



wwPDB X-ray Structure Validation Summary Report

Jul 23, 2014 – 09:43 AM EDT

PDB ID : 4V9L
Title : 70S Ribosome translocation intermediate FA-3.6A containing elongation factor EFG/FUSIDIC ACID/GDP, 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>

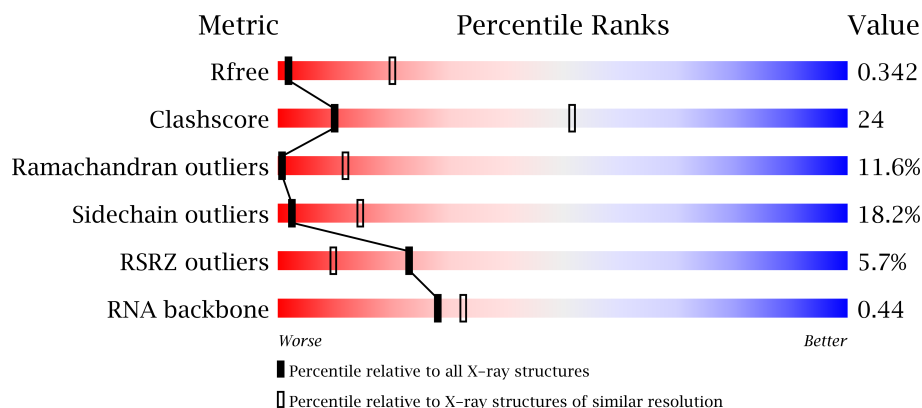
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : **FAILED**
EDS : stable23489
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) : stable23489

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	

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Mol	Chain	Length	Quality of chain
6	CG	155	
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	AA	1511	
20	CA	1511	
21	AW	77	
21	CW	77	
22	AV	23	
22	CV	23	
23	AY	687	
23	CY	687	
24	AU	6	
24	CU	6	
25	BC	228	
25	DC	228	
26	BD	275	
26	DD	275	
27	BE	205	

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Mol	Chain	Length	Quality of chain
27	DE	205	
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	

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Mol	Chain	Length	Quality of chain
48	D3	60	
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	Be	102	
54	De	102	
55	Bf	31	
55	Bg	31	
55	Df	31	
55	Dg	31	
56	Bh	30	
56	Dh	30	
57	B1	93	
57	D1	93	
58	B4	35	
58	D4	35	
59	BA	2879	
59	DA	2879	
60	BB	119	
60	DB	119	

2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 308166 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
			1010	639	197	174			
8	CI	127	Total	C	N	O	0	0	0
			1010	639	197	174			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	58	HIS	ARG	CONFLICT	UNP P62669
CI	58	HIS	ARG	CONFLICT	UNP P62669

- 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			
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	155	144	2			
16	CQ	100	Total	C	N	O	S	0	0	0
			835	534	155	144	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AQ	96	GLU	GLN	CONFLICT	UNP P62658
CQ	96	GLU	GLN	CONFLICT	UNP P62658

- 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
			763	470	162	129	2			
19	CT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AT	41	ILE	VAL	CONFLICT	UNP P62661
CT	41	ILE	VAL	CONFLICT	UNP P62661

- Molecule 20 is a RNA chain called ribosomal RNA 16S.

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

- Molecule 21 is a RNA chain called transfer RNA.

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

- Molecule 22 is a RNA chain called messenger RNA.

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

- Molecule 23 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AY	667	Total	C	N	O	S	0	0	0
			5219	3318	893	990	18			
23	CY	667	Total	C	N	O	S	0	0	0
			5219	3318	893	990	18			

There are 4 discrepancies between the modelled and reference sequences:

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

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

- 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			
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
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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			
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			

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

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

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

- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L7/L12.

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

- Molecule 57 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	B1	93	Total	C	N	O	S	0	0	0
			732	460	145	126	1			
57	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 58 is a protein called 50S ribosomal protein L31.

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

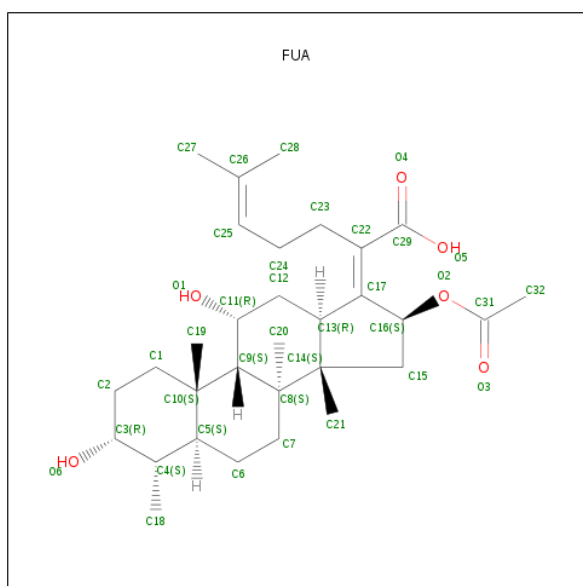
- Molecule 59 is a RNA chain called 23S ribosomal RNA.

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

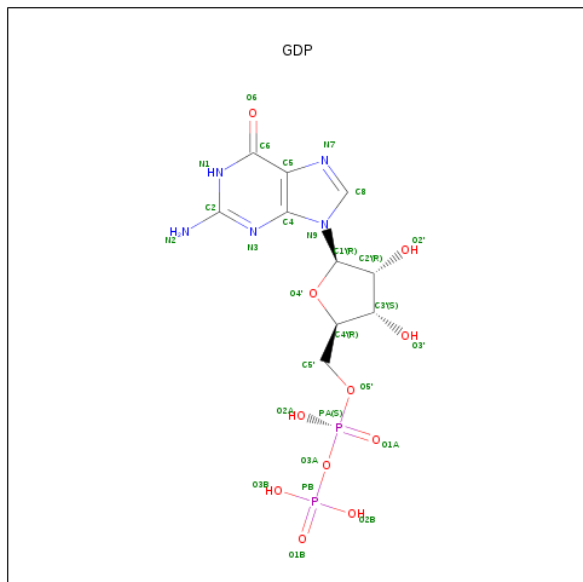
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
60	BB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			
60	DB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

- Molecule 61 is FUSIDIC ACID (three-letter code: FUA) (formula: $C_{31}H_{48}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
61	AY	1	Total	C	O	0	0
			37	31	6		
61	CY	1	Total	C	O	0	0
			37	31	6		

- Molecule 62 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
62	AY	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
62	CY	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

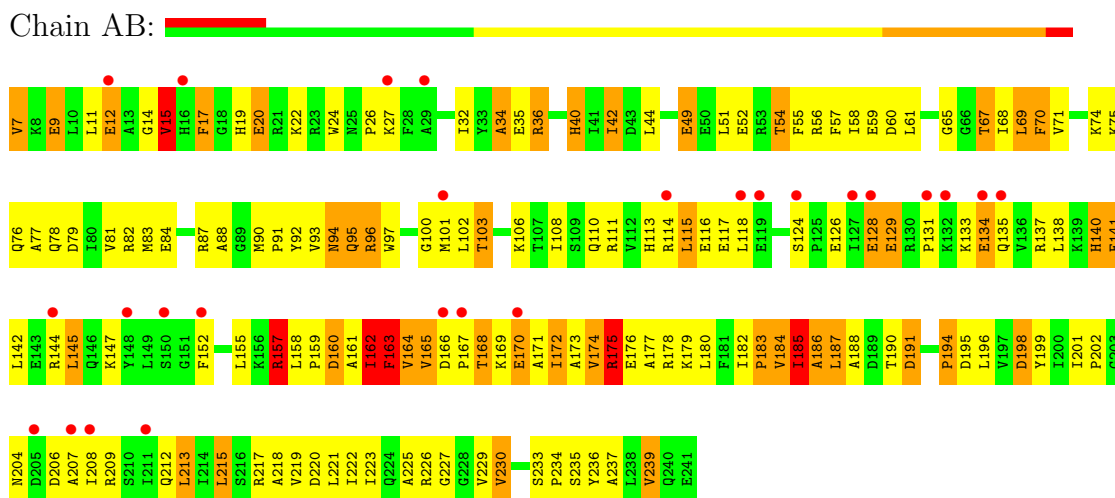
- Molecule 63 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	BA	1	Total	Mg	0	0
			1	1		
63	CY	1	Total	Mg	0	0
			1	1		

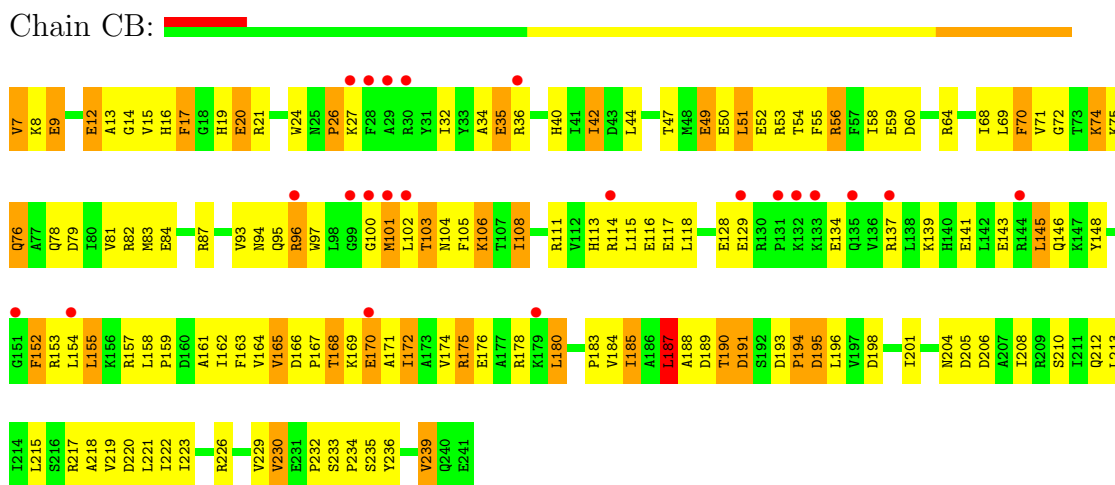
3 Residue-property plots

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.

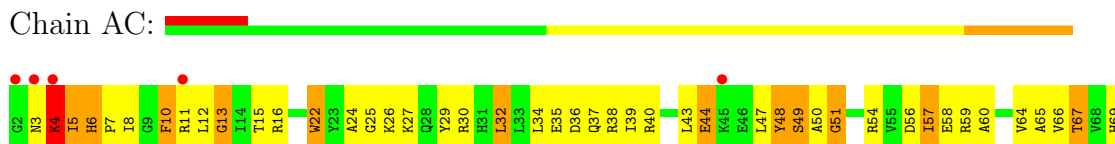
• Molecule 1: 30S ribosomal protein S2

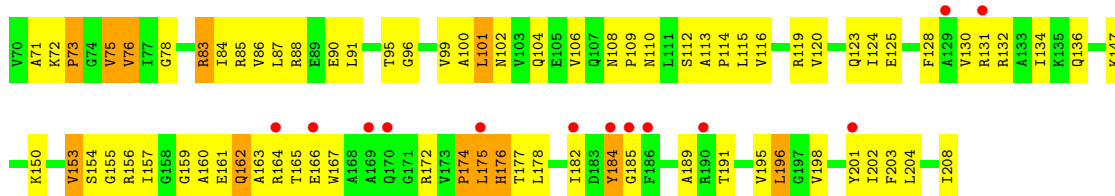


• Molecule 1: 30S ribosomal protein S2



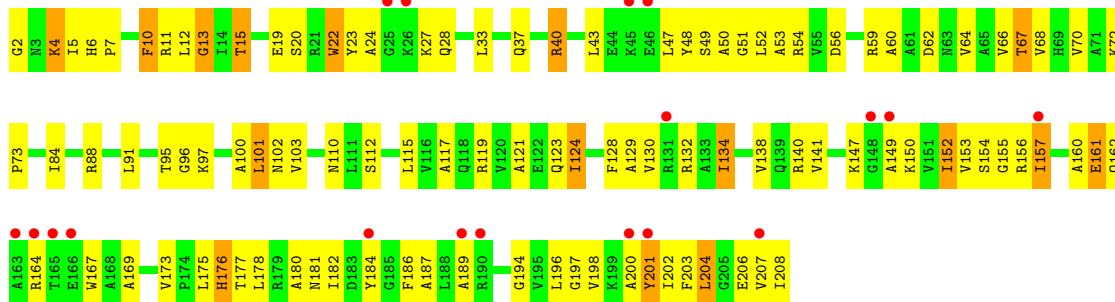
• Molecule 2: 30S ribosomal protein S3





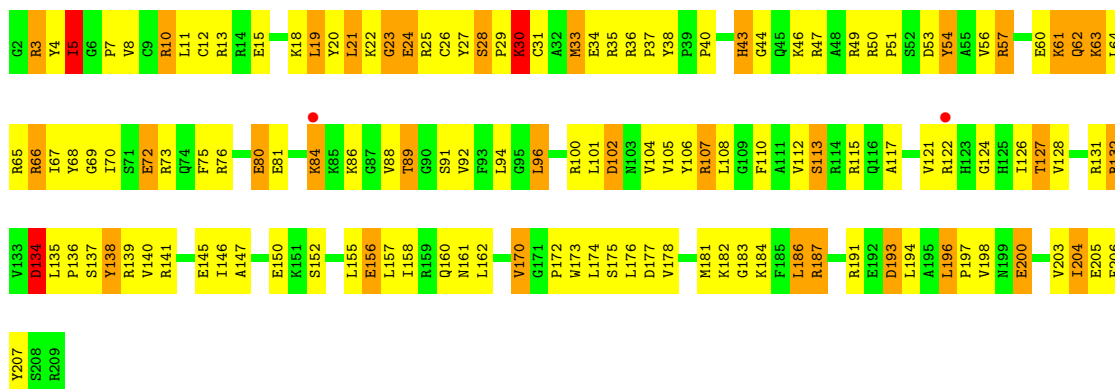
• Molecule 2: 30S ribosomal protein S3

Chain CC:



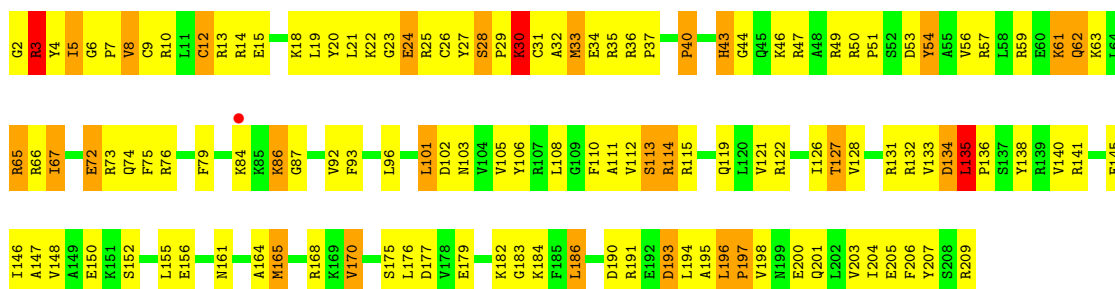
• Molecule 3: 30S ribosomal protein S4

Chain AD:



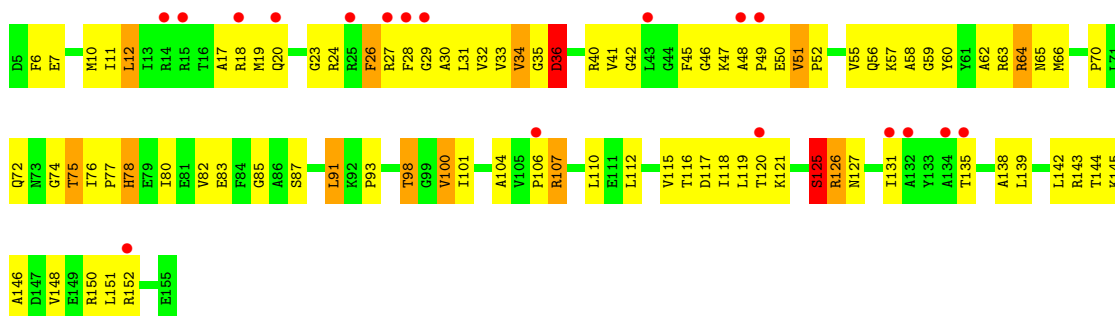
• Molecule 3: 30S ribosomal protein S4

Chain CD:



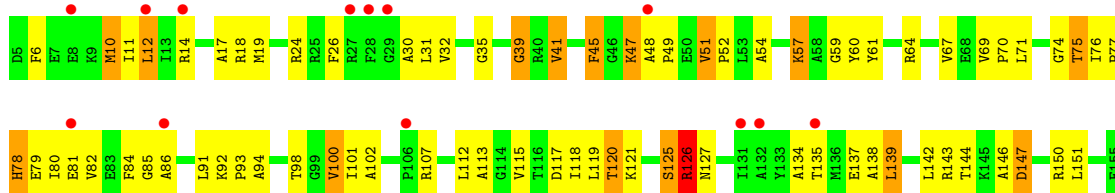
• Molecule 4: 30S ribosomal protein S5

Chain AE:



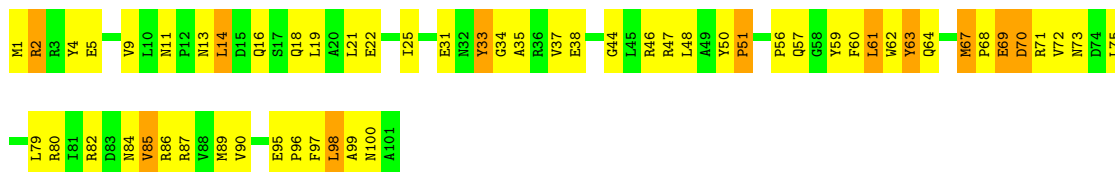
- Molecule 4: 30S ribosomal protein S5

Chain CE:



- Molecule 5: 30S ribosomal protein S6

Chain AF:



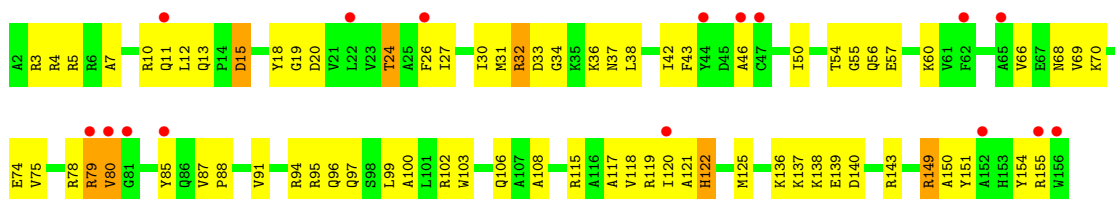
- Molecule 5: 30S ribosomal protein S6

Chain CF:



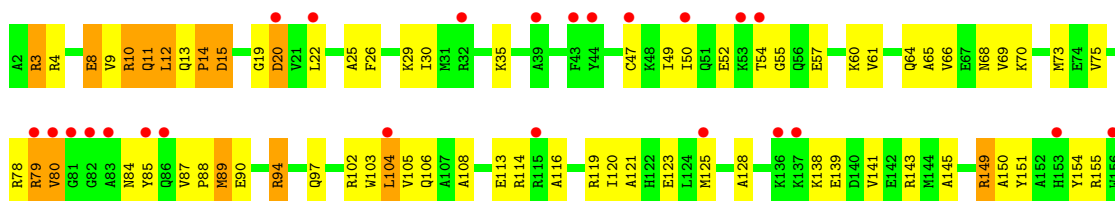
- Molecule 6: 30S ribosomal protein S7

Chain AG:



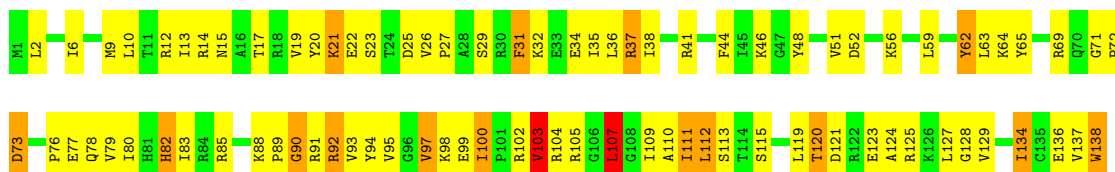
- Molecule 6: 30S ribosomal protein S7

Chain CG:



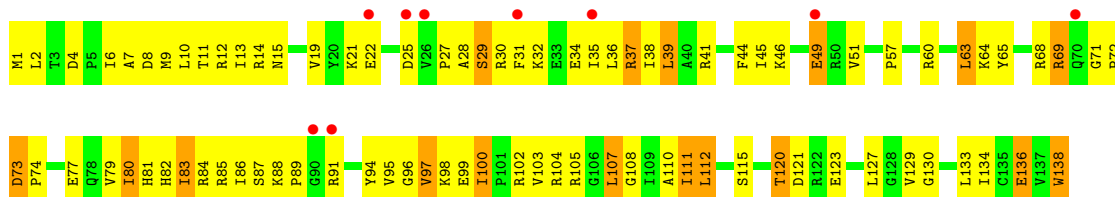
• Molecule 7: 30S ribosomal protein S8

Chain AH:



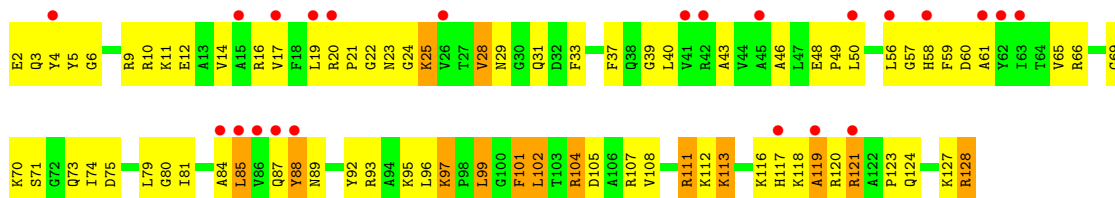
• Molecule 7: 30S ribosomal protein S8

Chain CH:



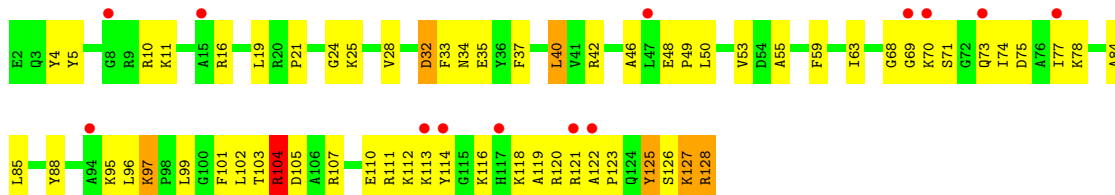
• Molecule 8: 30S ribosomal protein S9

Chain AI:



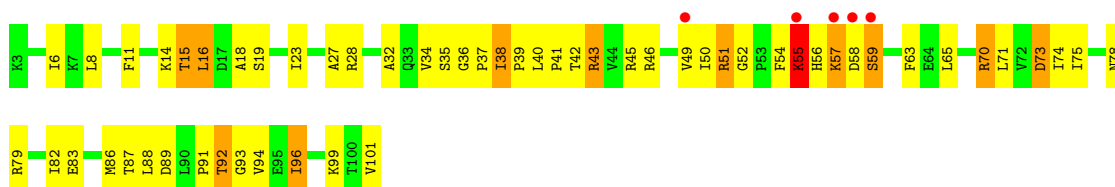
• Molecule 8: 30S ribosomal protein S9

Chain CI:



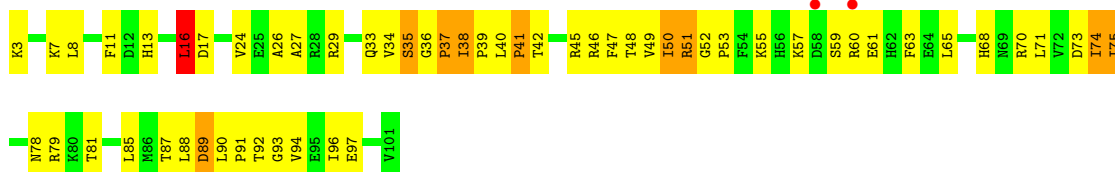
• Molecule 9: 30S ribosomal protein S10

Chain AJ:



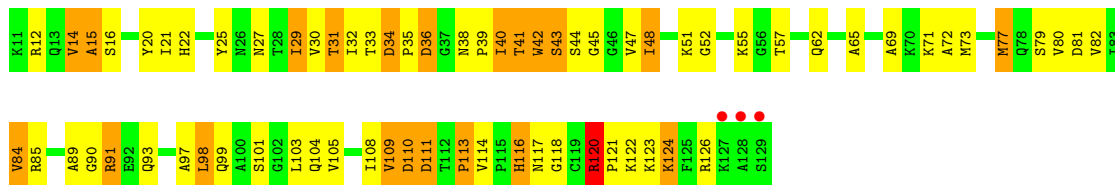
• Molecule 9: 30S ribosomal protein S10

Chain CJ:



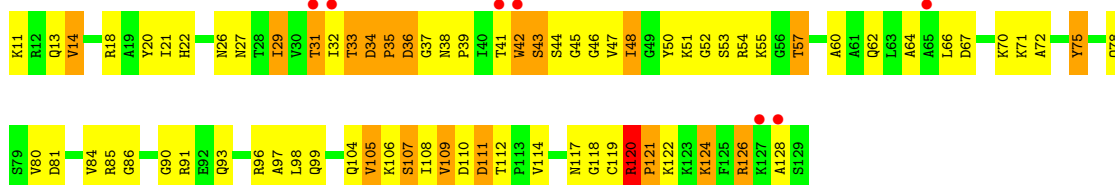
• Molecule 10: 30S ribosomal protein S11

Chain AK:



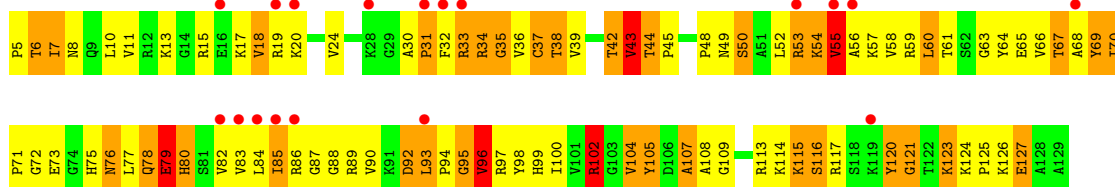
• Molecule 10: 30S ribosomal protein S11

Chain CK:



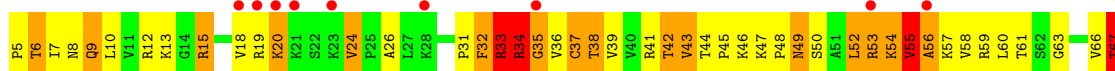
• Molecule 11: 30S ribosomal protein S12

Chain AL:



• Molecule 11: 30S ribosomal protein S12

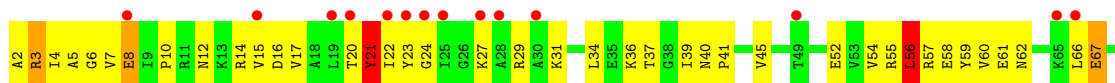
Chain CL:





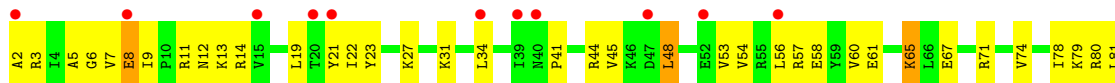
• Molecule 12: 30S ribosomal protein S13

Chain AM:



• Molecule 12: 30S ribosomal protein S13

Chain CM:



• Molecule 13: 30S ribosomal protein S14 type Z

Chain AN:



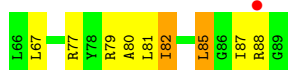
• Molecule 13: 30S ribosomal protein S14 type Z

Chain CN:



• Molecule 14: 30S ribosomal protein S15

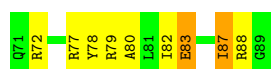
Chain AO:



• Molecule 14: 30S ribosomal protein S15

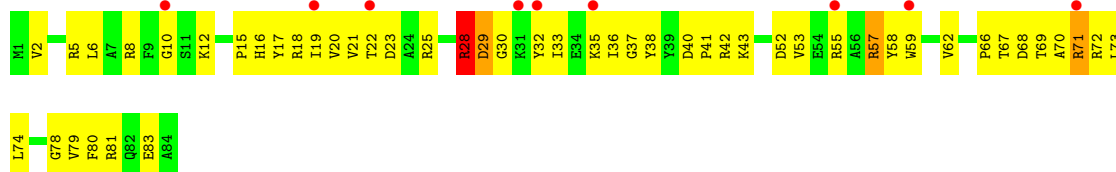
Chain CO:





- Molecule 15: 30S ribosomal protein S16

Chain AP:



- Molecule 17: 30S ribosomal protein S18

Chain CR:



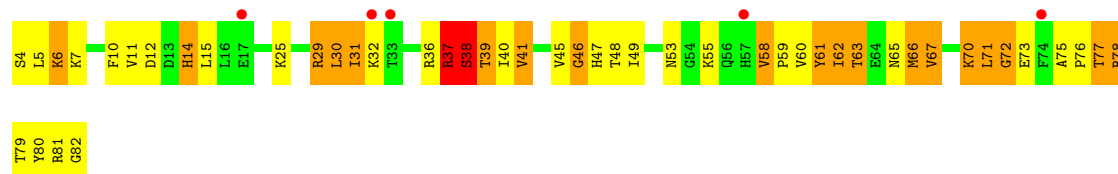
- Molecule 18: 30S ribosomal protein S19

Chain AS:



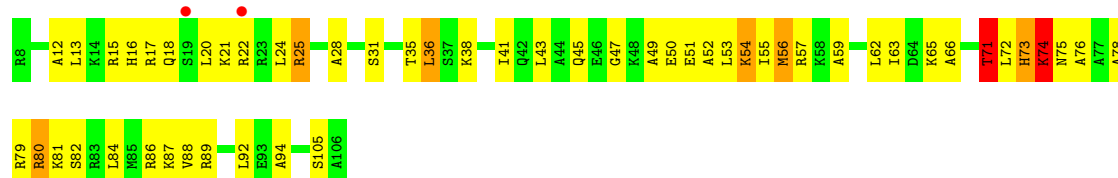
- Molecule 18: 30S ribosomal protein S19

Chain CS:



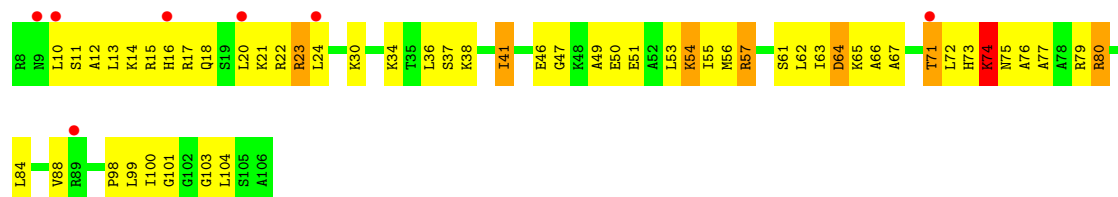
- Molecule 19: 30S ribosomal protein S20

Chain AT:



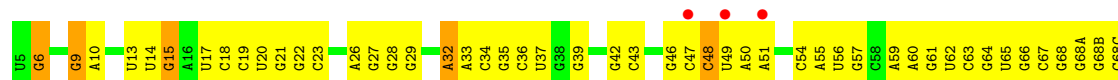
- Molecule 19: 30S ribosomal protein S20

Chain CT:



- Molecule 20: ribosomal RNA 16S

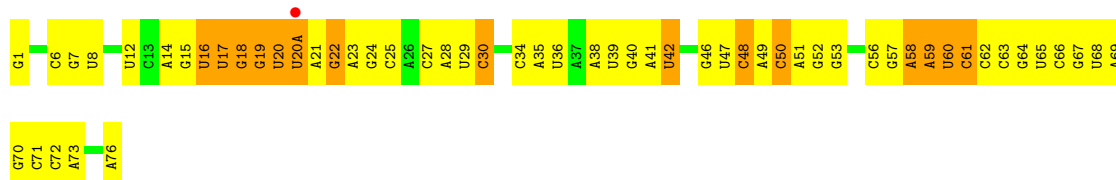
Chain AA:





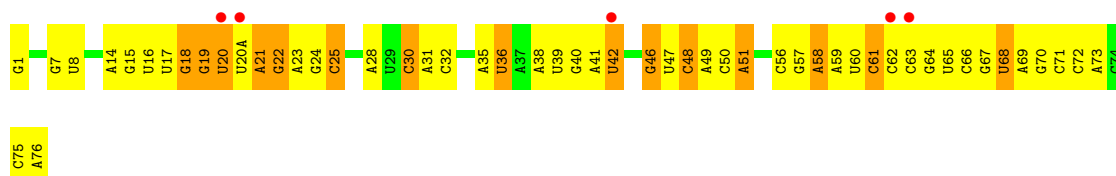






• Molecule 21: transfer RNA

Chain CW:



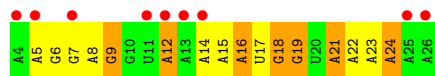
• Molecule 22: messenger RNA

Chain AV:



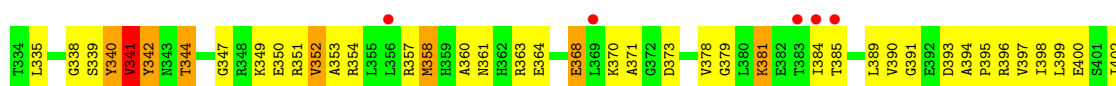
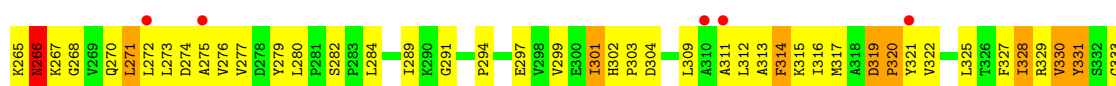
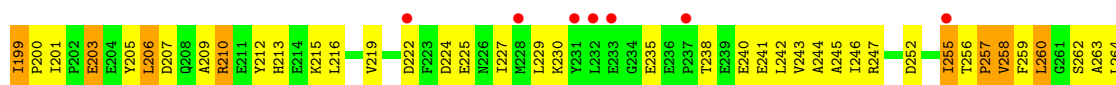
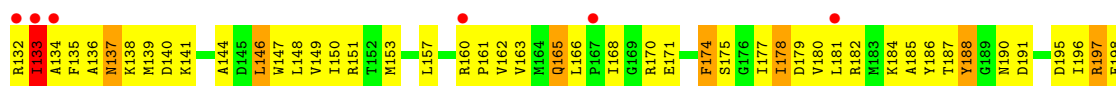
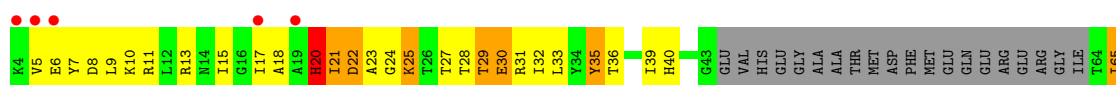
• Molecule 22: messenger RNA

Chain CV:



• Molecule 23: Elongation factor G

Chain AY:







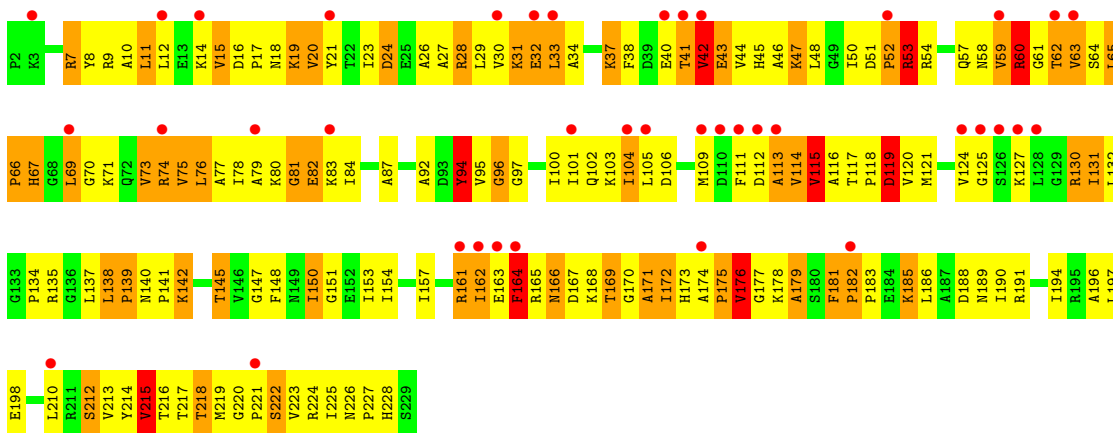
• Molecule 24: VIOMYCIN

Chain CU:



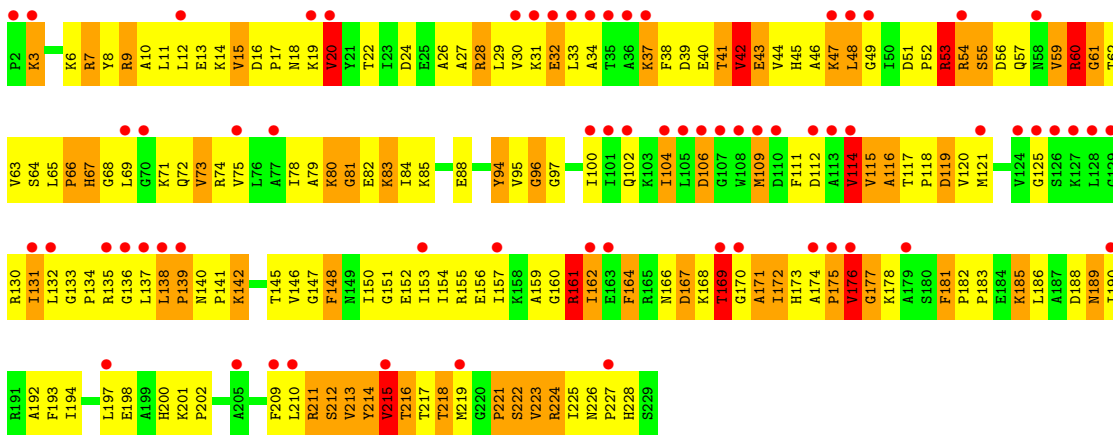
• Molecule 25: 50S ribosomal protein L1

Chain BC:



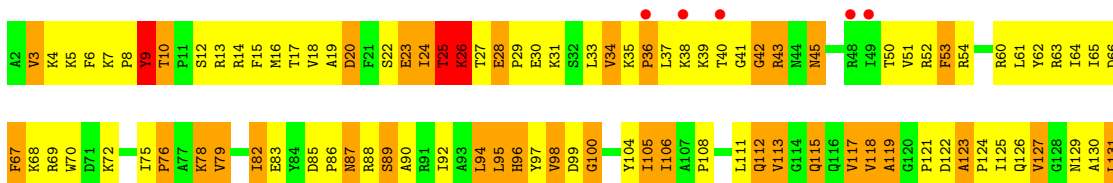
• Molecule 25: 50S ribosomal protein L1

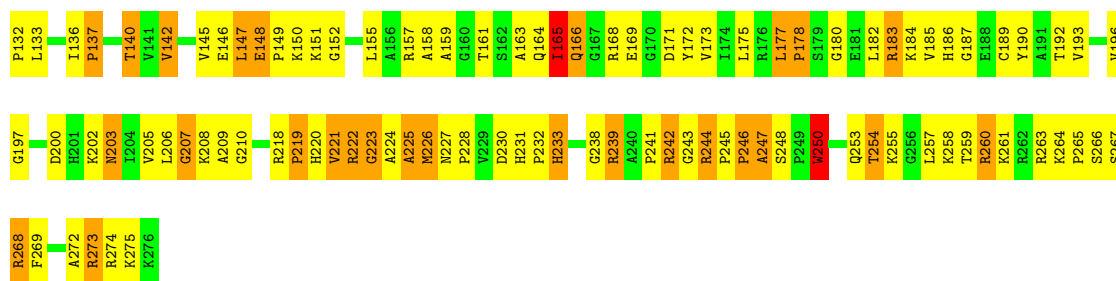
Chain DC:



• Molecule 26: 50S ribosomal protein L2

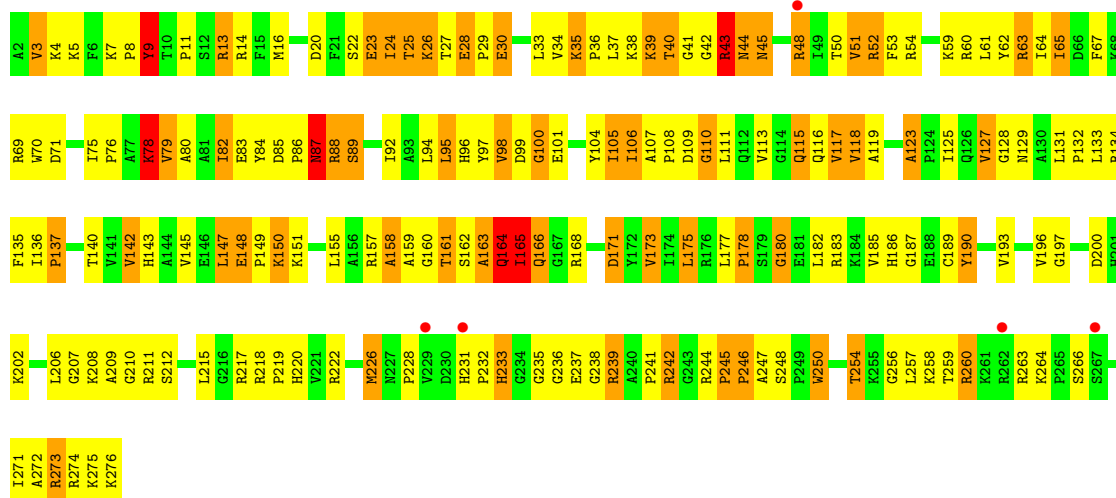
Chain BD:





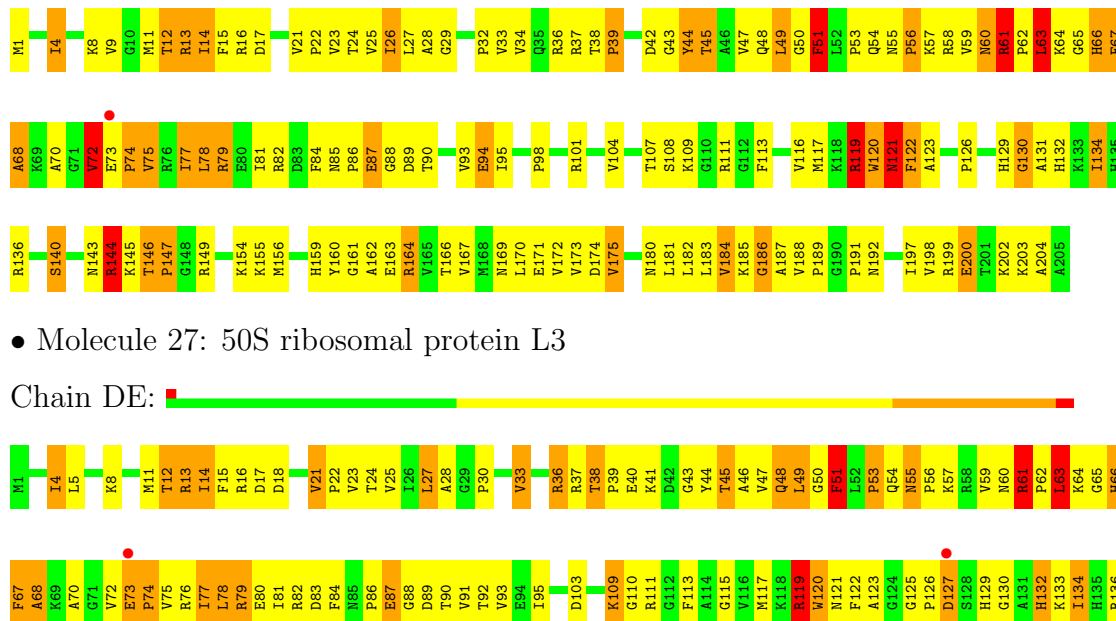
• Molecule 26: 50S ribosomal protein L2

Chain DD:



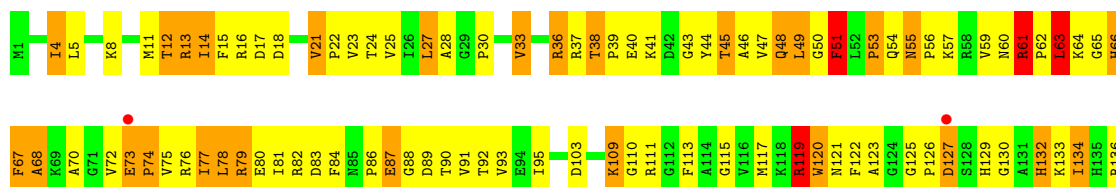
• Molecule 27: 50S ribosomal protein L3

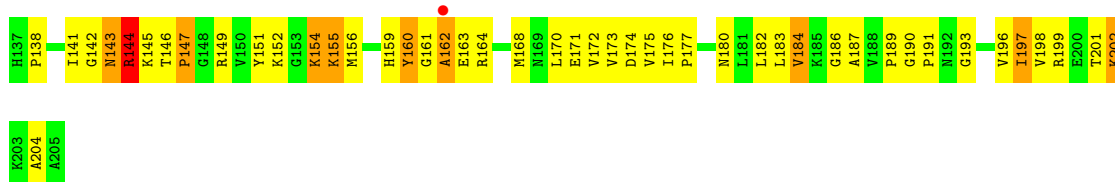
Chain BE:



• Molecule 27: 50S ribosomal protein L3

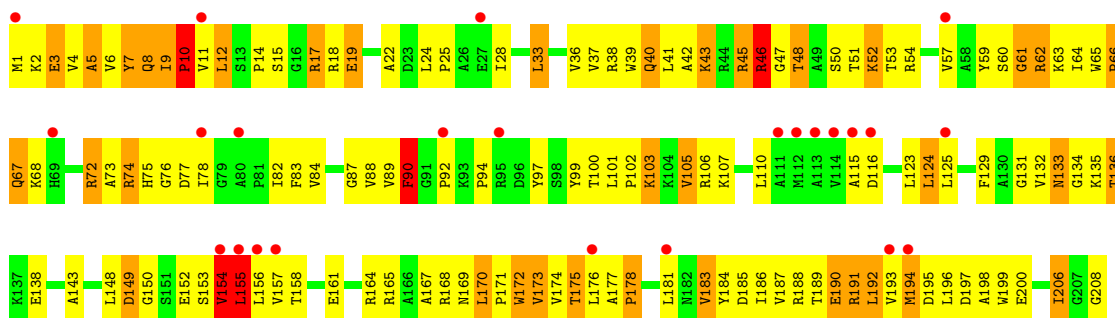
Chain DE:





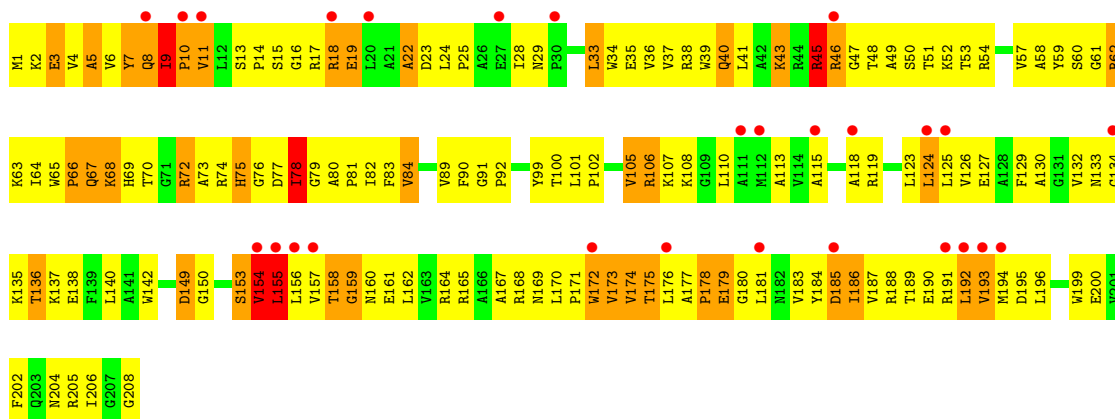
• Molecule 28: 50S ribosomal protein L4

Chain BF:



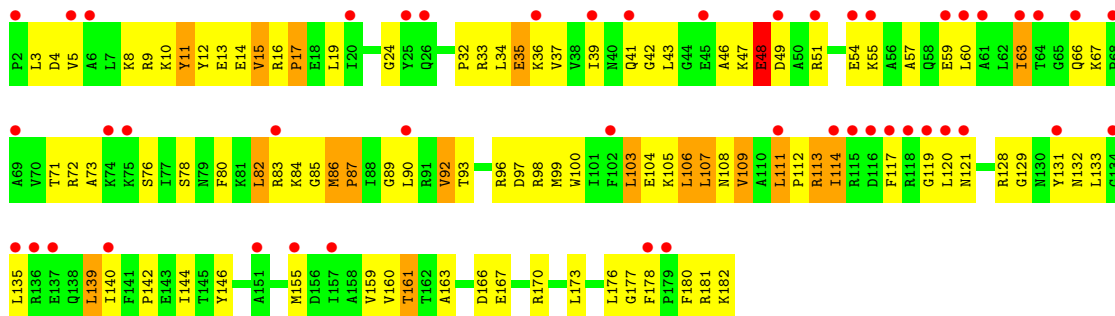
• Molecule 28: 50S ribosomal protein L4

Chain DF:

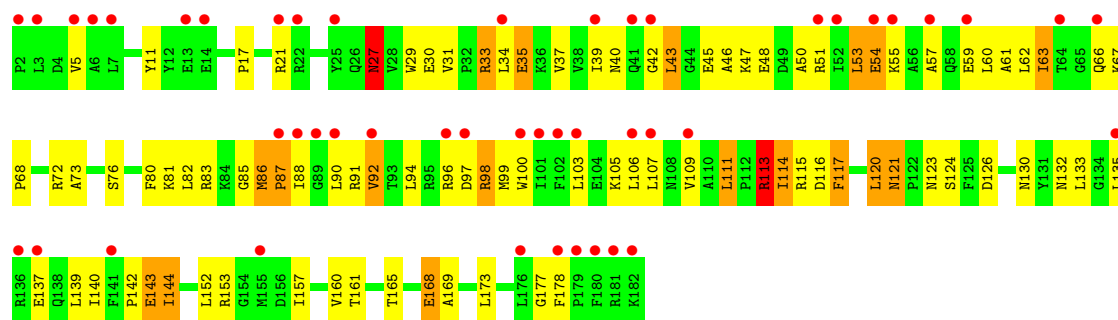


• Molecule 29: 50S ribosomal protein L5

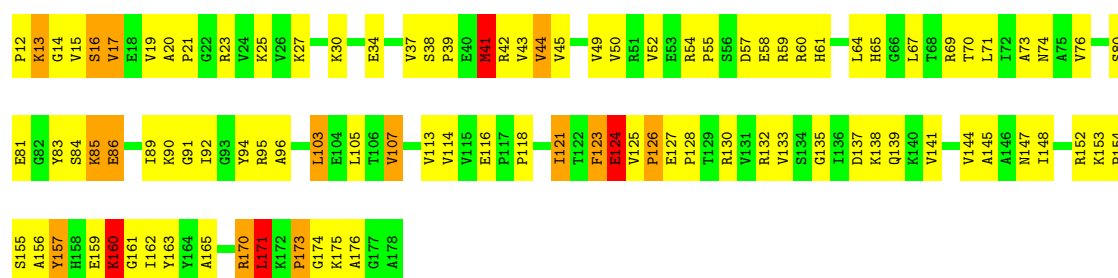
Chain BG:



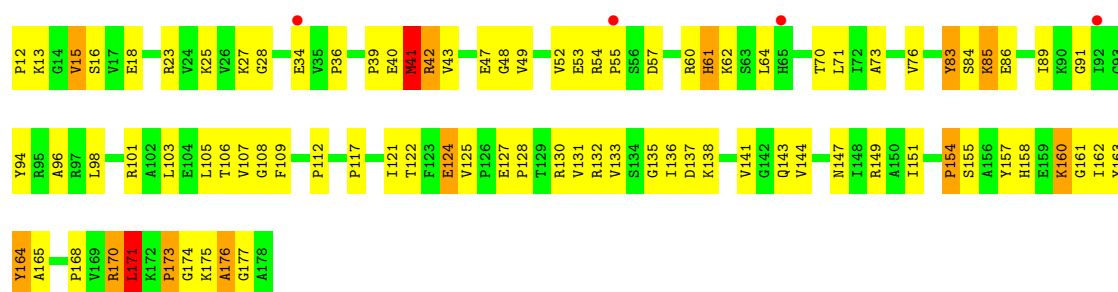
• Molecule 29: 50S ribosomal protein L5

Chain DG: 

- Molecule 30: 50S ribosomal protein L6

Chain BH: 

- Molecule 30: 50S ribosomal protein L6

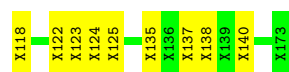
Chain DH: 

- Molecule 31: 50S RIBOSOMAL PROTEIN L10

Chain BJ: 

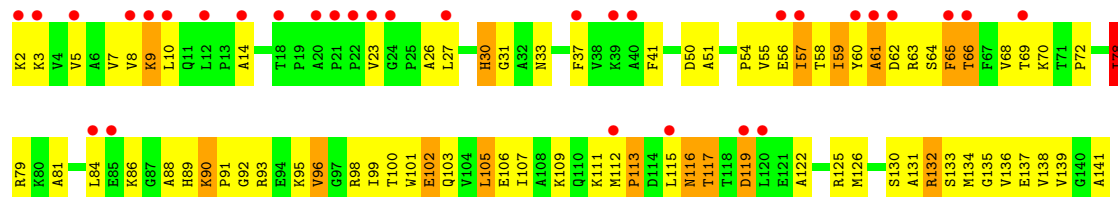
- Molecule 31: 50S RIBOSOMAL PROTEIN L10

Chain DJ: 



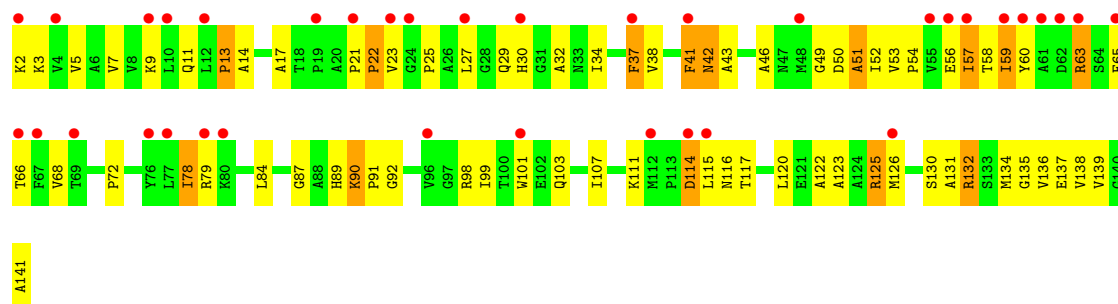
- Molecule 32: 50S ribosomal protein L11

Chain BK:



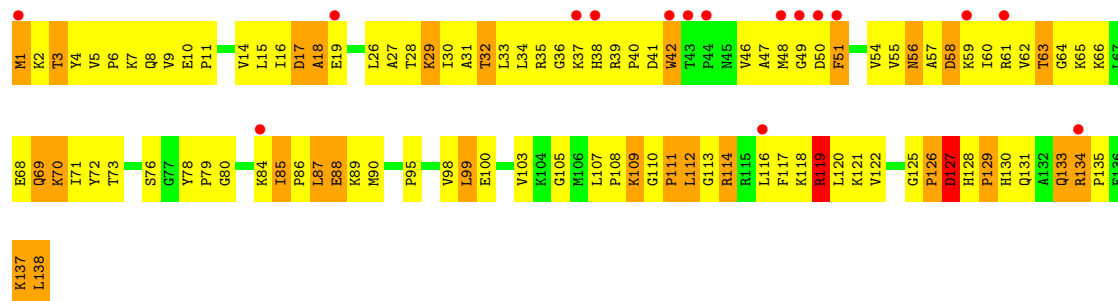
- Molecule 32: 50S ribosomal protein L11

Chain DK:



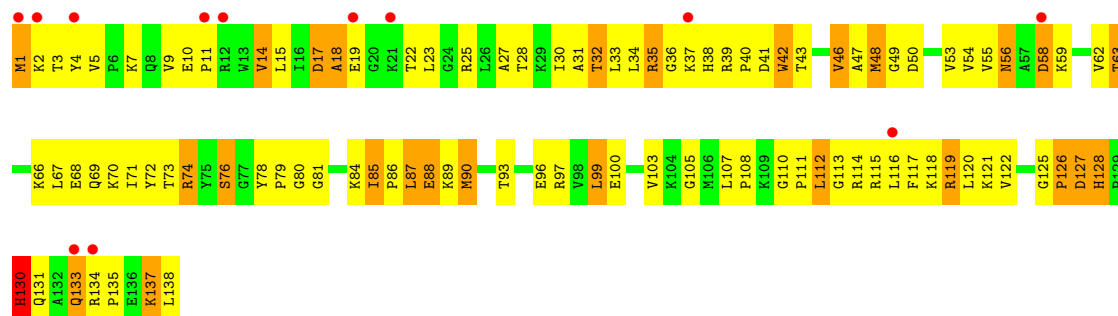
- Molecule 33: 50S ribosomal protein L13

Chain BN:

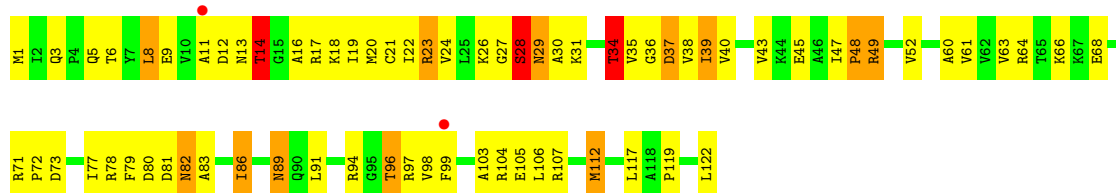


- Molecule 33: 50S ribosomal protein L13

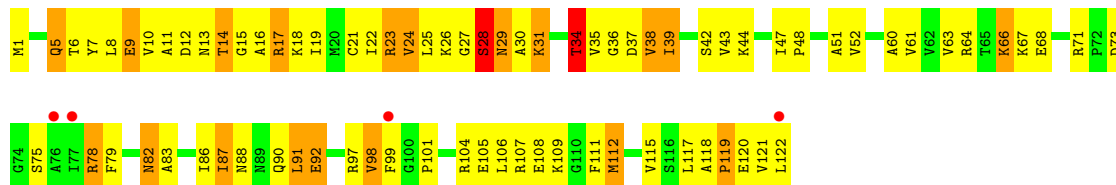
Chain DN:



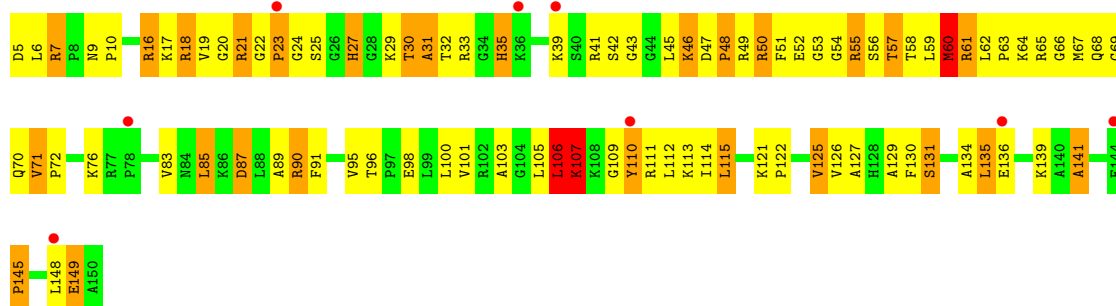
- Molecule 34: 50S ribosomal protein L14

Chain BO: 

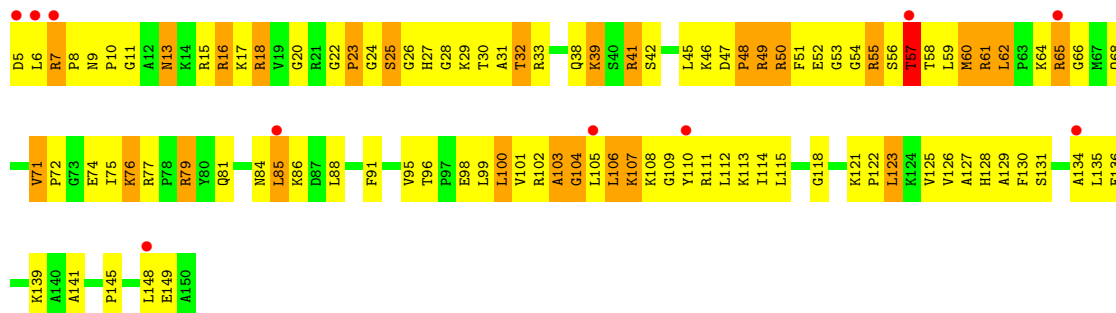
- Molecule 34: 50S ribosomal protein L14

Chain DO: 

- Molecule 35: 50S ribosomal protein L15

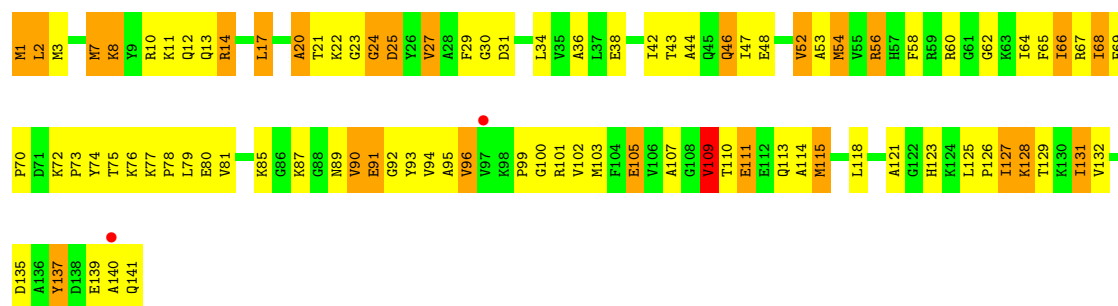
Chain BP: 

- Molecule 35: 50S ribosomal protein L15

Chain DP: 

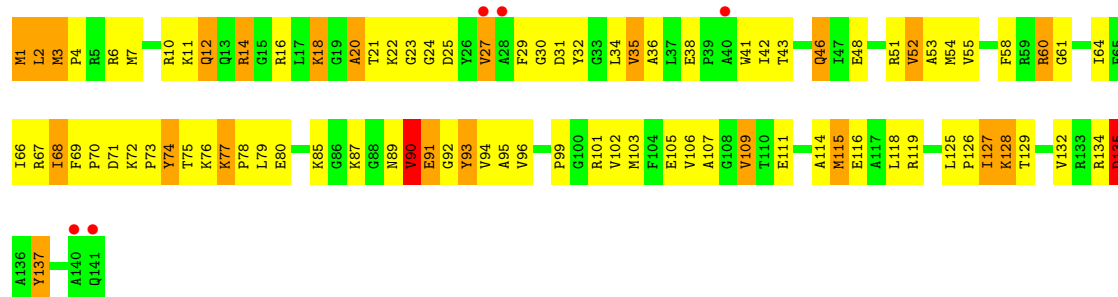
- Molecule 36: 50S ribosomal protein L16

Chain BQ: 



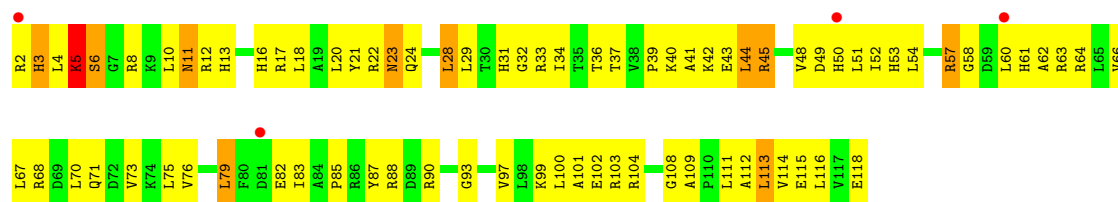
- Molecule 36: 50S ribosomal protein L16

Chain DQ:



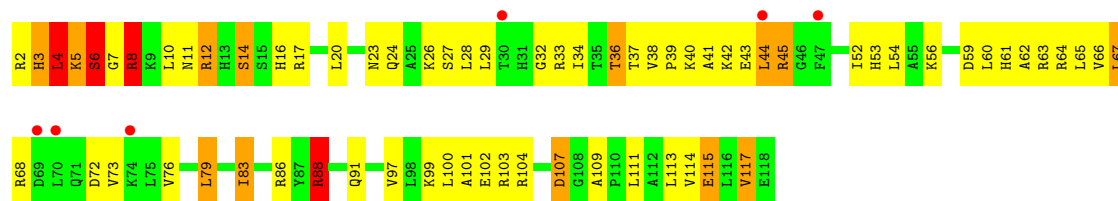
- Molecule 37: 50S ribosomal protein L17

Chain BR:



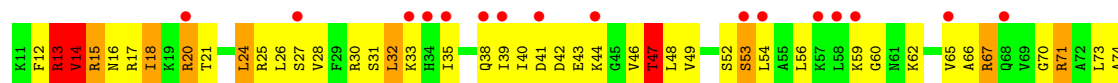
- Molecule 37: 50S ribosomal protein L17

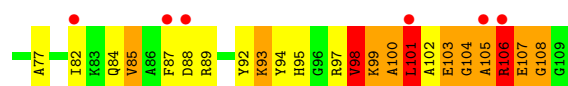
Chain DR:



- Molecule 38: 50S ribosomal protein L18

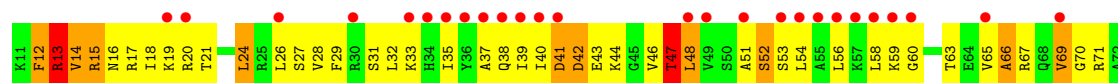
Chain BS:





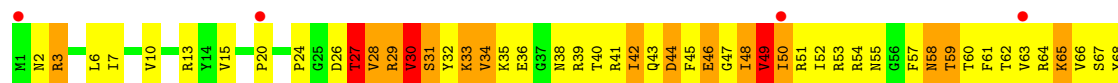
• Molecule 38: 50S ribosomal protein L18

Chain DS:



• Molecule 39: 50S ribosomal protein L19

Chain BT:



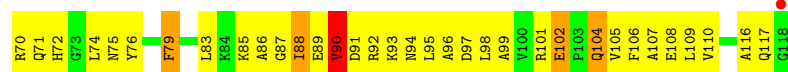
• Molecule 39: 50S ribosomal protein L19

Chain DT:



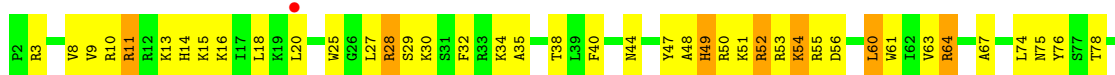
• Molecule 40: 50S ribosomal protein L20

Chain BU:



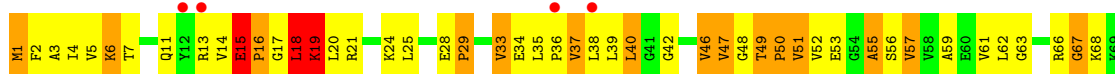
• Molecule 40: 50S ribosomal protein L20

Chain DU: 

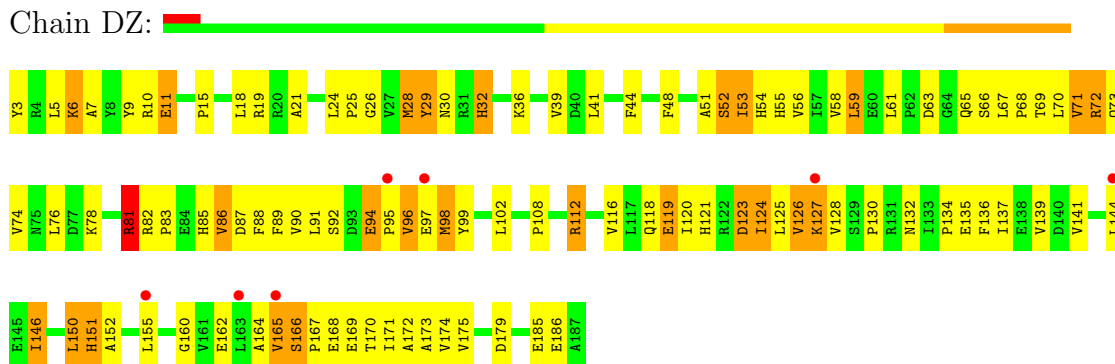


- Molecule 41: 50S ribosomal protein L21

Chain BV: 

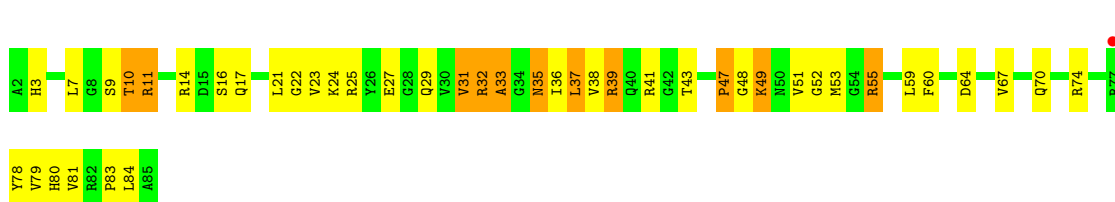


Chain DZ:



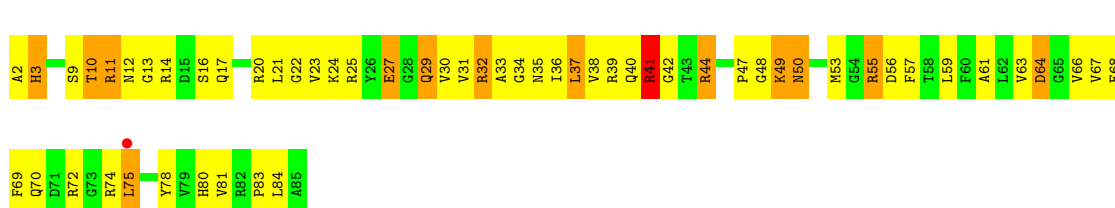
- Molecule 46: 50S ribosomal protein L27

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

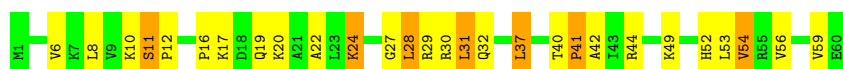
Chain B3:



- Molecule 48: 50S ribosomal protein L30

Chain D3:





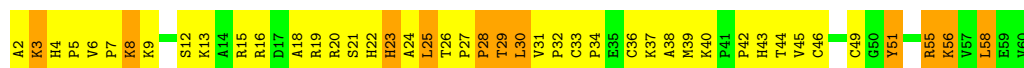
- Molecule 49: 50S ribosomal protein L32

Chain B5:



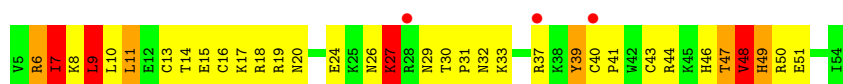
- Molecule 49: 50S ribosomal protein L32

Chain D5:



- Molecule 50: 50S ribosomal protein L33

Chain B6:



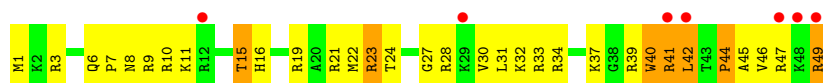
- Molecule 50: 50S ribosomal protein L33

Chain D6:



- Molecule 51: 50S ribosomal protein L34

Chain B7:



- Molecule 51: 50S ribosomal protein L34

Chain D7:



- Molecule 52: 50S ribosomal protein L35

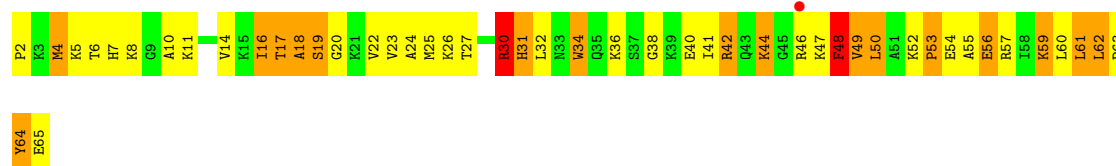
Chain B8:



E65

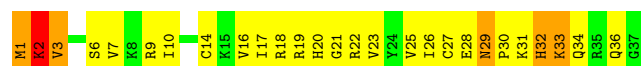
- Molecule 52: 50S ribosomal protein L35

Chain D8: 



- Molecule 53: 50S ribosomal protein L36

Chain B9: 



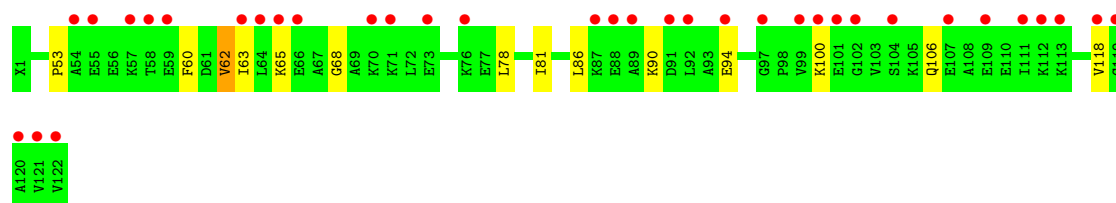
- Molecule 53: 50S ribosomal protein L36

Chain D9: 



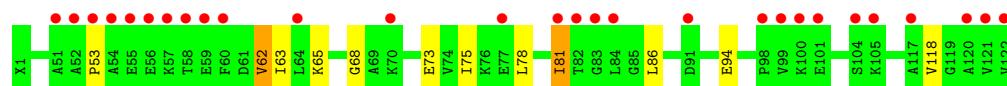
- Molecule 54: 50S ribosomal protein L7/L12

Chain Be: 



- Molecule 54: 50S ribosomal protein L7/L12

Chain De: 



- Molecule 55: 50S RIBOSOMAL PROTEIN L7/L12

Chain Bf: 

There are no outlier residues recorded for this chain.

- Molecule 55: 50S RIBOSOMAL PROTEIN L7/L12

Chain Bg: 

There are no outlier residues recorded for this chain.

- Molecule 55: 50S RIBOSOMAL PROTEIN L7/L12

Chain Df: 

There are no outlier residues recorded for this chain.

- Molecule 55: 50S RIBOSOMAL PROTEIN L7/L12

Chain Dg: 

There are no outlier residues recorded for this chain.

- Molecule 56: 50S RIBOSOMAL PROTEIN L7/L12

Chain Bh: 

There are no outlier residues recorded for this chain.

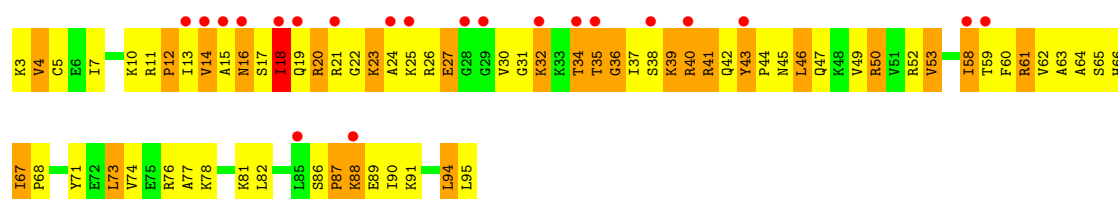
- Molecule 56: 50S RIBOSOMAL PROTEIN L7/L12

Chain Dh: 


There are no outlier residues recorded for this chain.

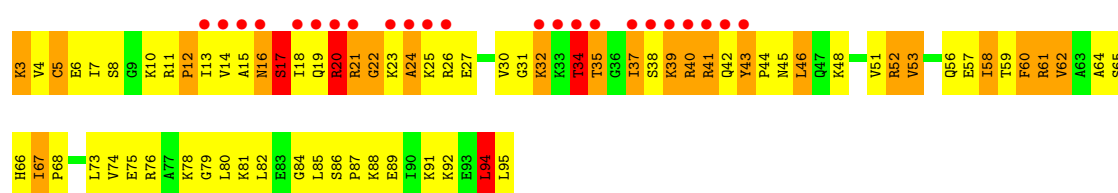
- Molecule 57: 50S ribosomal protein L28

Chain B1: 




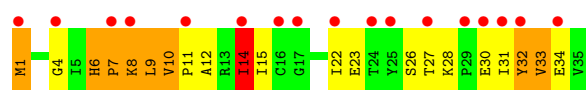
- Molecule 57: 50S ribosomal protein L28

Chain D1: 



- Molecule 58: 50S ribosomal protein L31

Chain B4: 



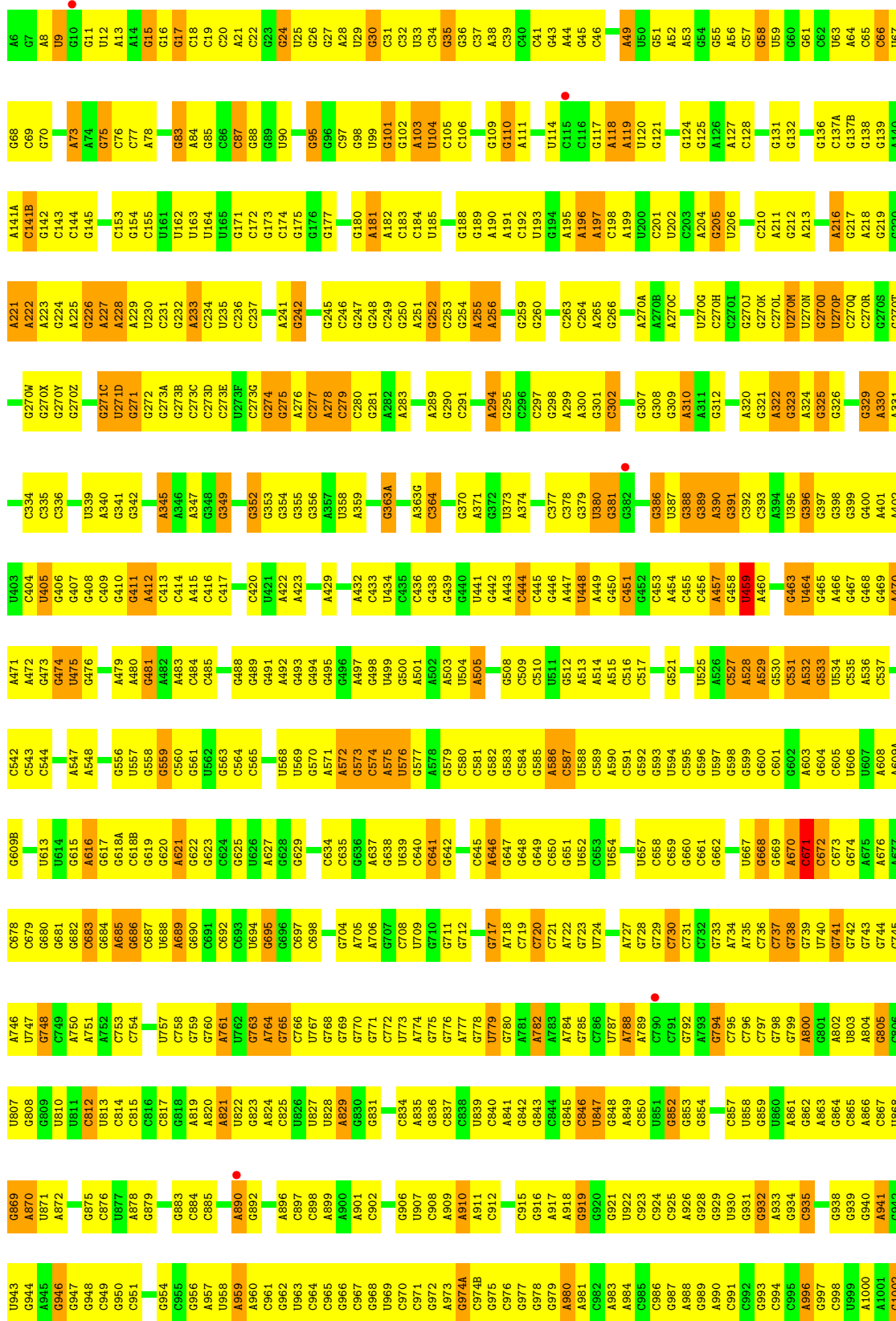
- Molecule 58: 50S ribosomal protein L31

Chain D4: 

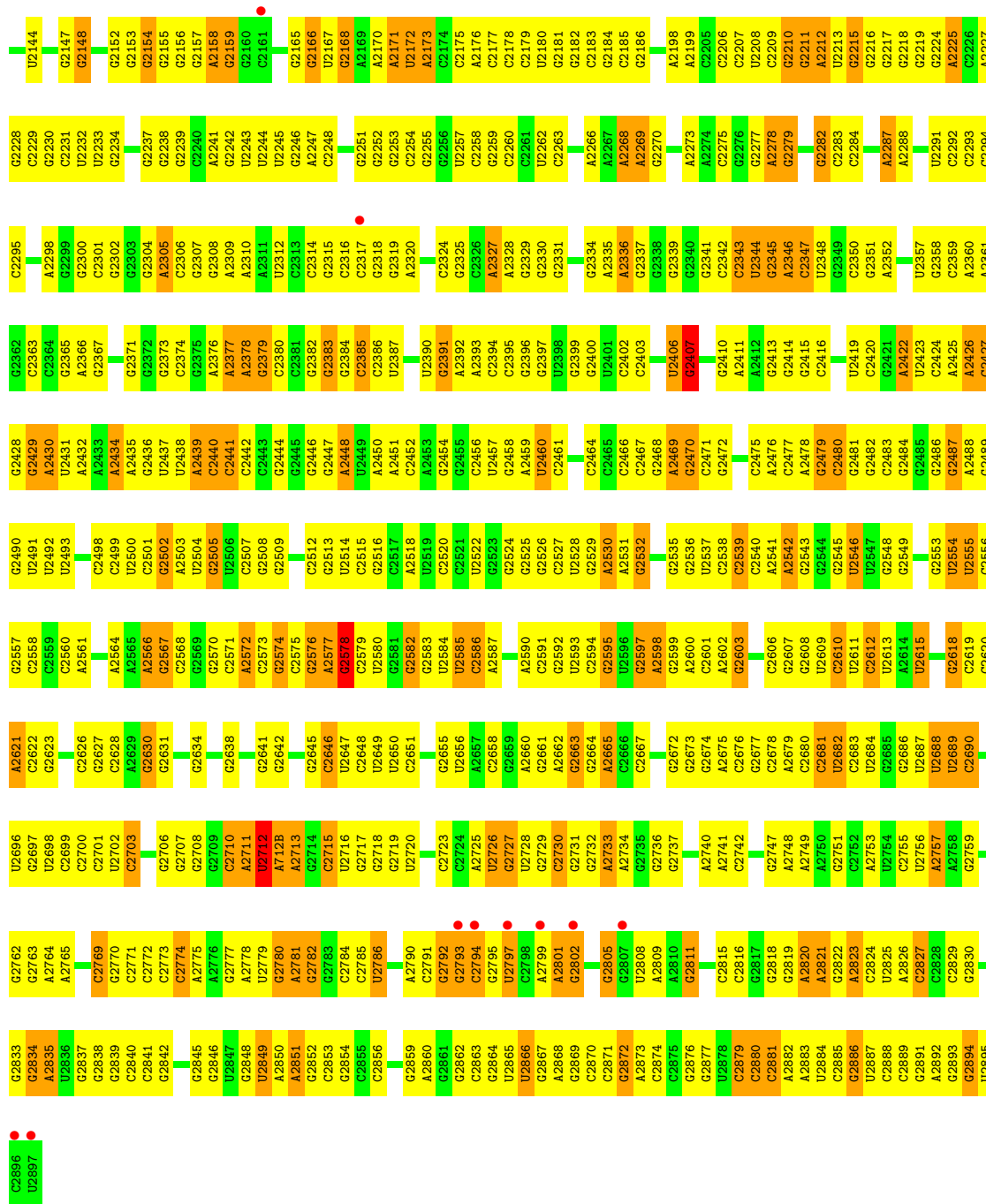


- Molecule 59: 23S ribosomal RNA

Chain BA:

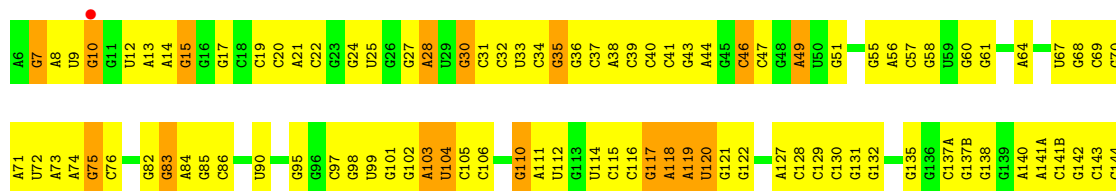


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U2074	U2011	G1949	G1861	U1798	C1710	A1641	A1570	G1500	G1429	G1356	U1288	C1221	G1144	C1076	C1006
U2075	G2012	G1950	G1862	G1799	C1711	G1642	A1571	C1502	C1430	U1357	C1289	C1222	C1145	A1077	C1007
U2076	A2013	U1951	G1863	C1800	G1801	C1643	A1572	C1502		G1358	C1290	G1223	A1148	U1078	C1008
C2077	A2014	A1952	U1864	G1801	G1717	C1644	U1576	A1508	A1434	A1359	C1291	A1226	G1149	C1079	A1009
U2078	A2015	A1953	G1869	A1802	G1718	C1645	U1577	A1509	G1435	A1360	U1292	A1226	G1150	C1080	A1010
U2079	U2016	G1954	C1870	A1803	G1725	C1646	C1577	A1509	G1436	G1363	C1293		G1151	U1081	G1011
G2080	U2017	U1955	A1871	C1804	G1726	G1647	U1578	A1510	C1437	C1362	C1293		G1152	U1082	G1012
C2081	G2018	U1956	A1872	U1805	G1727	C1648	A1579	A1511	U1438	C1363	U1294	C1230	C1153	U1083	C1013
A2082	A2019	C1957	C1806	G1806	G1728	G1649	U1579	A1512	U1439	G1364	G1295	G1230	C1154	U1084	U1014
G2083	G2020	G1958	C1807	G1807	A1729	G1650	G1581	C1513	A1439	A1365	G1296	G1232	G1155	A1084	
C2084	C2021	U1959	C1881	U1808	G1730	G1651	C1582	U1514	G1440	C1366		C1233	A1155	A1085	G1015
G2085	U2022	A1960	C1891	G1809	G1731	A1652	C1583	C1514	G1443	U1234	U1300	U1234	A1156	G1016	
U2086	C2023	C1961	A1884	A1810	A1732	G1853	C1585	U1516	G1444	G1371	A1301	G1235	G1157	G1017	
G2087	G2024	G1962	A1885	G1811	G1733	G1854	A1586	G1517	A1448		A1302	G1236		A1088	U1019
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U2089	G1964	G1887	G1813	C1742	G1742	C1656	C1588	G1519	G1446	G1376	C1306	U1240	G1163	U1090	A1020
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U2092	C1967	A1890	G1816	A1749	A1749	U1859	C1591	G1524	A1498	A1379	G1309	G1243	U1167	G1024	G1024
G2093	G1969	G1891	G1817				C1592	G1525			G1310	G1244		U1097	
C2094	A1970	A1819	U1818					G1526			G1311			A1098	
G2095	G1971	G1896	U1820								U1312			U1101	A1027
U2096	A1972	C1972	G1897								U1313			C1102	A1028
	G1973	G1973	U1898								C1314			A1103	A1029
	C1974	C1974	U1899												
	G1975	G1975	A1900	G1824	G1753	A1665	A1596	A1529			A1317				U1033
	U1976	A1901	G1825	U1825	C1754	G1666	A1597	A1530			A1321			G1034	U1035
	A1977	C1902	G1826	G1826	G1755	G1667	C1598	C1531			A1322			U1108	G1036
	C1978	G1903	G1828	G1828	U1762	C1672	A1603	U1535			U1323			G1109	G1037
	C1979	G1906	A1829	A1829	G1763	U1673	C1537	C1537			G1324			G1110	C1038
	G1980		C1830	C1830	G1764	G1674	C1605	U1539			G1325			G1111	G1039
	A1981		G1831	G1831	G1765	A1675	C1606	G1540			U1326			G1112	C1040
	C1982		A1912	C1832	U1766	A1676	C1607	G1541			G1327			G1125	C1041
			A1913	U1833		A1677	A1608	U1541			G1328			G1126	G1042
			C1914	U1834		G1678	A1609	G1542			G1329			G1127	C1043
			U1915	U1834			A1610	A1543			U1330			G1128	C1044
			A1916	C1838		G1681	C1611	C1544			C1402			G1129	A1045
			U1917	A1773		G1682	C1612	A1545			A1331			A1204	A1046
			C1920	C1774		C1683	G1613	A1546			C1333			G1124	G1047
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				U1779			C1615	C1547			U1335			A1126	C1049
				A1780			A1616	C1548			A1336			A1127	
				C1781			C1617				A1337			G1128	
				C1782				C1551			G1337			A1129	A1054
				A1783			G1623	G1552			G1338			U1130	G1055
				A1784			A1614	A1553			U1339			G1131	G1056
				A1785			G1626	A1554			U1340			A1132	A1057
				A1786			G1626	A1554			U1341			U1133	G1058
				A1787			C163B	C1557			A1342			U1133	G1059
				A1788			A1631	A1558			G1343			C1135	U1060
				C1789			G1632	G1559			G1344			G1136	U1061
				A1790			A1633				C1345			G1137	G1062
				C1790			G1633				A1278			G1138	G1063
				A1791			A1634	G1563			G1279			A1213	C1064
				G1702			G1635	C1564			G1281			G1139	
				G1705			C1636	C1565			G1281			C1140	
				U1706			C1637	A1566			G1282			U1141	A1070
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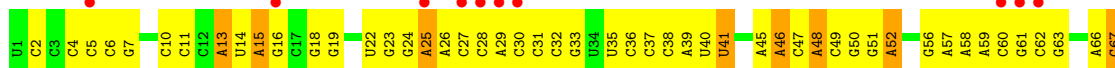
• Molecule 59: 23S ribosomal RNA

Chain DA:



G1107	A1045	G978	C915	G848	A784	A722	G656	U597	A528	C462	G333	G272	A228	G146
G1112	A1046	G979	G916	A849	G785	G723	U657	G598	A529	G463	C334	G273A	A229	C148
U1113	G1047	A980	A917	C950	C796	U724	C658	G600	G530	U464	C335	G273B	U230	C149
G1114	A1048	A983	G919	A852	A788	G725	C659	G601	G531	G465	C336	C273C	C231	C150
G1115	C1049	A984	G920	G853	A789	A726	C660	G602	A532	A466	C337	C273D	G232	
C1116	A1050	C985	G921	G854	C790	G728	G662	A603	G533	G467	C340	U273E	A233	
G1117	G1051	C986	U922	G855	C791	G729	G663	G604	U534	G468	A340	C273F	C234	C153
	C1052	A987	C923	C956	G792	C730	C664	C605	C535	G469	G341	C273G	U235	G154
G1120	C1053	A988	C924	C957	A793	G731	U667	U606	A536	A470	G342	G274	C236	C155
G1122	A1054	C989	C925	U858	G794	C732	G668	A608	G539	A471	G343	A275	C237	
C1123	G1055	A990	A926	G859	C795	G733	G669	G609A	G540	A472	G344	G276		G171
G1124	C1056	C991	G928		C796	A734	A670	G609B	C542	G473	U350	A278	U243	G172
	A1057	C992	G929	G862	C797	A735	C671	G609C	C543	G474	U351	C279	G245	G173
G1125	G1058	G993	U930	A863	G798	C736	C672	G609D	C544	U475	G351		G246	C174
A1126	C1059	C994	G931	G864	C799	C737	C673	C610	C545	G476	G352	C287	G247	G175
A1127	U1060	C995	G932	C865	A800	G738	C674	G612	G546	A477	G353	C288	G248	
A1128	U1061	A996	A933	A866	G801	G739	G675	U613	C547	A478	G354	C290	C249	G179
A1129	G1062	C997	G934	C867	A804	U740	A676	U614	G548	A479	G355	G291	G250	A181
U1130	G1063	C998	C935	U868	A805	G741	C678	G615	A547	A480	U358	C292	G251	A182
G1131	C1064	U999		G869	G805	G742	C679	A616	G549	A481	A359		G252	C183
	U1065	A1000	G938	A870	C806	G743	G680	G617	G556	A482	C419	A294	G253	
C1135	G1136	A1001	G939	U871	U807	G744	G681	G618A	G557	A483	C420	G295		C184
G1137	A1002	G1002	G940	A872	G808	G745	G682	C618B	U557	C484	U421	C296	A256	U185
G1138	A1003	G809	A941	G873	G809	A746	C683	G619	G558	C485	A422	C297	A257	G186
G1139	A1004		G942	G874	U747		C684	G620	G559	C486	A423	G298	G258	G187
	C1005		U943	G875			C685	A621	C560	G487	G424	G299	G259	G188
C1140	C1006		A945	A878	U813	C749	A685	G622	C561	G488	G425	A300	G260	G189
U1141	U1007	C1007	G946	G879	C814	A750	G686	G623	U562	G489	C426	G301	G261	
U1142	G1008	C1008	G947	G880	C817	A751	C687	G624	G563	G491		C302	A262	U193
A1148	C1009	A1009	G948	G881	U688	C752	U689	G625	C564	A492	U431	U303	G304	G194
A1143	C1076	G1076	G949	G882	A689	C753	U690	U626	G565	G493	A432	G305	A265	A195
G1144	U1077	G1144	C950	G883	C691	C754	A627	G628		G494	C433	U306	G266	A196
C1145	U1078	C1078	G951	G884	C692	U757	C692	G628	G570	G496	U434	G307	A270C	C198
	G1149	C1080	G952		A821	U757	C693	A631	A571	U499	C435	U373	A270D	A199
C1150	U1081	G1016		A887	G823	G758	U694	A632	A572	G500	C436	G308	C270E	U200
G1151	U1082	G1017	C955	C988	A824	G759	G695	A633	G573	A501	C438	G309	G270F	G201
C1152	U1083	C1018	G956	C889	C825	G760	G696	C634	C574	A502	G440	A310	U270G	U202
G1154	A1085	U1019	A957	A890	U826	U762	C697	C635	U576	A503	U441	G311	U270H	C203
	C1086	A1020	U958	G892	U827	G763	C698	G636	G577	U504	G442	C313	C270I	A204
	A1087	A1021	A959	C893	A828	A764	A699	A637	A578	A505	A443	A314	G270J	G205
G1157	C1088	G1022	A960	C894	A829	G765	G700	G638	G579	A506	C444	G315	G270K	
	U1089	C1023	C961	U895		C766		U639	C580	A507	C445	C316	C270L	C210
	G1089	G1024	G962	A896	G832	U767	A705	C640	C581	G508	G446	G317	U270M	A211
	U1090	G1025	U963	C997	U833	G768	A706	C641	C582	G509	A447	C318	U270N	A212
G1162	G1091	U1026	C964		C834	G769	G707	G642	C583	C510	U448	C319	G270O	G213
G1163	C1092	A1027	G965	A900	A835	G770	C708	A643	C584	C511	A449	A320	U270P	G214
U1164	G1093	A1028	G966	A901	G836	G771	U709	A644	G585	A513	G450	G321	C270Q	G215
C1165	U1094	A1029	C967	C902	C837	C772	G710	C645	A586	A514	C451	A322	G270R	A216
C1166	A1095	G1030	G968	C903	C838	U773	G711	A646	C587	A515	G452	G323	G270S	G217
U1167	U1097		U969	C904	U839	A774	G712	G647	U588	C516	A453	A324	G270T	A218
	G1168	C971	C970	U905	C840	G775	G715	G648	A590	C517	A454	G325	G270U	G219
G1169		G972	G971	G906	A841	G776	A716	G649	A591	G518	C455	G326	G270V	G220
	U1101	A973	G972	G907	G842	U779	G717	C650	C591	C521	C456	G327	G270Y	A221
G1173	A1102	G1037	A973	A909	G843		G718	G651	C592	G522	A457	U328	A222	A223
A1174	C1038		G974A	A910	C844	G780	A718	U652	G593	U525	G458	G329	C271B	G226
U1175	G1039		C974B	A911	C845	A781	C719	C853	U594	A526	U459	G330	U271D	
G1176	C1104		G975	A912	C846	A782	C720	U654	C595	C527	G461	A332	G271	
A1177	G1106	G1042			U847	A783	C721	A655	G596					





C68	G69	A73	U74	G75	G76	U77	A78	C79	U80	G81	C82	G83	C84	G85	G86	G87	C88	G89A	A89B	C90	U95	A99	G100	A101	G102	U103	A104	G105	G106	U107	C108	G109	G110	U111	G112	G118
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4 Data and refinement statistics

Xtriage (Phenix) failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	308.96Å 670.66Å 347.77Å 90.00° 92.52° 90.00°	Depositor
Resolution (Å)	40.00 – 3.50 140.20 – 3.57	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.50) 74.7 (140.20-3.57)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.284 , 0.328 0.304 , 0.342	Depositor DCC
R_{free} test set	33495 reflections (5.25%)	DCC
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 52.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	308166	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, MG, DPP, KBE, UAL, FUA, 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	0.38	0/1945	0.72	1/2621 (0.0%)
1	CB	0.37	0/1945	0.67	1/2621 (0.0%)
2	AC	0.28	0/1645	0.53	0/2216
2	CC	0.28	0/1645	0.52	0/2216
3	AD	0.30	0/1733	0.58	0/2318
3	CD	0.30	0/1733	0.58	1/2318 (0.0%)
4	AE	0.32	0/1172	0.58	1/1576 (0.1%)
4	CE	0.31	0/1172	0.58	1/1576 (0.1%)
5	AF	0.31	0/856	0.59	0/1154
5	CF	0.31	0/856	0.56	1/1154 (0.1%)
6	AG	0.29	0/1276	0.51	0/1709
6	CG	0.28	0/1276	0.52	0/1709
7	AH	0.30	0/1136	0.57	0/1527
7	CH	0.28	0/1136	0.55	0/1527
8	AI	0.29	0/1029	0.53	0/1379
8	CI	0.27	0/1029	0.49	0/1379
9	AJ	0.27	0/815	0.54	0/1095
9	CJ	0.28	0/815	0.57	1/1095 (0.1%)
10	AK	0.33	0/900	0.61	0/1213
10	CK	0.36	0/900	0.65	0/1213
11	AL	0.40	0/992	0.83	2/1327 (0.2%)
11	CL	0.40	0/992	0.82	1/1327 (0.1%)
12	AM	0.29	0/1008	0.59	1/1347 (0.1%)
12	CM	0.28	0/1008	0.54	0/1347
13	AN	0.30	0/501	0.52	0/664
13	CN	0.26	0/501	0.46	0/664
14	AO	0.31	0/745	0.52	0/992
14	CO	0.31	0/745	0.53	0/992
15	AP	0.28	0/722	0.50	0/970
15	CP	0.27	0/722	0.52	0/970
16	AQ	0.36	0/848	0.65	0/1131
16	CQ	0.37	0/848	0.71	0/1131

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AR	0.31	0/579	0.59	0/768
17	CR	0.30	0/579	0.55	0/768
18	AS	0.31	0/647	0.60	0/870
18	CS	0.31	0/647	0.61	0/870
19	AT	0.33	0/765	0.56	0/1007
19	CT	0.32	0/765	0.55	0/1007
20	AA	0.37	0/36351	1.02	61/56736 (0.1%)
20	CA	0.36	0/36351	0.99	53/56736 (0.1%)
21	AW	0.33	0/1827	1.03	0/2845
21	CW	0.33	0/1827	1.01	5/2845 (0.2%)
22	AV	0.27	0/568	0.81	0/886
22	CV	0.29	0/568	0.92	0/886
23	AY	0.34	1/5317 (0.0%)	0.66	7/7198 (0.1%)
23	CY	0.37	2/5317 (0.0%)	0.61	1/7198 (0.0%)
24	AU	0.95	0/11	1.28	0/13
24	CU	0.92	0/11	1.04	0/13
25	BC	0.41	0/1774	0.74	1/2391 (0.0%)
25	DC	0.43	0/1774	0.72	1/2391 (0.0%)
26	BD	0.33	0/2195	0.65	1/2955 (0.0%)
26	DD	0.35	0/2195	0.65	0/2955
27	BE	0.32	0/1602	0.66	0/2160
27	DE	0.31	0/1602	0.66	0/2160
28	BF	0.35	0/1663	0.73	2/2249 (0.1%)
28	DF	0.37	0/1663	0.76	3/2249 (0.1%)
29	BG	0.40	1/1499 (0.1%)	0.59	0/2016
29	DG	0.38	1/1499 (0.1%)	0.61	0/2016
30	BH	0.30	0/1298	0.60	0/1751
30	DH	0.29	0/1298	0.57	0/1751
32	BK	0.27	0/1054	0.51	0/1427
32	DK	0.27	0/1054	0.50	0/1427
33	BN	0.45	0/1131	0.77	0/1525
33	DN	0.48	0/1131	0.74	0/1525
34	BO	0.30	0/943	0.57	0/1269
34	DO	0.29	0/943	0.55	0/1269
35	BP	0.30	0/1131	0.62	0/1504
35	DP	0.29	0/1131	0.62	0/1504
36	BQ	0.35	0/1143	0.63	0/1527
36	DQ	0.34	0/1143	0.60	0/1527
37	BR	0.30	0/974	0.60	0/1302
37	DR	0.31	0/974	0.61	0/1302
38	BS	0.34	0/783	0.69	0/1041
38	DS	0.33	0/783	0.70	0/1041
39	BT	0.34	0/1161	0.67	0/1549

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	DT	0.36	0/1161	0.66	0/1549
40	BU	0.36	0/982	0.57	0/1306
40	DU	0.40	0/982	0.60	0/1306
41	BV	0.38	0/790	0.70	1/1057 (0.1%)
41	DV	0.38	0/790	0.67	0/1057
42	BW	0.31	0/911	0.59	0/1220
42	DW	0.31	0/911	0.61	1/1220 (0.1%)
43	BX	0.30	0/748	0.55	0/1004
43	DX	0.29	0/748	0.54	1/1004 (0.1%)
44	BY	0.32	0/831	0.62	0/1108
44	DY	0.33	0/831	0.66	0/1108
45	BZ	0.29	0/1505	0.58	0/2042
45	DZ	0.28	0/1505	0.58	0/2042
46	B0	0.28	0/671	0.49	0/892
46	D0	0.28	0/671	0.54	0/892
47	B2	0.31	0/600	0.55	0/793
47	D2	0.32	0/600	0.55	0/793
48	B3	0.27	0/482	0.53	0/646
48	D3	0.27	0/482	0.55	0/646
49	B5	0.33	0/473	0.59	0/639
49	D5	0.31	0/473	0.57	0/639
50	B6	0.29	0/440	0.70	1/586 (0.2%)
50	D6	0.30	0/440	0.66	0/586
51	B7	0.33	0/438	0.64	0/575
51	D7	0.31	0/438	0.59	0/575
52	B8	0.34	0/525	0.68	0/691
52	D8	0.30	0/525	0.64	0/691
53	B9	0.30	0/310	0.55	0/407
53	D9	0.32	0/310	0.52	0/407
54	Be	0.28	0/538	0.50	0/715
54	De	0.26	0/538	0.49	0/715
57	B1	0.46	0/739	0.82	0/981
57	D1	0.47	0/739	0.84	1/981 (0.1%)
58	B4	0.32	0/276	0.58	0/372
58	D4	0.35	0/276	0.62	0/372
59	BA	0.40	0/69437	1.04	158/108401 (0.1%)
59	DA	0.40	3/69437 (0.0%)	1.03	149/108401 (0.1%)
60	BB	0.37	0/2853	1.08	11/4451 (0.2%)
60	DB	0.35	0/2853	1.03	5/4451 (0.1%)
All	All	0.37	8/330576 (0.0%)	0.92	474/492228 (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	3
1	CB	0	1
11	CL	0	2
23	AY	0	3
23	CY	0	2
25	BC	0	1
25	DC	0	3
26	BD	0	1
26	DD	0	2
28	BF	0	2
28	DF	0	2
29	BG	0	2
29	DG	0	2
31	BJ	0	1
31	DJ	0	1
35	DP	0	1
38	BS	0	3
38	DS	0	3
42	BW	0	1
42	DW	0	1
57	B1	0	2
57	D1	0	2
All	All	0	41

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	CY	506	GLN	C-N	8.35	1.53	1.34
29	BG	114	ILE	N-CA	-7.50	1.31	1.46
29	DG	114	ILE	N-CA	-7.47	1.31	1.46
23	CY	25	LYS	C-N	6.18	1.48	1.34
23	AY	506	GLN	C-N	-5.48	1.21	1.34

The worst 5 of 474 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	DA	1006	C	C6-N1-C2	-13.61	114.86	120.30
59	DA	459	U	N1-C2-N3	12.63	122.48	114.90
59	BA	1006	C	C6-N1-C2	-12.54	115.28	120.30
23	AY	506	GLN	O-C-N	-12.49	102.72	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	AA	815	A	C5-C6-N6	11.75	133.10	123.70

There are no chirality outliers.

5 of 41 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AB	162	ILE	Peptide
1	AB	170	GLU	Peptide
1	AB	185	ILE	Peptide
23	AY	133	ILE	Peptide
23	AY	503	GLY	Mainchain

5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AB	1910	0	1957	135	0
1	CB	1910	0	1957	107	0
2	AC	1621	0	1688	87	0
2	CC	1621	0	1688	64	0
3	AD	1703	0	1763	104	0
3	CD	1703	0	1763	104	0
4	AE	1156	0	1213	70	0
4	CE	1156	0	1213	57	0
5	AF	843	0	857	42	0
5	CF	843	0	857	32	0
6	AG	1257	0	1296	54	0
6	CG	1257	0	1296	53	0
7	AH	1116	0	1177	67	0
7	CH	1116	0	1177	73	0
8	AI	1010	0	1037	78	0
8	CI	1010	0	1037	57	0
9	AJ	802	0	849	44	0
9	CJ	802	0	849	48	0
10	AK	885	0	904	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	CK	885	0	904	60	0
11	AL	976	0	1062	113	0
11	CL	976	0	1062	103	0
12	AM	997	0	1072	67	0
12	CM	997	0	1072	49	0
13	AN	492	0	529	37	0
13	CN	492	0	529	26	0
14	AO	734	0	771	47	0
14	CO	734	0	771	43	0
15	AP	706	0	725	45	0
15	CP	706	0	725	28	0
16	AQ	835	0	904	64	0
16	CQ	835	0	904	57	0
17	AR	574	0	644	36	0
17	CR	574	0	644	37	0
18	AS	634	0	655	34	0
18	CS	634	0	655	45	0
19	AT	763	0	861	38	0
19	CT	763	0	861	37	0
20	AA	32474	0	16393	1002	0
20	CA	32474	0	16393	1036	0
21	AW	1635	0	831	63	0
21	CW	1635	0	831	53	0
22	AV	503	0	252	12	0
22	CV	503	0	252	15	0
23	AY	5219	0	5290	315	0
23	CY	5219	0	5291	323	0
24	AU	48	0	39	1	0
24	CU	48	0	39	3	0
25	BC	1742	0	1798	168	0
25	DC	1742	0	1798	180	0
26	BD	2145	0	2234	202	0
26	DD	2145	0	2234	199	0
27	BE	1569	0	1634	124	0
27	DE	1569	0	1634	121	0
28	BF	1628	0	1680	132	0
28	DF	1628	0	1680	153	0
29	BG	1474	0	1535	72	0
29	DG	1474	0	1535	71	0
30	BH	1274	0	1342	57	0
30	DH	1274	0	1342	49	0
31	BJ	851	0	197	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	DJ	851	0	193	39	0
32	BK	1035	0	1082	58	0
32	DK	1035	0	1082	53	0
33	BN	1104	0	1180	84	0
33	DN	1104	0	1180	97	0
34	BO	933	0	996	64	0
34	DO	933	0	996	77	0
35	BP	1114	0	1187	87	0
35	DP	1114	0	1187	87	0
36	BQ	1122	0	1179	74	0
36	DQ	1122	0	1179	71	0
37	BR	960	0	1021	70	0
37	DR	960	0	1021	61	0
38	BS	775	0	835	68	0
38	DS	775	0	835	62	0
39	BT	1147	0	1207	101	0
39	DT	1147	0	1207	100	0
40	BU	964	0	1022	84	0
40	DU	964	0	1022	60	1
41	BV	779	0	852	66	0
41	DV	779	0	852	69	0
42	BW	900	0	964	69	0
42	DW	900	0	964	49	0
43	BX	734	0	789	44	0
43	DX	734	0	789	42	0
44	BY	818	0	908	58	0
44	DY	818	0	908	59	0
45	BZ	1473	0	1497	80	0
45	DZ	1473	0	1497	69	0
46	B0	662	0	688	33	0
46	D0	662	0	688	46	0
47	B2	598	0	653	28	0
47	D2	598	0	653	31	0
48	B3	477	0	529	23	0
48	D3	477	0	529	19	0
49	B5	459	0	477	46	0
49	D5	459	0	477	47	0
50	B6	433	0	461	26	0
50	D6	433	0	461	38	0
51	B7	430	0	480	38	0
51	D7	430	0	480	37	0
52	B8	517	0	582	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	D8	517	0	582	47	0
53	B9	307	0	338	22	0
53	D9	307	0	335	17	0
54	Be	686	0	615	0	0
54	De	686	0	616	0	0
55	Bf	156	0	40	0	0
55	Bg	156	0	41	0	0
55	Df	156	0	40	0	0
55	Dg	156	0	37	0	0
56	Bh	151	0	39	0	0
56	Dh	151	0	40	0	0
57	B1	732	0	808	72	0
57	D1	732	0	808	81	0
58	B4	271	0	284	19	0
58	D4	271	0	284	18	0
59	BA	61997	0	31250	2039	1
59	DA	61997	0	31250	2203	0
60	BB	2551	0	1295	85	0
60	DB	2551	0	1295	85	0
61	AY	37	0	47	6	0
61	CY	37	0	47	7	0
62	AY	28	0	12	12	0
62	CY	28	0	12	13	0
63	BA	1	0	0	0	0
63	CY	1	0	0	0	0
All	All	308166	0	213086	12302	1

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 24.

The worst 5 of 12302 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:CY:19:ALA:H	23:CY:25:LYS:CE	1.38	1.34
59:DA:2405:G:H21	59:DA:2412:A:N6	1.28	1.26
23:CY:19:ALA:N	23:CY:25:LYS:HE3	1.49	1.26
59:DA:2405:G:N2	59:DA:2412:A:H62	1.29	1.25
21:AW:15:G:N2	21:AW:48:C:H42	1.36	1.24

All (1) 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)
59:BA:1015:G:O2'	40:DU:118:GLY:O[3_545]	2.09	0.11

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%)	154 (66%)	51 (22%)	28 (12%)	1	11
1	CB	233/235 (99%)	159 (68%)	50 (22%)	24 (10%)	1	14
2	AC	205/207 (99%)	154 (75%)	32 (16%)	19 (9%)	1	18
2	CC	205/207 (99%)	156 (76%)	36 (18%)	13 (6%)	2	29
3	AD	206/208 (99%)	149 (72%)	31 (15%)	26 (13%)	0	10
3	CD	206/208 (99%)	153 (74%)	32 (16%)	21 (10%)	1	14
4	AE	149/151 (99%)	117 (78%)	22 (15%)	10 (7%)	2	28
4	CE	149/151 (99%)	117 (78%)	25 (17%)	7 (5%)	4	39
5	AF	99/101 (98%)	75 (76%)	15 (15%)	9 (9%)	1	18
5	CF	99/101 (98%)	74 (75%)	16 (16%)	9 (9%)	1	18
6	AG	153/155 (99%)	121 (79%)	25 (16%)	7 (5%)	4	39
6	CG	153/155 (99%)	124 (81%)	22 (14%)	7 (5%)	4	39
7	AH	136/138 (99%)	97 (71%)	27 (20%)	12 (9%)	1	19
7	CH	136/138 (99%)	97 (71%)	28 (21%)	11 (8%)	1	21
8	AI	125/127 (98%)	93 (74%)	27 (22%)	5 (4%)	5	44
8	CI	125/127 (98%)	99 (79%)	22 (18%)	4 (3%)	6	51
9	AJ	97/99 (98%)	75 (77%)	13 (13%)	9 (9%)	1	18
9	CJ	97/99 (98%)	75 (77%)	17 (18%)	5 (5%)	3	35
10	AK	117/119 (98%)	82 (70%)	21 (18%)	14 (12%)	1	11
10	CK	117/119 (98%)	82 (70%)	22 (19%)	13 (11%)	1	13
11	AL	123/125 (98%)	38 (31%)	52 (42%)	33 (27%)	0	1
11	CL	123/125 (98%)	47 (38%)	43 (35%)	33 (27%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	AM	123/125 (98%)	93 (76%)	20 (16%)	10 (8%)	1	21
12	CM	123/125 (98%)	91 (74%)	25 (20%)	7 (6%)	3	33
13	AN	58/60 (97%)	44 (76%)	7 (12%)	7 (12%)	1	11
13	CN	58/60 (97%)	44 (76%)	10 (17%)	4 (7%)	2	27
14	AO	86/88 (98%)	65 (76%)	14 (16%)	7 (8%)	1	21
14	CO	86/88 (98%)	60 (70%)	21 (24%)	5 (6%)	3	32
15	AP	82/84 (98%)	66 (80%)	15 (18%)	1 (1%)	19	75
15	CP	82/84 (98%)	64 (78%)	14 (17%)	4 (5%)	3	37
16	AQ	98/100 (98%)	70 (71%)	18 (18%)	10 (10%)	1	14
16	CQ	98/100 (98%)	70 (71%)	18 (18%)	10 (10%)	1	14
17	AR	68/70 (97%)	51 (75%)	10 (15%)	7 (10%)	1	14
17	CR	68/70 (97%)	48 (71%)	13 (19%)	7 (10%)	1	14
18	AS	77/79 (98%)	41 (53%)	23 (30%)	13 (17%)	0	4
18	CS	77/79 (98%)	46 (60%)	17 (22%)	14 (18%)	0	3
19	AT	97/99 (98%)	82 (84%)	11 (11%)	4 (4%)	4	44
19	CT	97/99 (98%)	79 (81%)	12 (12%)	6 (6%)	2	30
23	AY	663/687 (96%)	451 (68%)	138 (21%)	74 (11%)	1	13
23	CY	663/687 (96%)	461 (70%)	134 (20%)	68 (10%)	1	14
24	AU	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
24	CU	2/6 (33%)	1 (50%)	0	1 (50%)	0	0
25	BC	226/228 (99%)	110 (49%)	66 (29%)	50 (22%)	0	1
25	DC	226/228 (99%)	123 (54%)	59 (26%)	44 (20%)	0	2
26	BD	273/275 (99%)	174 (64%)	47 (17%)	52 (19%)	0	3
26	DD	273/275 (99%)	165 (60%)	61 (22%)	47 (17%)	0	4
27	BE	203/205 (99%)	128 (63%)	40 (20%)	35 (17%)	0	4
27	DE	203/205 (99%)	122 (60%)	45 (22%)	36 (18%)	0	4
28	BF	206/208 (99%)	130 (63%)	46 (22%)	30 (15%)	0	7
28	DF	206/208 (99%)	128 (62%)	44 (21%)	34 (16%)	0	5
29	BG	179/181 (99%)	122 (68%)	48 (27%)	9 (5%)	3	37
29	DG	179/181 (99%)	134 (75%)	36 (20%)	9 (5%)	3	37
30	BH	165/167 (99%)	118 (72%)	27 (16%)	20 (12%)	1	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	DH	165/167 (99%)	111 (67%)	33 (20%)	21 (13%)	0	10
32	BK	138/140 (99%)	96 (70%)	30 (22%)	12 (9%)	1	19
32	DK	138/140 (99%)	97 (70%)	34 (25%)	7 (5%)	3	36
33	BN	136/138 (99%)	86 (63%)	28 (21%)	22 (16%)	0	5
33	DN	136/138 (99%)	88 (65%)	35 (26%)	13 (10%)	1	17
34	BO	120/122 (98%)	86 (72%)	24 (20%)	10 (8%)	1	20
34	DO	120/122 (98%)	87 (72%)	25 (21%)	8 (7%)	2	28
35	BP	144/146 (99%)	85 (59%)	39 (27%)	20 (14%)	0	8
35	DP	144/146 (99%)	81 (56%)	38 (26%)	25 (17%)	0	4
36	BQ	139/141 (99%)	96 (69%)	27 (19%)	16 (12%)	1	12
36	DQ	139/141 (99%)	97 (70%)	29 (21%)	13 (9%)	1	17
37	BR	115/117 (98%)	80 (70%)	27 (24%)	8 (7%)	2	26
37	DR	115/117 (98%)	83 (72%)	20 (17%)	12 (10%)	1	14
38	BS	97/99 (98%)	56 (58%)	21 (22%)	20 (21%)	0	2
38	DS	97/99 (98%)	56 (58%)	21 (22%)	20 (21%)	0	2
39	BT	136/138 (99%)	80 (59%)	31 (23%)	25 (18%)	0	3
39	DT	136/138 (99%)	85 (62%)	29 (21%)	22 (16%)	0	5
40	BU	115/117 (98%)	84 (73%)	25 (22%)	6 (5%)	3	35
40	DU	115/117 (98%)	90 (78%)	16 (14%)	9 (8%)	1	22
41	BV	99/101 (98%)	66 (67%)	16 (16%)	17 (17%)	0	4
41	DV	99/101 (98%)	63 (64%)	22 (22%)	14 (14%)	0	8
42	BW	111/113 (98%)	85 (77%)	11 (10%)	15 (14%)	0	8
42	DW	111/113 (98%)	85 (77%)	15 (14%)	11 (10%)	1	15
43	BX	91/93 (98%)	72 (79%)	15 (16%)	4 (4%)	4	41
43	DX	91/93 (98%)	72 (79%)	14 (15%)	5 (6%)	3	34
44	BY	105/107 (98%)	51 (49%)	30 (29%)	24 (23%)	0	1
44	DY	105/107 (98%)	46 (44%)	26 (25%)	33 (31%)	0	0
45	BZ	183/185 (99%)	132 (72%)	33 (18%)	18 (10%)	1	16
45	DZ	183/185 (99%)	132 (72%)	32 (18%)	19 (10%)	1	14
46	B0	82/84 (98%)	59 (72%)	16 (20%)	7 (8%)	1	20
46	D0	82/84 (98%)	57 (70%)	15 (18%)	10 (12%)	1	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	B2	69/71 (97%)	51 (74%)	14 (20%)	4 (6%)	3	32
47	D2	69/71 (97%)	56 (81%)	10 (14%)	3 (4%)	4	42
48	B3	58/60 (97%)	48 (83%)	6 (10%)	4 (7%)	2	27
48	D3	58/60 (97%)	42 (72%)	10 (17%)	6 (10%)	1	14
49	B5	57/59 (97%)	43 (75%)	11 (19%)	3 (5%)	3	35
49	D5	57/59 (97%)	41 (72%)	12 (21%)	4 (7%)	2	26
50	B6	48/50 (96%)	28 (58%)	13 (27%)	7 (15%)	0	7
50	D6	48/50 (96%)	29 (60%)	8 (17%)	11 (23%)	0	1
51	B7	47/49 (96%)	35 (74%)	8 (17%)	4 (8%)	1	20
51	D7	47/49 (96%)	32 (68%)	9 (19%)	6 (13%)	0	10
52	B8	62/64 (97%)	35 (56%)	17 (27%)	10 (16%)	0	5
52	D8	62/64 (97%)	36 (58%)	18 (29%)	8 (13%)	0	10
53	B9	35/37 (95%)	18 (51%)	12 (34%)	5 (14%)	0	7
53	D9	35/37 (95%)	24 (69%)	8 (23%)	3 (9%)	1	19
54	Be	70/102 (69%)	38 (54%)	24 (34%)	8 (11%)	1	12
54	De	70/102 (69%)	41 (59%)	23 (33%)	6 (9%)	1	19
57	B1	91/93 (98%)	60 (66%)	19 (21%)	12 (13%)	0	9
57	D1	91/93 (98%)	56 (62%)	18 (20%)	17 (19%)	0	3
58	B4	33/35 (94%)	15 (46%)	13 (39%)	5 (15%)	0	6
58	D4	33/35 (94%)	17 (52%)	9 (27%)	7 (21%)	0	2
All	All	13260/13576 (98%)	9009 (68%)	2708 (20%)	1543 (12%)	1	12

5 of 1543 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AB	9	GLU
1	AB	76	GLN
1	AB	165	VAL
1	AB	194	PRO
2	AC	4	LYS

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%)	167 (82%)	36 (18%)	3	16
2	AC	161/161 (100%)	132 (82%)	29 (18%)	2	15
2	CC	161/161 (100%)	136 (84%)	25 (16%)	4	24
3	AD	180/180 (100%)	145 (81%)	35 (19%)	2	12
3	CD	180/180 (100%)	150 (83%)	30 (17%)	3	19
4	AE	116/116 (100%)	93 (80%)	23 (20%)	2	11
4	CE	116/116 (100%)	98 (84%)	18 (16%)	4	24
5	AF	90/90 (100%)	78 (87%)	12 (13%)	6	31
5	CF	90/90 (100%)	82 (91%)	8 (9%)	14	56
6	AG	126/126 (100%)	113 (90%)	13 (10%)	10	47
6	CG	126/126 (100%)	115 (91%)	11 (9%)	15	57
7	AH	119/119 (100%)	98 (82%)	21 (18%)	3	16
7	CH	119/119 (100%)	105 (88%)	14 (12%)	8	38
8	AI	98/98 (100%)	82 (84%)	16 (16%)	3	21
8	CI	98/98 (100%)	84 (86%)	14 (14%)	5	28
9	AJ	89/89 (100%)	75 (84%)	14 (16%)	4	23
9	CJ	89/89 (100%)	72 (81%)	17 (19%)	2	13
10	AK	90/90 (100%)	71 (79%)	19 (21%)	1	9
10	CK	90/90 (100%)	73 (81%)	17 (19%)	2	13
11	AL	104/104 (100%)	77 (74%)	27 (26%)	1	5
11	CL	104/104 (100%)	72 (69%)	32 (31%)	0	4
12	AM	100/100 (100%)	83 (83%)	17 (17%)	3	18
12	CM	100/100 (100%)	89 (89%)	11 (11%)	9	43
13	AN	49/49 (100%)	43 (88%)	6 (12%)	7	36
13	CN	49/49 (100%)	43 (88%)	6 (12%)	7	36
14	AO	79/79 (100%)	71 (90%)	8 (10%)	11	48
14	CO	79/79 (100%)	65 (82%)	14 (18%)	3	16
15	AP	72/72 (100%)	66 (92%)	6 (8%)	16	59
15	CP	72/72 (100%)	62 (86%)	10 (14%)	5	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	AQ	95/95 (100%)	81 (85%)	14 (15%)	4	26
16	CQ	95/95 (100%)	79 (83%)	16 (17%)	3	19
17	AR	61/61 (100%)	51 (84%)	10 (16%)	3	20
17	CR	61/61 (100%)	53 (87%)	8 (13%)	6	32
18	AS	69/69 (100%)	55 (80%)	14 (20%)	2	11
18	CS	69/69 (100%)	54 (78%)	15 (22%)	1	9
19	AT	76/76 (100%)	64 (84%)	12 (16%)	4	23
19	CT	76/76 (100%)	67 (88%)	9 (12%)	8	38
23	AY	563/579 (97%)	470 (84%)	93 (16%)	3	20
23	CY	563/579 (97%)	463 (82%)	100 (18%)	2	16
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%)	140 (78%)	40 (22%)	1	8
25	DC	180/180 (100%)	138 (77%)	42 (23%)	1	7
26	BD	217/217 (100%)	169 (78%)	48 (22%)	1	8
26	DD	217/217 (100%)	164 (76%)	53 (24%)	1	6
27	BE	165/165 (100%)	134 (81%)	31 (19%)	2	13
27	DE	165/165 (100%)	127 (77%)	38 (23%)	1	7
28	BF	165/165 (100%)	133 (81%)	32 (19%)	2	12
28	DF	165/165 (100%)	135 (82%)	30 (18%)	2	14
29	BG	155/155 (100%)	130 (84%)	25 (16%)	3	22
29	DG	155/155 (100%)	127 (82%)	28 (18%)	2	15
30	BH	136/136 (100%)	116 (85%)	20 (15%)	4	26
30	DH	136/136 (100%)	125 (92%)	11 (8%)	17	61
32	BK	105/105 (100%)	90 (86%)	15 (14%)	5	28
32	DK	105/105 (100%)	89 (85%)	16 (15%)	4	25
33	BN	117/117 (100%)	95 (81%)	22 (19%)	2	13
33	DN	117/117 (100%)	94 (80%)	23 (20%)	2	11
34	BO	100/100 (100%)	80 (80%)	20 (20%)	2	11
34	DO	100/100 (100%)	81 (81%)	19 (19%)	2	13
35	BP	112/112 (100%)	87 (78%)	25 (22%)	1	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	DP	112/112 (100%)	94 (84%)	18 (16%)	3	22
36	BQ	111/111 (100%)	82 (74%)	29 (26%)	1	5
36	DQ	111/111 (100%)	86 (78%)	25 (22%)	1	8
37	BR	100/100 (100%)	87 (87%)	13 (13%)	6	33
37	DR	100/100 (100%)	82 (82%)	18 (18%)	2	15
38	BS	77/77 (100%)	62 (80%)	15 (20%)	2	12
38	DS	77/77 (100%)	58 (75%)	19 (25%)	1	6
39	BT	120/120 (100%)	94 (78%)	26 (22%)	1	9
39	DT	120/120 (100%)	92 (77%)	28 (23%)	1	7
40	BU	93/93 (100%)	72 (77%)	21 (23%)	1	8
40	DU	93/93 (100%)	73 (78%)	20 (22%)	1	9
41	BV	82/82 (100%)	60 (73%)	22 (27%)	1	5
41	DV	82/82 (100%)	59 (72%)	23 (28%)	0	4
42	BW	92/92 (100%)	68 (74%)	24 (26%)	1	5
42	DW	92/92 (100%)	72 (78%)	20 (22%)	1	9
43	BX	75/75 (100%)	64 (85%)	11 (15%)	4	26
43	DX	75/75 (100%)	60 (80%)	15 (20%)	2	11
44	BY	88/88 (100%)	69 (78%)	19 (22%)	1	9
44	DY	88/88 (100%)	72 (82%)	16 (18%)	2	14
45	BZ	162/162 (100%)	133 (82%)	29 (18%)	2	15
45	DZ	162/162 (100%)	134 (83%)	28 (17%)	3	17
46	B0	66/66 (100%)	54 (82%)	12 (18%)	2	14
46	D0	66/66 (100%)	51 (77%)	15 (23%)	1	7
47	B2	66/66 (100%)	62 (94%)	4 (6%)	26	73
47	D2	66/66 (100%)	60 (91%)	6 (9%)	14	54
48	B3	52/52 (100%)	45 (86%)	7 (14%)	6	30
48	D3	52/52 (100%)	45 (86%)	7 (14%)	6	30
49	B5	51/51 (100%)	44 (86%)	7 (14%)	5	29
49	D5	51/51 (100%)	41 (80%)	10 (20%)	2	11
50	B6	49/49 (100%)	38 (78%)	11 (22%)	1	8
50	D6	49/49 (100%)	37 (76%)	12 (24%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	B7	42/42 (100%)	35 (83%)	7 (17%)	3	19
51	D7	42/42 (100%)	38 (90%)	4 (10%)	12	51
52	B8	54/54 (100%)	39 (72%)	15 (28%)	0	4
52	D8	54/54 (100%)	37 (68%)	17 (32%)	0	3
53	B9	34/34 (100%)	28 (82%)	6 (18%)	3	16
53	D9	34/34 (100%)	32 (94%)	2 (6%)	28	75
54	Be	54/54 (100%)	47 (87%)	7 (13%)	6	33
54	De	54/54 (100%)	46 (85%)	8 (15%)	4	26
57	B1	78/78 (100%)	59 (76%)	19 (24%)	1	6
57	D1	78/78 (100%)	58 (74%)	20 (26%)	1	5
58	B4	31/31 (100%)	23 (74%)	8 (26%)	1	5
58	D4	31/31 (100%)	26 (84%)	5 (16%)	3	22
All	All	11142/11174 (100%)	9117 (82%)	2025 (18%)	2	14

5 of 2025 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
46	B0	27	GLU
5	CF	67	MET
43	DX	76	ARG
49	B5	46	CYS
1	CB	68	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 70 such sidechains are listed below:

Mol	Chain	Res	Type
39	BT	58	ASN
10	CK	93	GLN
40	DU	71	GLN
39	BT	84	GLN
3	CD	119	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
20	AA	1510/1511 (99%)	305 (20%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
20	CA	1510/1511 (99%)	285 (18%)	0
21	AW	76/77 (98%)	23 (30%)	0
21	CW	76/77 (98%)	22 (28%)	0
22	AV	22/23 (95%)	8 (36%)	0
22	CV	22/23 (95%)	8 (36%)	0
59	BA	2878/2879 (99%)	665 (23%)	0
59	DA	2878/2879 (99%)	666 (23%)	0
60	BB	118/119 (99%)	21 (17%)	0
60	DB	118/119 (99%)	17 (14%)	0
All	All	9208/9218 (99%)	2020 (21%)	0

5 of 2020 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
20	AA	6	G
20	AA	9	G
20	AA	13	U
20	AA	15	G
20	AA	29	G

There are no RNA pucker outliers to report.

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	8.26	1 (12%)	6,8,10	0.86	0
24	DPP	AU	2	24	5,5,6	6.95	1 (20%)	3,5,7	2.11	1 (33%)
24	UAL	AU	5	24	7,8,9	2.23	3 (42%)	6,9,11	1.35	1 (16%)
24	5OH	AU	6	24	12,12,13	5.56	4 (33%)	13,16,18	2.28	3 (23%)
24	KBE	CU	1	24	8,8,9	8.34	1 (12%)	6,8,10	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	DPP	CU	2	24	5,5,6	7.11	1 (20%)	3,5,7	1.97	1 (33%)
24	UAL	CU	5	24	7,8,9	2.18	3 (42%)	6,9,11	1.18	1 (16%)
24	5OH	CU	6	24	12,12,13	5.49	4 (33%)	13,16,18	2.55	4 (30%)

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 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	CU	1	KBE	O-C	23.57	1.27	1.11
24	AU	1	KBE	O-C	23.33	1.27	1.11
24	AU	6	5OH	O-C	17.99	1.23	1.11
24	CU	6	5OH	O-C	17.80	1.23	1.11
24	CU	2	DPP	O-C	15.86	1.22	1.11

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AU	6	5OH	CR-CB-CA	5.29	117.65	112.81
24	CU	6	5OH	C-CA-N	5.07	120.18	111.94
24	CU	6	5OH	CR-CB-NP	5.02	116.02	108.69
24	AU	6	5OH	CR-CB-NP	3.93	114.43	108.69
24	AU	6	5OH	CR-CS-NR	3.76	120.78	109.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
61	FUA	AY	701	-	40,40,40	1.71	8 (20%)	64,64,64	2.00	13 (20%)
62	GDP	AY	702	-	30,30,30	1.41	5 (16%)	45,47,47	2.05	9 (20%)
61	FUA	CY	701	-	40,40,40	1.70	8 (20%)	64,64,64	2.19	17 (26%)
62	GDP	CY	702	-	30,30,30	1.42	5 (16%)	45,47,47	2.03	9 (20%)

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	FUA	AY	701	-	-	1/18/92/92	0/4/4/4
62	GDP	AY	702	-	-	0/16/32/32	0/3/3/3
61	FUA	CY	701	-	-	1/18/92/92	0/4/4/4
62	GDP	CY	702	-	-	0/16/32/32	0/3/3/3

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	CY	701	FUA	C29-C22	5.02	1.54	1.47
61	AY	701	FUA	C29-C22	4.50	1.53	1.47
61	AY	701	FUA	C23-C22	-4.15	1.40	1.51
61	AY	701	FUA	C23-C24	-4.05	1.39	1.53
62	CY	702	GDP	C5-N7	-3.97	1.33	1.38

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	AY	702	GDP	C6-C5-N7	-6.72	133.24	134.14
61	CY	701	FUA	C13-C12-C11	-6.64	102.94	112.00
62	CY	702	GDP	C6-C5-N7	-6.45	133.27	134.14
61	CY	701	FUA	C23-C22-C17	-6.38	115.26	123.78
61	AY	701	FUA	C23-C22-C17	-6.37	115.27	123.78

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
61	AY	701	FUA	C16-C17-C22-C29
61	CY	701	FUA	C16-C17-C22-C29

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
54	Be	1
54	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	37.69
1	Be	30:UNK	C	51:ALA	N	36.65

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%)	0.60	26 (11%) 6 4	4, 59, 144, 223	0
1	CB	235/235 (100%)	0.62	22 (9%) 9 5	5, 60, 155, 214	0
2	AC	207/207 (100%)	0.43	18 (8%) 10 6	4, 63, 136, 190	0
2	CC	207/207 (100%)	0.56	18 (8%) 10 6	3, 57, 130, 186	0
3	AD	208/208 (100%)	-0.20	2 (0%) 79 47	4, 57, 142, 206	0
3	CD	208/208 (100%)	-0.10	1 (0%) 88 64	14, 72, 144, 196	0
4	AE	151/151 (100%)	0.54	18 (11%) 5 4	5, 34, 122, 151	0
4	CE	151/151 (100%)	0.36	13 (8%) 11 6	4, 35, 133, 165	0
5	AF	101/101 (100%)	-0.45	0 100 100	4, 27, 93, 145	0
5	CF	101/101 (100%)	-0.45	0 100 100	5, 37, 115, 163	0
6	AG	155/155 (100%)	0.66	16 (10%) 7 5	10, 78, 153, 229	0
6	CG	155/155 (100%)	1.06	24 (15%) 3 2	3, 84, 172, 210	0
7	AH	138/138 (100%)	0.27	0 100 100	3, 31, 89, 166	0
7	CH	138/138 (100%)	0.39	9 (6%) 18 8	1, 37, 130, 199	0
8	AI	127/127 (100%)	1.07	23 (18%) 2 2	6, 72, 140, 199	0
8	CI	127/127 (100%)	0.70	13 (10%) 7 5	14, 84, 152, 237	0
9	AJ	99/99 (100%)	0.09	5 (5%) 27 11	9, 68, 136, 163	0
9	CJ	99/99 (100%)	-0.01	2 (2%) 62 30	13, 65, 154, 217	0
10	AK	119/119 (100%)	0.11	3 (2%) 54 25	7, 56, 137, 180	0
10	CK	119/119 (100%)	0.26	7 (5%) 22 9	8, 55, 145, 175	0
11	AL	125/125 (100%)	0.60	18 (14%) 3 3	5, 39, 105, 171	0
11	CL	125/125 (100%)	0.73	17 (13%) 4 3	8, 52, 134, 176	0
12	AM	125/125 (100%)	1.01	24 (19%) 2 2	23, 90, 167, 199	0
12	CM	125/125 (100%)	0.69	18 (14%) 3 3	14, 90, 166, 190	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AN	60/60 (100%)	0.65	6 (10%) 8 5	8, 38, 114, 139	0
13	CN	60/60 (100%)	0.33	0 100 100	8, 42, 131, 166	0
14	AO	88/88 (100%)	-0.28	1 (1%) 77 44	5, 37, 108, 158	0
14	CO	88/88 (100%)	-0.16	0 100 100	8, 49, 130, 197	0
15	AP	84/84 (100%)	0.68	9 (10%) 6 4	18, 68, 131, 171	0
15	CP	84/84 (100%)	0.62	9 (10%) 6 4	8, 79, 159, 224	0
16	AQ	100/100 (100%)	0.33	5 (5%) 28 12	9, 43, 120, 169	0
16	CQ	100/100 (100%)	0.42	7 (7%) 16 7	5, 43, 118, 142	0
17	AR	70/70 (100%)	-0.17	1 (1%) 72 38	7, 30, 134, 185	0
17	CR	70/70 (100%)	-0.01	4 (5%) 23 10	7, 28, 130, 193	0
18	AS	79/79 (100%)	0.64	9 (11%) 6 4	15, 78, 159, 206	0
18	CS	79/79 (100%)	0.28	5 (6%) 19 8	10, 80, 154, 204	0
19	AT	99/99 (100%)	0.11	2 (2%) 62 30	4, 64, 120, 187	0
19	CT	99/99 (100%)	0.28	7 (7%) 16 7	16, 71, 155, 187	0
20	AA	1511/1511 (100%)	-0.28	31 (2%) 60 29	3, 62, 163, 289	0
20	CA	1511/1511 (100%)	-0.30	24 (1%) 68 35	5, 63, 173, 323	0
21	AW	77/77 (100%)	-0.43	1 (1%) 74 40	21, 91, 179, 234	0
21	CW	77/77 (100%)	-0.05	5 (6%) 18 8	44, 97, 221, 273	0
22	AV	23/23 (100%)	0.85	4 (17%) 2 2	56, 136, 187, 205	0
22	CV	23/23 (100%)	2.03	9 (39%) 1 1	66, 119, 215, 230	0
23	AY	667/687 (97%)	0.15	39 (5%) 22 9	5, 64, 147, 208	0
23	CY	667/687 (97%)	0.24	53 (7%) 13 7	4, 68, 150, 203	0
24	AU	2/6 (33%)	0.14	0 100 100	155, 155, 155, 155	0
24	CU	2/6 (33%)	-0.02	0 100 100	81, 81, 81, 88	0
25	BC	228/228 (100%)	0.87	39 (17%) 2 2	45, 128, 217, 259	0
25	DC	228/228 (100%)	1.49	67 (29%) 1 1	33, 153, 230, 287	0
26	BD	275/275 (100%)	-0.11	5 (1%) 65 33	4, 26, 103, 166	0
26	DD	275/275 (100%)	-0.19	5 (1%) 65 33	4, 25, 107, 210	0
27	BE	205/205 (100%)	-0.12	1 (0%) 88 64	1, 31, 135, 229	0
27	DE	205/205 (100%)	-0.02	3 (1%) 70 36	6, 41, 144, 221	0
28	BF	208/208 (100%)	0.59	24 (11%) 5 4	6, 49, 162, 216	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DF	208/208 (100%)	0.68	27 (12%) 4 3	10, 62, 162, 266	0
29	BG	181/181 (100%)	1.31	47 (25%) 1 2	11, 91, 152, 197	0
29	DG	181/181 (100%)	1.29	47 (25%) 1 2	33, 105, 176, 209	0
30	BH	167/167 (100%)	-0.17	0 100 100	3, 47, 130, 224	0
30	DH	167/167 (100%)	-0.03	4 (2%) 56 26	6, 56, 141, 187	0
31	BJ	0/170	-	-	-	-
31	DJ	0/170	-	-	-	-
32	BK	140/140 (100%)	1.09	32 (22%) 1 2	17, 104, 194, 230	0
32	DK	140/140 (100%)	1.40	36 (25%) 1 2	37, 124, 205, 244	0
33	BN	138/138 (100%)	0.68	16 (11%) 5 4	59, 83, 108, 111	0
33	DN	138/138 (100%)	0.62	12 (8%) 10 6	59, 81, 104, 111	0
34	BO	122/122 (100%)	0.19	2 (1%) 68 35	5, 33, 94, 148	0
34	DO	122/122 (100%)	0.09	4 (3%) 44 20	4, 30, 131, 183	0
35	BP	146/146 (100%)	0.38	8 (5%) 24 10	7, 55, 131, 173	0
35	DP	146/146 (100%)	0.24	10 (6%) 17 8	1, 60, 152, 204	0
36	BQ	141/141 (100%)	-0.30	2 (1%) 72 38	20, 43, 113, 170	0
36	DQ	141/141 (100%)	-0.17	5 (3%) 42 19	8, 32, 107, 219	0
37	BR	117/117 (100%)	0.07	4 (3%) 43 19	7, 38, 125, 156	0
37	DR	117/117 (100%)	0.03	6 (5%) 27 11	2, 38, 126, 213	0
38	BS	99/99 (100%)	0.98	22 (22%) 1 2	27, 104, 191, 225	0
38	DS	99/99 (100%)	1.80	34 (34%) 1 1	11, 106, 194, 248	0
39	BT	138/138 (100%)	0.13	7 (5%) 27 11	6, 53, 139, 225	0
39	DT	138/138 (100%)	0.30	10 (7%) 15 7	3, 68, 141, 201	0
40	BU	117/117 (100%)	0.15	3 (2%) 53 24	11, 22, 80, 175	0
40	DU	117/117 (100%)	0.03	2 (1%) 67 34	6, 20, 94, 136	0
41	BV	101/101 (100%)	0.35	6 (5%) 22 9	0, 32, 104, 143	0
41	DV	101/101 (100%)	0.05	2 (1%) 62 30	2, 32, 117, 147	0
42	BW	113/113 (100%)	0.18	3 (2%) 52 24	8, 32, 103, 140	0
42	DW	113/113 (100%)	0.20	5 (4%) 33 14	2, 31, 116, 157	0
43	BX	93/93 (100%)	-0.02	2 (2%) 59 28	5, 51, 118, 172	0
43	DX	93/93 (100%)	0.30	5 (5%) 25 10	7, 50, 136, 198	0
44	BY	107/107 (100%)	0.01	8 (7%) 14 7	12, 69, 151, 213	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
44	DY	107/107 (100%)	0.11	5 (4%)	30	13	6, 70, 150, 196	0
45	BZ	185/185 (100%)	-0.09	2 (1%)	77	44	13, 52, 123, 175	0
45	DZ	185/185 (100%)	0.07	7 (3%)	38	17	10, 61, 135, 194	0
46	B0	84/84 (100%)	-0.16	1 (1%)	75	42	6, 53, 127, 163	0
46	D0	84/84 (100%)	-0.01	1 (1%)	75	42	7, 58, 132, 217	0
47	B2	71/71 (100%)	-0.33	0	100	100	12, 61, 137, 175	0
47	D2	71/71 (100%)	-0.34	0	100	100	9, 60, 127, 145	0
48	B3	60/60 (100%)	-0.12	0	100	100	8, 31, 96, 111	0
48	D3	60/60 (100%)	0.04	0	100	100	13, 29, 101, 126	0
49	B5	59/59 (100%)	-0.21	0	100	100	8, 37, 148, 208	0
49	D5	59/59 (100%)	-0.08	0	100	100	6, 44, 156, 223	0
50	B6	50/50 (100%)	0.27	3 (6%)	21	9	12, 92, 147, 163	0
50	D6	50/50 (100%)	0.93	9 (18%)	2	2	31, 89, 175, 242	0
51	B7	49/49 (100%)	1.06	7 (14%)	3	3	9, 16, 135, 218	0
51	D7	49/49 (100%)	1.52	11 (22%)	1	2	11, 32, 107, 180	0
52	B8	64/64 (100%)	0.21	1 (1%)	68	35	5, 46, 98, 130	0
52	D8	64/64 (100%)	0.30	1 (1%)	68	35	7, 56, 123, 178	0
53	B9	37/37 (100%)	-0.20	0	100	100	10, 26, 148, 246	0
53	D9	37/37 (100%)	-0.25	0	100	100	8, 19, 104, 158	0
54	Be	72/102 (70%)	2.36	35 (48%)	1	1	24, 113, 183, 201	0
54	De	72/102 (70%)	2.37	28 (38%)	1	1	18, 114, 206, 259	0
55	Bf	0/31	-	-	-	-	-	-
55	Bg	0/31	-	-	-	-	-	-
55	Df	0/31	-	-	-	-	-	-
55	Dg	0/31	-	-	-	-	-	-
56	Bh	0/30	-	-	-	-	-	-
56	Dh	0/30	-	-	-	-	-	-
57	B1	93/93 (100%)	0.93	21 (22%)	1	2	1, 79, 187, 243	0
57	D1	93/93 (100%)	1.03	23 (24%)	1	2	8, 72, 174, 241	0
58	B4	35/35 (100%)	2.20	17 (48%)	1	1	74, 144, 233, 266	0
58	D4	35/35 (100%)	2.57	21 (60%)	0	1	64, 158, 226, 275	0
59	BA	2879/2879 (100%)	-0.46	18 (0%)	86	59	3, 43, 145, 276	0
59	DA	2879/2879 (100%)	-0.42	25 (0%)	81	51	0, 47, 163, 315	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
60	BB	119/119 (100%)	-0.36	4 (3%) 43 19	21, 108, 175, 210	0
60	DB	119/119 (100%)	0.08	10 (8%) 11 6	23, 97, 186, 258	0
All	All	22686/23318 (97%)	0.07	1293 (5%) 23 10	0, 57, 160, 323	0

The worst 5 of 1293 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
54	De	59	GLU	10.8
51	D7	48	LYS	9.7
54	Be	58	THR	9.5
54	De	100	LYS	9.2
54	De	99	VAL	9.0

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	UAL	AU	5	9/10	0.36	-	149,151,153,154	0
24	DPP	AU	2	6/7	0.23	-	153,153,154,154	0
24	KBE	AU	1	9/10	0.20	-	154,155,156,156	0
24	KBE	CU	1	9/10	0.30	-	69,74,77,77	0
24	DPP	CU	2	6/7	0.17	-	77,79,80,82	0
24	5OH	AU	6	12/13	0.51	-	151,153,154,154	0
24	5OH	CU	6	12/13	0.33	-	84,88,89,89	0
24	UAL	CU	5	9/10	0.33	-	89,90,91,91	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	GDP	CY	702	28/28	0.29	-	78,82,83,84	0
63	MG	CY	703	1/1	0.18	-	1,1,1,1	0
62	GDP	AY	702	28/28	0.19	-	78,82,83,84	0
63	MG	BA	2901	1/1	0.27	-	5,5,5,5	0
61	FUA	AY	701	37/37	0.44	-	154,155,156,156	0
61	FUA	CY	701	37/37	0.69	-	199,200,202,202	0

6.5 Other polymers ⓘ

There are no such residues in this entry.