



wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 07:48 PM BST

PDB ID : 4V9K
Title : 70S ribosome translocation intermediate GDPNP-I containing elongation factor EFG/GDPNP, mRNA, and tRNA bound in the pe*/E state.
Authors : Zhou, J.; Lancaster, L.; Donohue, J.P.; Noller, H.F.
Deposited on : 2013-04-24
Resolution : 3.50 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

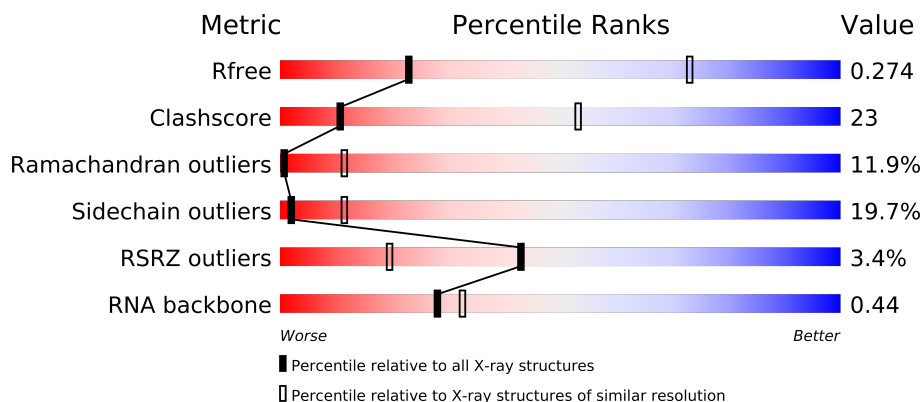
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 3.50 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	AB	235	
1	CB	235	
2	AC	207	
2	CC	207	
3	AD	208	
3	CD	208	
4	AE	151	
4	CE	151	
5	AF	101	
5	CF	101	
6	AG	155	
6	CG	155	

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Mol	Chain	Length	Quality of chain
7	AH	138	
7	CH	138	
8	AI	127	
8	CI	127	
9	AJ	99	
9	CJ	99	
10	AK	119	
10	CK	119	
11	AL	125	
11	CL	125	
12	AM	125	
12	CM	125	
13	AN	60	
13	CN	60	
14	AO	88	
14	CO	88	
15	AP	84	
15	CP	84	
16	AQ	100	
16	CQ	100	
17	AR	70	
17	CR	70	
18	AS	79	
18	CS	79	
19	AT	99	
19	CT	99	
20	AY	687	
20	CY	687	
21	AA	1511	
21	CA	1511	
22	AW	77	
22	CW	77	
23	AV	23	
23	CV	23	
24	AU	6	
24	CU	6	
25	BC	228	
25	DC	228	
26	BD	275	
26	DD	275	
27	BE	205	
27	DE	205	

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Mol	Chain	Length	Quality of chain
28	BF	208	
28	DF	208	
29	BG	181	
29	DG	181	
30	BH	167	
30	DH	167	
31	BJ	170	
31	DJ	170	
32	BK	140	
32	DK	140	
33	BN	138	
33	DN	138	
34	BO	122	
34	DO	122	
35	BP	146	
35	DP	146	
36	BQ	141	
36	DQ	141	
37	BR	117	
37	DR	117	
38	BS	99	
38	DS	99	
39	BT	138	
39	DT	138	
40	BU	117	
40	DU	117	
41	BV	101	
41	DV	101	
42	BW	113	
42	DW	113	
43	BX	93	
43	DX	93	
44	BY	107	
44	DY	107	
45	BZ	185	
45	DZ	185	
46	B0	84	
46	D0	84	
47	B2	71	
47	D2	71	
48	B3	60	
48	D3	60	

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Mol	Chain	Length	Quality of chain
49	B5	59	
49	D5	59	
50	B6	50	
50	D6	50	
51	B7	49	
51	D7	49	
52	B8	64	
52	D8	64	
53	B9	37	
53	D9	37	
54	Bf	31	
54	Bg	31	
54	Df	31	
54	Dg	31	
55	Bh	30	
55	Dh	30	
56	B1	93	
56	D1	93	
57	B4	35	
57	D4	35	
58	Be	102	
58	De	102	
59	BA	2879	
59	DA	2879	
60	BB	119	
60	DB	119	

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 308422 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 protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AB	235	Total	C	N	O	S	0	0	0
			1910	1218	342	345	5			
1	CB	235	Total	C	N	O	S	0	0	0
			1910	1218	342	345	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AC	207	Total	C	N	O	S	0	0	0
			1621	1022	315	283	1			
2	CC	207	Total	C	N	O	S	0	0	0
			1621	1022	315	283	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
3	CD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AE	151	Total	C	N	O	S	0	0	0
			1156	729	218	205	4			
4	CE	151	Total	C	N	O	S	0	0	0
			1156	729	218	205	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
5	CF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
6	CG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
7	CH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	AI	127	Total	C	N	O	0	0	0
			1011	639	198	174			
8	CI	127	Total	C	N	O	0	0	0
			1011	639	198	174			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AJ	99	Total	C	N	O	S	0	0	0
			802	504	157	140	1			
9	CJ	99	Total	C	N	O	S	0	0	0
			802	504	157	140	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AL	125	Total	C	N	O	S	0	0	0
			976	614	196	165	1			
11	CL	125	Total	C	N	O	S	0	0	0
			976	614	196	165	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AM	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			
12	CM	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			

- Molecule 13 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
13	CN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
14	CO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AP	84	Total	C	N	O	S	0	0	0
			706	446	140	119	1			
15	CP	84	Total	C	N	O	S	0	0	0
			706	446	140	119	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AQ	100	Total	C	N	O	S	0	0	0
			835	534	156	143	2			
16	CQ	100	Total	C	N	O	S	0	0	0
			835	534	156	143	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	AR	70	Total	C	N	O	0	0	0
			574	367	112	95			
17	CR	70	Total	C	N	O	0	0	0
			574	367	112	95			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AS	79	Total	C	N	O	S	0	0	0
			634	405	115	112	2			
18	CS	79	Total	C	N	O	S	0	0	0
			634	405	115	112	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AT	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			
19	CT	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

- Molecule 20 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AY	687	Total	C	N	O	S	0	0	0
			5380	3414	922	1024	20			
20	CY	687	Total	C	N	O	S	0	0	0
			5380	3414	922	1024	20			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AY	129	LYS	HIS	CONFLICT	UNP Q72I01

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Chain	Residue	Modelled	Actual	Comment	Reference
AY	226	ASN	HIS	CONFLICT	UNP Q72I01
CY	129	LYS	HIS	CONFLICT	UNP Q72I01
CY	226	ASN	HIS	CONFLICT	UNP Q72I01

- Molecule 21 is a RNA chain called ribosomal RNA 16S.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AA	1511	Total	C	N	O	P	0	0	0
			32474	14455	6015	10494	1510			
21	CA	1511	Total	C	N	O	P	0	0	0
			32474	14455	6015	10494	1510			

- Molecule 22 is a RNA chain called transfer RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AW	77	Total	C	N	O	P	0	0	0
			1635	732	291	536	76			
22	CW	77	Total	C	N	O	P	0	0	0
			1635	732	291	536	76			

- Molecule 23 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AV	23	Total	C	N	O	P	0	0	0
			503	227	106	148	22			
23	CV	23	Total	C	N	O	P	0	0	0
			503	227	106	148	22			

- Molecule 24 is a protein called VIOMYCIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	AU	6	Total	C	N	O	0	0	0
			48	25	13	10			
24	CU	6	Total	C	N	O	0	0	0
			48	25	13	10			

- Molecule 25 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BC	228	Total	C	N	O	S	0	0	0
			1742	1101	319	319	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	DC	228	Total	C	N	O	S	0	0	0
			1742	1101	319	319	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BC	20	VAL	ILE	CONFLICT	UNP Q72GV9
BC	28	ARG	HIS	CONFLICT	UNP Q72GV9
DC	20	VAL	ILE	CONFLICT	UNP Q72GV9
DC	28	ARG	HIS	CONFLICT	UNP Q72GV9

- Molecule 26 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BD	275	Total	C	N	O	S	0	0	0
			2145	1353	428	361	3			
26	DD	275	Total	C	N	O	S	0	0	0
			2145	1353	428	361	3			

- Molecule 27 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BE	205	Total	C	N	O	S	0	0	0
			1569	991	300	272	6			
27	DE	205	Total	C	N	O	S	0	0	0
			1569	991	300	272	6			

- Molecule 28 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BF	208	Total	C	N	O	S	0	0	0
			1628	1037	304	284	3			
28	DF	208	Total	C	N	O	S	0	0	0
			1628	1037	304	284	3			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BF	2	LYS	-	INSERTION	UNP Q72I05
BF	3	GLU	-	INSERTION	UNP Q72I05
BF	4	VAL	-	INSERTION	UNP Q72I05

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Chain	Residue	Modelled	Actual	Comment	Reference
BF	5	ALA	-	INSERTION	UNP Q72I05
BF	6	VAL	-	INSERTION	UNP Q72I05
DF	2	LYS	-	INSERTION	UNP Q72I05
DF	3	GLU	-	INSERTION	UNP Q72I05
DF	4	VAL	-	INSERTION	UNP Q72I05
DF	5	ALA	-	INSERTION	UNP Q72I05
DF	6	VAL	-	INSERTION	UNP Q72I05

- Molecule 29 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			
29	DG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BG	5	VAL	LEU	CONFLICT	UNP Q72I16
DG	5	VAL	LEU	CONFLICT	UNP Q72I16

- Molecule 30 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BH	167	Total	C	N	O	S	0	0	0
			1274	806	238	229	1			
30	DH	167	Total	C	N	O	S	0	0	0
			1274	806	238	229	1			

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
31	BJ	170	Total	C	N	O	0	0	0
			851	510	170	171			
31	DJ	170	Total	C	N	O	0	0	0
			851	510	170	171			

- Molecule 32 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BK	140	Total	C	N	O	S	0	0	0
			1035	659	183	188	5			
32	DK	140	Total	C	N	O	S	0	0	0
			1035	659	183	188	5			

- Molecule 33 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
33	DN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 34 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
34	DO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BO	69	ILE	VAL	CONFLICT	UNP Q72I14
DO	69	ILE	VAL	CONFLICT	UNP Q72I14

- Molecule 35 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			
35	DP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 36 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
36	DQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BQ	32	TYR	PHE	CONFLICT	UNP Q72I11
DQ	32	TYR	PHE	CONFLICT	UNP Q72I11

- Molecule 37 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
37	BR	117	Total	C	N	O	0	0	0
			960	599	202	159			
37	DR	117	Total	C	N	O	0	0	0
			960	599	202	159			

- Molecule 38 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
38	BS	99	Total	C	N	O	0	0	0
			775	488	155	132			
38	DS	99	Total	C	N	O	0	0	0
			775	488	155	132			

- Molecule 39 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BT	138	Total	C	N	O	S	0	0	0
			1147	713	235	198	1			
39	DT	138	Total	C	N	O	S	0	0	0
			1147	713	235	198	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BT	123	GLN	LYS	CONFLICT	UNP Q72JU9
BT	135	ALA	VAL	CONFLICT	UNP Q72JU9
DT	123	GLN	LYS	CONFLICT	UNP Q72JU9
DT	135	ALA	VAL	CONFLICT	UNP Q72JU9

- Molecule 40 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BU	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	DU	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 41 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
41	DV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 42 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BW	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			
42	DW	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			

- Molecule 43 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
43	BX	93	Total	C	N	O	0	0	0
			734	477	132	125			
43	DX	93	Total	C	N	O	0	0	0
			734	477	132	125			

- Molecule 44 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BY	107	Total	C	N	O	S	0	0	0
			818	524	155	134	5			
44	DY	107	Total	C	N	O	S	0	0	0
			818	524	155	134	5			

- Molecule 45 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BZ	185	Total	C	N	O	S	0	0	0
			1473	939	262	270	2			
45	DZ	185	Total	C	N	O	S	0	0	0
			1473	939	262	270	2			

- Molecule 46 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	B0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			
46	D0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B0	11	ARG	LYS	CONFLICT	UNP Q72HR3
D0	11	ARG	LYS	CONFLICT	UNP Q72HR3

- Molecule 47 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	B2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			
47	D2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			

- Molecule 48 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	B3	60	Total	C	N	O	S	0	0	0
			477	303	91	82	1			
48	D3	60	Total	C	N	O	S	0	0	0
			477	303	91	82	1			

- Molecule 49 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
49	D5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B5	29	THR	ILE	CONFLICT	UNP P62652
D5	29	THR	ILE	CONFLICT	UNP P62652

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B6	50	Total	C	N	O	S	0	0	0
			433	270	88	71	4			
50	D6	50	Total	C	N	O	S	0	0	0
			433	270	88	71	4			

- Molecule 51 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			
51	D7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			

- Molecule 52 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			
52	D8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 53 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
53	D9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L7/L12.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
54	Bf	31	Total	C	N	O	0	0	0
			156	93	31	32			
54	Bg	31	Total	C	N	O	0	0	0
			156	93	31	32			
54	Df	31	Total	C	N	O	0	0	0
			156	93	31	32			
54	Dg	31	Total	C	N	O	0	0	0
			156	93	31	32			

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L7/L12.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
55	Bh	30	Total	C	N	O	0	0	0
			151	90	30	31			
55	Dh	30	Total	C	N	O	0	0	0
			151	90	30	31			

- Molecule 56 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	B1	93	Total	C	N	O	S	0	0	0
			732	460	145	126	1			
56	D1	93	Total	C	N	O	S	0	0	0
			732	460	145	126	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B1	81	LYS	ARG	CONFLICT	UNP Q72G84
D1	81	LYS	ARG	CONFLICT	UNP Q72G84

- Molecule 57 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	B4	35	Total	C	N	O	S	0	0	0
			271	174	44	50	3			
57	D4	35	Total	C	N	O	S	0	0	0
			271	174	44	50	3			

- Molecule 58 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
58	Be	102	Total	C	N	O	0	0	0
			686	430	119	137			
58	De	102	Total	C	N	O	0	0	0
			686	430	119	137			

- Molecule 59 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	BA	2879	Total	C	N	O	P	0	0	0
			61997	27594	11582	19943	2878			

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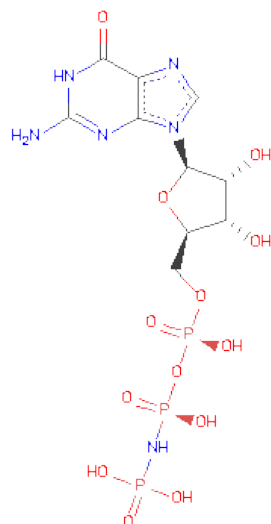
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	DA	2879	Total	C	N	O	P	0	0	0
			61997	27594	11582	19943	2878			

- Molecule 60 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
60	BB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			
60	DB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

- Molecule 61 is PHOSPHOAMINOPHOSPHONICACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
61	AY	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
61	CY	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

- Molecule 62 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	AY	1	Total	Mg	0	0
			1	1		

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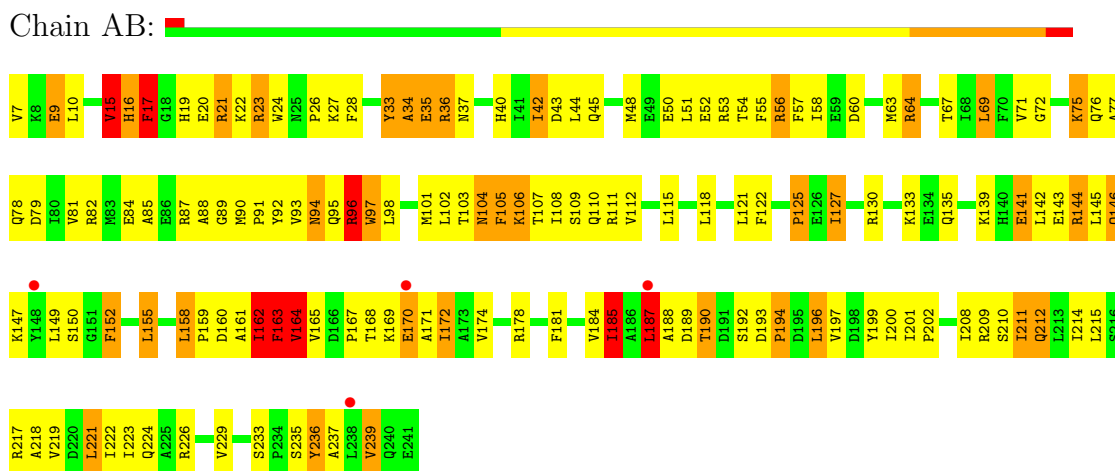
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	CY	1	Total	Mg	0	0
			1	1		

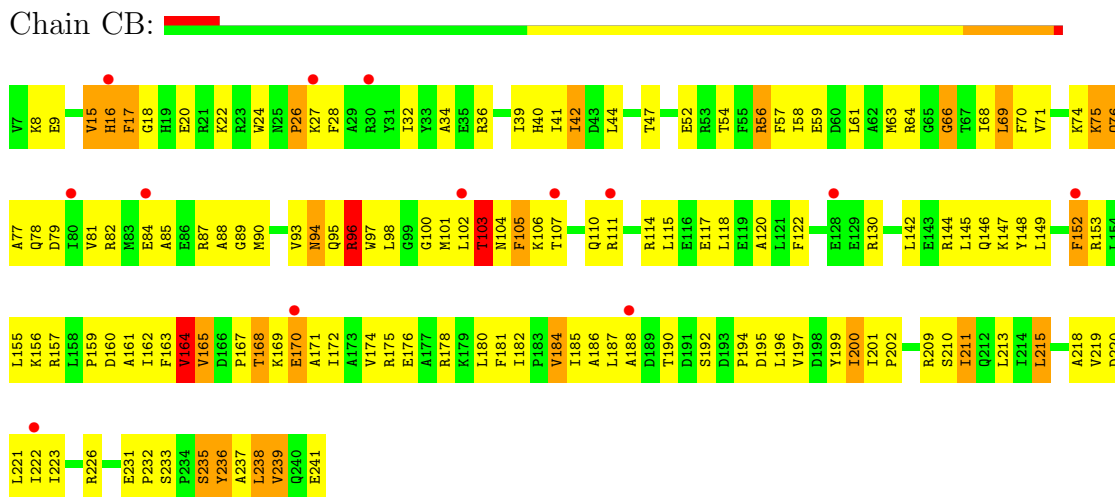
3 Residue-property plots

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

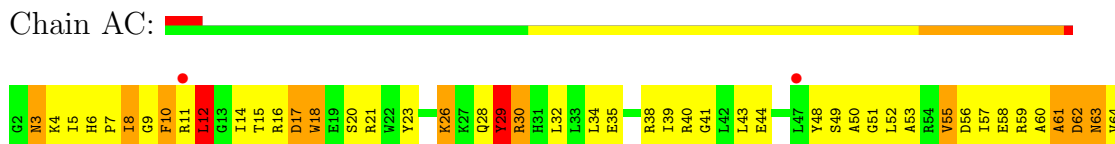
• Molecule 1: 30S ribosomal protein S2

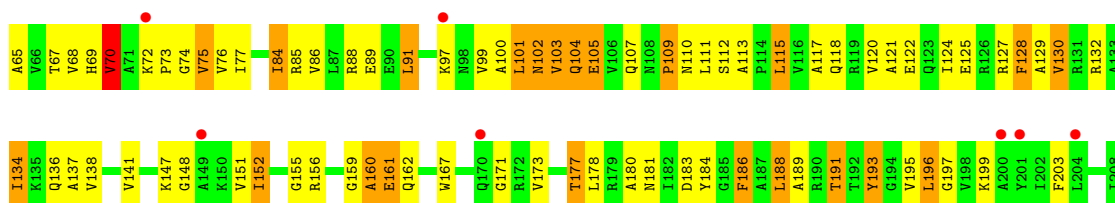


• Molecule 1: 30S ribosomal protein S2



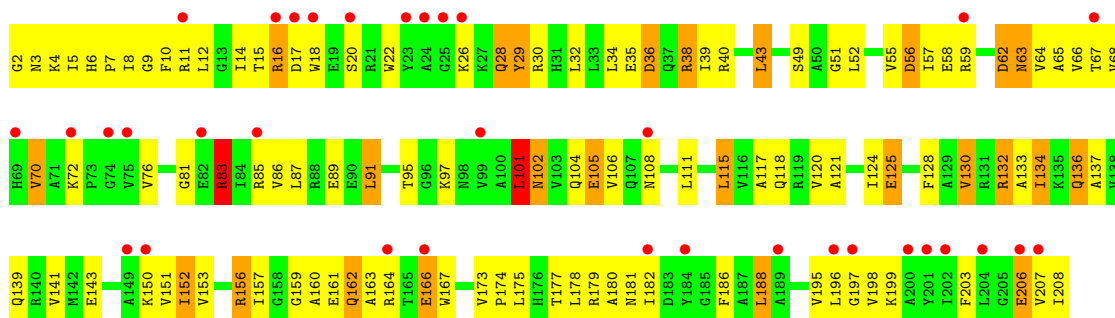
• Molecule 2: 30S ribosomal protein S3





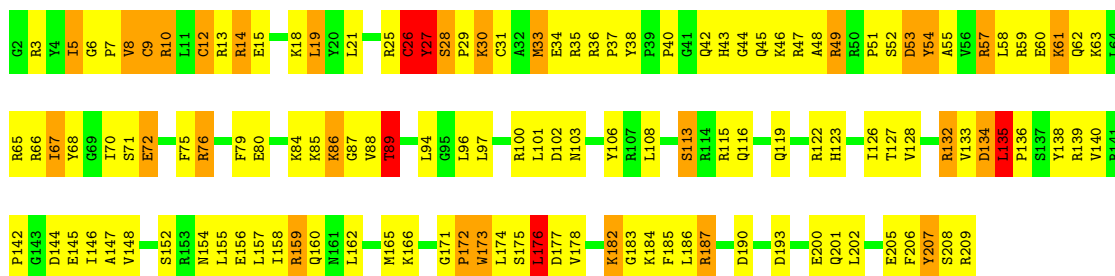
• Molecule 2: 30S ribosomal protein S3

Chain CC:



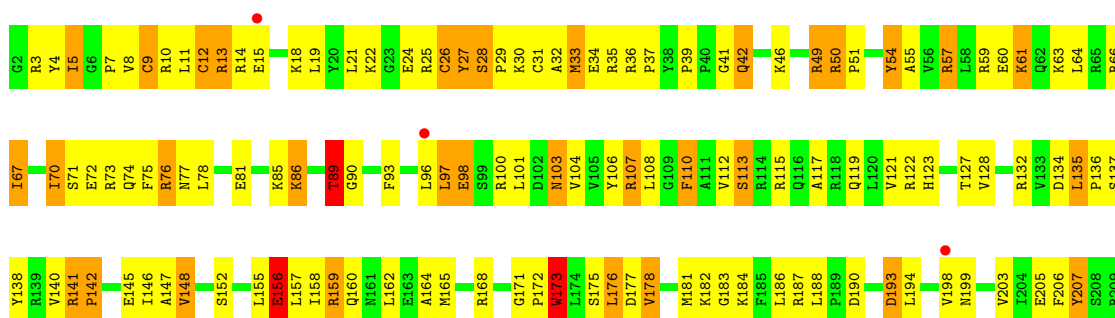
• Molecule 3: 30S ribosomal protein S4

Chain AD:



• Molecule 3: 30S ribosomal protein S4

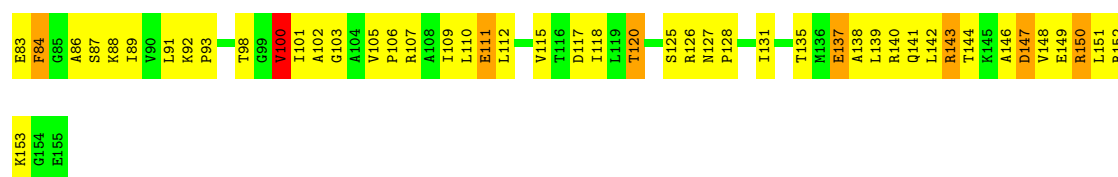
Chain CD:



• Molecule 4: 30S ribosomal protein S5

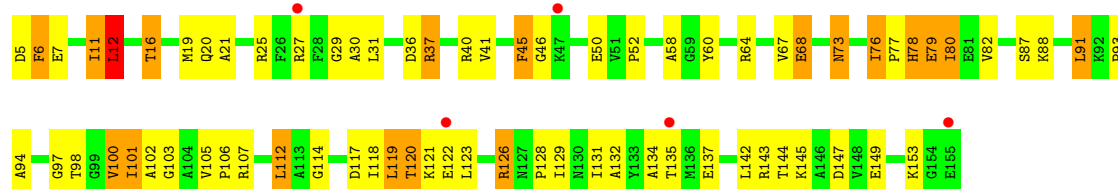
Chain AE:





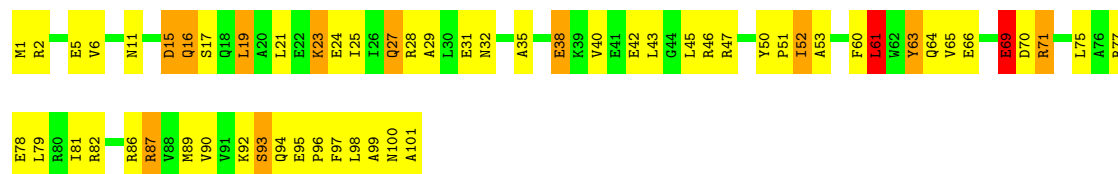
- Molecule 4: 30S ribosomal protein S5

Chain CE:



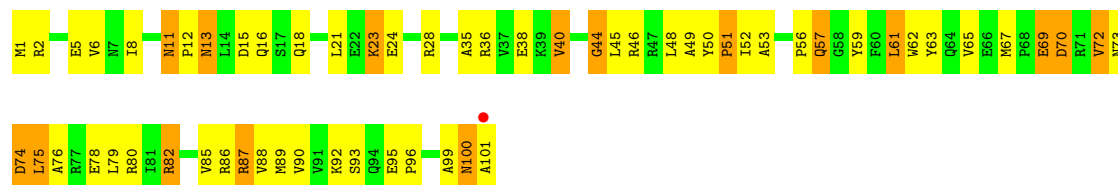
- Molecule 5: 30S ribosomal protein S6

Chain AF:



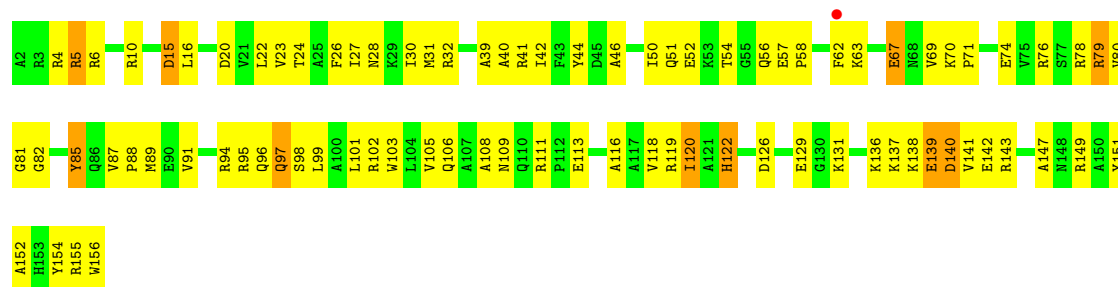
- Molecule 5: 30S ribosomal protein S6

Chain CF:



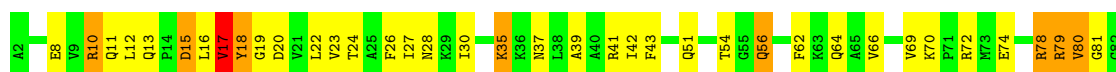
- Molecule 6: 30S ribosomal protein S7

Chain AG:



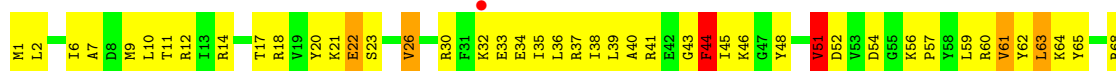
- Molecule 6: 30S ribosomal protein S7

Chain CG:



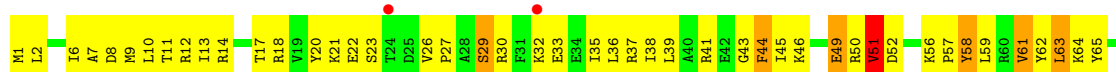
• Molecule 7: 30S ribosomal protein S8

Chain AH:



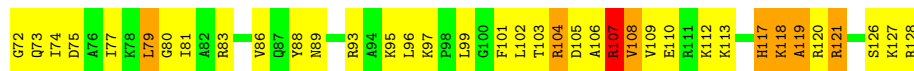
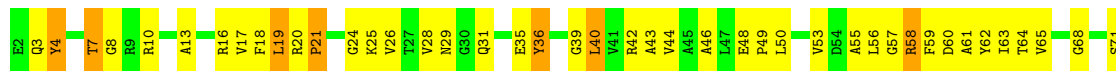
• Molecule 7: 30S ribosomal protein S8

Chain CH:



• Molecule 8: 30S ribosomal protein S9

Chain AI:



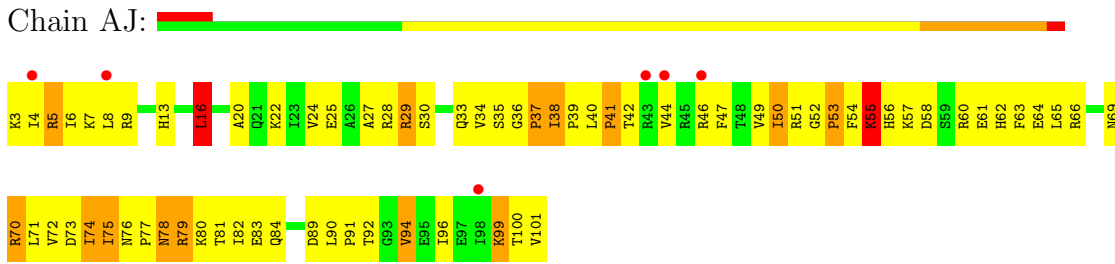
• Molecule 8: 30S ribosomal protein S9

Chain CI:



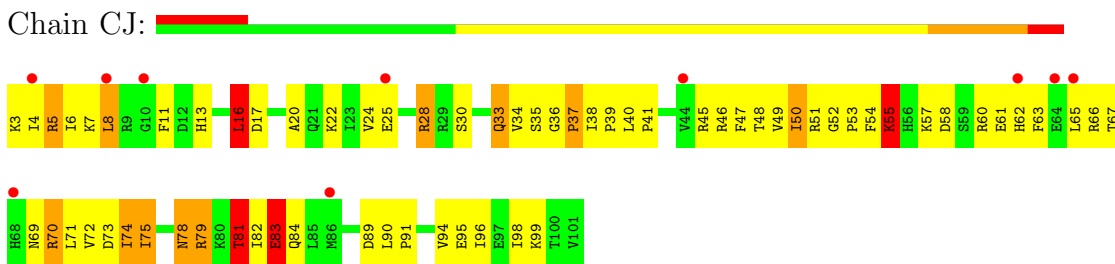
• Molecule 9: 30S ribosomal protein S10

Chain AJ:



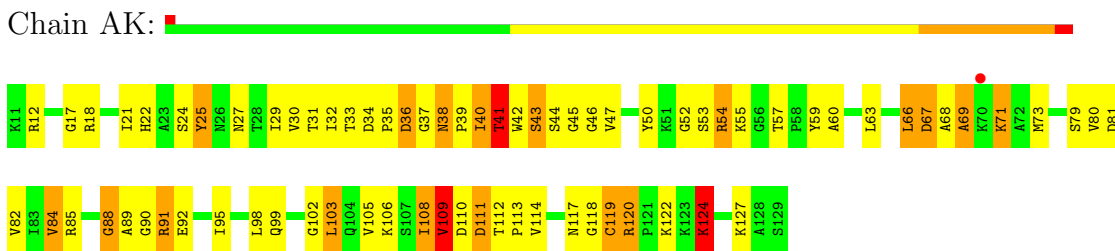
- Molecule 9: 30S ribosomal protein S10

Chain CJ:



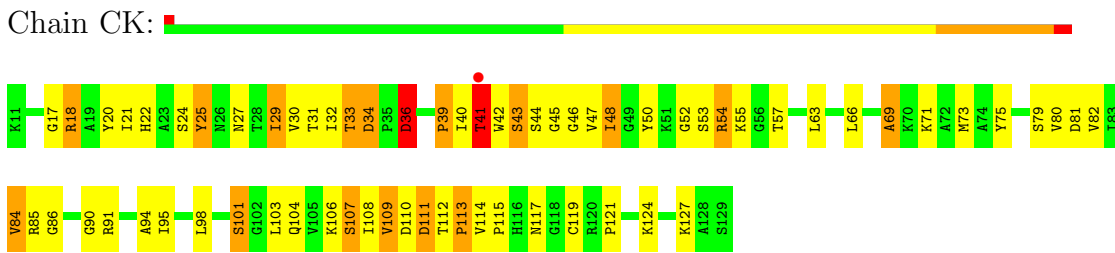
- Molecule 10: 30S ribosomal protein S11

Chain AK:



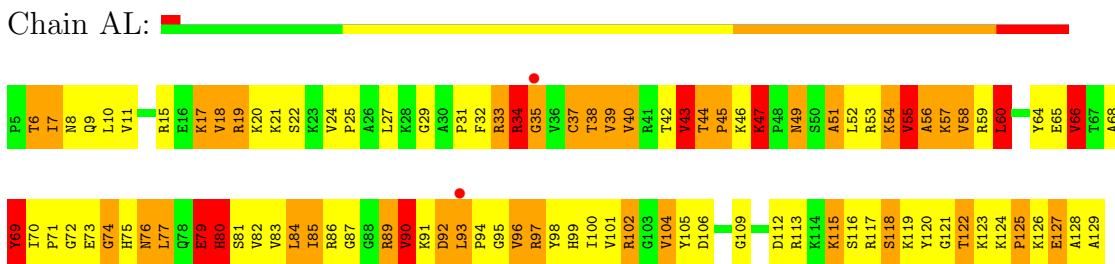
- Molecule 10: 30S ribosomal protein S11

Chain CK:



- Molecule 11: 30S ribosomal protein S12

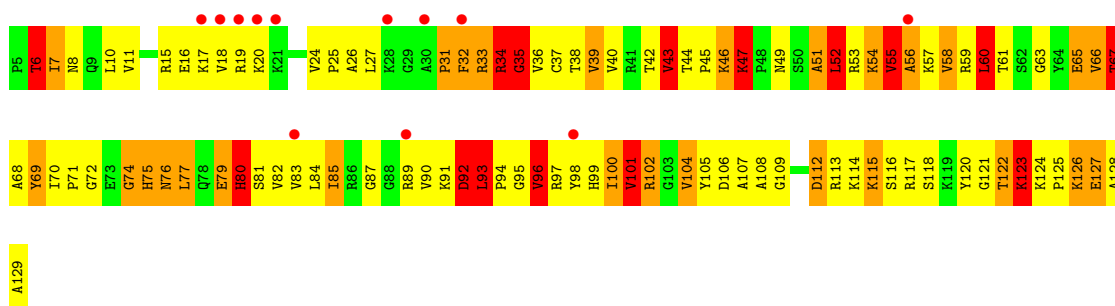
Chain AL:



- Molecule 11: 30S ribosomal protein S12

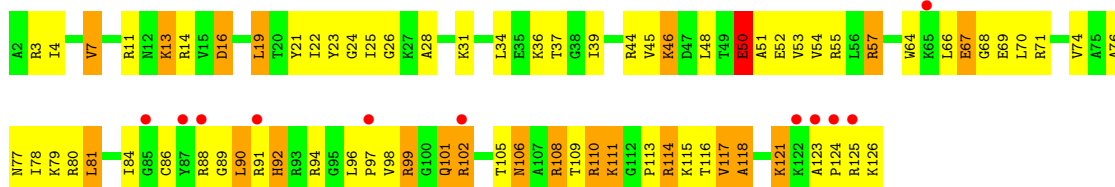
Chain CL:





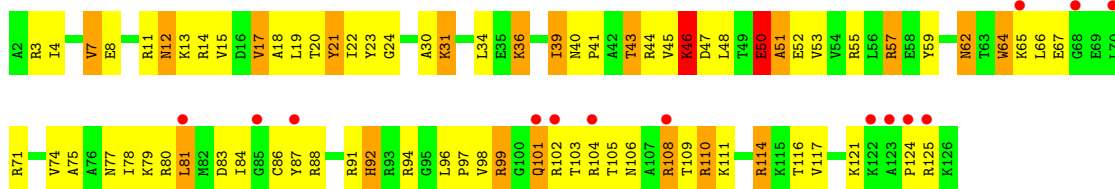
- Molecule 12: 30S ribosomal protein S13

Chain AM:



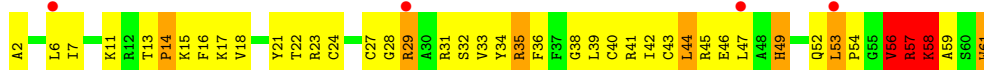
- Molecule 12: 30S ribosomal protein S13

Chain CM:



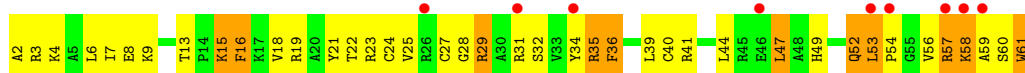
- Molecule 13: 30S ribosomal protein S14 type Z

Chain AN:



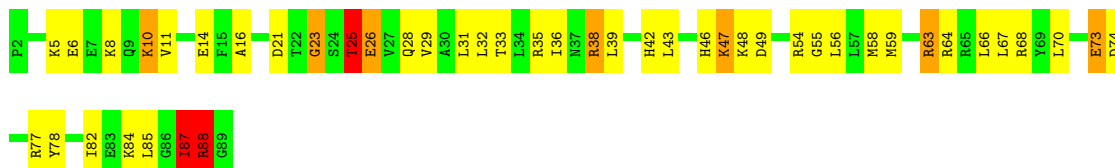
- Molecule 13: 30S ribosomal protein S14 type Z

Chain CN:

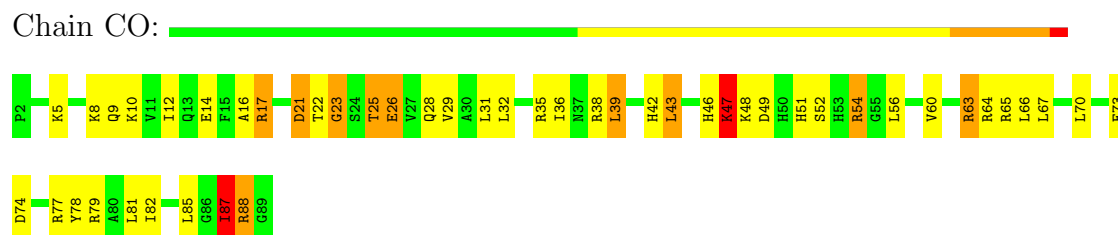


- Molecule 14: 30S ribosomal protein S15

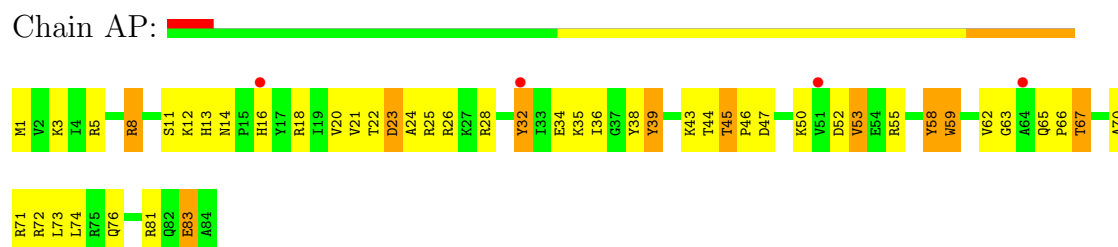
Chain AO:



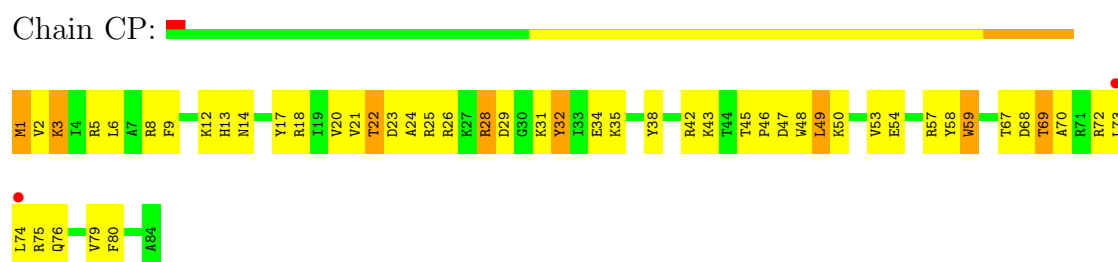
- Molecule 14: 30S ribosomal protein S15



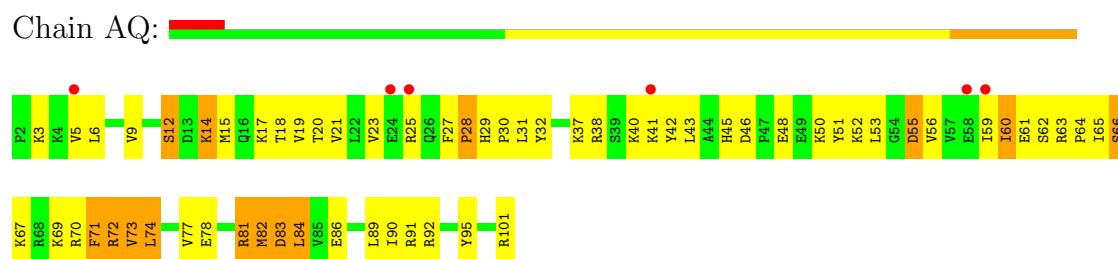
- Molecule 15: 30S ribosomal protein S16



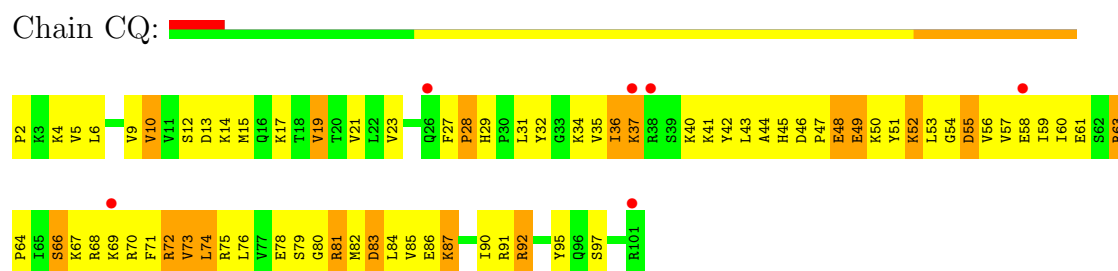
- Molecule 15: 30S ribosomal protein S16



- Molecule 16: 30S ribosomal protein S17



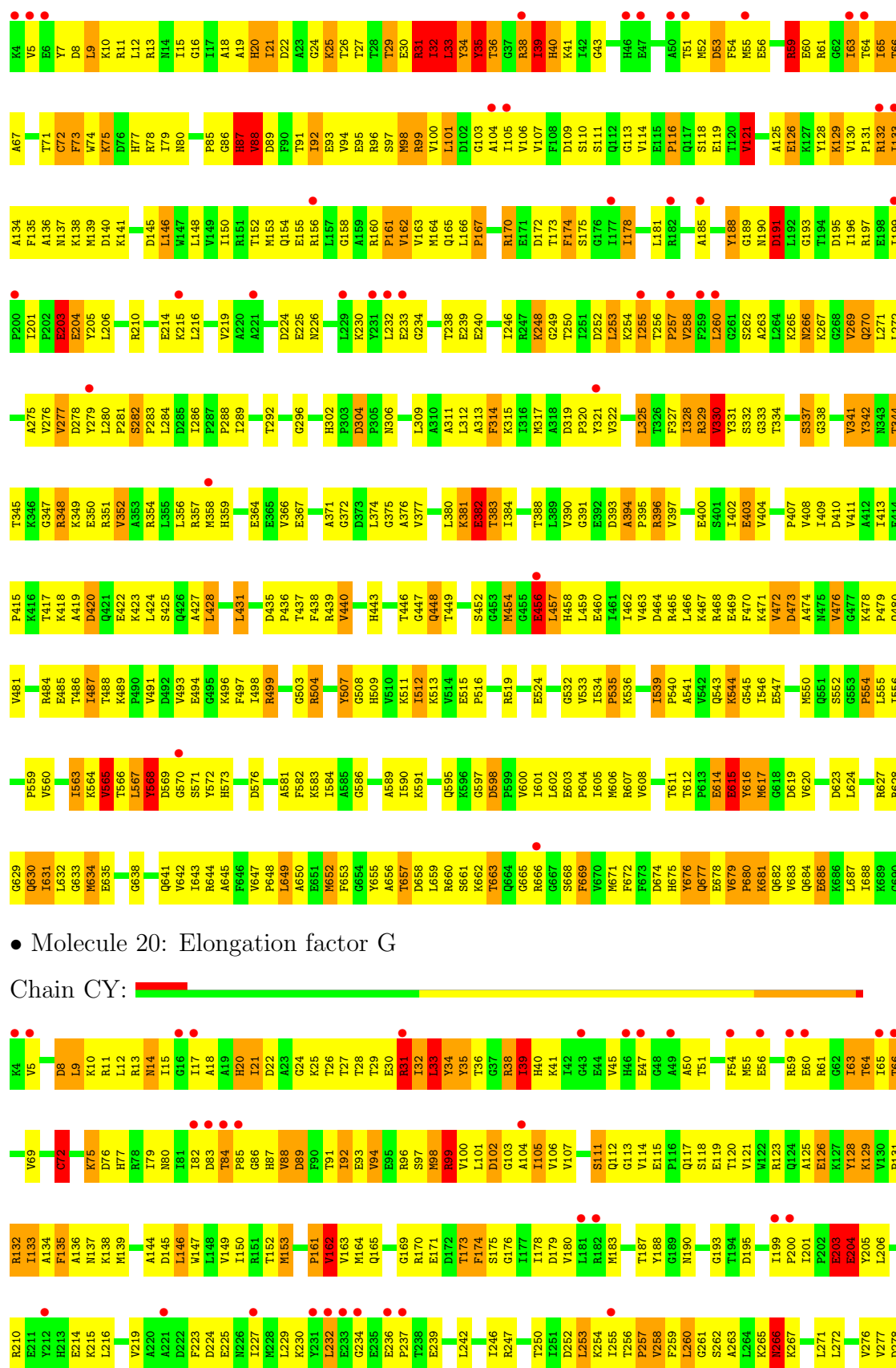
- Molecule 16: 30S ribosomal protein S17

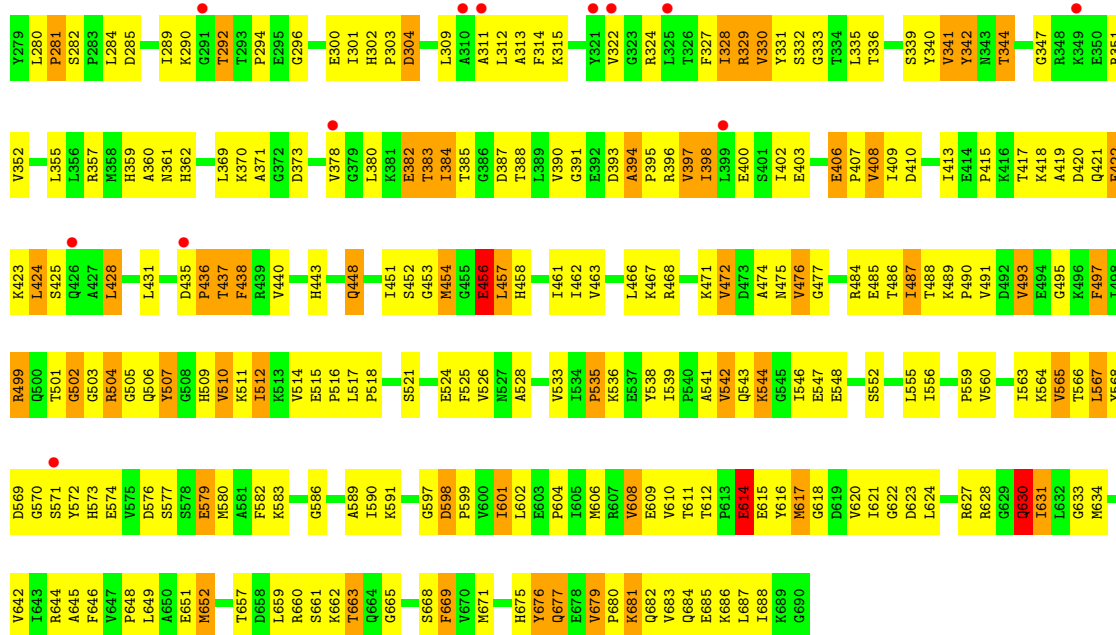


- Molecule 17: 30S ribosomal protein S18



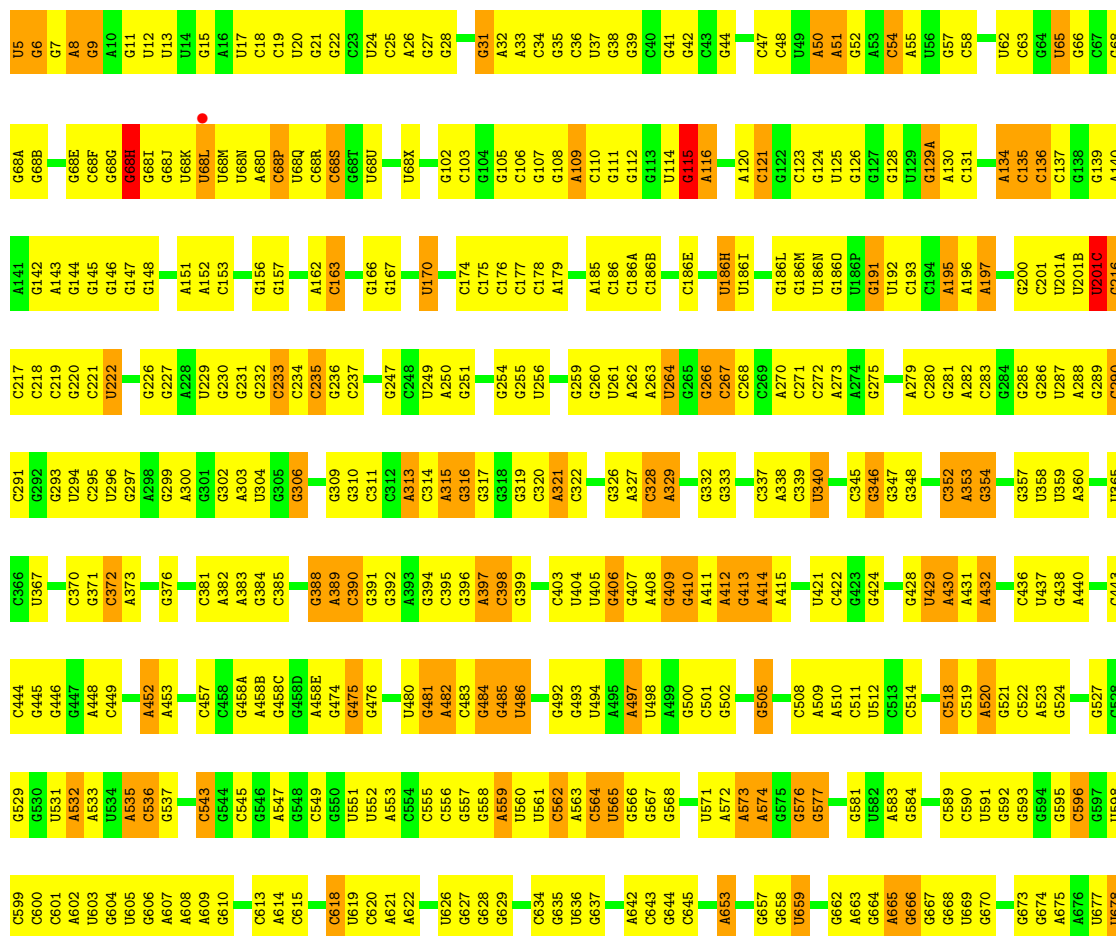


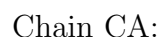




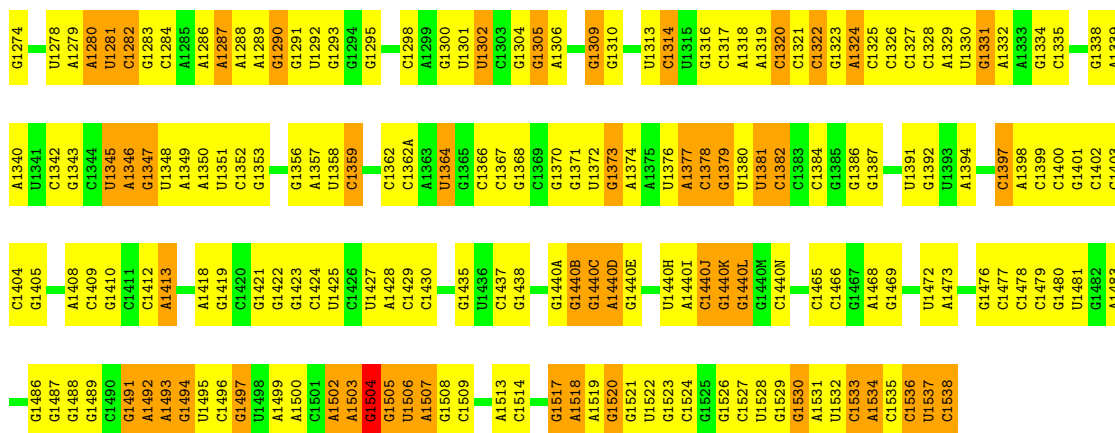
• Molecule 21: ribosomal RNA 16S

Chain AA:



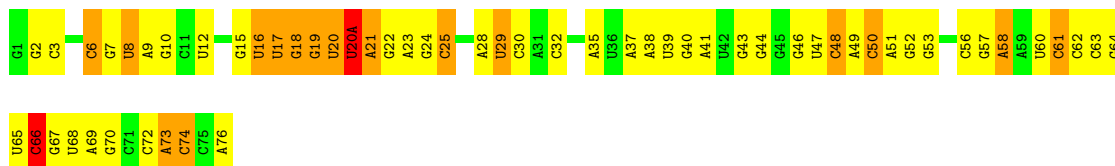


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U1212	A1130	C1045	A977	A908	U833	U757	C680	C600	U551	A441	U365	C295	C219	A152	C68F
A1213	G1131	U1049	C978	A909	U834	G758	A687	U603	A532	C442	U366	U296	C220	C153	G68G
G1214	C834	C834	C979	C910	G835	C762	G688	U604	A533	C443	U367	A298	C221	G156	G68H
G1215	U1135	U835	C980	U911	G836	G763	G689	U605	U534	C444	U368	A299	G226	G157	G68I
G1216	G1063	G837	U981	C912	G837	C764	G690	U606	A535	C445	U369	A300	G227	G158	G68J
C1217	C1054	G838	C985	G916	G838	G765	G691	A608	A536	C446	C372	G301	U229	G159	G68K
U1218	A1055	U838	A986	G917	U838A	A766	U692	A609	A537	C447	A373	G302	G230	A160	U68L
U1219	G1138	C838B	C987	A918	C838B	A767	G693	G610	A538	C448	A374	A303	G231	A161	U68M
G1220	G1057	U839	U992	A919	U839C	A768	G694	G611	A539	A452	A375	U304	G232	A162	U68N
G1221	C1140	G1058	C993	U920	C848	G769	A696	A611	A540	A453	G376	G305	C233	A163	G68O
G1222	G1141	C1059	A994	U921	C849	G770	A697	C612	C543	C457	A382	G306	G234	A164	G68P
G1223	G1142	C1060	C995	G922	U850	C771	U697	C613	C544	C458	A383	G307	G235	C165	U68Q
G1224	G1143	G1061	C996	A923	G851	G772	C701	A614	G545	C459	A384	C308	G236	G166	U68R
A1225	G1144	U1062	U999	C924	G852	G773	A702	C615	C546	C459A	C385	G310	C240	G167	C68S
C1226	C1145	U1063	A1000	G925	G858	G774	A703	G616	A547	C459B	C386	C311	C241	G168	G68T
A1227	G1146	U1064	G1001	G926	A859	G775	G703	G617	A548	C459C	U387	A312	C242	C169	C68Y
C1228	C1147	U1065	G1002	G927	A860	A777	A704	C620	C549	G475	G388	A313	C243	A171	G104
A1229	U1148	G1068	G1003	G928	G861	G778	U705	A621	U551	U480	A389	A314	C244	A172	G105
C1230	C1149	U1069	A1004	G929	G862	C779	A706	G628	U552	U481	C390	G315	C245	U173	C106
G1231	U1150	C1069	A1005	G933	U863	A780	C707	U710	A553	A482	C391	G316	G251	C176	G107
U1232	A1151	U1070	C1006	G934	A864	A781	G711	C634	C554	A483	G392	A321	G252	C177	G108
C1234	A1152	U1071	A1007	A935	A865	C784	A712	G635	C555	A484	G396	C322	G253	C178	A109
U1235	A1080	G1008	C1008	A936	C866	G785	G713	U636	C556	G485	A397	U323	G254	C179	C110
A1286	U1159	U1085	G1009	A937	C867	G786	G714	G637	A559	G490	C398	G324	U256	G112	G111
C1237	G1160	U1086	G1010	A938	C868	A787	G715	G637	C562	G491	C401	A325	G257	G113	G113
A1238	C1161	G1087	U1012	G939	U870	U788	A716	A642	C563	G492	G402	A326	G258	C185	G114
U1240	C1162	U1088	G1013	C940	U871	U789	C717	A643	C564	G493	G403	A327	G259	C186	G115
G1241	G1089	A872	A1014	G941	A873	A792	G721	C644	C565	U494	C404	C328	A262	C187	G116
A1245	G1171	G1094	A1015	G942	A874	U793	A722	C645	U565	A495	G407	C330	A263	C188	G117
C1246	G1173	U1095	C1017	G943	C875	A794	U723	U646	C566	A496	G408	C331	A264	C189	G118
U1247	C1096	C876	C1018	G945	C877	A802	U724	C647	G567	U498	A409	G332	U265	C190	U119
A1248	C1097	A946	C1019	A947	C878	G803	G725	A648	C568	C501	G410	G333	G266	C191	A120
C1249	U1020	G879	U1020	G947	C879	U804	A737	G649	C569	G505	A411	A338	C267	C192	C121
A1250	G1021	U950	G1021	G950	C880	C805	A728	A653	A572	G506	A412	A339	C268	C193	G122
A1251	G1022	G881	G1022	G951	C881	C806	A729	G657	A573	C507	A413	U340	C269	C194	C123
C1253	C1103	C882	G1023	U952	C882	G809	G730	G658	A574	C508	A414	C341	G270	C195	G124
G1254	A1105	G953	U1025	C953	C883	C810	C735	U659	G575	A509	A415	C342	C271	U125	U126
C1255	G1106	U884	G1026	G954	U884	C811	C736	G660	G576	A510	U423	A344	C272	G126	G127
A1256	C1027	G955	C1027	U955	G955	C812	A737	G661	C577	C511	C422	C345	A273	U127	G128
U1257	G1028	U956	C1028	U956	A889	U813	C738	A663	C578	U512	C423	G346	C277	U129	U129
G1258	C1028A	U960	C1028A	U961	C889	A814	G741	G664	U580	C513	G424	G347	C278	C193	G129A
C1259	U1028B	C962	C1028B	C962	U891	A815	G742	A665	G581	C514	G425	G348	A279	C194	A130
U1194	A1111	G963	G1028C	G963	A892	C817	U743	G666	U582	C518	U427	A351	C280	A195	C131
C1195	C1114	C993	A1028F	G966	C894	G818	C744	G667	A583	G521	U428	C352	C281	A196	A134
U1196	C1115	G995	G1028G	C967	G894	A819	C745	G668	G584	C522	U429	A353	G285	C197	C135
G1197	C1118	G996	G1028H	A968	G895	U820	G746	U669	C586	C523	A431	A354	G286	C136	C136
C1198	C1119	C999	A1035	A969	C999	G821	C748	G671	G590	C524	A432	C355	U287	G200	C137
A1204	U1205	G1036	A1036	C970	A900	G821	C749	G672	C591	G525	A433	A356	C288	C201	C201
U1206	G1124	G971	G1037	G971	A901	G822	G750	U673	G592	C526	A434	G357	G289	U201A	U201A
G1207	U1125	C972	G902	C972	G902	G823	G751	G674	G592	C527	C435	U358	C290	U201B	U201B
C1208	U1126	G973	G903	A974	A974	G824	A753	G675	G597	C528	C436	U359	C291	U201C	U201C
G1209	G1127	U1040	G903	A975	A975	G825	C754	A676	G597	C529	U437	A360	C292	G145	G145
C1210	C1128	G906	G906	A976	A976	A828	G755	U677	U598	G529	G438	G361	G293	C217	C217



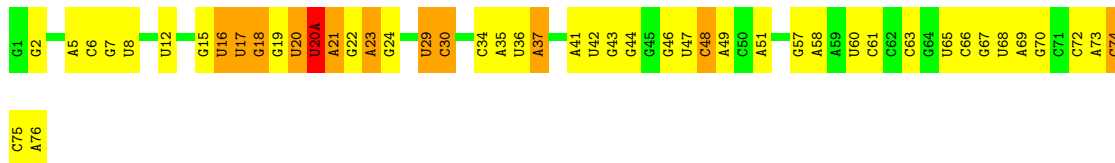
- Molecule 22: transfer RNA

Chain AW:



- Molecule 22: transfer RNA

Chain CW:



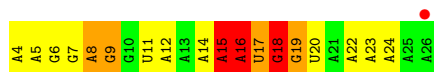
- Molecule 23: messenger RNA

Chain AV:



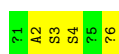
- Molecule 23: messenger RNA

Chain CV:



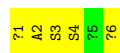
- Molecule 24: VIOMYCIN

Chain AU:



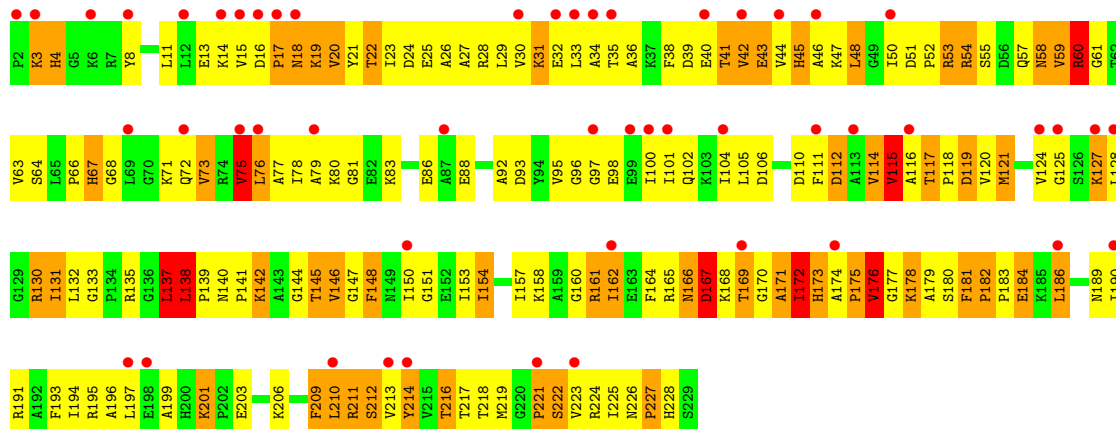
- Molecule 24: VIOMYCIN

Chain CU:



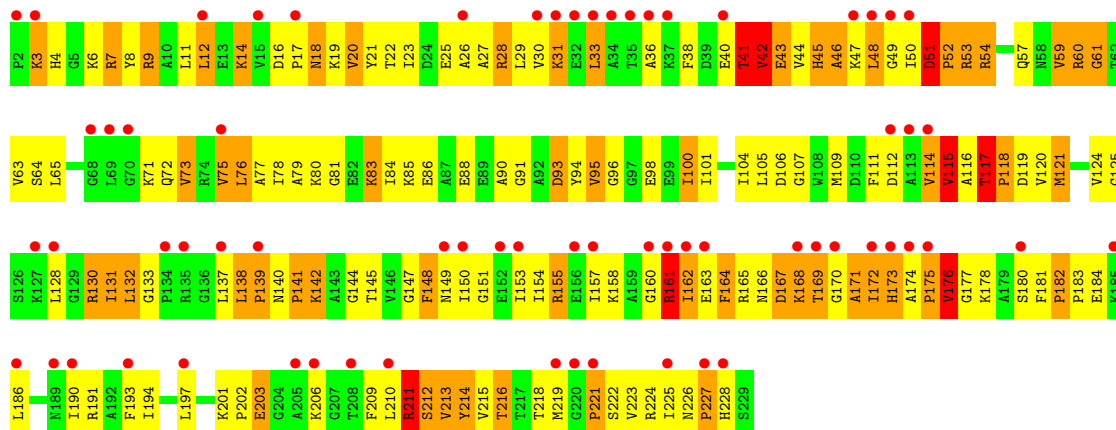
- Molecule 25: 50S ribosomal protein L1

Chain BC:



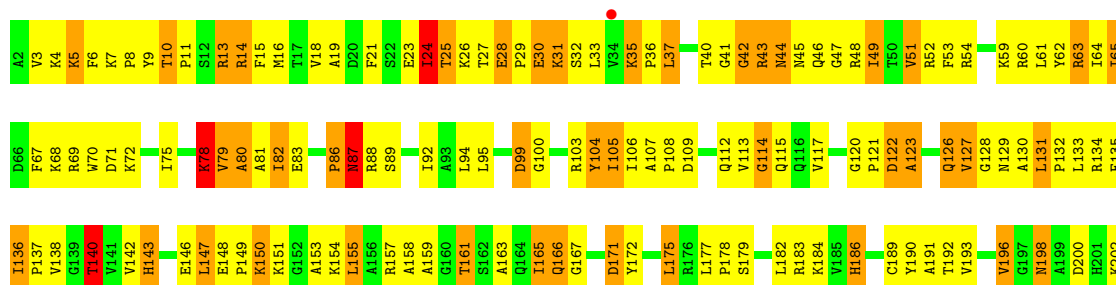
- Molecule 25: 50S ribosomal protein L1

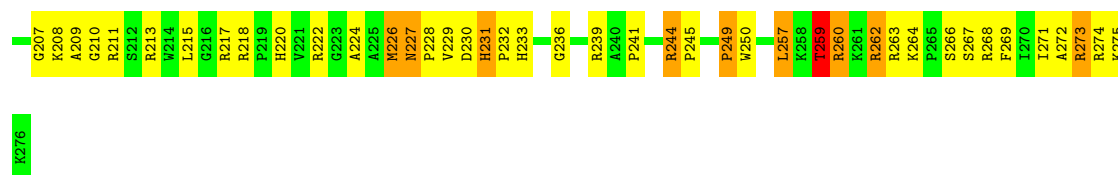
Chain DC:



- Molecule 26: 50S ribosomal protein L2

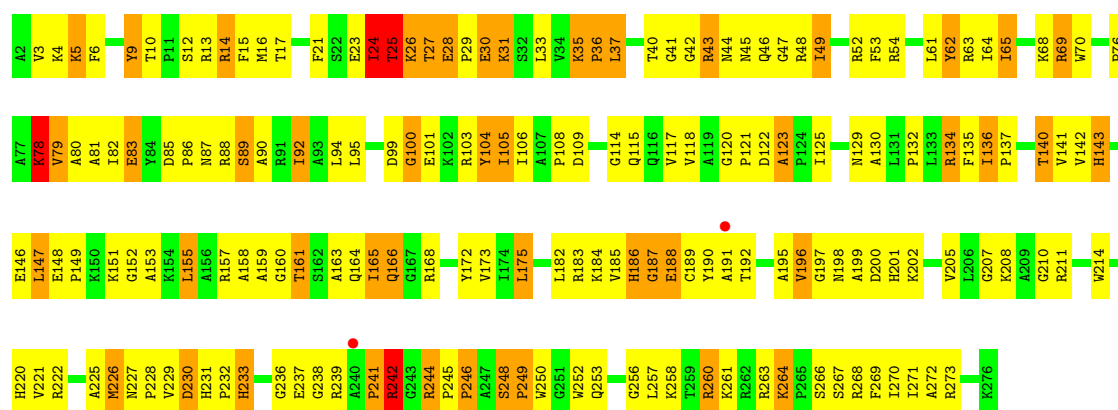
Chain BD:





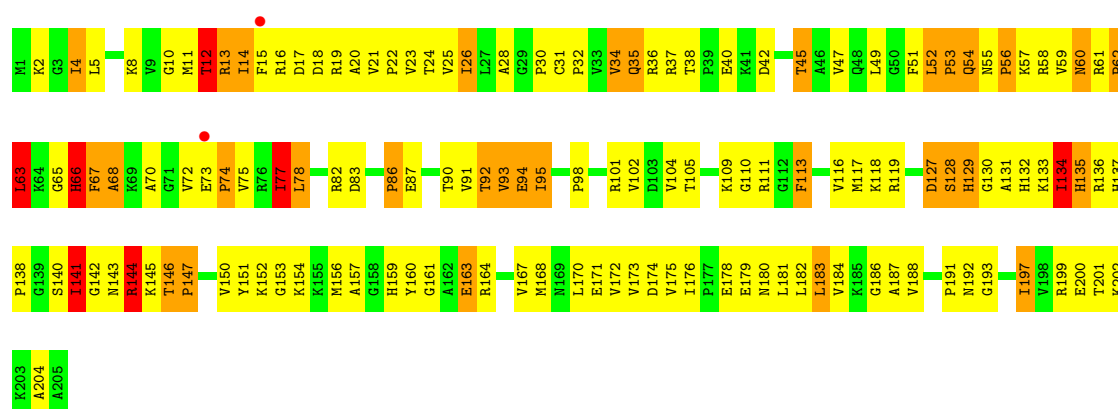
- Molecule 26: 50S ribosomal protein L2

Chain DD:



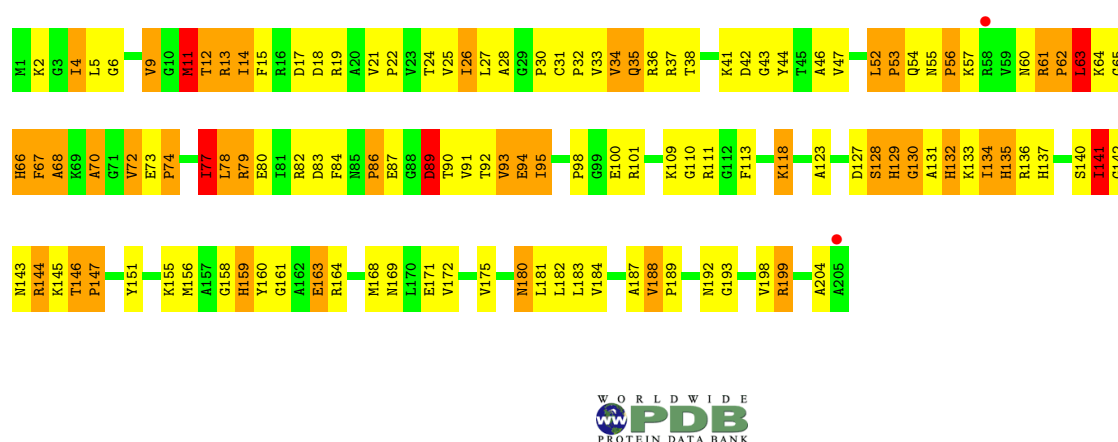
- Molecule 27: 50S ribosomal protein L3

Chain BE:



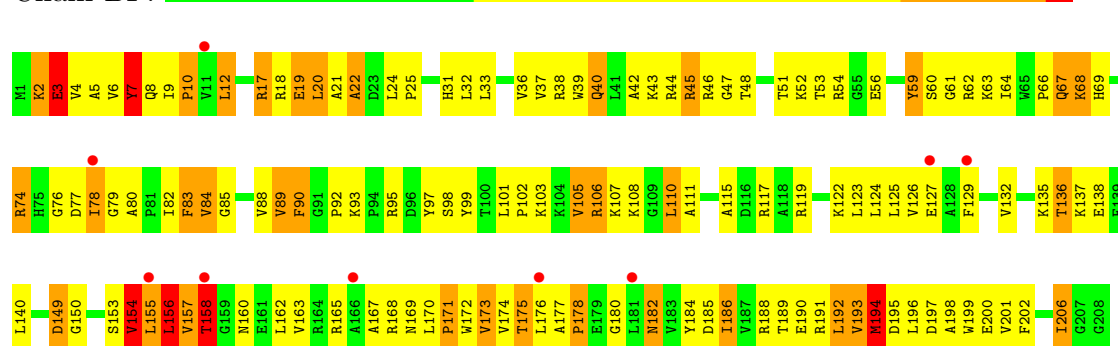
- Molecule 27: 50S ribosomal protein L3

Chain DE:



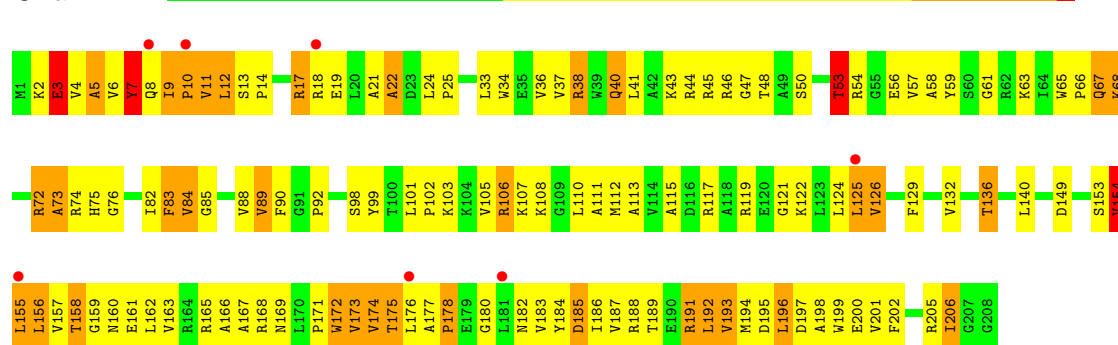
- Molecule 28: 50S ribosomal protein L4

Chain BF:



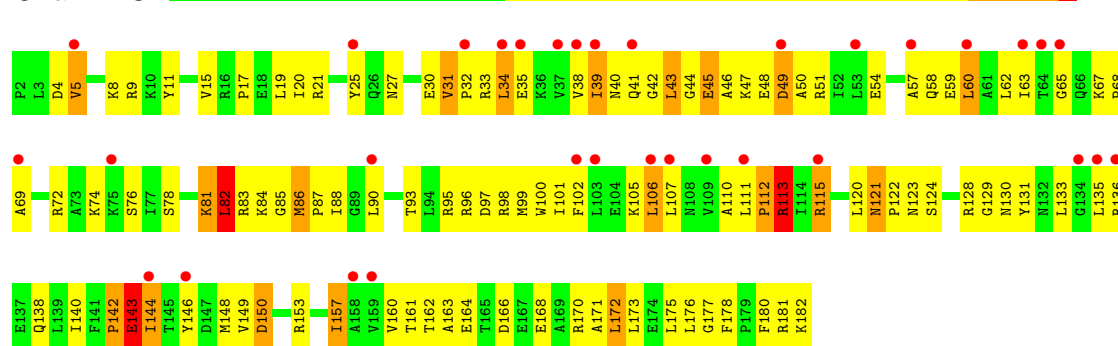
- Molecule 28: 50S ribosomal protein L4

Chain DF:



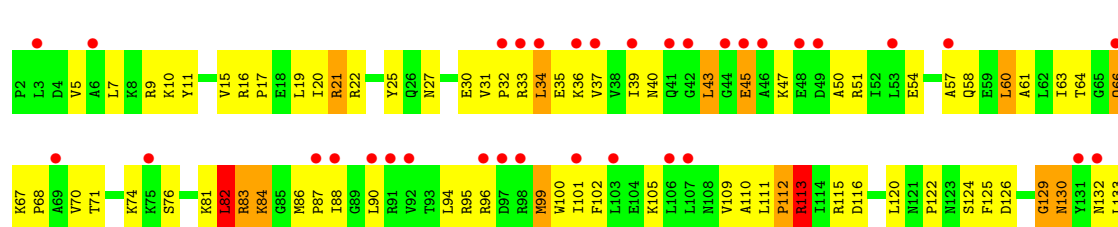
- Molecule 29: 50S ribosomal protein L5

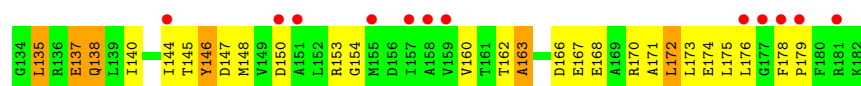
Chain BG:



- Molecule 29: 50S ribosomal protein L5

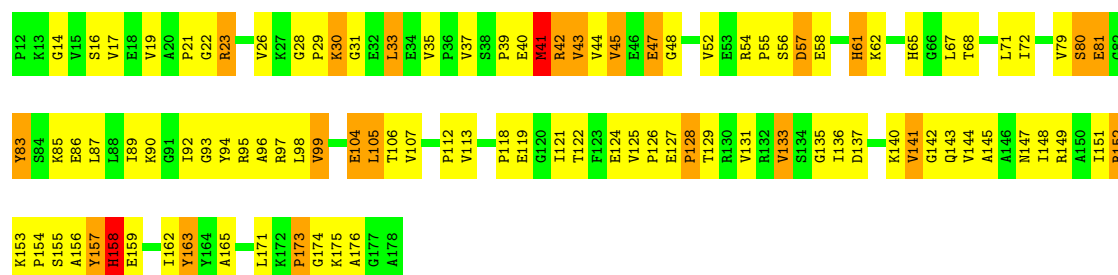
Chain DG:





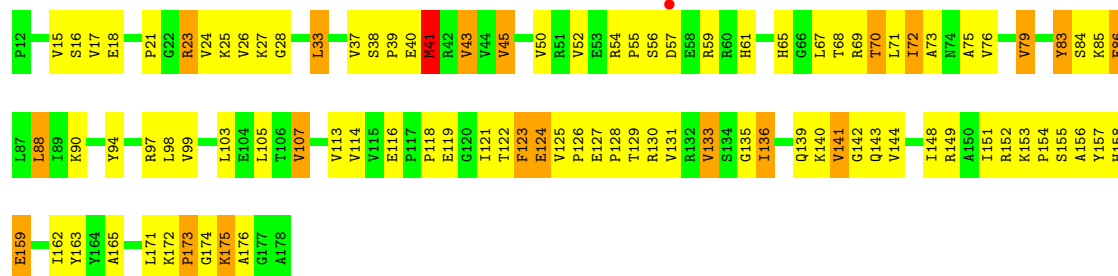
- Molecule 30: 50S ribosomal protein L6

Chain BH:



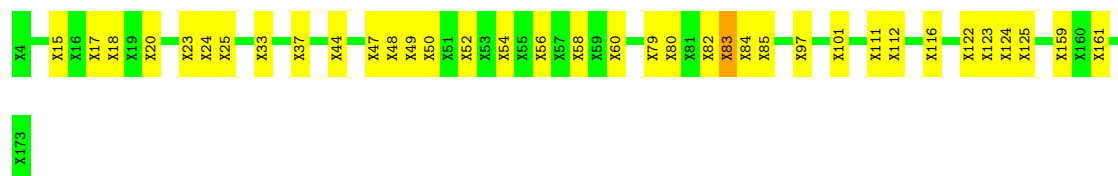
- Molecule 30: 50S ribosomal protein L6

Chain DH:



- Molecule 31: 50S RIBOSOMAL PROTEIN L10

Chain BJ:



- Molecule 31: 50S RIBOSOMAL PROTEIN L10

Chain DJ:



- Molecule 32: 50S ribosomal protein L11

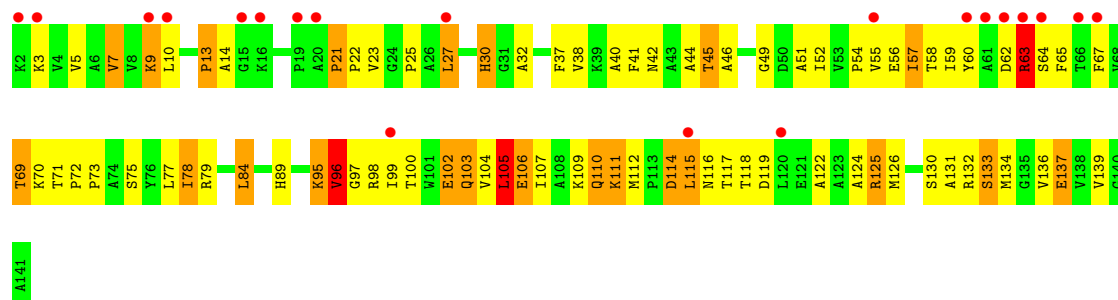
Chain BK:





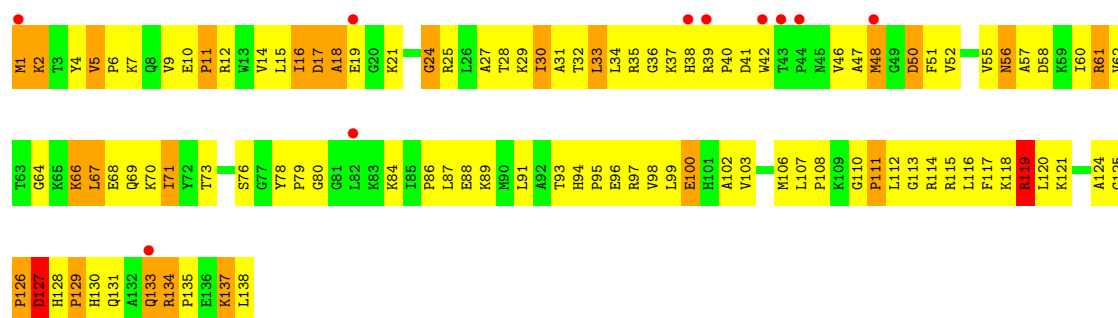
• Molecule 32: 50S ribosomal protein L11

Chain DK:



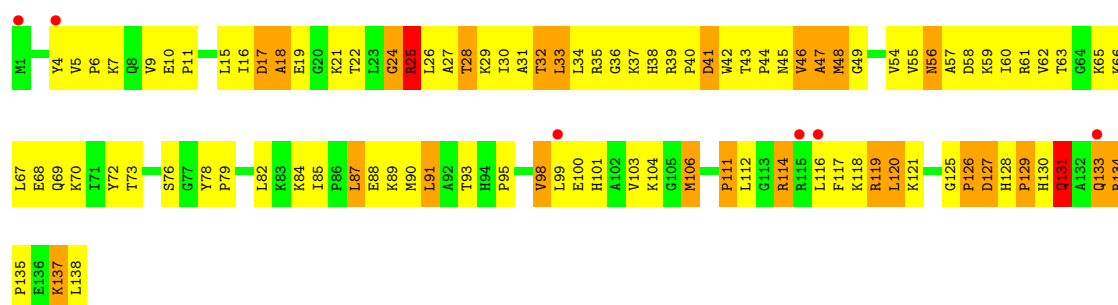
• Molecule 33: 50S ribosomal protein L13

Chain BN:



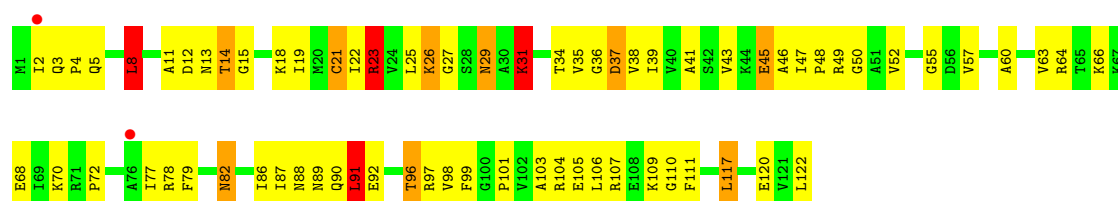
• Molecule 33: 50S ribosomal protein L13

Chain DN:

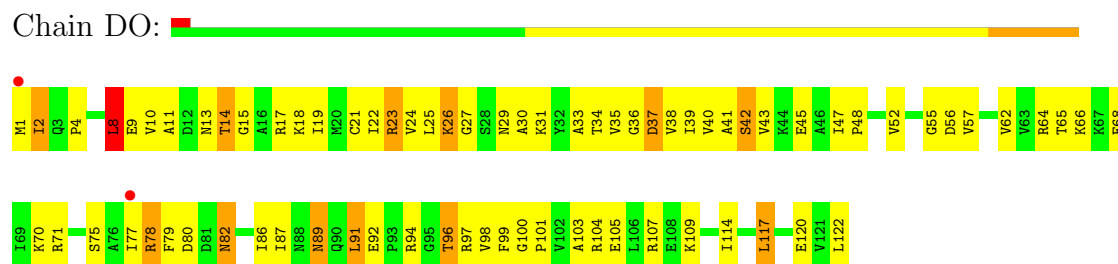


• Molecule 34: 50S ribosomal protein L14

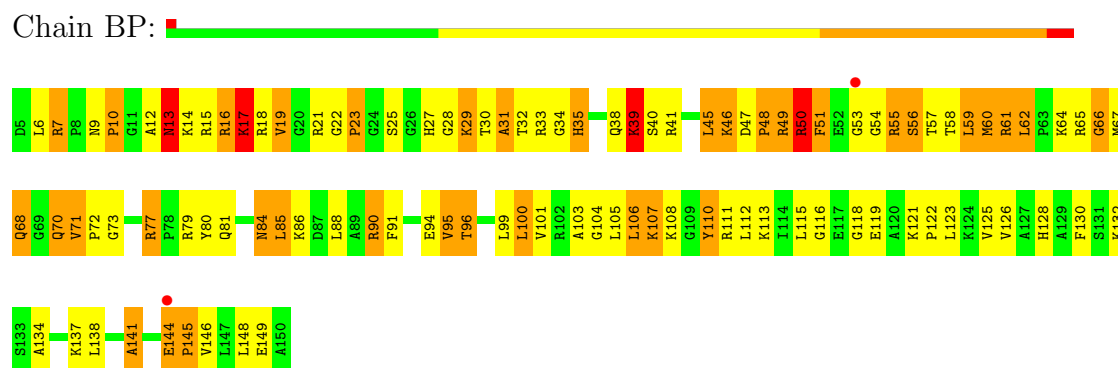
Chain BO:



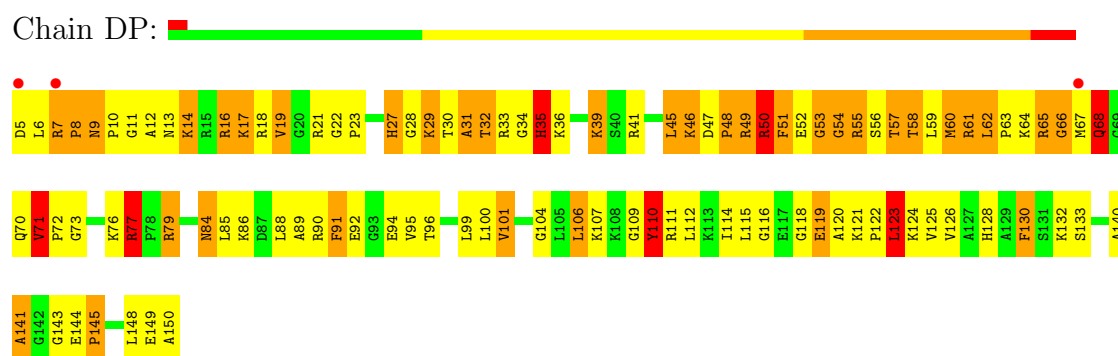
- Molecule 34: 50S ribosomal protein L14



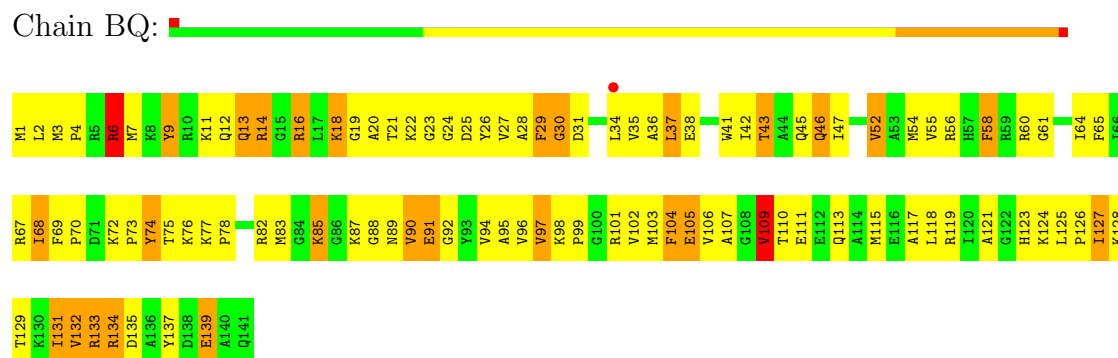
- Molecule 35: 50S ribosomal protein L15



- Molecule 35: 50S ribosomal protein L15

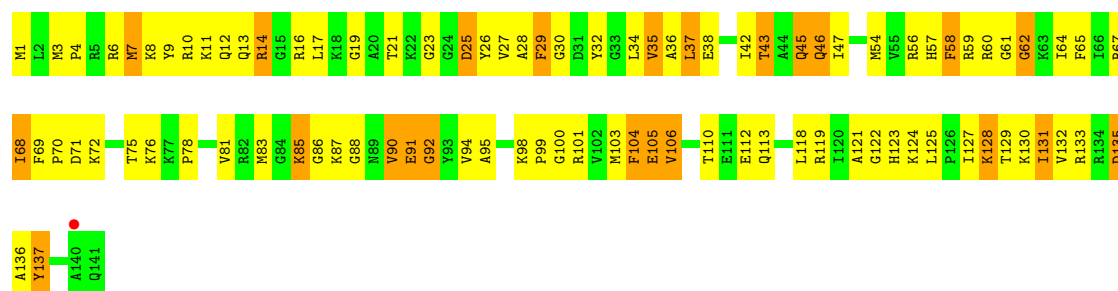


- Molecule 36: 50S ribosomal protein L16



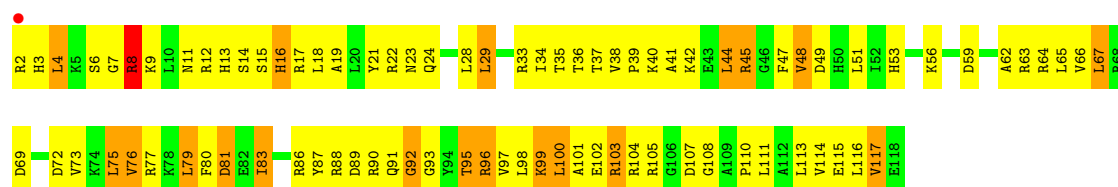
- Molecule 36: 50S ribosomal protein L16





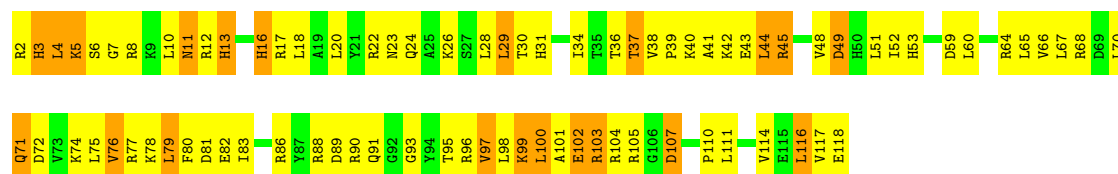
- Molecule 37: 50S ribosomal protein L17

Chain BR:



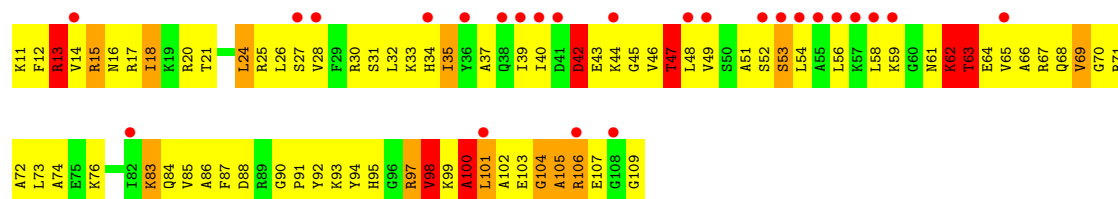
- Molecule 37: 50S ribosomal protein L17

Chain DR:



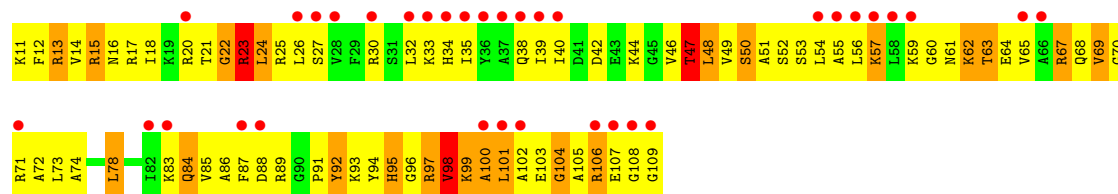
- Molecule 38: 50S ribosomal protein L18

Chain BS:



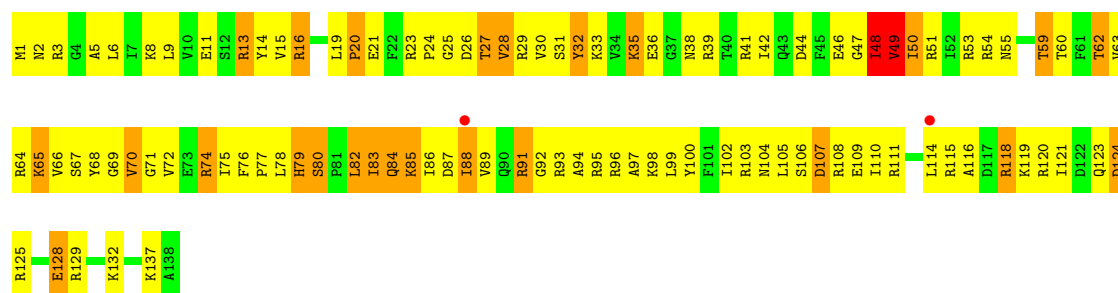
- Molecule 38: 50S ribosomal protein L18

Chain DS:



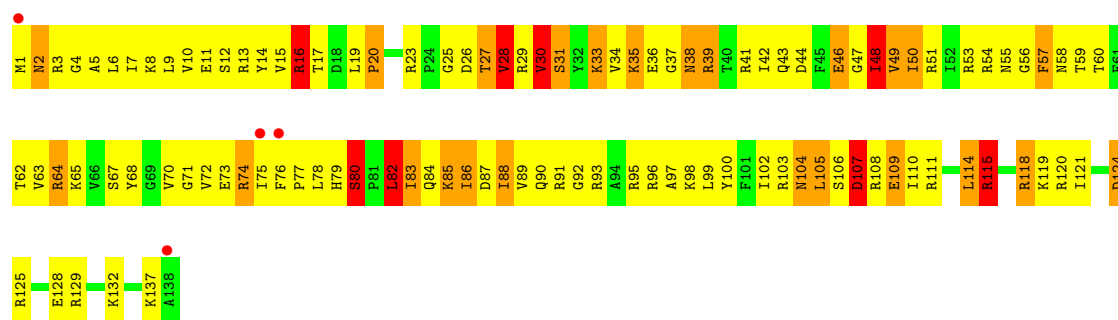
- Molecule 39: 50S ribosomal protein L19

Chain BT:



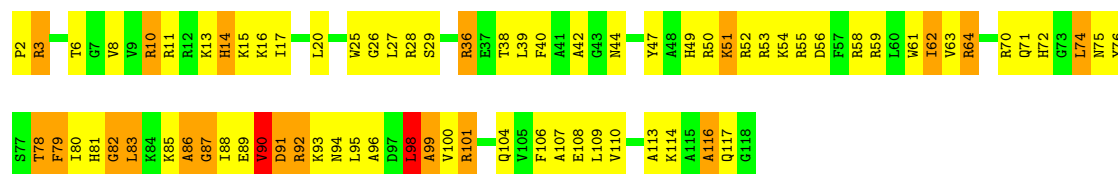
- Molecule 39: 50S ribosomal protein L19

Chain DT:



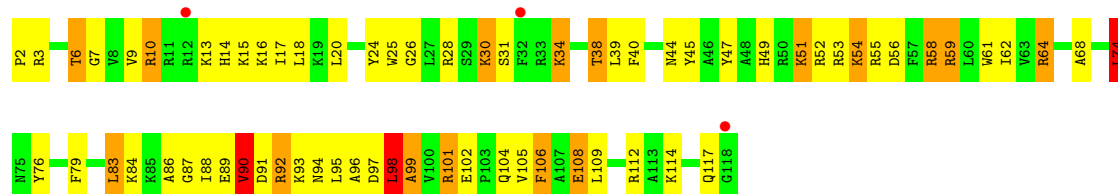
- Molecule 40: 50S ribosomal protein L20

Chain BU:



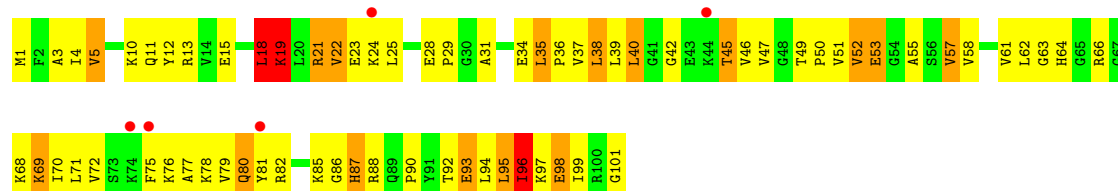
- Molecule 40: 50S ribosomal protein L20

Chain DU:

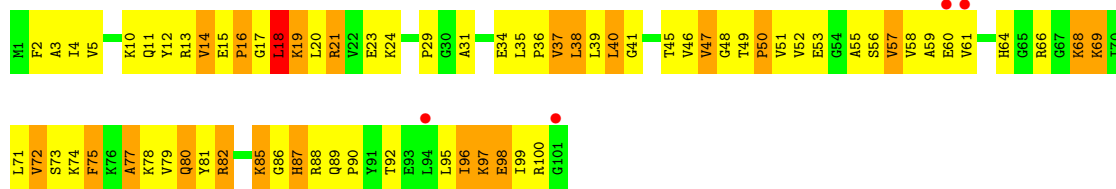


- Molecule 41: 50S ribosomal protein L21

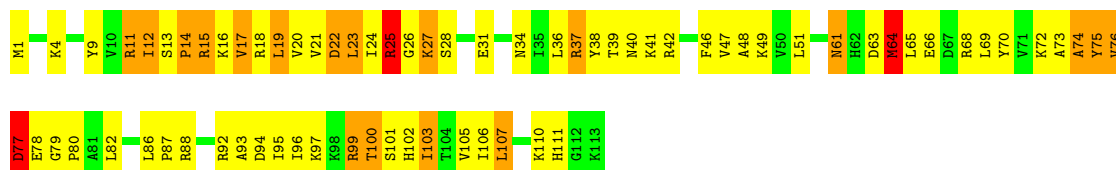
Chain BV:



- Molecule 41: 50S ribosomal protein L21

Chain DV: 

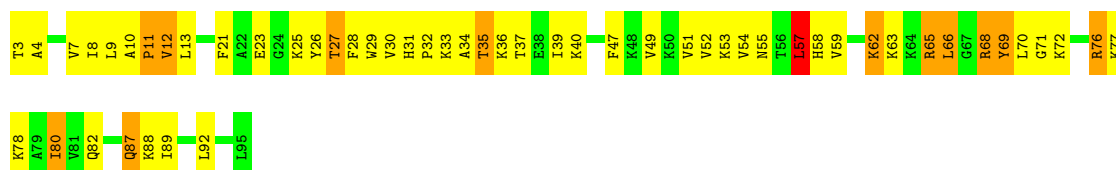
- Molecule 42: 50S ribosomal protein L22

Chain BW: 

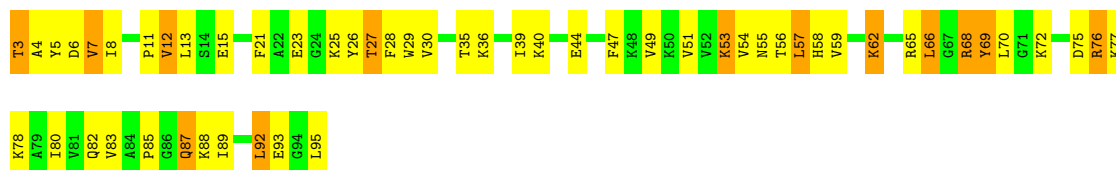
- Molecule 42: 50S ribosomal protein L22

Chain DW: 

- Molecule 43: 50S ribosomal protein L23

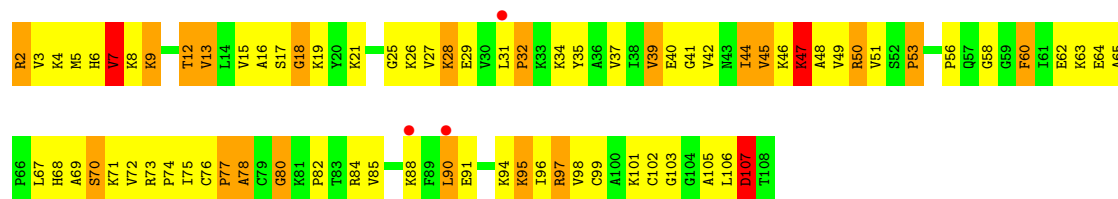
Chain BX: 

- Molecule 43: 50S ribosomal protein L23

Chain DX: 

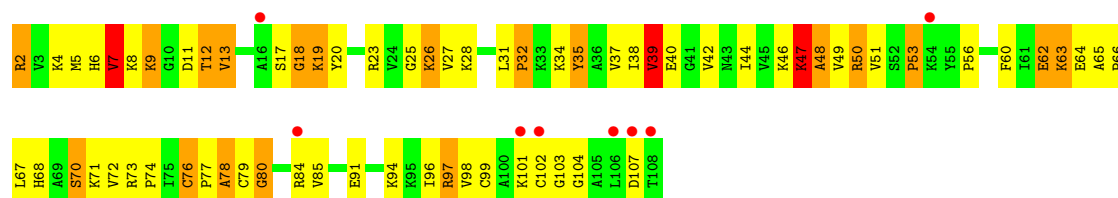
- Molecule 44: 50S ribosomal protein L24

Chain BY: 



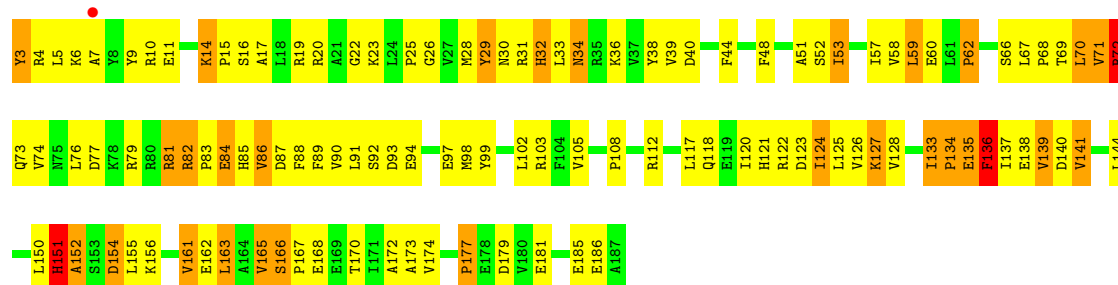
• Molecule 44: 50S ribosomal protein L24

Chain DY:



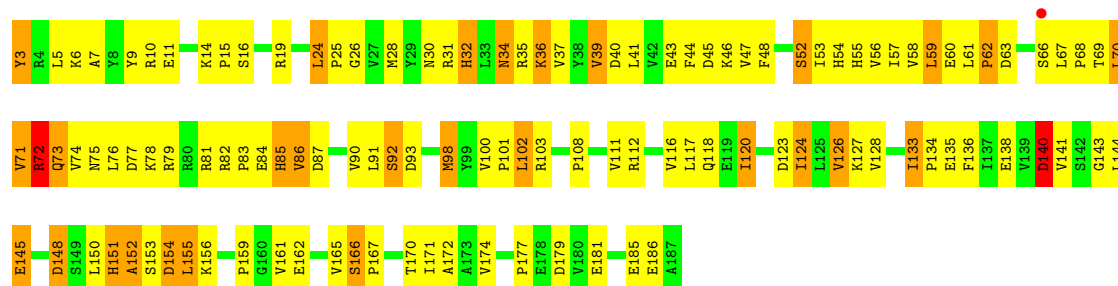
• Molecule 45: 50S ribosomal protein L25

Chain BZ:



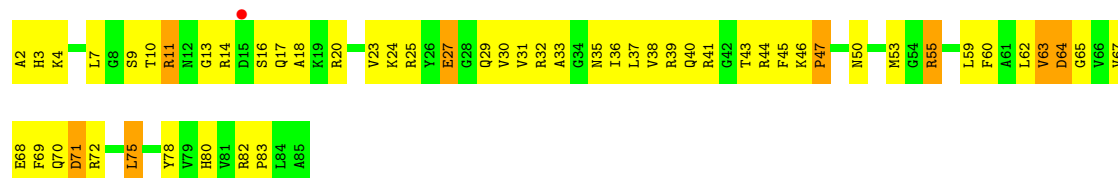
• Molecule 45: 50S ribosomal protein L25

Chain DZ:



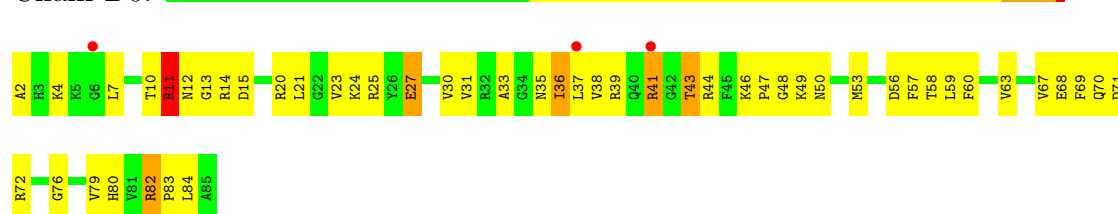
• Molecule 46: 50S ribosomal protein L27

Chain B0:



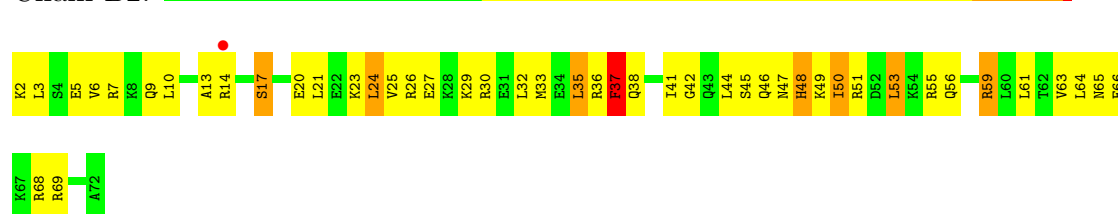
- Molecule 46: 50S ribosomal protein L27

Chain D0:



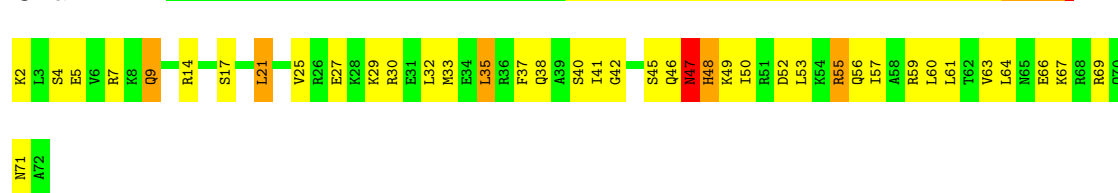
- Molecule 47: 50S ribosomal protein L29

Chain B2:



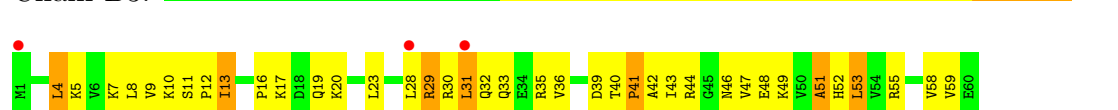
- Molecule 47: 50S ribosomal protein L29

Chain D2:



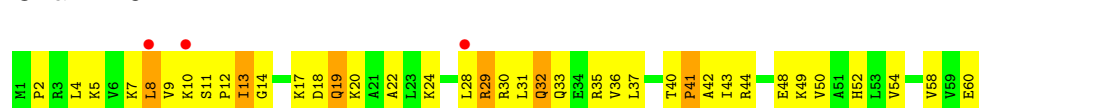
- Molecule 48: 50S ribosomal protein L30

Chain B3:



- Molecule 48: 50S ribosomal protein L30

Chain D3:



- Molecule 49: 50S ribosomal protein L32

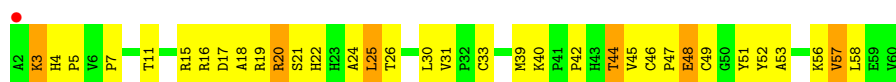
Chain B5:



- Molecule 49: 50S ribosomal protein L32

Chain D5:





- Molecule 50: 50S ribosomal protein L33

Chain B6:



- Molecule 50: 50S ribosomal protein L33

Chain D6:



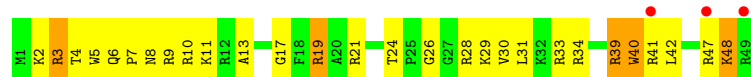
- Molecule 51: 50S ribosomal protein L34

Chain B7:



- Molecule 51: 50S ribosomal protein L34

Chain D7:



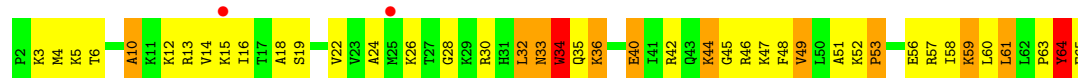
- Molecule 52: 50S ribosomal protein L35

Chain B8:



- Molecule 52: 50S ribosomal protein L35

Chain D8:



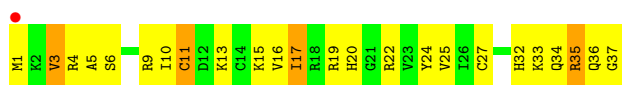
- Molecule 53: 50S ribosomal protein L36

Chain B9:



- Molecule 53: 50S ribosomal protein L36

Chain D9: 



- Molecule 54: 50S RIBOSOMAL PROTEIN L7/L12

Chain Bf: 

There are no outlier residues recorded for this chain.

- Molecule 54: 50S RIBOSOMAL PROTEIN L7/L12

Chain Bg: 

There are no outlier residues recorded for this chain.

- Molecule 54: 50S RIBOSOMAL PROTEIN L7/L12

Chain Df: 

There are no outlier residues recorded for this chain.

- Molecule 54: 50S RIBOSOMAL PROTEIN L7/L12

Chain Dg: 

There are no outlier residues recorded for this chain.

- Molecule 55: 50S RIBOSOMAL PROTEIN L7/L12

Chain Bh: 

There are no outlier residues recorded for this chain.

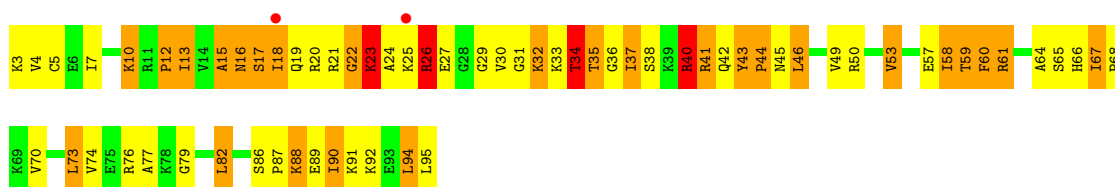
- Molecule 55: 50S RIBOSOMAL PROTEIN L7/L12

Chain Dh: 

There are no outlier residues recorded for this chain.

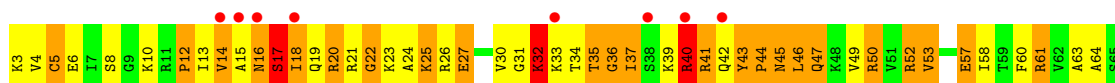
- Molecule 56: 50S ribosomal protein L28

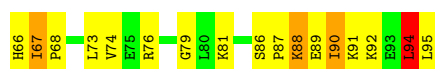
Chain B1: 



- Molecule 56: 50S ribosomal protein L28

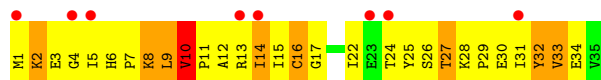
Chain D1: 





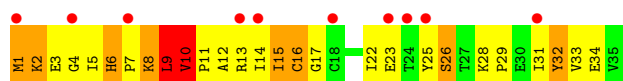
- Molecule 57: 50S ribosomal protein L31

Chain B4:



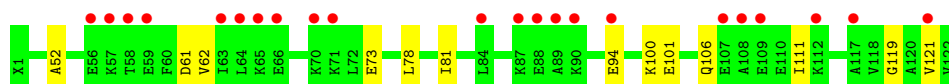
- Molecule 57: 50S ribosomal protein L31

Chain D4:



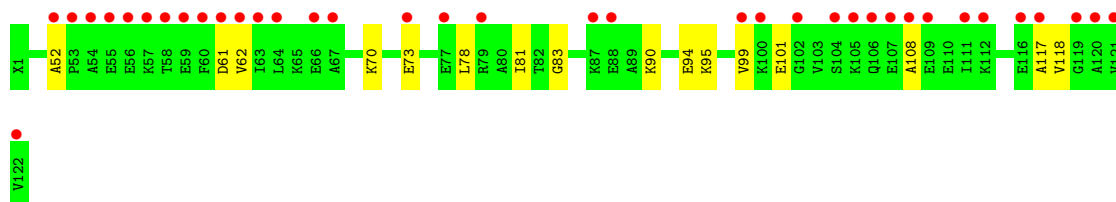
- Molecule 58: 50S ribosomal protein L7/L12

Chain Be:



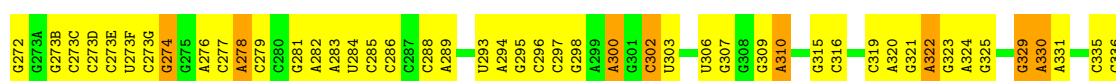
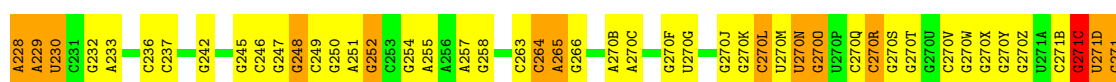
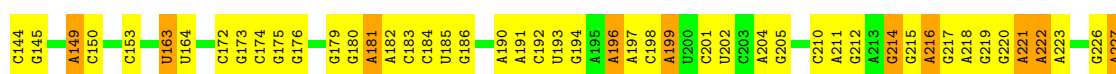
- Molecule 58: 50S ribosomal protein L7/L12

Chain De:



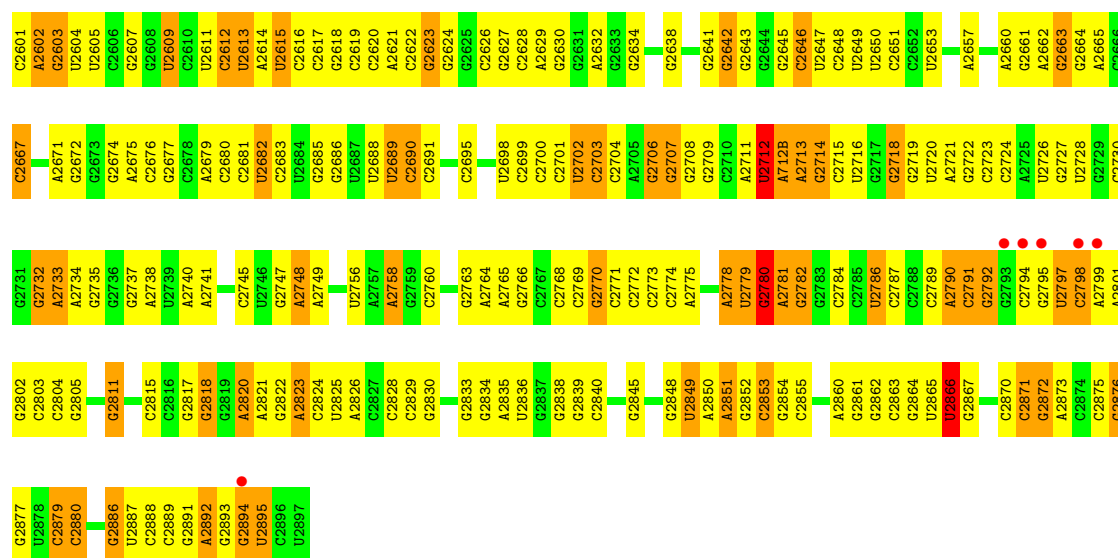
- Molecule 59: 23S ribosomal RNA

Chain BA:



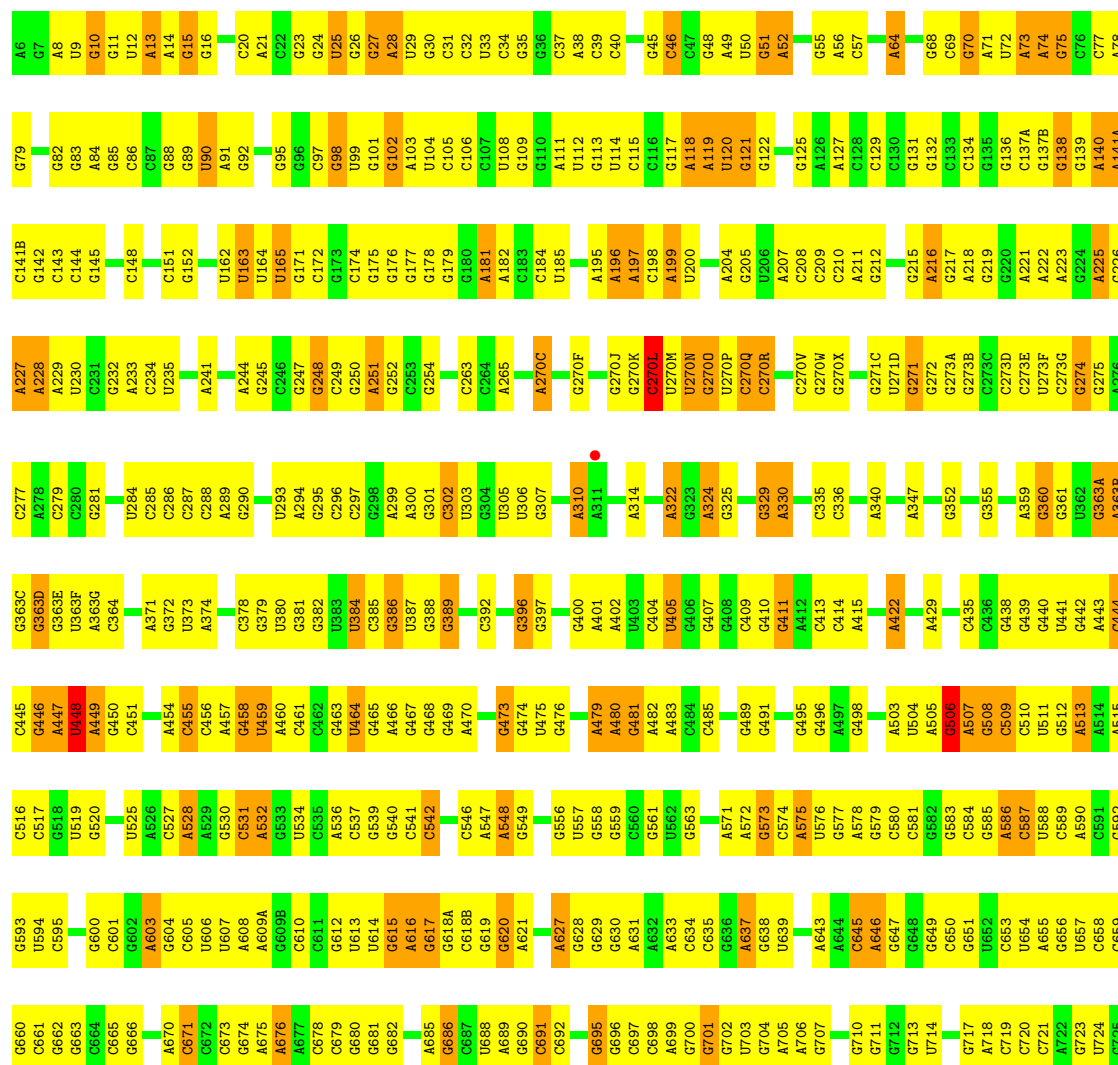
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U2167	G2168	A2171	U2172	A2173	C2174	C2175	A2176	C2177	C2178	C2179	G2182	C2183	G2184	C2195	A2198	A2199	C2207	U2208	C2209	G2283	G2284	C2285	A2286	A2287	A2288	G2289	G2290	U2291	C2292	C2293	G2299	G2300	C2301	G2302	G2303	G2304	A2305	A2306	G2307	G2308	A2311	C2316	A2320	G2321	A2322	G2323	G2324	A2325	C2326	A2327	G2328																										
G2252	C2258	G2259	C2260	U2265	A2266	A2267	A2268	A2269	G2270	G2271	U2272	A2273	A2274	C2275	G2276	G2277	A2278	G2279	G2280	G2281	G2282	G2283	G2284	C2285	A2286	A2287	A2288	G2289	G2290	U2291	C2292	C2293	G2299	G2300	C2301	G2302	G2303	G2304	A2305	A2306	G2307	G2308	A2311	C2316	A2320	G2321	A2322	G2323	G2324	A2325	C2326	A2327	G2328																								
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G2464	G2465	G2466	G2467	G2468	G2469	G2470	G2475	G2476	G2477	G2478	G2479	G2480	G2481	G2482	G2483	G2484	G2485	G2486	G2487	G2488	G2489	G2490	U2491	G2494	G2495	G2496	G2497	U2500	U2501	G2502	G2503	G2504	G2505	G2510	U2511	U2514	G2515	G2516	G2517	U2518	G2519	G2520	G2521	U2522	G2523	G2524	G2525	G2526	G2527	G2528	G2529	A2530	A2531	G2532	A2600																						
C2533	A2534	G2535	G2536	U2537	C2538	C2539	C2540	U2541	A2542	G2543	G2544	G2549	U2552	G2553	U2554	U2555	G2556	G2557	G2558	U2562	U2563	A2564	A2565	A2566	G2567	G2570	G2571	A2572	G2573	G2574	G2575	G2576	A2577	G2578	G2579	U2580	G2581	G2582	G2583	U2584	U2585	G2586	A2587	G2588	A2589	A2590	G2591	G2592	U2593	G2594	G2595	U2596	G2597	A2600																							
C1432	U1433	A1434	G1435	G1436	C1437	U1438	A1439	G1440	G1441	G1442	A1443	C1444	C1445	G1448	A1498	G1449	A1453	U1454	G1455	G1458	G1459	A1460	G1461	G1462	C1463	C1464	G1465	A1536	A1538	A1528	C1598	C1599	C1531	G1601	C1532	C1533	C1534	U1535	A1536	C1476	C1477	G1478	G1479	A1480	U1481	G1483	A1486	G1487	A1490	G1491	G1492	G1493	A1494	A1495	A1496	U1497																					
C1498	C1499	C1499	C1501	A1508	A1509	A1510	A1511	G1512	G1583	C1513	U1514	U1515	U1516	G1517	G1448	A1498	G1449	A1453	U1454	G1455	G1458	G1459	A1460	G1461	G1462	C1463	C1464	G1465	A1536	A1538	A1528	C1598	C1599	C1531	G1601	C1532	C1533	C1534	U1535	A1536	C1476	C1477	G1478	G1479	A1480	U1481	G1483	A1486	G1487	A1490	G1491	G1492	G1493	A1494	A1495	A1496	U1497																				
G1642	G1643	G1644	G1645	G1646	G1647	C1648	G1651	G1654	A1655	U1654	C1656	C1657	C1658	C1659	U1660	G1661	C1662	G1663	A1664	A1665	G1666	G1667	A1668	A1669	C1672	U1673	C1674	G1675	A1676	G1677	G1678	G1681	G1682	C1683	C1684	G1687	C1688	C1691	C1694	C1695	G1696	G1697	A1698	G1699	A1700	G1692	G1708	U1709	G1710	C1711	C1712	U1727																									
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C1800	G1801	A1802	A1803	A1809	G1810	G1811	A1812	A1815	G1816	U1817	U1818	A1819	G1820	U1821	G1822	G1823	G1824	A1825	G1826	C1827	G1828	A1829	C1836	C1837	U1838	G1839	G1840	U1841	G1842	C1843	C1844	A1845	G1846	A1847	A1848	G1849	G1850	U1851	C1852	A1853	A1854	G1855	G1856	G1857	G1858	A1859	A1871	A1872	G1878	C1879	C1882	G1883	U1884	A1885																							
C1886	C1887	G1888	A1889	A1890	C1895	G1896	G1897	U1898	G1899	A1900	A1901	C1902	G1903	G1904	C1905	G1906	G1907	C1908	C1909	G1910	U1911	A1912	A1913	C1914	U1915	A1916	U1917	G1922	U1923	C1924	G1925	C1932	G1933	C1934	G1935	A1936	A1937	A1938	U1939	U1940	C1941	C1942	U1943	U1944	A1952	C1955	U1956	C1957	C1958	G1959	A1960																										
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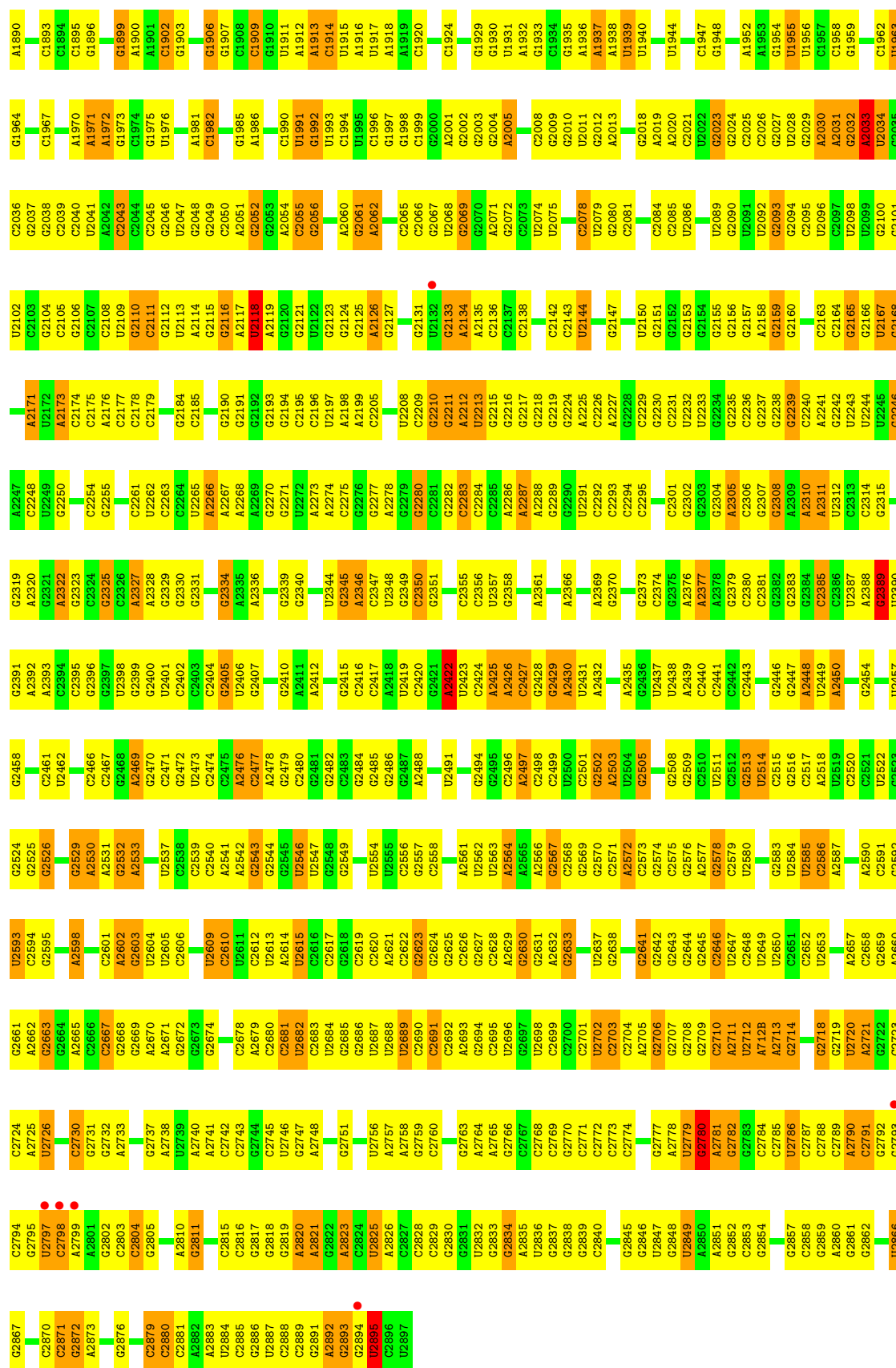


• Molecule 59: 23S ribosomal RNA

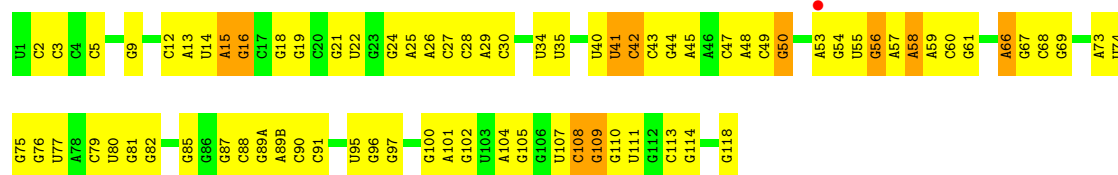
Chain DA:



U1806	G1707	A1631	C1550	G1484	G1418	G1348	G1277	G1212	U1141	G1071	U999	G938	U871	A804	G726
C1806	C1708	A1632	C1551	G1485	A1419	A1349	A1278	A1213	U1142	C1072	A1000	G939	A872	G805	G729
A1810	A1709	G1633	C1556	A1486	A1420	U1352	G1279	G1214	A114B	C1076	A1001	G940	G873	C730	C730
A1812	C1710	G1634	C1557	G1488	G1421	A1353	A1286	G1215	G1143	U1077	C1002	A941	G808	C731	C731
G1813	C1711	G1636	A1558	G1492	G1422	A1354	A1287	G1216	G1144	U1078	C1005	G942	G809	C732	C732
G1814	C1712	A1637	G1559	G1491	G1424	G1355	U1288	G1217	A1148	C1079	C1006	U943	G878	C733	C733
A1815	U1727	G1638	C1565	G1492	A1427	G1356	C1291	C1221	G1149	U1080	C1007	G944	A879	A734	A734
G1816	G1728	C1639	A1566	G1493	G1428	U1357	U1292	C1224	C1152	U1081	C1008	A945	C812	G738	G738
G1817	A1729	A1640	A1567	A1494	C1428	G1358	C1293	G1225	C1153	U1082	A1009	G946	U813	G739	G739
U1818	U1730	G1641	G1568	A1495	G1429	A1359	C1294	G1226	C1154	U1083	A1010	G947	C814	U740	U740
A1819	A1732	G1642	G1569	G1496	C1430	A1360	U1294	A1226	G1154	U1084	G1011	G948	C815	G741	G741
U1820	G1733	G1643	A1570	U1497	U1431	G1361	C1295	G1227	A1155	A1085	U1012	C949	C816	G742	G742
A1821	G1733	C1644	A1570	C1498	C1432	C1362	G1296	C1230	A1156	A1086	C1013	G950	C817	G743	G743
A1825	G1760	G1645	C1577	C1499	U1433	G1363	U1300	G1231	G1157	U1087	U1014	C951	A819	U747	U747
G1826	C1751	G1646	U1578	G1500	A1434	G1364	A1301	G1232	C1158	A1088	G1015	G952	A820	G748	G748
G1827	U1757	C1501	G1501	G1501	G1435	A1365	A1302	G1233	U1159	U1089	G1016	A953	A821	C749	C749
G1828	G1765	C1502	C1502	C1502	G1436	G1368	G1303	U1234	C1161	U1090	C1018	C955	U822	U762	U762
C1830	G1766	C1505	C1505	C1505	U1438	G1369	C1306	G1235	G1162	G1091	U1019	G956	U826	G763	G763
U1833	U1767	C1581	C1582	C1582	U1439	G1370	G1309	G1236	G1163	U1094	A1020	G957	U827	G764	G764
U1834	U1768	A1510	A1586	A1586	G1440	U1372	G1310	G1237	G1164	A1095	A1021	U958	U828	C766	C766
C1834	A1762	A1511	C1587	G1512	G1441	G1373	G1311	G1238	U1165	A1096	G1022	U959	U829	U767	U767
U1841	G1763	A1512	C1588	G1513	G1442	G1374	G1312	G1239	C1166	U1097	U1023	A960	A830	G768	G768
G1842	G1764	G1514	C1589	C1513	G1443	C1375	A1317	A1246	U1175	G1106	G1030	G968	U839	U769	U769
G1843	U1775	G1515	G1590	U1514	G1444	C1376	U1317	A1247	G1176	G1107	U1033	U969	C840	G771	G771
C1844	G1776	G1516	C1595	G1522	U1488	A1384	C1320	G1248	U1177	U1108	U1034	C970	A841	A774	A774
G1845	U1777	G1517	A1596	U1523	A1489	G1385	A1321	G1249	C1178	G1109	G1036	C971	G842	G775	G775
G1846	U1779	G1524	C1599	G1525	G1453	C1387	A1322	U1250	C1179	G1110	G1037	G972	G843	G776	G776
A1847	G1780	G1526	G1601	G1527	U1454	U1394	U1323	C1251	G1184	A1111	A1045	G973	C846	A777	A777
A1854	C1782	G1528	U1602	A1528	G1455	A1395	G1324	G1252	C1185	A1112	U1046	G974A	U847	G778	G778
G1858	U1783	A1529	A1603	A1529	C1458	U1396	U1325	A1253	G1186	U1113	A1046	G975	G848	G780	G780
A1859	A1785	G1530	C1604	G1530	G1459	U1397	U1326	G1254	C1187	U1114	G1047	G976	U849	U779	U779
G1860	A1786	C1531	G1605	C1531	A1460	C1398	G1327	U1255	G1188	G1115	A1048	G977	G852	A781	A781
G1861	G1787	C1532	C1606	C1532	G1461	G1399	G1328	G1256	G1189	C1116	C1049	G978	G853	A782	A782
G1862	U1788	G1533	G1607	G1533	C1462	U1400	U1329	C1257	G1190	U1119	A1050	G979	G854	A783	A783
G1863	C1788	G1534	A1608	G1534	C1463	G1401	A1331	C1258	G1193	G1120	G1051	A980	G855	A784	A784
U1869	U1789	U1535	A1609	U1535	C1464	C1402	A1332	G1259	G1196	C1121	G1055	A983	G856	G785	G785
U1870	C1790	A1536	A1610	A1536	G1465	C1403	G1333	C1261	C1197	G1122	G1056	A984	C857	G786	G786
G1871	A1791	C1537	C1611	C1537	G1466	C1404	U1334	U1263	U1198	C1123	A1057	C985	U858	U787	U787
C1870	G1792	G1538	G1612	G1538	C1467	U1405	A1335	G1264	U1199	C1124	G1058	C986	G859	A788	A788
A1871	U1794	G1539	C1613	G1539	G1468	U1406	U1336	G1265	C1200	G1125	G1059	G987	U860	A789	A789
A1872	C1795	U1540	U1541	U1540	A1469	C1407	U1337	A1265	C1201	A1126	U1060	G988	A861	C790	C790
G1882	U1796	G1542	C1614	G1542	G1470	C1408	G1338	U1266	C1202	G1127	U1061	A990	G862	C791	C791
G1883	C1797	U1543	A1543	U1543	A1471	G1409	U1339	G1267	U1203	A1132	G1062	A983	A863	G792	G792
A1884	U1798	C1544	C1544	C1544	C1476	G1410	U1340	U1268	A1203	U1133	G1063	C991	G864	A793	A793
A1885	G1799	U1545	A1545	U1545	A1477	C1411	A1341	A1269	A1204	U1134	G1064	C992	C865	G794	G794
C1886	U1800	G1546	U1621	A1546	G1478	G1413	A1342	C1270	U1205	G1135	U1065	C993	C866	C795	C795
G1887	G1801	C1547	C1622	C1547	G1479	G1414	G1343	A1271	G1206	G1136	U1066	C994	C867	C796	C796
A1888	A1802	C1548	G1624	C1548	G1480	U1415	G1344	A1272	C1207	G1137	U1067	A996	U868	G799	G799
U1889	G1804	C1549	C1549	C1549	U1481	G1416	G1346	A1275	A1210	G1138	A1067	G997	G869	G934	G934
					G1483	C1417	G1347	A1276	U1211	C1140	A1070	C998	C935	A800	A800

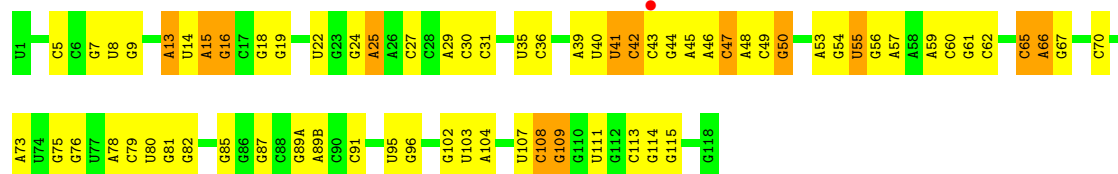


Chain BB:



- Molecule 60: 5S ribosomal RNA

Chain DB:



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	306.01Å 673.49Å 351.98Å 90.00° 92.69° 90.00°	Depositor
Resolution (Å)	40.00 – 3.50 131.34 – 3.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.50) 74.9 (131.34-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 3.49Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.262 , 0.309 0.259 , 0.274	Depositor DCC
R_{free} test set	38188 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	80.5	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 72.9	EDS
Estimated twinning fraction	0.247 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.26$, $\langle L^2 \rangle = 0.11$	Xtriage
Outliers	0 of 765681 reflections	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	308422	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GNP, DPP, MG, KBE, UAL, 5OH

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	AB	0.42	0/1945	0.73	4/2621 (0.2%)
1	CB	0.40	0/1945	0.69	1/2621 (0.0%)
2	AC	0.35	0/1645	0.60	0/2216
2	CC	0.33	0/1645	0.58	1/2216 (0.0%)
3	AD	0.37	0/1733	0.60	0/2318
3	CD	0.34	0/1733	0.61	0/2318
4	AE	0.35	0/1172	0.63	1/1576 (0.1%)
4	CE	0.34	0/1172	0.63	1/1576 (0.1%)
5	AF	0.38	0/856	0.67	2/1154 (0.2%)
5	CF	0.35	0/856	0.64	1/1154 (0.1%)
6	AG	0.34	0/1276	0.58	0/1709
6	CG	0.35	0/1276	0.58	0/1709
7	AH	0.34	0/1136	0.58	0/1527
7	CH	0.33	0/1136	0.57	0/1527
8	AI	0.36	0/1029	0.63	1/1378 (0.1%)
8	CI	0.36	0/1029	0.61	1/1378 (0.1%)
9	AJ	0.37	0/815	0.64	1/1095 (0.1%)
9	CJ	0.33	0/815	0.65	1/1095 (0.1%)
10	AK	0.40	0/900	0.65	0/1213
10	CK	0.37	0/900	0.63	0/1213
11	AL	0.47	0/992	0.89	3/1327 (0.2%)
11	CL	0.47	0/992	0.88	4/1327 (0.3%)
12	AM	0.33	0/1008	0.61	0/1347
12	CM	0.32	0/1008	0.58	0/1347
13	AN	0.37	0/501	0.57	0/664
13	CN	0.35	0/501	0.57	0/664
14	AO	0.39	0/745	0.62	0/992
14	CO	0.35	0/745	0.59	0/992
15	AP	0.34	0/722	0.58	0/970
15	CP	0.33	0/722	0.56	0/970
16	AQ	0.45	0/848	0.75	0/1131
16	CQ	0.42	0/848	0.71	0/1131

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AR	0.33	0/579	0.59	0/768
17	CR	0.31	0/579	0.57	0/768
18	AS	0.32	0/647	0.59	0/870
18	CS	0.31	0/647	0.56	0/870
19	AT	0.36	0/764	0.57	0/1006
19	CT	0.37	0/764	0.62	0/1006
20	AY	0.47	6/5481 (0.1%)	0.72	5/7418 (0.1%)
20	CY	0.52	7/5481 (0.1%)	0.76	12/7418 (0.2%)
21	AA	0.39	0/36351	0.97	36/56736 (0.1%)
21	CA	0.38	0/36351	0.95	35/56736 (0.1%)
22	AW	0.40	0/1827	1.06	9/2845 (0.3%)
22	CW	0.41	1/1827 (0.1%)	1.06	9/2845 (0.3%)
23	AV	0.78	1/568 (0.2%)	1.49	16/886 (1.8%)
23	CV	0.95	3/568 (0.5%)	1.74	19/886 (2.1%)
24	AU	1.05	0/11	1.28	0/13
24	CU	1.06	0/11	1.28	0/13
25	BC	0.44	0/1774	0.74	1/2391 (0.0%)
25	DC	0.50	1/1774 (0.1%)	0.76	0/2391
26	BD	0.38	0/2195	0.65	0/2955
26	DD	0.38	0/2195	0.67	0/2955
27	BE	0.39	0/1602	0.69	1/2160 (0.0%)
27	DE	0.35	0/1602	0.67	1/2160 (0.0%)
28	BF	0.41	0/1663	0.80	5/2249 (0.2%)
28	DF	0.41	0/1663	0.79	4/2249 (0.2%)
29	BG	0.57	1/1499 (0.1%)	0.60	0/2016
29	DG	0.59	1/1499 (0.1%)	0.67	3/2016 (0.1%)
30	BH	0.34	0/1298	0.59	0/1751
30	DH	0.34	0/1298	0.62	0/1751
32	BK	0.34	0/1054	0.60	0/1427
32	DK	0.34	0/1054	0.56	1/1427 (0.1%)
33	BN	0.58	0/1131	0.85	0/1525
33	DN	0.54	0/1131	0.80	0/1525
34	BO	0.36	0/943	0.65	1/1269 (0.1%)
34	DO	0.36	0/943	0.64	1/1269 (0.1%)
35	BP	0.34	0/1131	0.71	0/1504
35	DP	0.34	0/1131	0.71	0/1504
36	BQ	0.37	0/1143	0.64	0/1527
36	DQ	0.36	0/1143	0.60	0/1527
37	BR	0.38	0/974	0.65	0/1302
37	DR	0.34	0/974	0.62	1/1302 (0.1%)
38	BS	0.40	0/783	0.76	0/1041
38	DS	0.40	0/783	0.75	0/1041
39	BT	0.39	0/1161	0.76	3/1549 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	DT	0.37	0/1161	0.67	0/1549
40	BU	0.39	0/982	0.67	1/1306 (0.1%)
40	DU	0.42	0/982	0.68	1/1306 (0.1%)
41	BV	0.37	0/790	0.66	0/1057
41	DV	0.38	0/790	0.71	0/1057
42	BW	0.38	0/911	0.65	0/1220
42	DW	0.37	0/911	0.65	0/1220
43	BX	0.35	0/748	0.59	1/1004 (0.1%)
43	DX	0.35	0/748	0.60	0/1004
44	BY	0.35	0/831	0.65	0/1108
44	DY	0.34	0/831	0.60	0/1108
45	BZ	0.33	0/1505	0.60	0/2042
45	DZ	0.32	0/1505	0.59	0/2042
46	B0	0.33	0/671	0.55	0/892
46	D0	0.31	0/671	0.56	0/892
47	B2	0.37	0/600	0.65	1/793 (0.1%)
47	D2	0.34	0/600	0.60	0/793
48	B3	0.34	0/482	0.63	0/646
48	D3	0.31	0/482	0.58	0/646
49	B5	0.33	0/473	0.58	0/639
49	D5	0.34	0/473	0.60	0/639
50	B6	0.38	0/440	0.81	0/586
50	D6	0.35	0/440	0.79	1/586 (0.2%)
51	B7	0.38	0/438	0.62	0/575
51	D7	0.48	0/438	0.69	0/575
52	B8	0.37	0/525	0.67	0/691
52	D8	0.36	0/525	0.64	0/691
53	B9	0.32	0/310	0.55	0/407
53	D9	0.29	0/310	0.55	0/407
56	B1	0.53	0/739	0.83	1/981 (0.1%)
56	D1	0.54	0/739	0.84	2/981 (0.2%)
57	B4	0.40	0/276	0.65	0/372
57	D4	0.45	0/276	0.66	0/372
58	Be	0.36	0/538	0.55	0/715
58	De	0.35	0/538	0.61	0/715
59	BA	0.41	2/69437 (0.0%)	0.99	82/108401 (0.1%)
59	DA	0.40	1/69437 (0.0%)	0.97	72/108401 (0.1%)
60	BB	0.34	0/2853	0.93	0/4451
60	DB	0.34	0/2853	0.90	1/4451 (0.0%)
All	All	0.40	24/330902 (0.0%)	0.90	348/492664 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is

detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AB	0	2
1	CB	0	1
10	AK	0	1
11	AL	0	1
11	CL	0	1
20	AY	0	3
20	CY	0	8
25	BC	0	3
25	DC	0	2
26	DD	0	1
28	BF	0	2
28	DF	0	2
29	BG	0	1
29	DG	0	1
31	BJ	0	1
31	DJ	0	1
38	BS	0	2
38	DS	0	2
39	BT	0	2
39	DT	0	1
42	DW	0	1
56	B1	0	2
56	D1	0	3
All	All	0	44

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	CY	502	GLY	C-O	18.54	1.53	1.23
29	DG	112	PRO	CA-C	17.59	1.88	1.52
29	BG	112	PRO	CA-C	17.54	1.88	1.52
23	CV	16	A	O3'-P	-10.50	1.48	1.61
20	AY	499	ARG	C-N	9.84	1.56	1.34

The worst 5 of 348 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	CW	37	A	P-O3'-C3'	19.49	143.09	119.70
23	CV	16	A	P-O3'-C3'	18.93	142.41	119.70
20	CY	502	GLY	O-C-N	-12.85	101.35	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	CY	502	GLY	CA-C-N	12.59	141.38	116.20
20	CY	502	GLY	C-N-CA	11.35	146.14	122.30

There are no chirality outliers.

5 of 44 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AB	162	ILE	Peptide
1	AB	163	PHE	Peptide
10	AK	109	VAL	Peptide
11	AL	57	LYS	Peptide
20	AY	31	ARG	Peptide

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	AB	1910	0	1957	131	0
1	CB	1910	0	1957	98	0
2	AC	1621	0	1688	88	0
2	CC	1621	0	1688	67	0
3	AD	1703	0	1763	111	0
3	CD	1703	0	1763	120	0
4	AE	1156	0	1213	72	0
4	CE	1156	0	1213	54	0
5	AF	843	0	857	40	0
5	CF	843	0	857	40	0
6	AG	1257	0	1296	60	0
6	CG	1257	0	1296	61	0
7	AH	1116	0	1177	81	0
7	CH	1116	0	1177	73	0
8	AI	1011	0	1043	75	5
8	CI	1011	0	1043	54	0
9	AJ	802	0	849	71	0
9	CJ	802	0	849	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	AK	885	0	904	62	0
10	CK	885	0	904	61	0
11	AL	976	0	1062	110	0
11	CL	976	0	1062	113	0
12	AM	997	0	1072	76	0
12	CM	997	0	1072	72	5
13	AN	492	0	529	39	0
13	CN	492	0	529	35	0
14	AO	734	0	771	42	0
14	CO	734	0	771	42	0
15	AP	706	0	725	38	0
15	CP	706	0	725	39	0
16	AQ	835	0	906	63	0
16	CQ	835	0	906	63	0
17	AR	574	0	644	44	0
17	CR	574	0	644	36	0
18	AS	634	0	655	38	0
18	CS	634	0	655	33	0
19	AT	762	0	859	48	0
19	CT	762	0	859	32	0
20	AY	5380	0	5433	360	0
20	CY	5380	0	5435	346	0
21	AA	32474	0	16393	910	0
21	CA	32474	0	16393	851	0
22	AW	1635	0	831	64	0
22	CW	1635	0	831	55	0
23	AV	503	0	252	25	0
23	CV	503	0	252	34	0
24	AU	48	0	39	9	0
24	CU	48	0	39	9	0
25	BC	1742	0	1798	160	0
25	DC	1742	0	1798	148	0
26	BD	2145	0	2234	172	0
26	DD	2145	0	2234	164	0
27	BE	1569	0	1634	147	0
27	DE	1569	0	1634	122	0
28	BF	1628	0	1680	146	0
28	DF	1628	0	1680	141	0
29	BG	1474	0	1535	102	0
29	DG	1474	0	1535	82	0
30	BH	1274	0	1342	76	0
30	DH	1274	0	1342	73	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	BJ	851	0	197	29	0
31	DJ	851	0	196	25	0
32	BK	1035	0	1082	58	0
32	DK	1035	0	1082	57	0
33	BN	1104	0	1180	114	0
33	DN	1104	0	1180	115	0
34	BO	933	0	996	57	0
34	DO	933	0	996	71	0
35	BP	1114	0	1187	95	0
35	DP	1114	0	1187	111	0
36	BQ	1122	0	1179	81	0
36	DQ	1122	0	1179	65	0
37	BR	960	0	1021	77	0
37	DR	960	0	1021	71	0
38	BS	775	0	835	74	0
38	DS	775	0	835	76	0
39	BT	1147	0	1207	90	0
39	DT	1147	0	1207	111	0
40	BU	964	0	1022	85	0
40	DU	964	0	1022	76	0
41	BV	779	0	852	48	0
41	DV	779	0	852	62	0
42	BW	900	0	964	64	0
42	DW	900	0	964	57	0
43	BX	734	0	789	40	0
43	DX	734	0	789	42	0
44	BY	818	0	908	63	0
44	DY	818	0	908	58	0
45	BZ	1473	0	1497	89	0
45	DZ	1473	0	1497	81	0
46	B0	662	0	688	43	0
46	D0	662	0	688	40	0
47	B2	598	0	653	37	0
47	D2	598	0	653	28	0
48	B3	477	0	529	25	0
48	D3	477	0	529	25	0
49	B5	459	0	477	35	0
49	D5	459	0	477	34	0
50	B6	433	0	461	36	0
50	D6	433	0	461	36	0
51	B7	430	0	480	44	0
51	D7	430	0	480	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	B8	517	0	582	48	0
52	D8	517	0	582	50	0
53	B9	307	0	336	23	0
53	D9	307	0	335	20	0
54	Bf	156	0	41	0	0
54	Bg	156	0	39	0	0
54	Df	156	0	41	0	0
54	Dg	156	0	39	0	0
55	Bh	151	0	39	0	0
55	Dh	151	0	37	0	0
56	B1	732	0	808	88	0
56	D1	732	0	808	76	0
57	B4	271	0	284	31	0
57	D4	271	0	284	20	0
58	Be	686	0	620	0	0
58	De	686	0	619	0	0
59	BA	61997	0	31250	1815	0
59	DA	61997	0	31250	1738	0
60	BB	2551	0	1295	76	0
60	DB	2551	0	1295	70	0
61	AY	32	0	13	17	0
61	CY	32	0	13	32	0
62	AY	1	0	0	0	0
62	CY	1	0	0	0	0
All	All	308422	0	213301	11743	5

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 23.

The worst 5 of 11743 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
22:CW:37:A:C2	23:CV:16:A:C2	1.85	1.57
20:AY:33:LEU:HD21	20:AY:34:TYR:CE2	1.42	1.54
20:AY:33:LEU:HD21	20:AY:34:TYR:CD2	1.54	1.43
20:AY:33:LEU:CD2	20:AY:34:TYR:CD2	2.00	1.42
20:AY:138:LYS:NZ	61:AY:701:GNP:N3	1.61	1.42

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:AI:58:ARG:CZ	12:CM:46:LYS:CG[2_555]	1.66	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:AI:58:ARG:CD	12:CM:47:ASP:OD1[2_555]	1.74	0.46
8:AI:58:ARG:NH2	12:CM:46:LYS:CG[2_555]	1.88	0.32
8:AI:58:ARG:NE	12:CM:46:LYS:CG[2_555]	2.01	0.19
8:AI:58:ARG:NH2	12:CM:46:LYS:CD[2_555]	2.04	0.16

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	
1	AB	233/235 (99%)	173 (74%)	40 (17%)	20 (9%)	1	19
1	CB	233/235 (99%)	174 (75%)	36 (16%)	23 (10%)	1	15
2	AC	205/207 (99%)	137 (67%)	44 (22%)	24 (12%)	1	12
2	CC	205/207 (99%)	152 (74%)	34 (17%)	19 (9%)	1	18
3	AD	206/208 (99%)	146 (71%)	42 (20%)	18 (9%)	1	19
3	CD	206/208 (99%)	149 (72%)	46 (22%)	11 (5%)	3	35
4	AE	149/151 (99%)	107 (72%)	31 (21%)	11 (7%)	2	24
4	CE	149/151 (99%)	116 (78%)	24 (16%)	9 (6%)	2	31
5	AF	99/101 (98%)	75 (76%)	17 (17%)	7 (7%)	2	25
5	CF	99/101 (98%)	81 (82%)	7 (7%)	11 (11%)	1	13
6	AG	153/155 (99%)	120 (78%)	27 (18%)	6 (4%)	5	45
6	CG	153/155 (99%)	119 (78%)	27 (18%)	7 (5%)	4	39
7	AH	136/138 (99%)	98 (72%)	22 (16%)	16 (12%)	1	12
7	CH	136/138 (99%)	102 (75%)	21 (15%)	13 (10%)	1	17
8	AI	125/127 (98%)	88 (70%)	26 (21%)	11 (9%)	1	19
8	CI	125/127 (98%)	92 (74%)	25 (20%)	8 (6%)	2	29
9	AJ	97/99 (98%)	71 (73%)	17 (18%)	9 (9%)	1	18
9	CJ	97/99 (98%)	71 (73%)	16 (16%)	10 (10%)	1	14
10	AK	117/119 (98%)	74 (63%)	25 (21%)	18 (15%)	0	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	CK	117/119 (98%)	78 (67%)	26 (22%)	13 (11%)	1	13
11	AL	123/125 (98%)	42 (34%)	46 (37%)	35 (28%)	0	0
11	CL	123/125 (98%)	39 (32%)	44 (36%)	40 (32%)	0	0
12	AM	123/125 (98%)	86 (70%)	24 (20%)	13 (11%)	1	14
12	CM	123/125 (98%)	91 (74%)	18 (15%)	14 (11%)	1	12
13	AN	58/60 (97%)	40 (69%)	11 (19%)	7 (12%)	1	11
13	CN	58/60 (97%)	40 (69%)	14 (24%)	4 (7%)	2	27
14	AO	86/88 (98%)	65 (76%)	14 (16%)	7 (8%)	1	21
14	CO	86/88 (98%)	66 (77%)	15 (17%)	5 (6%)	3	32
15	AP	82/84 (98%)	55 (67%)	18 (22%)	9 (11%)	1	13
15	CP	82/84 (98%)	59 (72%)	18 (22%)	5 (6%)	2	30
16	AQ	98/100 (98%)	68 (69%)	18 (18%)	12 (12%)	1	11
16	CQ	98/100 (98%)	68 (69%)	20 (20%)	10 (10%)	1	14
17	AR	68/70 (97%)	50 (74%)	12 (18%)	6 (9%)	1	19
17	CR	68/70 (97%)	52 (76%)	10 (15%)	6 (9%)	1	19
18	AS	77/79 (98%)	51 (66%)	18 (23%)	8 (10%)	1	14
18	CS	77/79 (98%)	56 (73%)	12 (16%)	9 (12%)	1	12
19	AT	97/99 (98%)	72 (74%)	17 (18%)	8 (8%)	1	21
19	CT	97/99 (98%)	75 (77%)	14 (14%)	8 (8%)	1	21
20	AY	685/687 (100%)	431 (63%)	168 (24%)	86 (13%)	0	10
20	CY	685/687 (100%)	457 (67%)	156 (23%)	72 (10%)	1	14
24	AU	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
24	CU	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
25	BC	226/228 (99%)	108 (48%)	70 (31%)	48 (21%)	0	2
25	DC	226/228 (99%)	105 (46%)	75 (33%)	46 (20%)	0	2
26	BD	273/275 (99%)	180 (66%)	54 (20%)	39 (14%)	0	7
26	DD	273/275 (99%)	188 (69%)	47 (17%)	38 (14%)	0	8
27	BE	203/205 (99%)	130 (64%)	43 (21%)	30 (15%)	0	6
27	DE	203/205 (99%)	133 (66%)	36 (18%)	34 (17%)	0	5
28	BF	206/208 (99%)	126 (61%)	54 (26%)	26 (13%)	0	10
28	DF	206/208 (99%)	137 (66%)	47 (23%)	22 (11%)	1	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	BG	179/181 (99%)	120 (67%)	46 (26%)	13 (7%)	2	25
29	DG	179/181 (99%)	127 (71%)	44 (25%)	8 (4%)	4	40
30	BH	165/167 (99%)	118 (72%)	29 (18%)	18 (11%)	1	13
30	DH	165/167 (99%)	118 (72%)	32 (19%)	15 (9%)	1	18
32	BK	138/140 (99%)	88 (64%)	33 (24%)	17 (12%)	1	10
32	DK	138/140 (99%)	86 (62%)	33 (24%)	19 (14%)	0	8
33	BN	136/138 (99%)	93 (68%)	24 (18%)	19 (14%)	0	8
33	DN	136/138 (99%)	91 (67%)	27 (20%)	18 (13%)	0	9
34	BO	120/122 (98%)	92 (77%)	20 (17%)	8 (7%)	2	28
34	DO	120/122 (98%)	95 (79%)	20 (17%)	5 (4%)	4	43
35	BP	144/146 (99%)	81 (56%)	36 (25%)	27 (19%)	0	3
35	DP	144/146 (99%)	76 (53%)	35 (24%)	33 (23%)	0	1
36	BQ	139/141 (99%)	87 (63%)	32 (23%)	20 (14%)	0	7
36	DQ	139/141 (99%)	91 (66%)	31 (22%)	17 (12%)	1	11
37	BR	115/117 (98%)	83 (72%)	21 (18%)	11 (10%)	1	17
37	DR	115/117 (98%)	91 (79%)	17 (15%)	7 (6%)	2	30
38	BS	97/99 (98%)	56 (58%)	25 (26%)	16 (16%)	0	5
38	DS	97/99 (98%)	57 (59%)	25 (26%)	15 (16%)	0	5
39	BT	136/138 (99%)	76 (56%)	41 (30%)	19 (14%)	0	8
39	DT	136/138 (99%)	82 (60%)	28 (21%)	26 (19%)	0	3
40	BU	115/117 (98%)	79 (69%)	25 (22%)	11 (10%)	1	17
40	DU	115/117 (98%)	80 (70%)	23 (20%)	12 (10%)	1	14
41	BV	99/101 (98%)	57 (58%)	28 (28%)	14 (14%)	0	8
41	DV	99/101 (98%)	64 (65%)	22 (22%)	13 (13%)	0	9
42	BW	111/113 (98%)	82 (74%)	14 (13%)	15 (14%)	0	8
42	DW	111/113 (98%)	81 (73%)	16 (14%)	14 (13%)	0	10
43	BX	91/93 (98%)	73 (80%)	12 (13%)	6 (7%)	2	28
43	DX	91/93 (98%)	70 (77%)	16 (18%)	5 (6%)	3	34
44	BY	105/107 (98%)	50 (48%)	30 (29%)	25 (24%)	0	1
44	DY	105/107 (98%)	50 (48%)	34 (32%)	21 (20%)	0	2
45	BZ	183/185 (99%)	116 (63%)	46 (25%)	21 (12%)	1	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	DZ	183/185 (99%)	121 (66%)	44 (24%)	18 (10%)	1	16
46	B0	82/84 (98%)	59 (72%)	16 (20%)	7 (8%)	1	20
46	D0	82/84 (98%)	65 (79%)	13 (16%)	4 (5%)	3	37
47	B2	69/71 (97%)	49 (71%)	14 (20%)	6 (9%)	1	19
47	D2	69/71 (97%)	50 (72%)	17 (25%)	2 (3%)	7	54
48	B3	58/60 (97%)	46 (79%)	7 (12%)	5 (9%)	1	19
48	D3	58/60 (97%)	44 (76%)	9 (16%)	5 (9%)	1	19
49	B5	57/59 (97%)	44 (77%)	4 (7%)	9 (16%)	0	5
49	D5	57/59 (97%)	42 (74%)	11 (19%)	4 (7%)	2	26
50	B6	48/50 (96%)	28 (58%)	9 (19%)	11 (23%)	0	1
50	D6	48/50 (96%)	27 (56%)	8 (17%)	13 (27%)	0	1
51	B7	47/49 (96%)	30 (64%)	13 (28%)	4 (8%)	1	20
51	D7	47/49 (96%)	34 (72%)	11 (23%)	2 (4%)	4	42
52	B8	62/64 (97%)	42 (68%)	7 (11%)	13 (21%)	0	2
52	D8	62/64 (97%)	40 (64%)	11 (18%)	11 (18%)	0	4
53	B9	35/37 (95%)	28 (80%)	5 (14%)	2 (6%)	3	33
53	D9	35/37 (95%)	29 (83%)	4 (11%)	2 (6%)	3	33
56	B1	91/93 (98%)	56 (62%)	17 (19%)	18 (20%)	0	2
56	D1	91/93 (98%)	59 (65%)	18 (20%)	14 (15%)	0	6
57	B4	33/35 (94%)	15 (46%)	11 (33%)	7 (21%)	0	2
57	D4	33/35 (94%)	15 (46%)	9 (27%)	9 (27%)	0	1
58	Be	70/102 (69%)	36 (51%)	29 (41%)	5 (7%)	2	25
58	De	70/102 (69%)	40 (57%)	22 (31%)	8 (11%)	1	12
All	All	13304/13576 (98%)	8904 (67%)	2822 (21%)	1578 (12%)	1	11

5 of 1578 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AB	17	PHE
1	AB	22	LYS
1	AB	35	GLU
1	AB	75	LYS
1	AB	76	GLN

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	
1	AB	203/203 (100%)	164 (81%)	39 (19%)	2	12
1	CB	203/203 (100%)	177 (87%)	26 (13%)	6	33
2	AC	161/161 (100%)	125 (78%)	36 (22%)	1	8
2	CC	161/161 (100%)	122 (76%)	39 (24%)	1	6
3	AD	180/180 (100%)	143 (79%)	37 (21%)	2	10
3	CD	180/180 (100%)	142 (79%)	38 (21%)	1	9
4	AE	116/116 (100%)	96 (83%)	20 (17%)	3	18
4	CE	116/116 (100%)	95 (82%)	21 (18%)	2	15
5	AF	90/90 (100%)	76 (84%)	14 (16%)	4	23
5	CF	90/90 (100%)	74 (82%)	16 (18%)	2	16
6	AG	126/126 (100%)	111 (88%)	15 (12%)	8	37
6	CG	126/126 (100%)	112 (89%)	14 (11%)	9	42
7	AH	119/119 (100%)	94 (79%)	25 (21%)	1	9
7	CH	119/119 (100%)	91 (76%)	28 (24%)	1	7
8	AI	98/98 (100%)	82 (84%)	16 (16%)	3	21
8	CI	98/98 (100%)	77 (79%)	21 (21%)	1	9
9	AJ	89/89 (100%)	71 (80%)	18 (20%)	2	11
9	CJ	89/89 (100%)	66 (74%)	23 (26%)	1	5
10	AK	90/90 (100%)	73 (81%)	17 (19%)	2	13
10	CK	90/90 (100%)	72 (80%)	18 (20%)	2	11
11	AL	104/104 (100%)	74 (71%)	30 (29%)	0	4
11	CL	104/104 (100%)	77 (74%)	27 (26%)	1	5
12	AM	100/100 (100%)	83 (83%)	17 (17%)	3	18
12	CM	100/100 (100%)	86 (86%)	14 (14%)	5	28
13	AN	49/49 (100%)	39 (80%)	10 (20%)	2	10
13	CN	49/49 (100%)	35 (71%)	14 (29%)	0	4
14	AO	79/79 (100%)	70 (89%)	9 (11%)	8	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	CO	79/79 (100%)	66 (84%)	13 (16%)	3	20
15	AP	72/72 (100%)	59 (82%)	13 (18%)	2	15
15	CP	72/72 (100%)	61 (85%)	11 (15%)	4	25
16	AQ	95/95 (100%)	82 (86%)	13 (14%)	5	29
16	CQ	95/95 (100%)	80 (84%)	15 (16%)	4	23
17	AR	61/61 (100%)	53 (87%)	8 (13%)	6	32
17	CR	61/61 (100%)	53 (87%)	8 (13%)	6	32
18	AS	69/69 (100%)	58 (84%)	11 (16%)	4	22
18	CS	69/69 (100%)	52 (75%)	17 (25%)	1	6
19	AT	76/76 (100%)	66 (87%)	10 (13%)	6	32
19	CT	76/76 (100%)	68 (90%)	8 (10%)	10	46
20	AY	579/579 (100%)	459 (79%)	120 (21%)	2	10
20	CY	579/579 (100%)	483 (83%)	96 (17%)	3	19
24	AU	2/2 (100%)	2 (100%)	0	100	100
24	CU	2/2 (100%)	2 (100%)	0	100	100
25	BC	180/180 (100%)	132 (73%)	48 (27%)	1	5
25	DC	180/180 (100%)	128 (71%)	52 (29%)	0	4
26	BD	217/217 (100%)	167 (77%)	50 (23%)	1	7
26	DD	217/217 (100%)	175 (81%)	42 (19%)	2	12
27	BE	165/165 (100%)	137 (83%)	28 (17%)	3	18
27	DE	165/165 (100%)	136 (82%)	29 (18%)	3	16
28	BF	165/165 (100%)	133 (81%)	32 (19%)	2	12
28	DF	165/165 (100%)	140 (85%)	25 (15%)	4	25
29	BG	155/155 (100%)	130 (84%)	25 (16%)	3	22
29	DG	155/155 (100%)	130 (84%)	25 (16%)	3	22
30	BH	136/136 (100%)	111 (82%)	25 (18%)	2	14
30	DH	136/136 (100%)	117 (86%)	19 (14%)	5	28
32	BK	105/105 (100%)	74 (70%)	31 (30%)	0	4
32	DK	105/105 (100%)	77 (73%)	28 (27%)	1	5
33	BN	117/117 (100%)	98 (84%)	19 (16%)	3	21
33	DN	117/117 (100%)	93 (80%)	24 (20%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	BO	100/100 (100%)	85 (85%)	15 (15%)	4	26
34	DO	100/100 (100%)	86 (86%)	14 (14%)	5	28
35	BP	112/112 (100%)	82 (73%)	30 (27%)	1	5
35	DP	112/112 (100%)	85 (76%)	27 (24%)	1	6
36	BQ	111/111 (100%)	80 (72%)	31 (28%)	0	4
36	DQ	111/111 (100%)	84 (76%)	27 (24%)	1	6
37	BR	100/100 (100%)	79 (79%)	21 (21%)	1	9
37	DR	100/100 (100%)	78 (78%)	22 (22%)	1	8
38	BS	77/77 (100%)	60 (78%)	17 (22%)	1	8
38	DS	77/77 (100%)	59 (77%)	18 (23%)	1	7
39	BT	120/120 (100%)	94 (78%)	26 (22%)	1	9
39	DT	120/120 (100%)	93 (78%)	27 (22%)	1	8
40	BU	93/93 (100%)	75 (81%)	18 (19%)	2	12
40	DU	93/93 (100%)	70 (75%)	23 (25%)	1	6
41	BV	82/82 (100%)	60 (73%)	22 (27%)	1	5
41	DV	82/82 (100%)	62 (76%)	20 (24%)	1	6
42	BW	92/92 (100%)	69 (75%)	23 (25%)	1	6
42	DW	92/92 (100%)	76 (83%)	16 (17%)	3	17
43	BX	75/75 (100%)	56 (75%)	19 (25%)	1	6
43	DX	75/75 (100%)	58 (77%)	17 (23%)	1	7
44	BY	88/88 (100%)	69 (78%)	19 (22%)	1	9
44	DY	88/88 (100%)	73 (83%)	15 (17%)	3	18
45	BZ	162/162 (100%)	128 (79%)	34 (21%)	1	9
45	DZ	162/162 (100%)	125 (77%)	37 (23%)	1	7
46	B0	66/66 (100%)	56 (85%)	10 (15%)	4	25
46	D0	66/66 (100%)	56 (85%)	10 (15%)	4	25
47	B2	66/66 (100%)	59 (89%)	7 (11%)	10	45
47	D2	66/66 (100%)	58 (88%)	8 (12%)	7	36
48	B3	52/52 (100%)	42 (81%)	10 (19%)	2	12
48	D3	52/52 (100%)	45 (86%)	7 (14%)	6	30
49	B5	51/51 (100%)	39 (76%)	12 (24%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	D5	51/51 (100%)	41 (80%)	10 (20%)	2	11
50	B6	49/49 (100%)	37 (76%)	12 (24%)	1	6
50	D6	49/49 (100%)	34 (69%)	15 (31%)	0	4
51	B7	42/42 (100%)	35 (83%)	7 (17%)	3	19
51	D7	42/42 (100%)	36 (86%)	6 (14%)	5	28
52	B8	54/54 (100%)	42 (78%)	12 (22%)	1	8
52	D8	54/54 (100%)	44 (82%)	10 (18%)	2	13
53	B9	34/34 (100%)	32 (94%)	2 (6%)	28	75
53	D9	34/34 (100%)	30 (88%)	4 (12%)	8	38
56	B1	78/78 (100%)	58 (74%)	20 (26%)	1	5
56	D1	78/78 (100%)	58 (74%)	20 (26%)	1	5
57	B4	31/31 (100%)	22 (71%)	9 (29%)	0	4
57	D4	31/31 (100%)	21 (68%)	10 (32%)	0	3
58	Be	54/54 (100%)	46 (85%)	8 (15%)	4	26
58	De	54/54 (100%)	46 (85%)	8 (15%)	4	26
All	All	11174/11174 (100%)	8972 (80%)	2202 (20%)	2	11

5 of 2202 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
45	BZ	124	ILE
4	CE	73	ASN
43	DX	68	ARG
47	B2	53	LEU
58	Be	106	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 68 such sidechains are listed below:

Mol	Chain	Res	Type
50	B6	32	ASN
16	CQ	96	GLN
41	DV	89	GLN
3	CD	161	ASN
6	CG	148	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1511/1511 (100%)	326 (21%)	19 (1%)
21	CA	1511/1511 (100%)	310 (20%)	16 (1%)
22	AW	76/77 (98%)	22 (28%)	1 (1%)
22	CW	76/77 (98%)	19 (25%)	1 (1%)
23	AV	22/23 (95%)	11 (50%)	2 (9%)
23	CV	22/23 (95%)	9 (40%)	3 (13%)
59	BA	2878/2879 (99%)	666 (23%)	21 (0%)
59	DA	2878/2879 (99%)	629 (21%)	17 (0%)
60	BB	118/119 (99%)	20 (16%)	4 (3%)
60	DB	118/119 (99%)	19 (16%)	3 (2%)
All	All	9210/9218 (99%)	2031 (22%)	87 (0%)

5 of 2031 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	6	G
21	AA	7	G
21	AA	8	A
21	AA	9	G
21	AA	13	U

5 of 87 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
59	BA	2092	U
21	CA	115	G
59	DA	2092	U
59	BA	2422	A
60	BB	56	G

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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
24	KBE	AU	1	24	8,8,9	8.11	1 (12%)	6,8,10	0.70	0
24	DPP	AU	2	24	5,5,6	6.82	1 (20%)	3,5,7	2.62	2 (66%)
24	UAL	AU	5	24	7,8,9	2.10	3 (42%)	6,9,11	1.32	1 (16%)
24	5OH	AU	6	24	12,12,13	6.59	3 (25%)	13,16,18	0.81	0
24	KBE	CU	1	24	8,8,9	8.12	1 (12%)	6,8,10	0.70	0
24	DPP	CU	2	24	5,5,6	6.81	1 (20%)	3,5,7	2.64	2 (66%)
24	UAL	CU	5	24	7,8,9	2.09	3 (42%)	6,9,11	1.33	1 (16%)
24	5OH	CU	6	24	12,12,13	6.61	3 (25%)	13,16,18	0.81	0

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
24	KBE	AU	1	24	-	0/6/7/8	0/0/0/0
24	DPP	AU	2	24	-	0/2/4/6	0/0/0/0
24	UAL	AU	5	24	-	0/3/7/9	0/0/0/0
24	5OH	AU	6	24	-	0/2/18/20	0/1/1/1
24	KBE	CU	1	24	-	0/6/7/8	0/0/0/0
24	DPP	CU	2	24	-	0/2/4/6	0/0/0/0
24	UAL	CU	5	24	-	0/3/7/9	0/0/0/0
24	5OH	CU	6	24	-	0/2/18/20	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	CU	1	KBE	O-C	22.95	1.27	1.11
24	AU	1	KBE	O-C	22.92	1.27	1.11
24	CU	6	5OH	O-C	22.13	1.26	1.11
24	AU	6	5OH	O-C	22.04	1.26	1.11
24	AU	2	DPP	O-C	15.13	1.21	1.11

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	CU	2	DPP	C-CA-N	-3.74	110.10	113.83
24	AU	2	DPP	C-CA-N	-3.71	110.13	113.83
24	CU	5	UAL	CB-CA-N	2.39	127.80	122.88
24	AU	5	UAL	CB-CA-N	2.38	127.76	122.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	CU	2	DPP	CB-CA-N	-2.18	104.19	111.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates i

There are no carbohydrates in this entry.

5.6 Ligand geometry i

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
61	GNP	AY	701	62	34,34,34	1.85	6 (17%)	48,54,54	5.87	14 (29%)
61	GNP	CY	701	62	34,34,34	1.85	6 (17%)	48,54,54	5.87	14 (29%)

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
61	GNP	AY	701	62	-	0/18/38/38	0/3/3/3
61	GNP	CY	701	62	-	0/18/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	AY	701	GNP	PG-O1G	6.61	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	CY	701	GNP	PG-O1G	6.56	1.53	1.46
61	CY	701	GNP	PB-N3B	-4.55	1.60	1.64
61	AY	701	GNP	PB-N3B	-4.51	1.60	1.64
61	CY	701	GNP	PA-O3A	-2.84	1.54	1.59

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	CY	701	GNP	C6-C5-N7	-37.53	129.09	134.14
61	AY	701	GNP	C6-C5-N7	-37.52	129.09	134.14
61	AY	701	GNP	C6-N1-C2	8.74	125.14	120.20
61	CY	701	GNP	C6-N1-C2	8.68	125.10	120.20
61	CY	701	GNP	PA-O3A-PB	-4.68	115.98	132.05

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
58	Be	1
58	De	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	De	30:UNK	C	51:ALA	N	36.11
1	Be	30:UNK	C	51:ALA	N	35.10

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	AB	235/235 (100%)	0.17	4 (1%) 67 34	30, 75, 127, 171	0
1	CB	235/235 (100%)	0.57	13 (5%) 24 10	34, 86, 153, 201	0
2	AC	207/207 (100%)	0.45	9 (4%) 34 14	27, 59, 115, 156	0
2	CC	207/207 (100%)	1.00	34 (16%) 2 2	23, 75, 130, 190	0
3	AD	208/208 (100%)	-0.21	0 100 100	24, 72, 124, 159	0
3	CD	208/208 (100%)	0.00	3 (1%) 72 38	23, 85, 142, 184	0
4	AE	151/151 (100%)	-0.10	0 100 100	17, 48, 101, 156	0
4	CE	151/151 (100%)	0.22	5 (3%) 44 20	14, 58, 106, 151	0
5	AF	101/101 (100%)	-0.15	0 100 100	15, 50, 100, 133	0
5	CF	101/101 (100%)	-0.25	1 (0%) 79 47	29, 61, 123, 148	0
6	AG	155/155 (100%)	-0.31	1 (0%) 86 59	30, 80, 139, 199	0
6	CG	155/155 (100%)	-0.41	0 100 100	38, 82, 137, 180	0
7	AH	138/138 (100%)	0.09	1 (0%) 84 56	28, 59, 103, 142	0
7	CH	138/138 (100%)	0.35	4 (2%) 49 23	25, 75, 121, 155	0
8	AI	127/127 (100%)	-0.37	0 100 100	0, 71, 117, 134	0
8	CI	127/127 (100%)	-0.20	0 100 100	0, 84, 149, 220	0
9	AJ	99/99 (100%)	0.35	6 (6%) 21 9	25, 62, 116, 159	0
9	CJ	99/99 (100%)	0.91	10 (10%) 7 5	31, 75, 127, 166	0
10	AK	119/119 (100%)	-0.05	1 (0%) 83 53	31, 69, 116, 157	0
10	CK	119/119 (100%)	-0.23	1 (0%) 83 53	38, 72, 133, 151	0
11	AL	125/125 (100%)	0.13	2 (1%) 68 35	10, 66, 120, 181	0
11	CL	125/125 (100%)	0.44	12 (9%) 8 5	29, 69, 136, 170	0
12	AM	125/125 (100%)	0.29	11 (8%) 10 6	49, 86, 144, 212	0
12	CM	125/125 (100%)	0.44	14 (11%) 6 4	53, 100, 158, 223	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AN	60/60 (100%)	0.54	4 (6%) 17 8	28, 52, 87, 120	0
13	CN	60/60 (100%)	0.95	9 (15%) 3 3	39, 69, 117, 135	0
14	AO	88/88 (100%)	-0.02	0 100 100	22, 60, 114, 139	0
14	CO	88/88 (100%)	-0.03	0 100 100	25, 68, 119, 170	0
15	AP	84/84 (100%)	0.25	4 (4%) 29 13	26, 66, 109, 117	0
15	CP	84/84 (100%)	0.25	2 (2%) 56 26	52, 81, 127, 153	0
16	AQ	100/100 (100%)	0.39	6 (6%) 21 9	0, 67, 117, 139	0
16	CQ	100/100 (100%)	0.56	6 (6%) 21 9	0, 68, 126, 150	0
17	AR	70/70 (100%)	0.08	3 (4%) 34 14	14, 54, 120, 154	0
17	CR	70/70 (100%)	0.01	0 100 100	39, 63, 113, 155	0
18	AS	79/79 (100%)	0.91	13 (16%) 2 2	47, 92, 136, 169	0
18	CS	79/79 (100%)	0.70	7 (8%) 10 6	44, 99, 145, 189	0
19	AT	99/99 (100%)	-0.17	0 100 100	0, 77, 128, 159	0
19	CT	99/99 (100%)	-0.00	1 (1%) 79 47	0, 79, 131, 166	0
20	AY	687/687 (100%)	0.22	37 (5%) 25 10	23, 84, 139, 174	0
20	CY	687/687 (100%)	0.25	46 (6%) 17 8	40, 92, 149, 204	0
21	AA	1511/1511 (100%)	-0.56	3 (0%) 93 80	15, 67, 145, 258	0
21	CA	1511/1511 (100%)	-0.56	1 (0%) 93 84	18, 70, 157, 272	0
22	AW	77/77 (100%)	-0.67	0 100 100	32, 90, 174, 205	0
22	CW	77/77 (100%)	-0.69	0 100 100	39, 101, 193, 240	0
23	AV	23/23 (100%)	-0.64	0 100 100	41, 100, 156, 172	0
23	CV	23/23 (100%)	-0.22	1 (4%) 34 14	41, 118, 186, 216	0
24	AU	2/6 (33%)	-0.31	0 100 100	114, 114, 114, 114	0
24	CU	2/6 (33%)	-0.40	0 100 100	119, 119, 119, 119	0
25	BC	228/228 (100%)	1.30	51 (22%) 1 2	81, 124, 178, 222	0
25	DC	228/228 (100%)	1.42	66 (28%) 1 1	102, 162, 214, 247	0
26	BD	275/275 (100%)	-0.16	1 (0%) 90 71	11, 47, 102, 126	0
26	DD	275/275 (100%)	-0.13	2 (0%) 84 56	23, 54, 107, 147	0
27	BE	205/205 (100%)	-0.08	2 (0%) 79 47	19, 55, 101, 193	0
27	DE	205/205 (100%)	0.06	2 (0%) 79 47	12, 60, 120, 175	0
28	BF	208/208 (100%)	0.19	9 (4%) 34 14	16, 69, 131, 178	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DF	208/208 (100%)	0.18	7 (3%) 43 19	34, 83, 176, 205	0
29	BG	181/181 (100%)	0.95	33 (18%) 2 2	41, 90, 132, 195	0
29	DG	181/181 (100%)	1.30	46 (25%) 1 2	44, 104, 159, 196	0
30	BH	167/167 (100%)	-0.14	0 100 100	21, 68, 123, 159	0
30	DH	167/167 (100%)	-0.12	1 (0%) 86 59	36, 73, 140, 192	0
31	BJ	0/170	-	-	-	-
31	DJ	0/170	-	-	-	-
32	BK	140/140 (100%)	0.17	6 (4%) 34 14	60, 114, 165, 206	0
32	DK	140/140 (100%)	0.53	20 (14%) 3 3	72, 142, 197, 229	0
33	BN	138/138 (100%)	0.51	10 (7%) 15 7	59, 83, 108, 111	0
33	DN	138/138 (100%)	0.43	6 (4%) 34 14	61, 89, 110, 118	0
34	BO	122/122 (100%)	0.17	2 (1%) 68 35	23, 44, 90, 158	0
34	DO	122/122 (100%)	0.26	2 (1%) 68 35	26, 47, 96, 121	0
35	BP	146/146 (100%)	-0.13	2 (1%) 72 38	23, 71, 132, 167	0
35	DP	146/146 (100%)	-0.03	3 (2%) 60 29	19, 88, 140, 212	0
36	BQ	141/141 (100%)	-0.22	1 (0%) 84 56	32, 53, 103, 155	0
36	DQ	141/141 (100%)	-0.29	1 (0%) 84 56	34, 58, 126, 178	0
37	BR	117/117 (100%)	0.12	1 (0%) 81 51	22, 57, 106, 123	0
37	DR	117/117 (100%)	0.10	0 100 100	34, 67, 108, 138	0
38	BS	99/99 (100%)	1.14	25 (25%) 1 2	41, 104, 177, 190	0
38	DS	99/99 (100%)	1.50	34 (34%) 1 1	44, 114, 168, 203	0
39	BT	138/138 (100%)	0.02	2 (1%) 72 38	23, 68, 126, 162	0
39	DT	138/138 (100%)	0.02	4 (2%) 49 23	25, 71, 133, 177	0
40	BU	117/117 (100%)	0.12	0 100 100	20, 45, 102, 140	0
40	DU	117/117 (100%)	0.30	3 (2%) 53 24	29, 54, 89, 222	0
41	BV	101/101 (100%)	0.46	5 (4%) 28 12	22, 58, 105, 172	0
41	DV	101/101 (100%)	0.31	4 (3%) 36 16	28, 60, 114, 177	0
42	BW	113/113 (100%)	0.09	0 100 100	14, 43, 101, 135	0
42	DW	113/113 (100%)	0.23	1 (0%) 81 51	11, 60, 133, 215	0
43	BX	93/93 (100%)	-0.18	0 100 100	16, 55, 107, 137	0
43	DX	93/93 (100%)	-0.32	0 100 100	16, 66, 134, 180	0
44	BY	107/107 (100%)	0.13	3 (2%) 50 23	38, 88, 141, 193	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	DY	107/107 (100%)	0.36	8 (7%) 14 7	45, 96, 167, 200	0
45	BZ	185/185 (100%)	-0.22	1 (0%) 88 64	36, 70, 124, 167	0
45	DZ	185/185 (100%)	-0.22	1 (0%) 88 64	48, 82, 136, 193	0
46	B0	84/84 (100%)	-0.06	1 (1%) 75 42	24, 65, 112, 142	0
46	D0	84/84 (100%)	0.43	3 (3%) 41 18	47, 77, 140, 162	0
47	B2	71/71 (100%)	0.02	1 (1%) 72 38	34, 64, 118, 140	0
47	D2	71/71 (100%)	0.08	0 100 100	33, 85, 127, 141	0
48	B3	60/60 (100%)	0.26	3 (5%) 28 12	28, 61, 116, 135	0
48	D3	60/60 (100%)	0.31	3 (5%) 28 12	32, 73, 137, 160	0
49	B5	59/59 (100%)	-0.02	1 (1%) 67 34	22, 55, 125, 138	0
49	D5	59/59 (100%)	0.18	1 (1%) 67 34	29, 75, 130, 161	0
50	B6	50/50 (100%)	-0.24	0 100 100	36, 74, 120, 139	0
50	D6	50/50 (100%)	0.36	3 (6%) 21 9	49, 81, 143, 164	0
51	B7	49/49 (100%)	-0.04	1 (2%) 62 30	43, 53, 102, 126	0
51	D7	49/49 (100%)	0.02	3 (6%) 21 9	34, 61, 112, 165	0
52	B8	64/64 (100%)	-0.10	1 (1%) 68 35	22, 66, 108, 137	0
52	D8	64/64 (100%)	0.14	2 (3%) 47 22	33, 70, 118, 139	0
53	B9	37/37 (100%)	0.22	2 (5%) 25 10	39, 60, 122, 134	0
53	D9	37/37 (100%)	-0.08	1 (2%) 52 24	46, 60, 134, 159	0
54	Bf	0/31	-	-	-	-
54	Bg	0/31	-	-	-	-
54	Df	0/31	-	-	-	-
54	Dg	0/31	-	-	-	-
55	Bh	0/30	-	-	-	-
55	Dh	0/30	-	-	-	-
56	B1	93/93 (100%)	0.10	2 (2%) 59 28	22, 78, 160, 236	0
56	D1	93/93 (100%)	0.34	8 (8%) 11 6	41, 89, 159, 194	0
57	B4	35/35 (100%)	1.28	8 (22%) 1 2	67, 116, 167, 189	0
57	D4	35/35 (100%)	1.46	10 (28%) 1 1	73, 136, 168, 196	0
58	Be	72/102 (70%)	1.50	22 (30%) 1 1	77, 113, 160, 174	0
58	De	72/102 (70%)	2.48	37 (51%) 0 1	87, 141, 192, 236	0
59	BA	2879/2879 (100%)	-0.54	11 (0%) 90 71	9, 59, 146, 260	0
59	DA	2879/2879 (100%)	-0.53	9 (0%) 91 76	5, 63, 160, 308	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
60	BB	119/119 (100%)	-0.52	1 (0%) 83 53	36, 103, 157, 192	0
60	DB	119/119 (100%)	-0.40	1 (0%) 83 53	33, 108, 159, 193	0
All	All	22726/23318 (97%)	-0.08	775 (3%) 43 19	0, 72, 150, 308	0

The worst 5 of 775 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
59	DA	2799	A	12.2
58	De	59	GLU	11.9
58	De	55	GLU	10.3
25	DC	2	PRO	8.7
20	CY	4	LYS	8.6

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

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
24	DPP	AU	2	6/7	0.21	-	114,114,114,114	0
24	5OH	AU	6	12/13	0.28	-	99,101,102,102	0
24	KBE	AU	1	9/10	0.30	-	114,114,114,114	0
24	5OH	CU	6	12/13	0.21	-	99,101,102,102	0
24	UAL	AU	5	9/10	0.16	-	114,114,114,114	0
24	UAL	CU	5	9/10	0.13	-	118,118,118,118	0
24	DPP	CU	2	6/7	0.18	-	118,118,118,118	0
24	KBE	CU	1	9/10	0.34	-	118,118,118,118	0

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
62	MG	CY	702	1/1	0.11	-	135,135,135,135	0
62	MG	AY	702	1/1	0.11	-	88,88,88,88	0
61	GNP	AY	701	32/32	0.22	-	58,71,81,83	0
61	GNP	CY	701	32/32	0.23	-	58,71,81,83	0

6.5 Other polymers ⓘ

There are no such residues in this entry.