARG	Mainchain

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	32895	0	16553	1994	0
2	AB	1705	0	1731	279	0
2	CB	1705	0	1732	233	0
3	AC	1625	0	1699	178	0
3	CC	1625	0	1699	193	0
4	AD	1643	0	1710	243	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	CD	1643	0	1710	224	0
5	AE	1106	0	1148	206	0
5	CE	1106	0	1148	145	0
6	AF	818	0	808	111	0
6	CF	818	0	808	117	0
7	AG	1182	0	1240	130	0
8	AH	979	0	1034	136	0
8	CH	979	0	1034	126	0
9	AI	1022	0	1070	133	0
9	CI	1022	0	1070	164	0
10	AJ	787	0	828	141	0
10	CJ	787	0	828	148	0
11	AK	877	0	887	140	0
11	CK	877	0	887	128	0
12	AL	955	0	1019	127	0
12	CL	955	0	1019	156	0
13	AM	884	0	944	94	0
14	AN	774	0	827	136	0
14	CN	769	0	822	130	0
15	AO	714	0	737	84	0
15	CO	714	0	737	61	0
16	AP	649	0	666	79	0
17	AQ	649	0	691	100	0
17	CQ	649	0	691	112	0
18	AR	456	0	478	53	0
18	CR	456	0	478	57	0
19	AS	638	0	665	74	0
19	CS	638	0	665	109	0
20	AT	665	0	714	97	0
20	CT	665	0	714	86	0
21	AU	426	0	449	116	0
21	CU	426	0	449	92	0
22	BA	61274	0	30819	3248	0
22	DA	60995	0	30679	5259	0
23	BB	2529	0	1281	118	0
24	BC	2083	0	2157	287	0
24	DC	2083	0	2157	345	0
25	BD	1565	0	1616	269	0
25	DD	1565	0	1616	291	0
26	BE	1552	0	1619	203	0
26	DE	1552	0	1619	266	0
27	BF	1411	0	1447	208	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	BG	1323	0	1374	211	0
28	DG	1323	0	1374	199	0
29	BH	1111	0	1148	166	0
29	DH	1111	0	1148	175	0
30	BI	1032	0	1088	114	0
30	DI	1032	0	1088	120	0
31	BJ	1129	0	1162	216	0
31	DJ	1129	0	1162	202	0
32	BK	939	0	1012	164	0
32	DK	939	0	1012	183	0
33	BL	1045	0	1117	169	0
33	DL	1045	0	1117	192	0
34	BM	1074	0	1157	146	0
34	DM	1074	0	1157	150	0
35	BN	961	0	1000	123	0
35	DN	961	0	1000	207	0
36	BO	892	0	923	92	0
36	DO	892	0	923	107	0
37	BP	917	0	965	195	0
37	DP	917	0	965	172	0
38	BQ	947	0	1022	191	0
38	DQ	947	0	1022	180	0
39	BR	816	0	839	138	0
39	DR	816	0	839	137	0
40	BS	857	0	922	110	0
40	DS	857	0	922	131	0
41	BT	739	0	807	156	0
41	DT	739	0	807	159	0
42	BU	780	0	834	84	0
42	DU	780	0	834	133	0
43	BV	753	0	780	76	0
43	DV	753	0	780	108	0
44	BW	596	0	610	229	0
44	DW	596	0	610	174	0
45	BX	625	0	655	104	0
45	DX	625	0	655	114	0
46	BY	509	0	543	69	0
46	DY	509	0	543	102	0
47	BZ	449	0	491	58	0
47	DZ	449	0	491	58	0
48	B0	444	0	461	32	0
48	D0	444	0	461	75	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	B1	410	0	440	57	0
49	D1	410	0	440	53	0
50	B2	377	0	418	36	0
50	D2	377	0	418	66	0
51	B3	504	0	574	53	0
51	D3	504	0	574	67	0
52	B4	302	0	340	47	0
52	D4	302	0	342	41	0
53	CA	32831	0	16521	2416	0
54	CG	1175	0	1230	194	0
55	CM	877	0	937	167	0
56	CP	639	0	656	101	0
57	DB	2507	0	1270	234	0
58	DF	1420	0	1460	282	0
59	AA	42	0	0	0	0
59	AN	1	0	0	0	0
59	BA	134	0	0	0	0
59	BB	4	0	0	0	0
59	BL	1	0	0	0	0
59	CA	42	0	0	0	0
59	DA	132	0	0	0	0
59	DB	1	0	0	0	0
59	DC	2	0	0	0	0
59	DE	1	0	0	0	0
59	DJ	1	0	0	0	0
60	BA	27	0	32	2	0
61	B4	1	0	0	0	0
61	D4	1	0	0	0	0
62	AA	197	0	0	5	0
62	AE	1	0	0	0	0
62	AL	1	0	0	0	0
62	AN	6	0	0	2	0
62	AT	2	0	0	0	0
62	AU	1	0	0	0	0
62	B2	2	0	0	0	0
62	B3	2	0	0	1	0
62	B4	1	0	0	0	0
62	BA	601	0	0	48	0
62	BB	20	0	0	1	0
62	BC	8	0	0	0	0
62	BD	4	0	0	1	0
62	BE	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	BL	3	0	0	1	0
62	BN	3	0	0	1	0
62	BQ	1	0	0	0	0
62	BR	1	0	0	1	0
62	BT	3	0	0	0	0
62	CA	193	0	0	7	0
62	CE	4	0	0	0	0
62	CI	1	0	0	0	0
62	CL	1	0	0	0	0
62	CN	3	0	0	0	0
62	CT	3	0	0	0	0
62	CU	2	0	0	0	0
62	D2	2	0	0	0	0
62	D3	1	0	0	0	0
62	D4	4	0	0	0	0
62	DA	599	0	0	28	0
62	DB	4	0	0	0	0
62	DC	9	0	0	2	0
62	DD	2	0	0	0	0
62	DE	3	0	0	0	0
62	DJ	5	0	0	0	0
62	DL	5	0	0	1	0
62	DN	3	0	0	0	0
62	DT	3	0	0	1	0
62	DU	2	0	0	0	0
62	DV	1	0	0	0	0
All	All	284501	0	190871	25099	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 53.

The worst 5 of 25099 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
22:BA:900:A:C2'	22:BA:901:C:H5'	1.40	1.46
2:AB:108:GLN:O	2:AB:110:ILE:N	1.58	1.37
22:BA:1073:A:C2'	22:BA:1074:G:H5''	1.54	1.35
2:CB:93:HIS:CG	2:CB:145:ASN:O	1.88	1.27
28:BG:84:LYS:HG3	28:BG:132:LEU:N	1.49	1.26

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	AB	216/218 (99%)	121 (56%)	65 (30%)	30 (14%)	0	2
2	CB	216/218 (99%)	145 (67%)	54 (25%)	17 (8%)	1	13
3	AC	204/206 (99%)	154 (76%)	33 (16%)	17 (8%)	1	12
3	CC	204/206 (99%)	147 (72%)	40 (20%)	17 (8%)	1	12
4	AD	203/205 (99%)	134 (66%)	42 (21%)	27 (13%)	0	3
4	CD	203/205 (99%)	139 (68%)	38 (19%)	26 (13%)	0	3
5	AE	148/150 (99%)	105 (71%)	26 (18%)	17 (12%)	1	5
5	CE	148/150 (99%)	110 (74%)	23 (16%)	15 (10%)	1	8
6	AF	98/100 (98%)	71 (72%)	19 (19%)	8 (8%)	1	12
6	CF	98/100 (98%)	62 (63%)	27 (28%)	9 (9%)	1	10
7	AG	149/151 (99%)	107 (72%)	34 (23%)	8 (5%)	3	26
8	AH	127/129 (98%)	92 (72%)	27 (21%)	8 (6%)	2	20
8	CH	127/129 (98%)	87 (68%)	30 (24%)	10 (8%)	1	13
9	AI	125/127 (98%)	83 (66%)	31 (25%)	11 (9%)	1	11
9	CI	125/127 (98%)	87 (70%)	29 (23%)	9 (7%)	2	16
10	AJ	96/98 (98%)	64 (67%)	19 (20%)	13 (14%)	0	3
10	CJ	96/98 (98%)	58 (60%)	24 (25%)	14 (15%)	0	2
11	AK	115/117 (98%)	85 (74%)	18 (16%)	12 (10%)	1	7
11	CK	115/117 (98%)	89 (77%)	17 (15%)	9 (8%)	1	13
12	AL	121/123 (98%)	84 (69%)	21 (17%)	16 (13%)	0	3
12	CL	121/123 (98%)	84 (69%)	25 (21%)	12 (10%)	1	8
13	AM	112/114 (98%)	87 (78%)	17 (15%)	8 (7%)	2	17
14	AN	92/100 (92%)	54 (59%)	23 (25%)	15 (16%)	0	1
14	CN	91/100 (91%)	58 (64%)	27 (30%)	6 (7%)	2	19
15	AO	86/88 (98%)	58 (67%)	22 (26%)	6 (7%)	2	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	CO	86/88 (98%)	68 (79%)	15 (17%)	3 (4%)	6	41
16	AP	80/82 (98%)	58 (72%)	13 (16%)	9 (11%)	1	5
17	AQ	78/80 (98%)	46 (59%)	20 (26%)	12 (15%)	0	2
17	CQ	78/80 (98%)	60 (77%)	8 (10%)	10 (13%)	0	3
18	AR	53/55 (96%)	39 (74%)	13 (24%)	1 (2%)	12	60
18	CR	53/55 (96%)	40 (76%)	11 (21%)	2 (4%)	5	37
19	AS	77/79 (98%)	56 (73%)	14 (18%)	7 (9%)	1	10
19	CS	77/79 (98%)	46 (60%)	24 (31%)	7 (9%)	1	10
20	AT	83/85 (98%)	54 (65%)	20 (24%)	9 (11%)	1	6
20	CT	83/85 (98%)	55 (66%)	21 (25%)	7 (8%)	1	12
21	AU	49/51 (96%)	25 (51%)	17 (35%)	7 (14%)	0	2
21	CU	49/51 (96%)	24 (49%)	11 (22%)	14 (29%)	0	0
24	BC	269/271 (99%)	197 (73%)	53 (20%)	19 (7%)	2	17
24	DC	269/271 (99%)	177 (66%)	55 (20%)	37 (14%)	0	3
25	BD	207/209 (99%)	140 (68%)	38 (18%)	29 (14%)	0	2
25	DD	207/209 (99%)	134 (65%)	39 (19%)	34 (16%)	0	1
26	BE	199/201 (99%)	143 (72%)	35 (18%)	21 (11%)	1	6
26	DE	199/201 (99%)	122 (61%)	51 (26%)	26 (13%)	0	3
27	BF	175/177 (99%)	127 (73%)	33 (19%)	15 (9%)	1	11
28	BG	174/176 (99%)	115 (66%)	32 (18%)	27 (16%)	0	2
28	DG	174/176 (99%)	100 (58%)	43 (25%)	31 (18%)	0	1
29	BH	147/149 (99%)	67 (46%)	46 (31%)	34 (23%)	0	0
29	DH	147/149 (99%)	71 (48%)	58 (40%)	18 (12%)	1	4
30	BI	139/141 (99%)	84 (60%)	41 (30%)	14 (10%)	1	8
30	DI	139/141 (99%)	78 (56%)	43 (31%)	18 (13%)	0	3
31	BJ	140/142 (99%)	101 (72%)	23 (16%)	16 (11%)	1	5
31	DJ	140/142 (99%)	90 (64%)	30 (21%)	20 (14%)	0	2
32	BK	120/122 (98%)	83 (69%)	15 (12%)	22 (18%)	0	1
32	DK	120/122 (98%)	83 (69%)	13 (11%)	24 (20%)	0	1
33	BL	141/143 (99%)	104 (74%)	28 (20%)	9 (6%)	2	20
33	DL	141/143 (99%)	81 (57%)	42 (30%)	18 (13%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	BM	134/136 (98%)	91 (68%)	25 (19%)	18 (13%)	0	3
34	DM	134/136 (98%)	93 (69%)	24 (18%)	17 (13%)	0	3
35	BN	118/120 (98%)	87 (74%)	21 (18%)	10 (8%)	1	11
35	DN	118/120 (98%)	72 (61%)	30 (25%)	16 (14%)	0	3
36	BO	114/116 (98%)	87 (76%)	20 (18%)	7 (6%)	2	22
36	DO	114/116 (98%)	76 (67%)	26 (23%)	12 (10%)	1	7
37	BP	112/114 (98%)	75 (67%)	21 (19%)	16 (14%)	0	2
37	DP	112/114 (98%)	65 (58%)	27 (24%)	20 (18%)	0	1
38	BQ	115/117 (98%)	91 (79%)	17 (15%)	7 (6%)	2	22
38	DQ	115/117 (98%)	78 (68%)	24 (21%)	13 (11%)	1	5
39	BR	101/103 (98%)	76 (75%)	16 (16%)	9 (9%)	1	10
39	DR	101/103 (98%)	67 (66%)	25 (25%)	9 (9%)	1	10
40	BS	108/110 (98%)	77 (71%)	25 (23%)	6 (6%)	3	25
40	DS	108/110 (98%)	75 (69%)	21 (19%)	12 (11%)	1	6
41	BT	91/93 (98%)	55 (60%)	19 (21%)	17 (19%)	0	1
41	DT	91/93 (98%)	47 (52%)	28 (31%)	16 (18%)	0	1
42	BU	100/102 (98%)	63 (63%)	22 (22%)	15 (15%)	0	2
42	DU	100/102 (98%)	50 (50%)	23 (23%)	27 (27%)	0	0
43	BV	92/94 (98%)	80 (87%)	10 (11%)	2 (2%)	10	56
43	DV	92/94 (98%)	61 (66%)	24 (26%)	7 (8%)	2	15
44	BW	77/79 (98%)	27 (35%)	25 (32%)	25 (32%)	0	0
44	DW	77/79 (98%)	34 (44%)	22 (29%)	21 (27%)	0	0
45	BX	75/77 (97%)	54 (72%)	15 (20%)	6 (8%)	1	13
45	DX	75/77 (97%)	46 (61%)	24 (32%)	5 (7%)	2	18
46	BY	61/63 (97%)	37 (61%)	16 (26%)	8 (13%)	0	3
46	DY	61/63 (97%)	40 (66%)	16 (26%)	5 (8%)	1	12
47	BZ	56/58 (97%)	44 (79%)	10 (18%)	2 (4%)	5	40
47	DZ	56/58 (97%)	35 (62%)	15 (27%)	6 (11%)	1	6
48	B0	54/56 (96%)	42 (78%)	8 (15%)	4 (7%)	2	15
48	D0	54/56 (96%)	37 (68%)	12 (22%)	5 (9%)	1	9
49	B1	48/50 (96%)	37 (77%)	6 (12%)	5 (10%)	1	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	D1	48/50 (96%)	33 (69%)	10 (21%)	5 (10%)	1	7
50	B2	44/46 (96%)	37 (84%)	6 (14%)	1 (2%)	10	54
50	D2	44/46 (96%)	32 (73%)	6 (14%)	6 (14%)	0	3
51	B3	62/64 (97%)	50 (81%)	8 (13%)	4 (6%)	2	19
51	D3	62/64 (97%)	40 (64%)	17 (27%)	5 (8%)	1	13
52	B4	36/38 (95%)	28 (78%)	4 (11%)	4 (11%)	1	6
52	D4	36/38 (95%)	24 (67%)	6 (17%)	6 (17%)	0	1
54	CG	148/150 (99%)	103 (70%)	34 (23%)	11 (7%)	2	15
55	CM	111/113 (98%)	63 (57%)	36 (32%)	12 (11%)	1	6
56	CP	78/80 (98%)	50 (64%)	19 (24%)	9 (12%)	1	5
58	DF	176/178 (99%)	98 (56%)	46 (26%)	32 (18%)	0	1
All	All	11238/11447 (98%)	7490 (67%)	2445 (22%)	1303 (12%)	1	5

5 of 1303 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	20	ARG
2	AB	21	TYR
2	AB	37	VAL
2	AB	40	ILE
2	AB	75	ALA

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	AB	180/180 (100%)	147 (82%)	33 (18%)	2	12
2	CB	180/180 (100%)	152 (84%)	28 (16%)	4	19
3	AC	170/170 (100%)	140 (82%)	30 (18%)	3	14
3	CC	170/170 (100%)	153 (90%)	17 (10%)	11	43
4	AD	172/172 (100%)	142 (83%)	30 (17%)	3	14
4	CD	172/172 (100%)	140 (81%)	32 (19%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	AE	113/113 (100%)	87 (77%)	26 (23%)	1	5
5	CE	113/113 (100%)	92 (81%)	21 (19%)	2	12
6	AF	87/87 (100%)	74 (85%)	13 (15%)	4	22
6	CF	87/87 (100%)	73 (84%)	14 (16%)	3	18
7	AG	124/124 (100%)	109 (88%)	15 (12%)	7	34
8	AH	104/104 (100%)	90 (86%)	14 (14%)	6	28
8	CH	104/104 (100%)	91 (88%)	13 (12%)	7	32
9	AI	105/105 (100%)	87 (83%)	18 (17%)	3	15
9	CI	105/105 (100%)	92 (88%)	13 (12%)	7	32
10	AJ	86/86 (100%)	74 (86%)	12 (14%)	5	25
10	CJ	86/86 (100%)	77 (90%)	9 (10%)	10	41
11	AK	90/90 (100%)	72 (80%)	18 (20%)	2	9
11	CK	90/90 (100%)	77 (86%)	13 (14%)	5	24
12	AL	103/103 (100%)	85 (82%)	18 (18%)	3	14
12	CL	103/103 (100%)	86 (84%)	17 (16%)	3	17
13	AM	92/92 (100%)	88 (96%)	4 (4%)	40	82
14	AN	79/83 (95%)	72 (91%)	7 (9%)	14	51
14	CN	79/83 (95%)	68 (86%)	11 (14%)	5	26
15	AO	76/76 (100%)	67 (88%)	9 (12%)	8	35
15	CO	76/76 (100%)	68 (90%)	8 (10%)	10	41
16	AP	65/65 (100%)	58 (89%)	7 (11%)	9	39
17	AQ	74/74 (100%)	60 (81%)	14 (19%)	2	11
17	CQ	74/74 (100%)	62 (84%)	12 (16%)	3	18
18	AR	48/48 (100%)	46 (96%)	2 (4%)	40	82
18	CR	48/48 (100%)	44 (92%)	4 (8%)	16	56
19	AS	70/70 (100%)	63 (90%)	7 (10%)	11	43
19	CS	70/70 (100%)	63 (90%)	7 (10%)	11	43
20	AT	65/65 (100%)	50 (77%)	15 (23%)	1	5
20	CT	65/65 (100%)	55 (85%)	10 (15%)	4	20
21	AU	44/44 (100%)	37 (84%)	7 (16%)	4	18
21	CU	44/44 (100%)	36 (82%)	8 (18%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	BC	216/216 (100%)	166 (77%)	50 (23%)	1	5
24	DC	216/216 (100%)	189 (88%)	27 (12%)	7	32
25	BD	164/164 (100%)	131 (80%)	33 (20%)	2	9
25	DD	164/164 (100%)	139 (85%)	25 (15%)	4	21
26	BE	165/165 (100%)	126 (76%)	39 (24%)	1	4
26	DE	165/165 (100%)	148 (90%)	17 (10%)	10	42
27	BF	148/148 (100%)	124 (84%)	24 (16%)	3	18
28	BG	137/137 (100%)	107 (78%)	30 (22%)	1	7
28	DG	137/137 (100%)	121 (88%)	16 (12%)	8	36
29	BH	114/114 (100%)	96 (84%)	18 (16%)	4	19
29	DH	114/114 (100%)	98 (86%)	16 (14%)	5	25
30	BI	109/109 (100%)	91 (84%)	18 (16%)	3	17
30	DI	109/109 (100%)	103 (94%)	6 (6%)	30	75
31	BJ	116/116 (100%)	84 (72%)	32 (28%)	0	2
31	DJ	116/116 (100%)	103 (89%)	13 (11%)	9	38
32	BK	103/103 (100%)	78 (76%)	25 (24%)	1	3
32	DK	103/103 (100%)	82 (80%)	21 (20%)	2	8
33	BL	102/102 (100%)	71 (70%)	31 (30%)	0	1
33	DL	102/102 (100%)	89 (87%)	13 (13%)	6	31
34	BM	109/109 (100%)	87 (80%)	22 (20%)	2	9
34	DM	109/109 (100%)	103 (94%)	6 (6%)	30	75
35	BN	100/100 (100%)	83 (83%)	17 (17%)	3	15
35	DN	100/100 (100%)	80 (80%)	20 (20%)	2	9
36	BO	86/86 (100%)	71 (83%)	15 (17%)	3	14
36	DO	86/86 (100%)	78 (91%)	8 (9%)	13	48
37	BP	99/99 (100%)	72 (73%)	27 (27%)	0	2
37	DP	99/99 (100%)	89 (90%)	10 (10%)	11	42
38	BQ	89/89 (100%)	72 (81%)	17 (19%)	2	10
38	DQ	89/89 (100%)	75 (84%)	14 (16%)	4	19
39	BR	84/84 (100%)	66 (79%)	18 (21%)	1	7
39	DR	84/84 (100%)	71 (84%)	13 (16%)	4	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	BS	93/93 (100%)	74 (80%)	19 (20%)	2	8
40	DS	93/93 (100%)	79 (85%)	14 (15%)	4	21
41	BT	80/80 (100%)	59 (74%)	21 (26%)	1	2
41	DT	80/80 (100%)	74 (92%)	6 (8%)	19	62
42	BU	83/83 (100%)	66 (80%)	17 (20%)	2	8
42	DU	83/83 (100%)	73 (88%)	10 (12%)	7	34
43	BV	78/78 (100%)	61 (78%)	17 (22%)	1	7
43	DV	78/78 (100%)	70 (90%)	8 (10%)	10	42
44	BW	59/59 (100%)	41 (70%)	18 (30%)	0	1
44	DW	59/59 (100%)	44 (75%)	15 (25%)	1	3
45	BX	67/67 (100%)	51 (76%)	16 (24%)	1	4
45	DX	67/67 (100%)	57 (85%)	10 (15%)	4	22
46	BY	55/55 (100%)	45 (82%)	10 (18%)	2	12
46	DY	55/55 (100%)	52 (94%)	3 (6%)	30	75
47	BZ	48/48 (100%)	32 (67%)	16 (33%)	0	1
47	DZ	48/48 (100%)	40 (83%)	8 (17%)	3	16
48	B0	47/47 (100%)	34 (72%)	13 (28%)	0	2
48	D0	47/47 (100%)	40 (85%)	7 (15%)	4	22
49	B1	45/45 (100%)	38 (84%)	7 (16%)	4	19
49	D1	45/45 (100%)	41 (91%)	4 (9%)	14	51
50	B2	38/38 (100%)	31 (82%)	7 (18%)	2	12
50	D2	38/38 (100%)	35 (92%)	3 (8%)	18	59
51	B3	51/51 (100%)	45 (88%)	6 (12%)	8	35
51	D3	51/51 (100%)	40 (78%)	11 (22%)	1	7
52	B4	34/34 (100%)	29 (85%)	5 (15%)	4	23
52	D4	34/34 (100%)	29 (85%)	5 (15%)	4	23
54	CG	123/123 (100%)	104 (85%)	19 (15%)	4	20
55	CM	91/91 (100%)	81 (89%)	10 (11%)	9	39
56	CP	65/65 (100%)	54 (83%)	11 (17%)	3	16
58	DF	149/149 (100%)	127 (85%)	22 (15%)	4	22
All	All	9331/9339 (100%)	7816 (84%)	1515 (16%)	3	18

5 of 1515 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
38	BQ	40	LYS
47	BZ	56	VAL
39	DR	13	ARG
39	BR	46	GLU
42	BU	86	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 355 such sidechains are listed below:

Mol	Chain	Res	Type
40	BS	61	ASN
3	CC	18	ASN
42	DU	52	ASN
42	BU	52	ASN
46	BY	41	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1532/1533 (99%)	482 (31%)	233 (15%)
22	BA	2850/2903 (98%)	900 (31%)	473 (16%)
22	DA	2839/2903 (97%)	1062 (37%)	506 (17%)
23	BB	117/118 (99%)	32 (27%)	18 (15%)
53	CA	1529/1530 (99%)	548 (35%)	236 (15%)
57	DB	116/117 (99%)	38 (32%)	15 (12%)
All	All	8983/9104 (98%)	3062 (34%)	1481 (16%)

5 of 3062 RNA backbone outliers are listed below:

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

5 of 1481 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	BA	2654	A

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Mol	Chain	Res	Type
53	CA	531	U
22	DA	2286	G
22	BA	2791	G
53	CA	116	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 364 ligands modelled in this entry, 363 are monoatomic - leaving 1 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	$\# Z > 2$
60	CLY	BA	3135	-	28,28,28	1.57	6 (21%)	40,40,40	1.64	9 (22%)

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
60	CLY	BA	3135	-	-	0/21/53/53	0/2/2/2

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	BA	3135	CLY	C14-N2	3.23	1.51	1.47
60	BA	3135	CLY	C15-N2	2.95	1.52	1.46
60	BA	3135	CLY	C5-S1	2.88	1.85	1.81
60	BA	3135	CLY	O5-C4	2.59	1.48	1.43
60	BA	3135	CLY	C11-N2	2.45	1.51	1.48

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	BA	3135	CLY	C8-C7-N1	-5.57	104.32	111.60
60	BA	3135	CLY	C11-C10-N1	-3.38	109.28	116.70
60	BA	3135	CLY	O4-C1-C2	-2.47	104.84	110.36
60	BA	3135	CLY	C10-C11-N2	-2.35	107.53	112.34
60	BA	3135	CLY	C5-O5-C4	-2.28	111.29	114.21

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	1533/1533 (100%)	-0.63	16 (1%) 79 32	26, 75, 180, 427	0
2	AB	218/218 (100%)	0.62	14 (6%) 19 4	111, 151, 210, 294	0
2	CB	218/218 (100%)	0.94	24 (11%) 6 2	125, 161, 248, 300	0
3	AC	206/206 (100%)	0.15	3 (1%) 70 23	51, 97, 147, 208	0
3	CC	206/206 (100%)	0.48	5 (2%) 56 14	74, 144, 225, 261	0
4	AD	205/205 (100%)	-0.13	2 (0%) 79 32	43, 83, 164, 311	0
4	CD	205/205 (100%)	-0.23	0 100 100	31, 59, 113, 227	0
5	AE	150/150 (100%)	0.06	1 (0%) 84 41	55, 78, 148, 255	0
5	CE	150/150 (100%)	0.06	0 100 100	55, 85, 149, 258	0
6	AF	100/100 (100%)	-0.05	0 100 100	53, 90, 143, 171	0
6	CF	100/100 (100%)	0.21	1 (1%) 79 32	72, 107, 167, 226	0
7	AG	151/151 (100%)	0.18	3 (1%) 62 18	67, 129, 199, 248	0
8	AH	129/129 (100%)	0.05	0 100 100	38, 71, 123, 214	0
8	CH	129/129 (100%)	0.25	0 100 100	53, 100, 161, 214	0
9	AI	127/127 (100%)	0.54	9 (7%) 16 4	66, 125, 243, 279	0
9	CI	127/127 (100%)	1.13	21 (16%) 2 1	111, 184, 282, 308	0
10	AJ	98/98 (100%)	0.43	6 (6%) 21 5	60, 114, 210, 262	0
10	CJ	98/98 (100%)	1.32	22 (22%) 1 1	103, 188, 266, 292	0
11	AK	117/117 (100%)	0.18	1 (0%) 81 36	36, 98, 174, 203	0
11	CK	117/117 (100%)	0.24	1 (0%) 81 36	55, 104, 165, 196	0
12	AL	123/123 (100%)	-0.21	1 (0%) 83 38	15, 54, 116, 167	0
12	CL	123/123 (100%)	0.09	1 (0%) 83 38	36, 73, 121, 188	0
13	AM	114/114 (100%)	0.17	1 (0%) 81 36	76, 125, 196, 274	0
14	AN	96/100 (96%)	0.18	2 (2%) 60 17	59, 102, 195, 267	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
14	CN	95/100 (95%)	1.31	21 (22%) 1 1	109, 221, 327, 373	0
15	AO	88/88 (100%)	-0.32	0 100 100	36, 70, 123, 182	0
15	CO	88/88 (100%)	-0.10	0 100 100	59, 103, 158, 277	0
16	AP	82/82 (100%)	0.32	4 (4%) 28 6	44, 74, 148, 243	0
17	AQ	80/80 (100%)	0.19	2 (2%) 54 13	29, 78, 141, 267	0
17	CQ	80/80 (100%)	0.39	3 (3%) 38 8	48, 106, 161, 199	0
18	AR	55/55 (100%)	-0.04	2 (3%) 41 9	60, 86, 161, 196	0
18	CR	55/55 (100%)	0.21	1 (1%) 65 20	47, 92, 186, 230	0
19	AS	79/79 (100%)	0.84	6 (7%) 14 4	79, 127, 199, 277	0
19	CS	79/79 (100%)	1.58	23 (29%) 1 1	181, 371, 451, 469	0
20	AT	85/85 (100%)	-0.01	0 100 100	43, 76, 116, 143	0
20	CT	85/85 (100%)	0.68	5 (5%) 22 5	58, 117, 197, 268	0
21	AU	51/51 (100%)	1.33	13 (25%) 1 1	88, 157, 204, 230	0
21	CU	51/51 (100%)	0.57	3 (5%) 22 5	58, 111, 182, 320	0
22	BA	2854/2903 (98%)	-0.60	32 (1%) 77 30	4, 28, 155, 403	0
22	DA	2841/2903 (97%)	0.11	69 (2%) 56 14	49, 122, 252, 460	0
23	BB	118/118 (100%)	-0.68	0 100 100	13, 43, 77, 106	0
24	BC	271/271 (100%)	-0.27	1 (0%) 90 55	5, 39, 81, 171	0
24	DC	271/271 (100%)	0.22	3 (1%) 77 30	51, 96, 147, 192	0
25	BD	209/209 (100%)	-0.30	0 100 100	3, 23, 72, 171	0
25	DD	209/209 (100%)	0.28	3 (1%) 72 25	50, 111, 176, 290	0
26	BE	201/201 (100%)	-0.23	0 100 100	2, 37, 98, 185	0
26	DE	201/201 (100%)	0.98	28 (13%) 4 2	62, 197, 395, 486	0
27	BF	177/177 (100%)	-0.01	1 (0%) 86 44	27, 70, 127, 197	0
28	BG	176/176 (100%)	-0.09	0 100 100	23, 60, 119, 205	0
28	DG	176/176 (100%)	0.92	27 (15%) 3 1	95, 195, 279, 335	0
29	BH	149/149 (100%)	1.43	46 (30%) 1 1	40, 177, 291, 362	0
29	DH	149/149 (100%)	1.73	46 (30%) 1 1	82, 181, 277, 319	0
30	BI	141/141 (100%)	1.75	38 (26%) 1 1	162, 269, 338, 374	0
30	DI	141/141 (100%)	1.73	43 (30%) 1 1	210, 324, 369, 408	0
31	BJ	142/142 (100%)	-0.36	0 100 100	6, 21, 60, 138	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
31	DJ	142/142 (100%)	0.49	5 (3%) 42 9	63, 102, 163, 184	0
32	BK	122/122 (100%)	-0.32	0 100 100	7, 26, 74, 263	0
32	DK	122/122 (100%)	0.54	4 (3%) 44 10	52, 95, 164, 236	0
33	BL	143/143 (100%)	-0.30	0 100 100	3, 35, 77, 103	0
33	DL	143/143 (100%)	0.77	14 (9%) 8 2	58, 159, 278, 348	0
34	BM	136/136 (100%)	-0.34	0 100 100	4, 26, 66, 135	0
34	DM	136/136 (100%)	0.38	4 (2%) 49 11	44, 105, 164, 196	0
35	BN	120/120 (100%)	-0.37	0 100 100	6, 20, 43, 151	0
35	DN	120/120 (100%)	0.79	10 (8%) 11 3	79, 127, 200, 268	0
36	BO	116/116 (100%)	-0.20	0 100 100	26, 43, 77, 126	0
36	DO	116/116 (100%)	1.17	24 (20%) 1 1	124, 169, 240, 292	0
37	BP	114/114 (100%)	-0.21	0 100 100	9, 35, 83, 148	0
37	DP	114/114 (100%)	0.54	6 (5%) 25 5	62, 114, 174, 238	0
38	BQ	117/117 (100%)	-0.39	0 100 100	3, 16, 43, 199	0
38	DQ	117/117 (100%)	0.65	5 (4%) 34 7	66, 103, 194, 288	0
39	BR	103/103 (100%)	-0.32	0 100 100	4, 31, 80, 180	0
39	DR	103/103 (100%)	0.93	11 (10%) 6 2	67, 130, 227, 316	0
40	BS	110/110 (100%)	-0.35	0 100 100	4, 17, 52, 175	0
40	DS	110/110 (100%)	1.03	13 (11%) 5 2	59, 130, 231, 279	0
41	BT	93/93 (100%)	-0.04	1 (1%) 77 30	19, 43, 128, 185	0
41	DT	93/93 (100%)	1.48	26 (27%) 1 1	123, 205, 306, 347	0
42	BU	102/102 (100%)	-0.02	0 100 100	18, 49, 120, 241	0
42	DU	102/102 (100%)	1.90	38 (37%) 1 0	123, 285, 434, 557	0
43	BV	94/94 (100%)	-0.13	0 100 100	15, 43, 86, 142	0
43	DV	94/94 (100%)	0.49	3 (3%) 45 10	97, 143, 194, 233	0
44	BW	79/79 (100%)	-0.02	0 100 100	10, 30, 105, 223	0
44	DW	79/79 (100%)	1.38	22 (27%) 1 1	82, 140, 238, 284	0
45	BX	77/77 (100%)	-0.24	0 100 100	11, 42, 84, 117	0
45	DX	77/77 (100%)	0.66	4 (5%) 26 6	78, 117, 171, 236	0
46	BY	63/63 (100%)	0.16	2 (3%) 45 10	30, 66, 136, 222	0
46	DY	63/63 (100%)	1.11	14 (22%) 1 1	143, 309, 433, 440	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
47	BZ	58/58 (100%)	-0.30	0 100 100	8, 22, 56, 111	0
47	DZ	58/58 (100%)	0.15	0 100 100	78, 119, 208, 217	0
48	B0	56/56 (100%)	-0.42	0 100 100	3, 24, 70, 159	0
48	D0	56/56 (100%)	0.71	2 (3%) 41 9	63, 139, 242, 298	0
49	B1	50/50 (100%)	0.04	0 100 100	22, 48, 99, 165	0
49	D1	50/50 (100%)	1.29	8 (16%) 3 1	99, 170, 210, 236	0
50	B2	46/46 (100%)	-0.36	0 100 100	7, 26, 52, 155	0
50	D2	46/46 (100%)	0.62	1 (2%) 59 16	81, 118, 175, 233	0
51	B3	64/64 (100%)	-0.41	0 100 100	5, 23, 44, 70	0
51	D3	64/64 (100%)	1.08	14 (21%) 1 1	65, 128, 183, 257	0
52	B4	38/38 (100%)	0.09	0 100 100	21, 45, 86, 124	0
52	D4	38/38 (100%)	1.69	15 (39%) 1 0	79, 137, 187, 227	0
53	CA	1530/1530 (100%)	-0.15	31 (2%) 62 18	34, 102, 281, 444	0
54	CG	150/150 (100%)	1.35	42 (28%) 1 1	107, 224, 298, 322	0
55	CM	113/113 (100%)	1.73	42 (37%) 1 0	182, 402, 494, 538	0
56	CP	80/80 (100%)	0.57	4 (5%) 28 6	51, 94, 155, 236	0
57	DB	117/117 (100%)	-0.13	1 (0%) 81 36	95, 169, 224, 274	0
58	DF	178/178 (100%)	1.04	24 (13%) 4 2	183, 225, 286, 338	0
All	All	20431/20551 (99%)	0.09	944 (4%) 31 7	2, 94, 269, 557	0

The worst 5 of 944 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
29	DH	92	GLY	15.4
22	BA	2179	C	12.7
29	DH	105	ALA	11.6
29	DH	124	THR	11.4
30	BI	2	LYS	10.1

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
59	MG	DA	3062	1/1	1.56	386.71	211,211,211,211	0
59	MG	DA	3019	1/1	2.15	106.35	247,247,247,247	0
59	MG	DA	3073	1/1	2.09	100.97	274,274,274,274	0
59	MG	BA	3024	1/1	0.51	76.83	166,166,166,166	0
59	MG	DA	3057	1/1	0.55	69.46	227,227,227,227	0
59	MG	DJ	201	1/1	2.33	68.94	230,230,230,230	0
59	MG	DA	3108	1/1	0.54	49.76	185,185,185,185	0
59	MG	DA	3005	1/1	1.33	47.32	309,309,309,309	0
59	MG	BA	3117	1/1	0.24	42.60	157,157,157,157	0
59	MG	BA	3033	1/1	0.30	31.74	162,162,162,162	0
59	MG	DA	3059	1/1	0.84	31.65	200,200,200,200	0
59	MG	BA	3054	1/1	0.40	28.99	189,189,189,189	0
59	MG	BA	3035	1/1	0.47	28.12	171,171,171,171	0
59	MG	DA	3061	1/1	1.01	25.05	229,229,229,229	0
59	MG	DA	3003	1/1	0.82	23.78	236,236,236,236	0
59	MG	BA	3129	1/1	0.92	23.08	214,214,214,214	0
59	MG	CA	1627	1/1	0.38	22.00	181,181,181,181	0
59	MG	AA	1618	1/1	0.59	20.85	197,197,197,197	0
59	MG	BA	3074	1/1	0.23	19.51	93,93,93,93	0
59	MG	CA	1628	1/1	1.51	19.13	260,260,260,260	0
59	MG	AA	1626	1/1	0.28	18.12	117,117,117,117	0
59	MG	DA	3021	1/1	0.36	17.79	199,199,199,199	0
59	MG	CA	1624	1/1	0.67	17.09	165,165,165,165	0
59	MG	DA	3077	1/1	0.48	16.98	222,222,222,222	0
59	MG	CA	1619	1/1	0.32	16.68	214,214,214,214	0
59	MG	DA	3131	1/1	0.32	16.25	212,212,212,212	0
59	MG	DA	3126	1/1	0.58	15.69	200,200,200,200	0
59	MG	BB	201	1/1	0.24	15.40	222,222,222,222	0
59	MG	BA	3069	1/1	0.32	14.08	151,151,151,151	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
59	MG	BA	3055	1/1	0.26	13.65	205,205,205,205	0
59	MG	BA	3026	1/1	0.29	13.24	133,133,133,133	0
59	MG	AA	1608	1/1	0.26	12.85	68,68,68,68	0
59	MG	BA	3085	1/1	0.22	12.44	100,100,100,100	0
59	MG	DA	3075	1/1	0.62	12.31	174,174,174,174	0
59	MG	BA	3096	1/1	0.17	12.14	102,102,102,102	0
59	MG	CA	1603	1/1	0.24	11.38	162,162,162,162	0
59	MG	DA	3025	1/1	1.41	11.33	278,278,278,278	0
59	MG	BA	3060	1/1	0.29	10.53	210,210,210,210	0
59	MG	BA	3018	1/1	0.28	10.47	6,6,6,6	0
59	MG	BA	3110	1/1	0.25	9.94	92,92,92,92	0
59	MG	CA	1612	1/1	0.32	9.87	136,136,136,136	0
59	MG	BA	3081	1/1	0.16	9.85	86,86,86,86	0
59	MG	CA	1626	1/1	0.23	9.58	23,23,23,23	0
59	MG	DA	3107	1/1	0.49	9.39	161,161,161,161	0
59	MG	BA	3100	1/1	0.25	8.92	89,89,89,89	0
59	MG	DE	301	1/1	0.50	8.62	131,131,131,131	0
59	MG	BA	3039	1/1	0.21	8.44	6,6,6,6	0
59	MG	DA	3035	1/1	0.42	7.78	194,194,194,194	0
59	MG	BA	3056	1/1	0.17	7.61	169,169,169,169	0
59	MG	CA	1614	1/1	0.38	7.51	210,210,210,210	0
59	MG	DA	3078	1/1	0.35	7.49	180,180,180,180	0
59	MG	DA	3129	1/1	1.64	6.88	233,233,233,233	0
59	MG	BA	3032	1/1	0.19	5.86	3,3,3,3	0
59	MG	DA	3002	1/1	0.36	5.81	180,180,180,180	0
59	MG	DA	3074	1/1	0.28	5.77	190,190,190,190	0
59	MG	DA	3114	1/1	0.31	5.68	167,167,167,167	0
59	MG	CA	1611	1/1	0.23	5.09	112,112,112,112	0
59	MG	AA	1614	1/1	0.27	5.04	194,194,194,194	0
59	MG	DA	3128	1/1	0.74	4.89	214,214,214,214	0
59	MG	DA	3084	1/1	0.42	4.79	144,144,144,144	0
59	MG	DA	3063	1/1	0.39	4.79	278,278,278,278	0
59	MG	BA	3027	1/1	0.17	4.57	46,46,46,46	0
59	MG	BA	3082	1/1	0.15	4.57	114,114,114,114	0
59	MG	AA	1625	1/1	0.23	4.42	30,30,30,30	0
59	MG	CA	1641	1/1	0.20	4.10	79,79,79,79	0
59	MG	DA	3090	1/1	0.42	4.07	165,165,165,165	0
59	MG	DA	3087	1/1	0.27	3.98	179,179,179,179	0
59	MG	DA	3027	1/1	0.70	3.94	253,253,253,253	0
59	MG	BA	3043	1/1	0.17	3.91	11,11,11,11	0
59	MG	DA	3122	1/1	0.33	3.87	153,153,153,153	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	BA	3102	1/1	0.17	3.69	3,3,3,3	0
60	CLY	BA	3135	27/27	0.19	3.56	11,17,22,22	0
59	MG	DA	3044	1/1	0.25	3.49	156,156,156,156	0
59	MG	CA	1607	1/1	0.22	3.43	121,121,121,121	0
59	MG	BA	3107	1/1	0.17	3.39	5,5,5,5	0
59	MG	BA	3131	1/1	0.29	3.38	154,154,154,154	0
59	MG	DC	302	1/1	0.27	3.35	129,129,129,129	0
59	MG	BA	3111	1/1	0.20	3.31	77,77,77,77	0
59	MG	DA	3007	1/1	0.37	3.27	254,254,254,254	0
59	MG	AA	1635	1/1	0.14	3.26	194,194,194,194	0
59	MG	AA	1612	1/1	0.20	3.19	105,105,105,105	0
59	MG	DA	3015	1/1	0.22	3.18	183,183,183,183	0
59	MG	CA	1608	1/1	0.22	3.16	41,41,41,41	0
59	MG	AA	1630	1/1	0.18	2.95	189,189,189,189	0
59	MG	DA	3034	1/1	0.32	2.92	125,125,125,125	0
59	MG	DA	3014	1/1	0.30	2.90	172,172,172,172	0
59	MG	DA	3068	1/1	0.47	2.78	209,209,209,209	0
59	MG	DA	3124	1/1	0.65	2.71	176,176,176,176	0
59	MG	BA	3073	1/1	0.16	2.65	8,8,8,8	0
59	MG	BA	3029	1/1	0.17	2.62	3,3,3,3	0
59	MG	BA	3002	1/1	0.15	2.50	85,85,85,85	0
59	MG	CA	1625	1/1	0.21	2.27	100,100,100,100	0
59	MG	DA	3048	1/1	0.28	2.17	218,218,218,218	0
59	MG	CA	1640	1/1	0.15	1.96	157,157,157,157	0
59	MG	AA	1641	1/1	0.16	1.91	22,22,22,22	0
59	MG	BA	3114	1/1	0.15	1.90	4,4,4,4	0
59	MG	BA	3105	1/1	0.17	1.84	42,42,42,42	0
59	MG	DA	3056	1/1	0.52	1.79	197,197,197,197	0
59	MG	CA	1615	1/1	0.17	1.76	172,172,172,172	0
59	MG	BA	3090	1/1	0.15	1.72	128,128,128,128	0
59	MG	DA	3110	1/1	0.28	1.72	153,153,153,153	0
59	MG	BA	3134	1/1	0.18	1.64	219,219,219,219	0
59	MG	DA	3020	1/1	0.20	1.51	49,49,49,49	0
59	MG	DA	3092	1/1	0.27	1.51	229,229,229,229	0
59	MG	DA	3013	1/1	0.24	1.51	126,126,126,126	0
59	MG	AA	1627	1/1	0.18	1.50	132,132,132,132	0
59	MG	BA	3047	1/1	0.16	1.48	111,111,111,111	0
59	MG	DA	3105	1/1	0.22	1.38	262,262,262,262	0
59	MG	DA	3132	1/1	0.29	1.32	174,174,174,174	0
59	MG	CA	1621	1/1	0.22	1.29	46,46,46,46	0
59	MG	BA	3038	1/1	0.15	1.19	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	DA	3028	1/1	0.36	1.18	143,143,143,143	0
59	MG	BA	3109	1/1	0.16	1.17	124,124,124,124	0
59	MG	DA	3103	1/1	0.20	1.07	44,44,44,44	0
59	MG	DA	3052	1/1	0.15	1.02	89,89,89,89	0
59	MG	BA	3011	1/1	0.22	0.99	102,102,102,102	0
59	MG	AA	1605	1/1	0.14	0.95	39,39,39,39	0
59	MG	AA	1621	1/1	0.15	0.94	25,25,25,25	0
59	MG	CA	1637	1/1	0.22	0.86	74,74,74,74	0
59	MG	AN	201	1/1	0.25	0.84	159,159,159,159	0
59	MG	BA	3123	1/1	0.15	0.83	11,11,11,11	0
59	MG	BA	3097	1/1	0.15	0.81	45,45,45,45	0
59	MG	DA	3102	1/1	0.18	0.78	86,86,86,86	0
59	MG	BA	3118	1/1	0.16	0.73	11,11,11,11	0
59	MG	BA	3041	1/1	0.14	0.70	13,13,13,13	0
59	MG	CA	1618	1/1	0.22	0.70	113,113,113,113	0
59	MG	DC	301	1/1	0.22	0.68	145,145,145,145	0
59	MG	AA	1617	1/1	0.16	0.65	115,115,115,115	0
59	MG	DA	3045	1/1	0.20	0.64	78,78,78,78	0
59	MG	BA	3058	1/1	0.16	0.62	107,107,107,107	0
59	MG	DA	3086	1/1	0.18	0.58	139,139,139,139	0
59	MG	CA	1633	1/1	0.15	0.53	63,63,63,63	0
59	MG	CA	1631	1/1	0.22	0.51	93,93,93,93	0
59	MG	BA	3040	1/1	0.15	0.44	11,11,11,11	0
59	MG	BA	3001	1/1	0.14	0.44	116,116,116,116	0
59	MG	BA	3130	1/1	0.24	0.38	97,97,97,97	0
59	MG	DA	3116	1/1	0.23	0.32	77,77,77,77	0
59	MG	AA	1629	1/1	0.18	0.31	180,180,180,180	0
59	MG	DA	3106	1/1	0.22	0.31	92,92,92,92	0
59	MG	CA	1636	1/1	0.29	0.31	181,181,181,181	0
59	MG	DA	3117	1/1	0.20	0.22	71,71,71,71	0
59	MG	BA	3120	1/1	0.15	0.22	4,4,4,4	0
59	MG	DA	3046	1/1	0.17	0.18	151,151,151,151	0
59	MG	DA	3058	1/1	0.16	0.18	204,204,204,204	0
59	MG	BA	3132	1/1	0.15	0.18	1,1,1,1	0
59	MG	DA	3119	1/1	0.20	0.15	93,93,93,93	0
59	MG	BL	201	1/1	0.13	0.06	53,53,53,53	0
59	MG	DA	3036	1/1	0.17	-0.06	82,82,82,82	0
59	MG	CA	1632	1/1	0.28	-0.08	156,156,156,156	0
59	MG	BA	3049	1/1	0.13	-0.09	66,66,66,66	0
59	MG	AA	1616	1/1	0.17	-0.10	98,98,98,98	0
59	MG	CA	1616	1/1	0.31	-0.16	254,254,254,254	0
59	MG	DA	3127	1/1	0.24	-0.17	142,142,142,142	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	BA	3068	1/1	0.13	-0.22	117,117,117,117	0
59	MG	DA	3047	1/1	0.18	-0.23	95,95,95,95	0
59	MG	CA	1617	1/1	0.27	-0.24	199,199,199,199	0
59	MG	DA	3080	1/1	0.22	-0.26	108,108,108,108	0
59	MG	BA	3122	1/1	0.14	-0.27	137,137,137,137	0
59	MG	CA	1601	1/1	0.17	-0.28	156,156,156,156	0
59	MG	DA	3049	1/1	0.23	-0.29	172,172,172,172	0
59	MG	BA	3099	1/1	0.14	-0.32	1,1,1,1	0
59	MG	AA	1607	1/1	0.15	-0.32	103,103,103,103	0
59	MG	DA	3076	1/1	0.17	-0.37	93,93,93,93	0
59	MG	AA	1632	1/1	0.11	-0.37	76,76,76,76	0
59	MG	BA	3072	1/1	0.16	-0.38	139,139,139,139	0
59	MG	DA	3088	1/1	0.21	-0.42	87,87,87,87	0
59	MG	AA	1636	1/1	0.16	-0.44	124,124,124,124	0
59	MG	CA	1610	1/1	0.10	-0.45	152,152,152,152	0
59	MG	DA	3042	1/1	0.27	-0.46	161,161,161,161	0
59	MG	AA	1619	1/1	0.11	-0.47	156,156,156,156	0
59	MG	BA	3062	1/1	0.13	-0.47	11,11,11,11	0
59	MG	DA	3104	1/1	0.17	-0.49	47,47,47,47	0
59	MG	BA	3103	1/1	0.14	-0.51	4,4,4,4	0
59	MG	CA	1602	1/1	0.15	-0.55	175,175,175,175	0
59	MG	AA	1604	1/1	0.10	-0.55	124,124,124,124	0
59	MG	DA	3081	1/1	0.19	-0.58	142,142,142,142	0
59	MG	DA	3125	1/1	0.17	-0.61	82,82,82,82	0
59	MG	DA	3094	1/1	0.21	-0.63	107,107,107,107	0
59	MG	BA	3061	1/1	0.15	-0.64	20,20,20,20	0
59	MG	DA	3017	1/1	0.17	-0.65	204,204,204,204	0
59	MG	DA	3109	1/1	0.23	-0.70	174,174,174,174	0
59	MG	DA	3001	1/1	0.17	-0.74	151,151,151,151	0
59	MG	AA	1637	1/1	0.14	-0.76	27,27,27,27	0
59	MG	DA	3029	1/1	0.18	-0.76	112,112,112,112	0
59	MG	BA	3021	1/1	0.14	-0.78	7,7,7,7	0
59	MG	AA	1610	1/1	0.08	-0.78	190,190,190,190	0
59	MG	DA	3115	1/1	0.17	-0.80	65,65,65,65	0
59	MG	DA	3039	1/1	0.21	-0.83	65,65,65,65	0
59	MG	DA	3091	1/1	0.21	-0.89	116,116,116,116	0
59	MG	DA	3083	1/1	0.15	-0.89	204,204,204,204	0
59	MG	DA	3043	1/1	0.19	-0.91	100,100,100,100	0
59	MG	DA	3120	1/1	0.19	-0.91	109,109,109,109	0
59	MG	DA	3111	1/1	0.14	-0.94	109,109,109,109	0
59	MG	AA	1628	1/1	0.12	-0.95	69,69,69,69	0
59	MG	BA	3007	1/1	0.09	-0.96	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	BA	3036	1/1	0.13	-1.01	4,4,4,4	0
59	MG	DA	3018	1/1	0.17	-1.01	226,226,226,226	0
59	MG	BA	3003	1/1	0.12	-1.01	69,69,69,69	0
59	MG	BA	3119	1/1	0.06	-1.02	51,51,51,51	0
59	MG	BA	3076	1/1	0.11	-1.03	114,114,114,114	0
59	MG	DA	3006	1/1	0.11	-1.04	211,211,211,211	0
59	MG	AA	1603	1/1	0.10	-1.05	111,111,111,111	0
59	MG	CA	1605	1/1	0.14	-1.07	37,37,37,37	0
59	MG	CA	1623	1/1	0.14	-1.09	124,124,124,124	0
59	MG	DA	3082	1/1	0.09	-1.10	197,197,197,197	0
59	MG	AA	1601	1/1	0.10	-1.10	70,70,70,70	0
59	MG	BA	3066	1/1	0.13	-1.14	10,10,10,10	0
59	MG	BA	3004	1/1	0.12	-1.16	138,138,138,138	0
59	MG	CA	1622	1/1	0.10	-1.18	226,226,226,226	0
59	MG	CA	1638	1/1	0.11	-1.21	130,130,130,130	0
59	MG	BA	3014	1/1	0.12	-1.27	68,68,68,68	0
59	MG	DA	3079	1/1	0.12	-1.28	142,142,142,142	0
59	MG	BA	3059	1/1	0.13	-1.29	190,190,190,190	0
59	MG	CA	1620	1/1	0.13	-1.31	168,168,168,168	0
59	MG	DA	3112	1/1	0.12	-1.42	131,131,131,131	0
59	MG	DA	3032	1/1	0.18	-1.42	121,121,121,121	0
59	MG	AA	1609	1/1	0.12	-1.45	46,46,46,46	0
59	MG	DA	3130	1/1	0.16	-1.46	85,85,85,85	0
59	MG	BA	3125	1/1	0.12	-1.49	27,27,27,27	0
59	MG	BB	204	1/1	0.12	-1.51	41,41,41,41	0
59	MG	DA	3031	1/1	0.16	-1.62	105,105,105,105	0
59	MG	DA	3041	1/1	0.16	-1.64	82,82,82,82	0
59	MG	DA	3012	1/1	0.13	-1.67	64,64,64,64	0
59	MG	AA	1602	1/1	0.12	-1.67	152,152,152,152	0
59	MG	DA	3069	1/1	0.13	-1.69	69,69,69,69	0
59	MG	AA	1634	1/1	0.06	-1.73	72,72,72,72	0
59	MG	BA	3008	1/1	0.13	-1.73	7,7,7,7	0
59	MG	DA	3050	1/1	0.15	-1.75	106,106,106,106	0
59	MG	DA	3033	1/1	0.14	-1.75	95,95,95,95	0
59	MG	DB	201	1/1	0.09	-1.79	104,104,104,104	0
59	MG	DA	3024	1/1	0.15	-1.80	89,89,89,89	0
59	MG	DA	3097	1/1	0.20	-1.84	144,144,144,144	0
59	MG	AA	1639	1/1	0.08	-1.85	108,108,108,108	0
59	MG	BB	202	1/1	0.10	-1.87	50,50,50,50	0
59	MG	BA	3089	1/1	0.10	-1.88	80,80,80,80	0
59	MG	CA	1629	1/1	0.13	-1.95	197,197,197,197	0
59	MG	DA	3099	1/1	0.14	-2.03	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	1631	1/1	0.12	-2.05	91,91,91,91	0
59	MG	AA	1606	1/1	0.10	-2.07	62,62,62,62	0
59	MG	BA	3044	1/1	0.13	-2.14	12,12,12,12	0
59	MG	AA	1640	1/1	0.09	-2.15	154,154,154,154	0
59	MG	CA	1634	1/1	0.15	-2.15	131,131,131,131	0
59	MG	DA	3067	1/1	0.11	-2.16	83,83,83,83	0
59	MG	DA	3096	1/1	0.16	-2.16	102,102,102,102	0
59	MG	BA	3098	1/1	0.07	-2.21	15,15,15,15	0
59	MG	BA	3124	1/1	0.11	-2.21	25,25,25,25	0
59	MG	DA	3118	1/1	0.10	-2.21	76,76,76,76	0
59	MG	BA	3092	1/1	0.09	-2.22	56,56,56,56	0
59	MG	DA	3064	1/1	0.14	-2.24	70,70,70,70	0
59	MG	DA	3121	1/1	0.12	-2.25	84,84,84,84	0
59	MG	BA	3013	1/1	0.12	-2.25	1,1,1,1	0
59	MG	BA	3045	1/1	0.12	-2.25	17,17,17,17	0
59	MG	DA	3060	1/1	0.11	-2.26	105,105,105,105	0
59	MG	BA	3078	1/1	0.12	-2.27	20,20,20,20	0
59	MG	AA	1638	1/1	0.09	-2.28	116,116,116,116	0
59	MG	BA	3063	1/1	0.11	-2.28	1,1,1,1	0
59	MG	DA	3066	1/1	0.11	-2.28	61,61,61,61	0
61	ZN	D4	101	1/1	0.07	-2.36	161,161,161,161	0
59	MG	BA	3112	1/1	0.10	-2.37	47,47,47,47	0
59	MG	CA	1639	1/1	0.12	-2.38	165,165,165,165	0
59	MG	DA	3009	1/1	0.08	-2.39	69,69,69,69	0
59	MG	BA	3079	1/1	0.12	-2.39	13,13,13,13	0
59	MG	DA	3070	1/1	0.13	-2.40	56,56,56,56	0
59	MG	DA	3026	1/1	0.12	-2.46	109,109,109,109	0
59	MG	BA	3048	1/1	0.10	-2.57	6,6,6,6	0
59	MG	BA	3020	1/1	0.10	-2.59	22,22,22,22	0
59	MG	BA	3086	1/1	0.15	-2.60	131,131,131,131	0
59	MG	BA	3115	1/1	0.10	-2.62	11,11,11,11	0
59	MG	DA	3016	1/1	0.14	-2.67	87,87,87,87	0
59	MG	BA	3023	1/1	0.09	-2.68	5,5,5,5	0
59	MG	BA	3017	1/1	0.10	-2.69	24,24,24,24	0
59	MG	AA	1633	1/1	0.10	-2.70	51,51,51,51	0
59	MG	AA	1624	1/1	0.11	-2.76	82,82,82,82	0
59	MG	BA	3108	1/1	0.10	-2.79	48,48,48,48	0
59	MG	DA	3123	1/1	0.14	-2.84	61,61,61,61	0
59	MG	DA	3071	1/1	0.07	-2.84	133,133,133,133	0
59	MG	BA	3031	1/1	0.13	-2.86	12,12,12,12	0
59	MG	AA	1611	1/1	0.07	-2.89	62,62,62,62	0
59	MG	CA	1642	1/1	0.08	-2.91	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	DA	3030	1/1	0.14	-2.92	68,68,68,68	0
59	MG	CA	1606	1/1	0.10	-2.94	64,64,64,64	0
59	MG	BA	3095	1/1	0.10	-2.95	77,77,77,77	0
59	MG	BA	3106	1/1	0.12	-2.96	13,13,13,13	0
59	MG	DA	3072	1/1	0.06	-3.00	187,187,187,187	0
59	MG	BA	3065	1/1	0.11	-3.03	17,17,17,17	0
59	MG	DA	3051	1/1	0.11	-3.10	57,57,57,57	0
59	MG	DA	3065	1/1	0.08	-3.11	49,49,49,49	0
61	ZN	B4	101	1/1	0.07	-3.14	80,80,80,80	0
59	MG	BA	3070	1/1	0.13	-3.15	53,53,53,53	0
59	MG	BA	3025	1/1	0.12	-3.21	26,26,26,26	0
59	MG	DA	3113	1/1	0.07	-3.22	148,148,148,148	0
59	MG	BA	3028	1/1	0.11	-3.23	77,77,77,77	0
59	MG	DA	3011	1/1	0.18	-3.24	127,127,127,127	0
59	MG	DA	3055	1/1	0.12	-3.45	120,120,120,120	0
59	MG	DA	3098	1/1	0.15	-3.47	172,172,172,172	0
59	MG	DA	3053	1/1	0.07	-3.48	67,67,67,67	0
59	MG	BA	3133	1/1	0.12	-3.65	139,139,139,139	0
59	MG	CA	1635	1/1	0.13	-3.70	95,95,95,95	0
59	MG	BA	3077	1/1	0.09	-3.71	30,30,30,30	0
59	MG	DA	3089	1/1	0.10	-3.71	99,99,99,99	0
59	MG	DA	3008	1/1	0.16	-3.85	148,148,148,148	0
59	MG	BA	3022	1/1	0.07	-3.99	8,8,8,8	0
59	MG	DA	3023	1/1	0.08	-4.14	87,87,87,87	0
59	MG	DA	3004	1/1	0.12	-4.28	114,114,114,114	0
59	MG	BA	3121	1/1	0.11	-4.42	15,15,15,15	0
59	MG	BA	3104	1/1	0.12	-4.51	3,3,3,3	0
59	MG	BA	3009	1/1	0.12	-4.54	6,6,6,6	0
59	MG	BA	3016	1/1	0.08	-4.66	2,2,2,2	0
59	MG	DA	3101	1/1	0.12	-4.66	67,67,67,67	0
59	MG	CA	1630	1/1	0.06	-4.73	131,131,131,131	0
59	MG	DA	3093	1/1	0.13	-4.75	114,114,114,114	0
59	MG	BA	3113	1/1	0.07	-4.77	114,114,114,114	0
59	MG	DA	3085	1/1	0.12	-4.78	87,87,87,87	0
59	MG	BA	3127	1/1	0.09	-4.81	3,3,3,3	0
59	MG	DA	3040	1/1	0.12	-4.83	70,70,70,70	0
59	MG	BA	3046	1/1	0.07	-4.90	149,149,149,149	0
59	MG	DA	3095	1/1	0.09	-4.93	95,95,95,95	0
59	MG	AA	1642	1/1	0.10	-4.96	37,37,37,37	0
59	MG	AA	1622	1/1	0.06	-4.97	76,76,76,76	0
59	MG	DA	3022	1/1	0.13	-5.02	69,69,69,69	0
59	MG	DA	3037	1/1	0.14	-5.04	197,197,197,197	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	BA	3005	1/1	0.09	-5.11	87,87,87,87	0
59	MG	BA	3037	1/1	0.10	-5.16	5,5,5,5	0
59	MG	BA	3075	1/1	0.06	-5.28	29,29,29,29	0
59	MG	BA	3091	1/1	0.08	-5.31	32,32,32,32	0
59	MG	BA	3084	1/1	0.11	-5.32	13,13,13,13	0
59	MG	BA	3128	1/1	0.10	-5.38	19,19,19,19	0
59	MG	AA	1623	1/1	0.06	-5.46	102,102,102,102	0
59	MG	DA	3054	1/1	0.10	-5.51	96,96,96,96	0
59	MG	BA	3080	1/1	0.06	-5.54	34,34,34,34	0
59	MG	BA	3051	1/1	0.10	-5.60	58,58,58,58	0
59	MG	CA	1604	1/1	0.06	-5.65	74,74,74,74	0
59	MG	BA	3064	1/1	0.08	-5.66	18,18,18,18	0
59	MG	DA	3100	1/1	0.11	-5.69	78,78,78,78	0
59	MG	AA	1613	1/1	0.07	-5.70	56,56,56,56	0
59	MG	BB	203	1/1	0.06	-5.85	17,17,17,17	0
59	MG	BA	3034	1/1	0.10	-5.90	5,5,5,5	0
59	MG	BA	3010	1/1	0.08	-5.90	29,29,29,29	0
59	MG	BA	3012	1/1	0.09	-6.09	1,1,1,1	0
59	MG	BA	3057	1/1	0.06	-6.10	48,48,48,48	0
59	MG	CA	1609	1/1	0.12	-6.43	83,83,83,83	0
59	MG	BA	3116	1/1	0.08	-6.47	76,76,76,76	0
59	MG	CA	1613	1/1	0.09	-6.48	105,105,105,105	0
59	MG	BA	3015	1/1	0.07	-6.48	55,55,55,55	0
59	MG	BA	3030	1/1	0.09	-6.60	21,21,21,21	0
59	MG	BA	3052	1/1	0.07	-7.27	5,5,5,5	0
59	MG	BA	3050	1/1	0.10	-7.50	10,10,10,10	0
59	MG	DA	3038	1/1	0.12	-7.61	102,102,102,102	0
59	MG	BA	3071	1/1	0.10	-7.62	7,7,7,7	0
59	MG	BA	3088	1/1	0.09	-7.64	50,50,50,50	0
59	MG	BA	3126	1/1	0.09	-7.93	9,9,9,9	0
59	MG	BA	3093	1/1	0.09	-7.99	36,36,36,36	0
59	MG	AA	1615	1/1	0.05	-8.18	120,120,120,120	0
59	MG	BA	3067	1/1	0.06	-8.76	18,18,18,18	0
59	MG	BA	3083	1/1	0.08	-9.85	28,28,28,28	0
59	MG	BA	3094	1/1	0.07	-9.95	9,9,9,9	0
59	MG	BA	3087	1/1	0.10	-10.12	35,35,35,35	0
59	MG	BA	3006	1/1	0.05	-10.57	39,39,39,39	0
59	MG	BA	3019	1/1	0.05	-11.78	15,15,15,15	0
59	MG	BA	3042	1/1	0.05	-12.31	41,41,41,41	0
59	MG	AA	1620	1/1	0.08	-24.00	117,117,117,117	0
59	MG	BA	3101	1/1	0.06	-28.70	11,11,11,11	0
59	MG	BA	3053	1/1	0.09	-31.97	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	DA	3010	1/1	0.70	-	218,218,218,218	0

6.5 Other polymers ⓘ

There are no such residues in this entry.