



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:08 PM GMT

PDB ID : 4W29
Title : 70S ribosome translocation intermediate containing elongation factor EFG/GDP/fusidic acid, mRNA, and tRNAs trapped in the AP/AP pe/E chimeric hybrid state.
Authors : Zhou, J.; Lancaster, L.; Donohue, J.P.; Noller, H.F.
Deposited on : 2014-07-02
Resolution : 3.80 Å(reported)

This is a wwPDB X-ray Structure 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/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

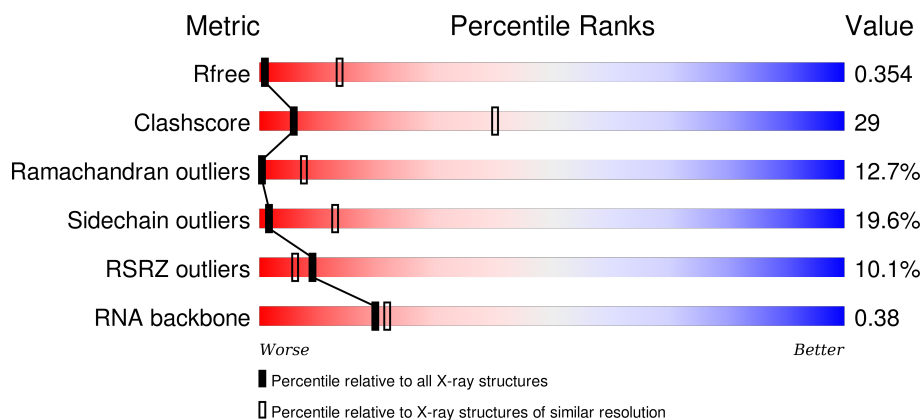
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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}	91344	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)
RNA backbone	2183	1070 (4.76-2.80)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AB	235	<div> <div>5%</div> <div>41%</div> <div>44%</div> <div>14%</div> </div>
1	CB	235	<div> <div>6%</div> <div>40%</div> <div>43%</div> <div>16%</div> </div>
2	AC	207	<div> <div>18%</div> <div>36%</div> <div>48%</div> <div>14%</div> </div>
2	CC	207	<div> <div>6%</div> <div>41%</div> <div>50%</div> <div>8%</div> </div>

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Mol	Chain	Length	Quality of chain
3	AD	208	
3	CD	208	
4	AE	151	
4	CE	151	
5	AF	101	
5	CF	101	
6	AG	155	
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	

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Mol	Chain	Length	Quality of chain
15	CP	84	
16	AQ	100	
16	CQ	100	
17	AR	70	
17	CR	70	
18	AS	79	
18	CS	79	
19	AT	99	
19	CT	99	
20	AY	687	
20	CY	687	
21	AA	1511	
21	CA	1511	
22	AW	77	
22	CW	77	
23	AV	36	
23	CV	36	
24	AX	78	
24	CX	78	
25	BC	228	
25	DC	228	
26	BD	275	
26	DD	275	
27	BE	205	
27	DE	205	

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Mol	Chain	Length	Quality of chain
28	BF	208	
28	DF	208	
29	BG	181	
29	DG	181	
30	BH	167	
30	DH	167	
31	BJ	170	
31	DJ	170	
32	BK	140	
32	DK	140	
33	BN	139	
33	DN	139	
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	

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Mol	Chain	Length	Quality of chain
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	B1	93	
47	D1	93	
48	B2	71	
48	D2	71	
49	B3	60	
49	D3	60	
50	B4	35	
50	D4	35	
51	B5	59	
51	D5	59	
52	B6	50	
52	D6	50	

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Mol	Chain	Length	Quality of chain
53	B7	49	
53	D7	49	
54	B8	64	
54	D8	64	
55	B9	37	
55	D9	37	
56	Be	103	
56	De	103	
57	Bf	31	
57	Bg	31	
57	Df	31	
57	Dg	31	
58	Bh	30	
58	Dh	30	
59	BA	2879	
59	DA	2879	
60	BB	119	
60	DB	119	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
61	GDP	CY	701	-	-	X	-
62	FUA	AY	702	-	-	X	X
62	FUA	CY	702	-	-	-	X
63	NMY	AA	1601	-	-	X	X
63	NMY	BA	2902	-	-	-	X
63	NMY	BA	2903	-	-	-	X
63	NMY	BA	2904	-	-	X	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
63	NMY	CA	1601	-	-	X	-
63	NMY	DA	2901	-	-	X	-

2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 312066 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 protein called Elongation factor G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AY	661	Total	C	N	O	S	0	0	0
			5173	3288	884	983	18			
20	CY	661	Total	C	N	O	S	0	0	0
			5173	3288	884	983	18			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AY	40	THR	HIS	CONFLICT	UNP Q72I01
AY	129	LYS	HIS	CONFLICT	UNP Q72I01
AY	226	ASN	HIS	CONFLICT	UNP Q72I01
CY	40	THR	HIS	CONFLICT	UNP Q72I01
CY	129	LYS	HIS	CONFLICT	UNP Q72I01
CY	226	ASN	HIS	CONFLICT	UNP Q72I01

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

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

- Molecule 22 is a RNA chain called tRNA.

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

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AV	36	Total	C	N	O	P	0	0	0
			783	351	159	237	36			
23	CV	36	Total	C	N	O	P	0	0	0
			781	352	159	235	35			

- Molecule 24 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AX	78	Total	C	N	O	P	0	0	0
			1629	730	293	531	75			
24	CX	78	Total	C	N	O	P	0	0	0
			1629	730	293	531	75			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AX	77	VAL	-	EXPRESSION TAG	GB U000096.3
AX	78	ACE	-	EXPRESSION TAG	GB U000096.3
CX	77	VAL	-	EXPRESSION TAG	GB U000096.3
CX	78	ACE	-	EXPRESSION TAG	GB U000096.3

- 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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	-	EXPRESSION TAG	UNP Q72I05
BF	3	GLU	-	EXPRESSION TAG	UNP Q72I05
BF	4	VAL	-	EXPRESSION TAG	UNP Q72I05
BF	5	ALA	-	EXPRESSION TAG	UNP Q72I05
BF	6	VAL	-	EXPRESSION TAG	UNP Q72I05
DF	2	LYS	-	EXPRESSION TAG	UNP Q72I05
DF	3	GLU	-	EXPRESSION TAG	UNP Q72I05
DF	4	VAL	-	EXPRESSION TAG	UNP Q72I05
DF	5	ALA	-	EXPRESSION TAG	UNP Q72I05
DF	6	VAL	-	EXPRESSION TAG	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	139	Total	C	N	O	S	0	0	0
			1114	717	207	186	4			
33	DN	139	Total	C	N	O	S	0	0	0
			1114	717	207	186	4			

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 47 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	B1	93	Total	C	N	O	S	0	0	0
			732	460	145	126	1			
47	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 48 is a protein called 50S ribosomal protein L29.

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

- Molecule 49 is a protein called 50S ribosomal protein L30.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
51	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 52 is a protein called 50S ribosomal protein L33.

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

- Molecule 53 is a protein called 50S ribosomal protein L34.

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

- Molecule 54 is a protein called 50S ribosomal protein L35.

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

- Molecule 55 is a protein called 50S ribosomal protein L36.

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

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

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

- Molecule 57 is a protein called 50S ribosomal protein L7/L12.

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

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

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

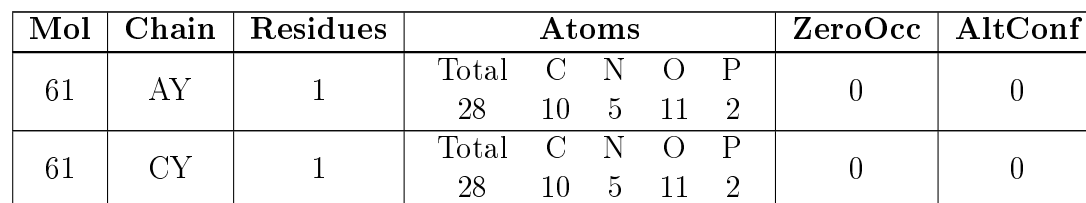
- Molecule 59 is a RNA chain called 23S RRNA.

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 RRNA.

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			

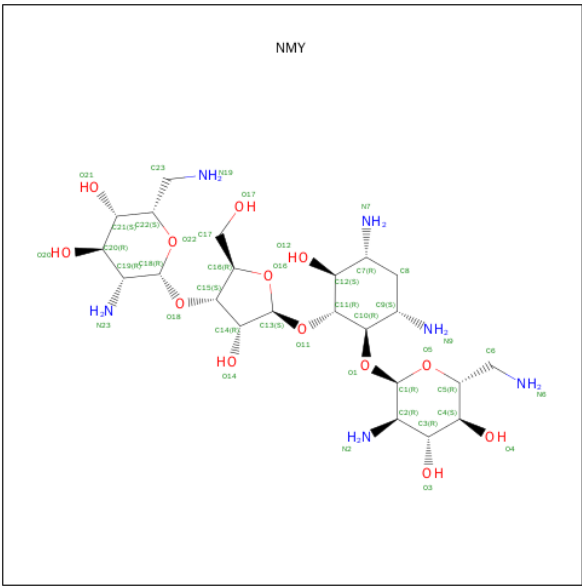
- Molecule 61 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



-
- The chemical structure of FUA (Furoic acid) is a complex polycyclic molecule. It features a central fused ring system with several stereocenters indicated by wedges and dashes. Key functional groups include a carboxylic acid group (C29, O4, O5) and a hydroxyl group (O1, H9). The structure is labeled with atom identifiers: C1 through C28, O1 through O6, and H5 through H13. The stereochemistry is defined by the following R/S configurations: C1(R), C2(R), C3(R), C4(S), C5(S), C6(S), C7(R), C8(S), C9(S), C10(S), C11(R), C12(R), C13(R), C14(S), C15(S), C16(S), C17(R), C18(S), C19(S), C20(S), C21(S), C22(R), C23(R), C24(R), C25(R), C26(R), C27(R), C28(R).

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

- Molecule 63 is NEOMYCIN (three-letter code: NMY) (formula: C₂₃H₄₆N₆O₁₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
63	AA	1	Total	C	N	O	0	0
			42	23	6	13		
63	BA	1	Total	C	N	O	0	0
			42	23	6	13		
63	BA	1	Total	C	N	O	0	0
			42	23	6	13		
63	BA	1	Total	C	N	O	0	0
			42	23	6	13		
63	CA	1	Total	C	N	O	0	0
			42	23	6	13		
63	DA	1	Total	C	N	O	0	0
			42	23	6	13		

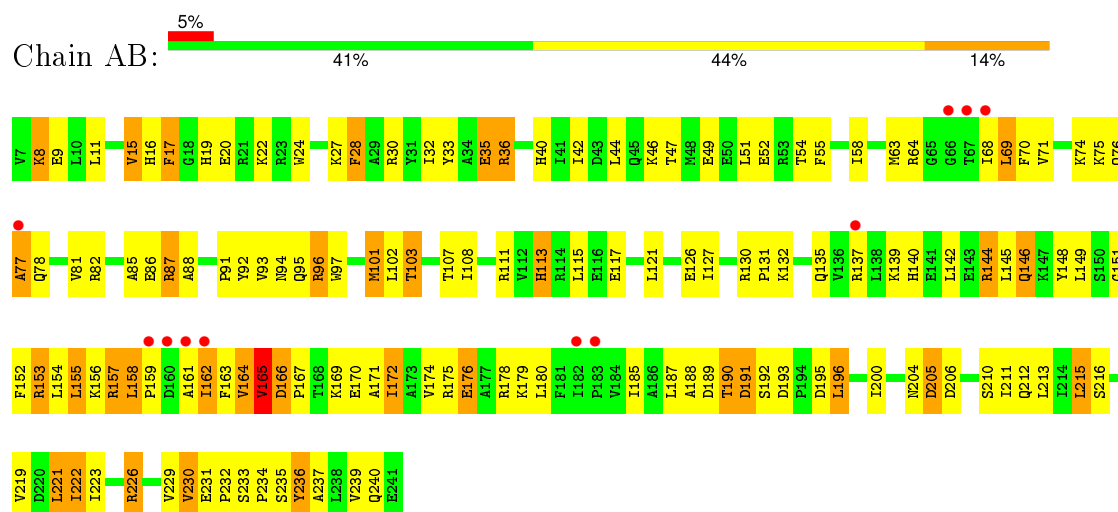
- Molecule 64 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

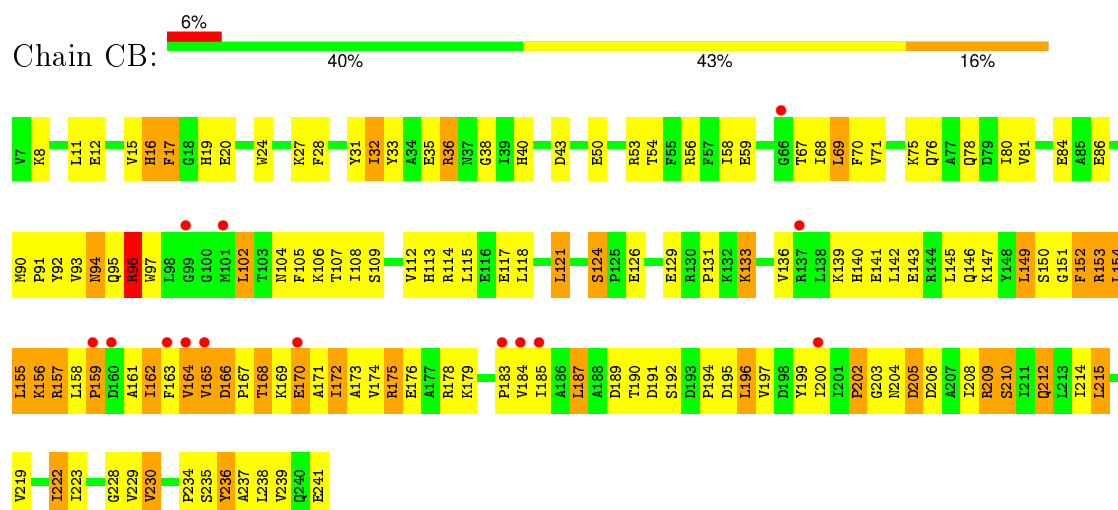
3 Residue-property plots

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 ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 30S ribosomal protein S2

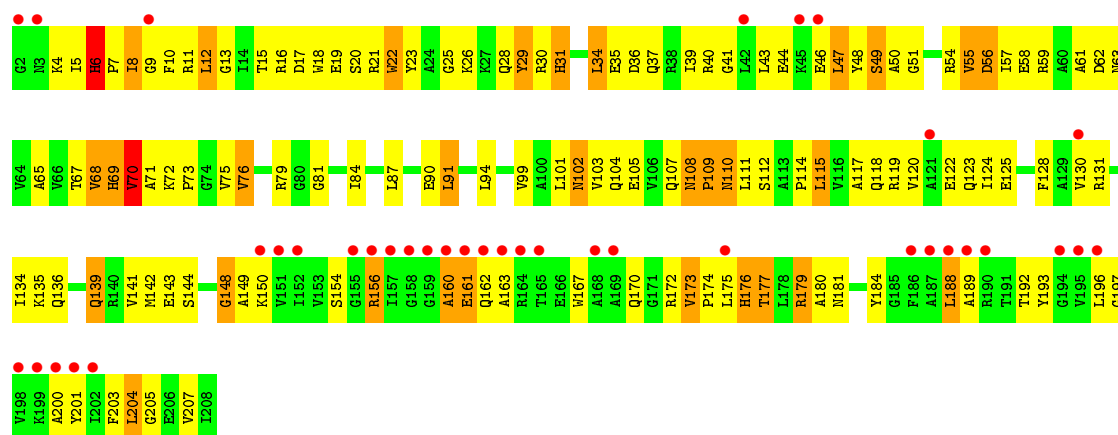


• Molecule 1: 30S ribosomal protein S2

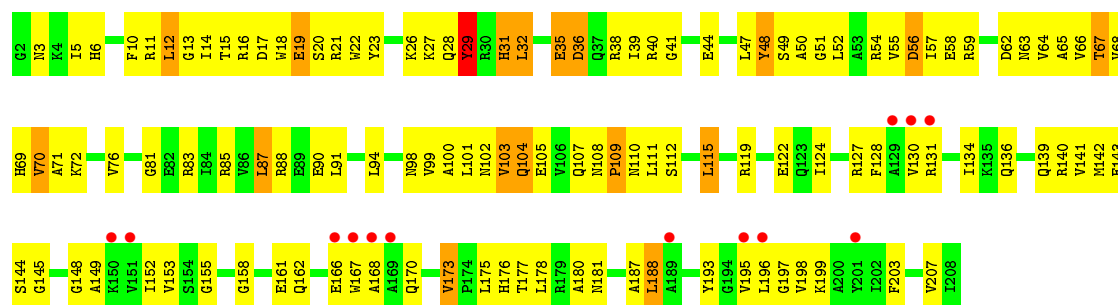
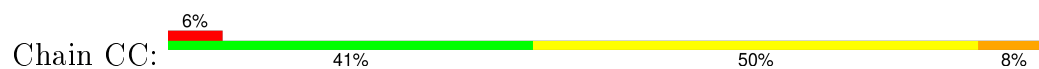


• Molecule 2: 30S ribosomal protein S3

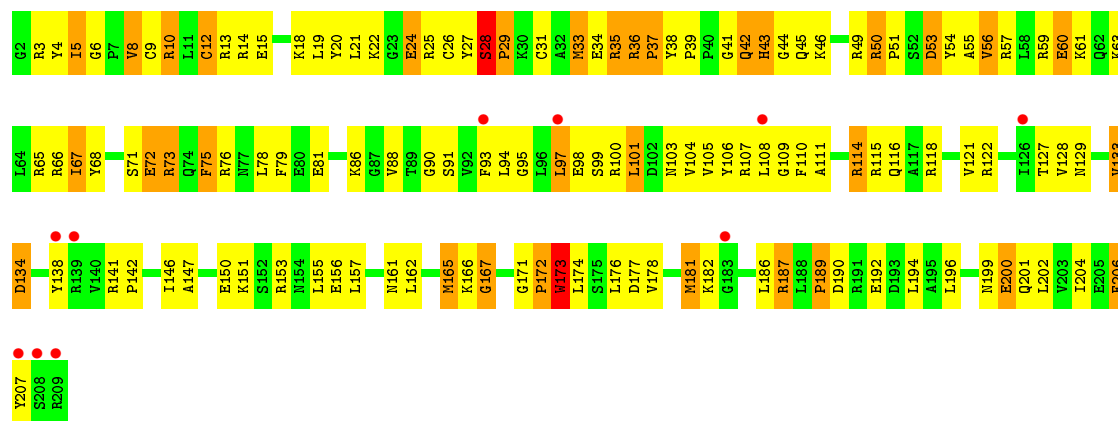




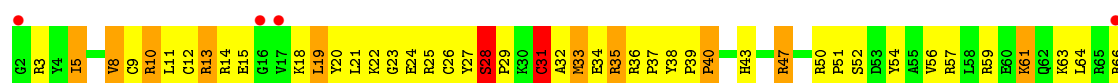
• Molecule 2: 30S ribosomal protein S3

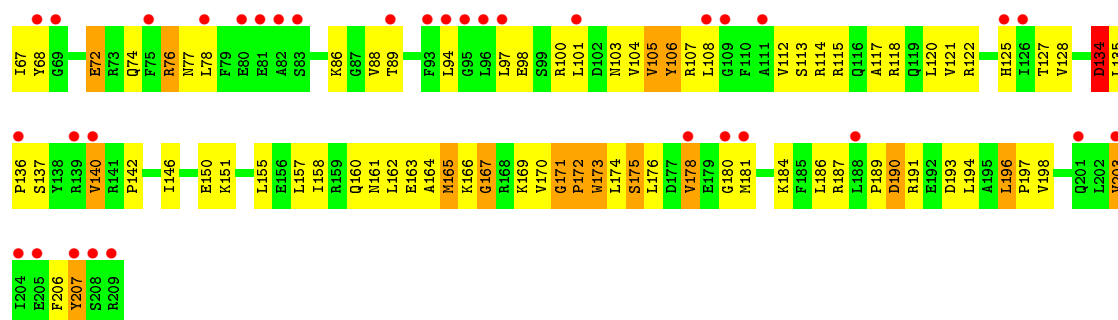


• Molecule 3: 30S ribosomal protein S4

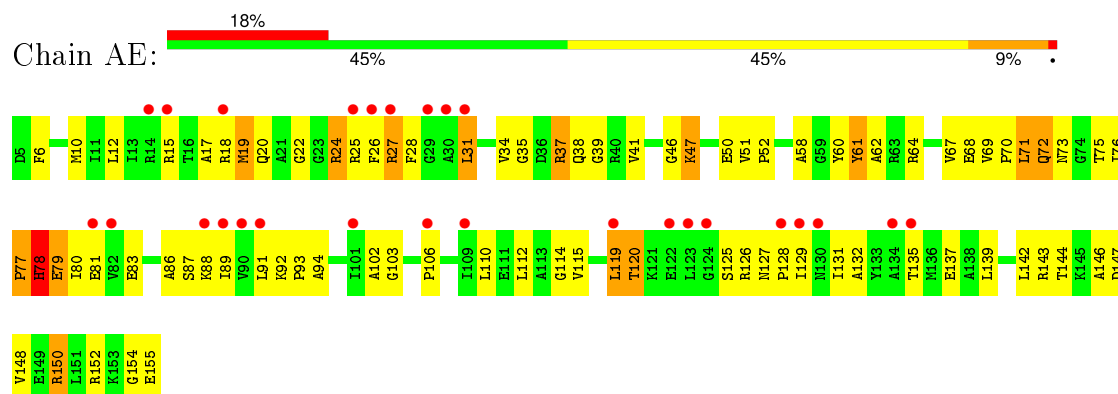


• Molecule 3: 30S ribosomal protein S4

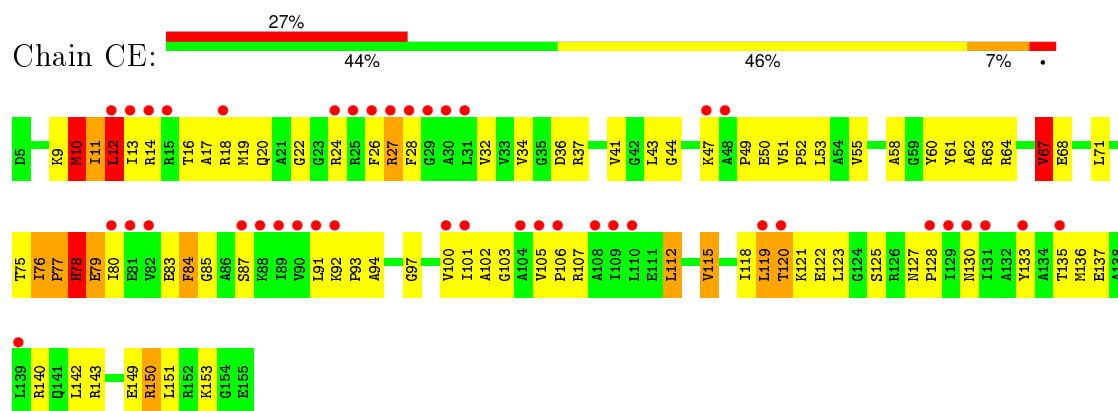




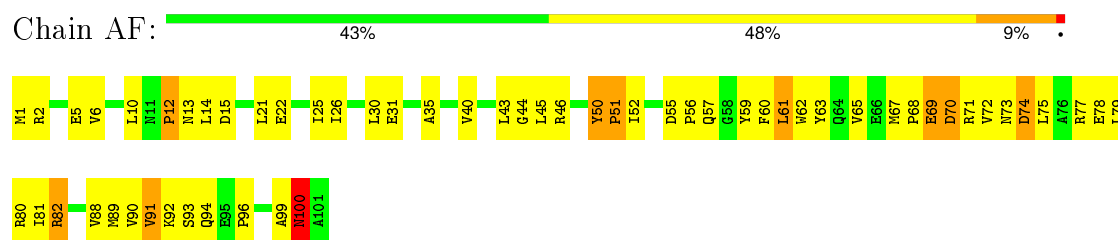
● Molecule 4: 30S ribosomal protein S5



● Molecule 4: 30S ribosomal protein S5

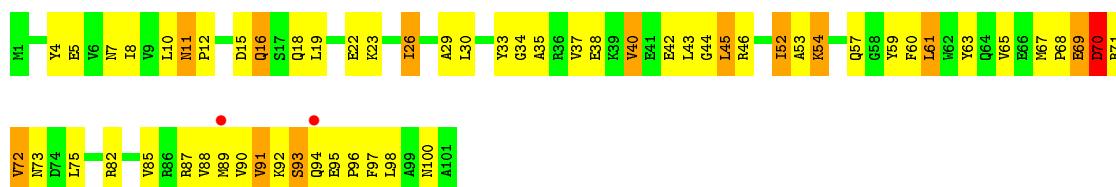


● Molecule 5: 30S ribosomal protein S6

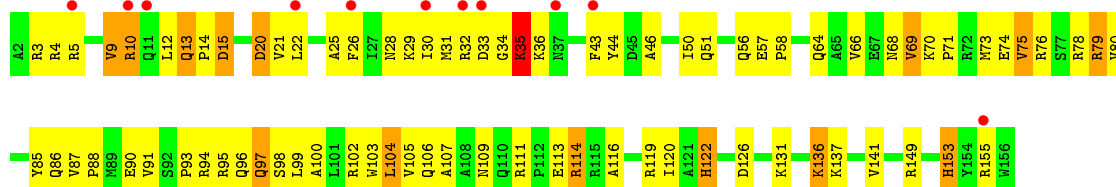


● Molecule 5: 30S ribosomal protein S6

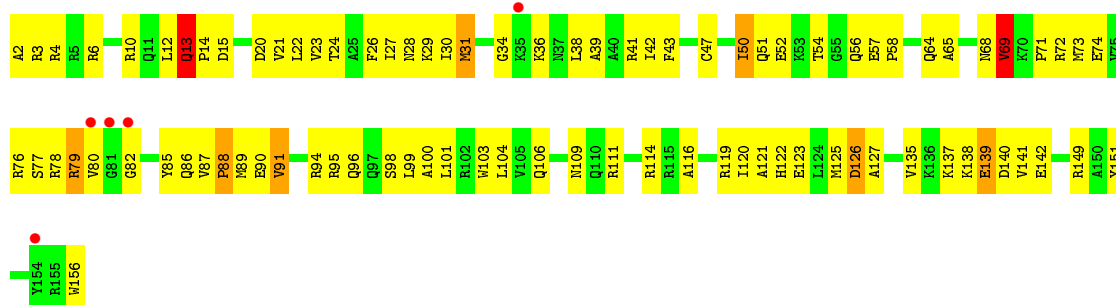
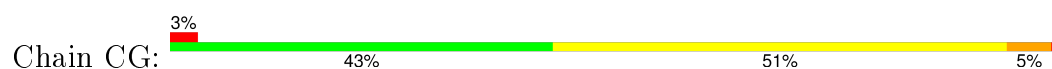




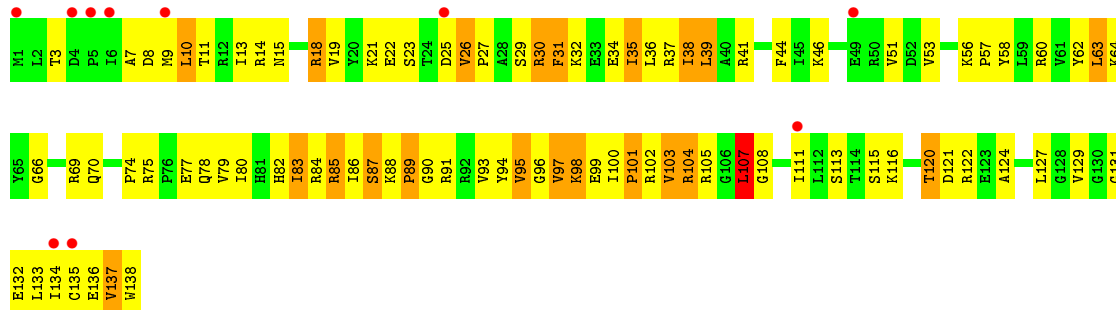
• Molecule 6: 30S ribosomal protein S7



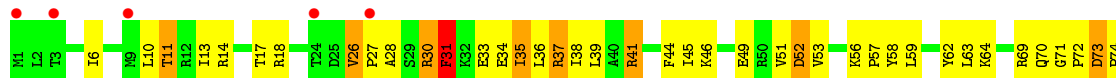
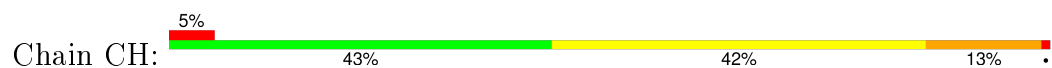
• Molecule 6: 30S ribosomal protein S7



• Molecule 7: 30S ribosomal protein S8

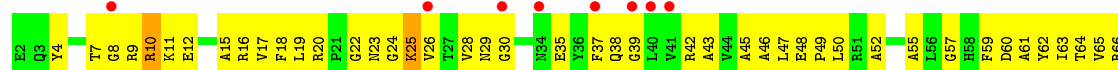


• Molecule 7: 30S ribosomal protein S8

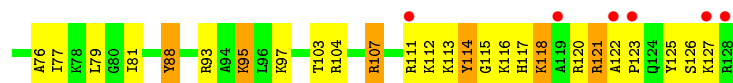
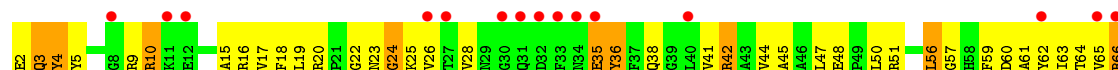




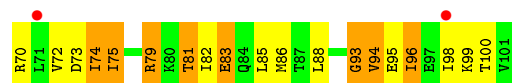
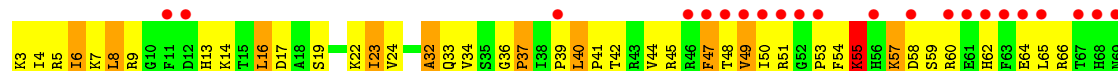
• Molecule 8: 30S ribosomal protein S9



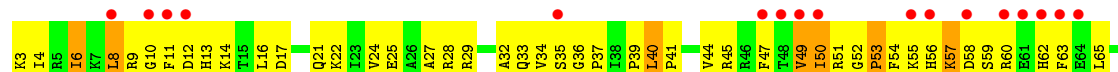
• Molecule 8: 30S ribosomal protein S9



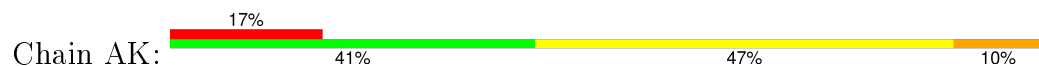
• Molecule 9: 30S ribosomal protein S10

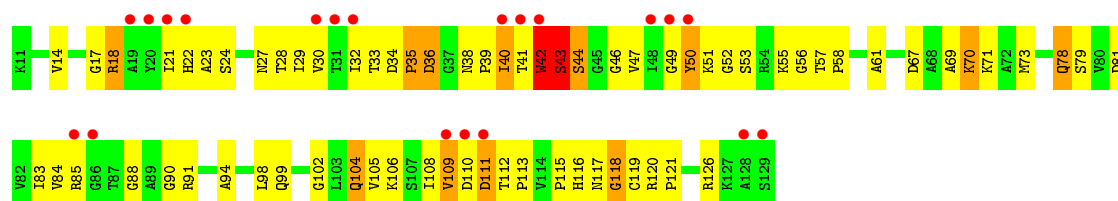


• Molecule 9: 30S ribosomal protein S10

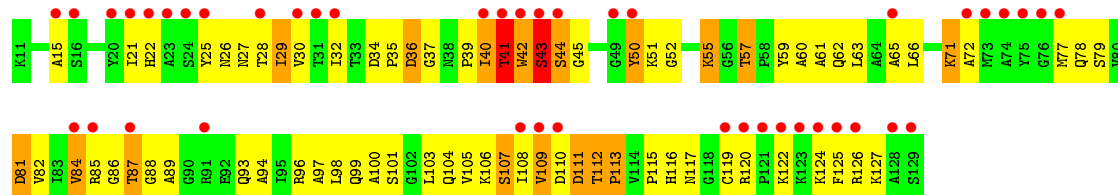


• Molecule 10: 30S ribosomal protein S11

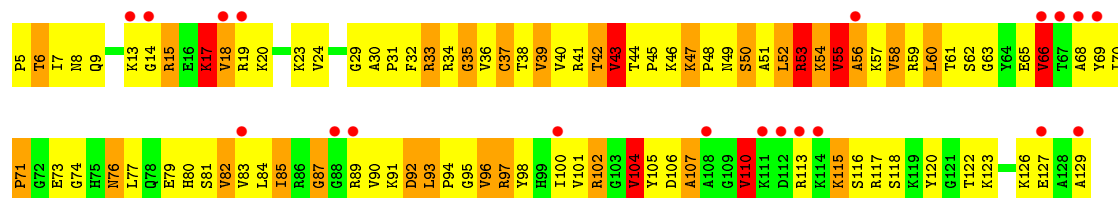




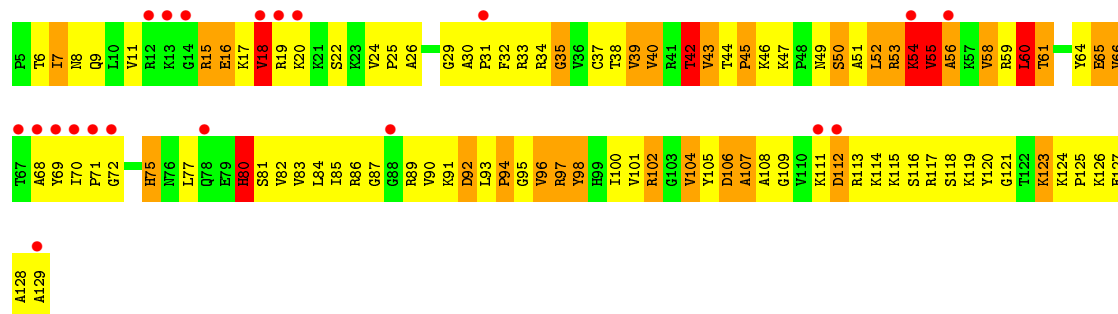
• Molecule 10: 30S ribosomal protein S11



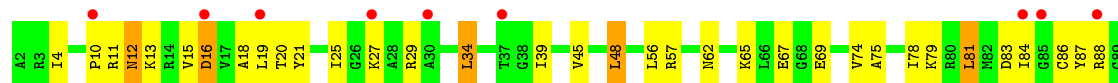
• Molecule 11: 30S ribosomal protein S12

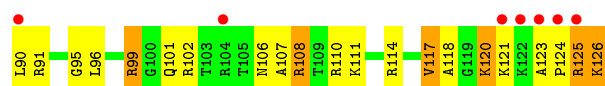


• Molecule 11: 30S ribosomal protein S12

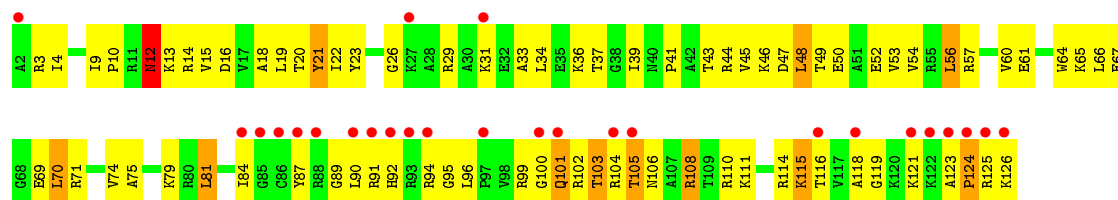


• Molecule 12: 30S ribosomal protein S13





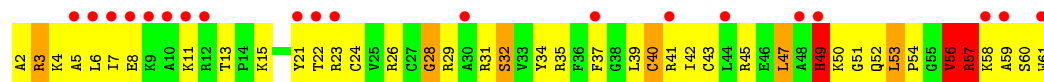
- Molecule 12: 30S ribosomal protein S13



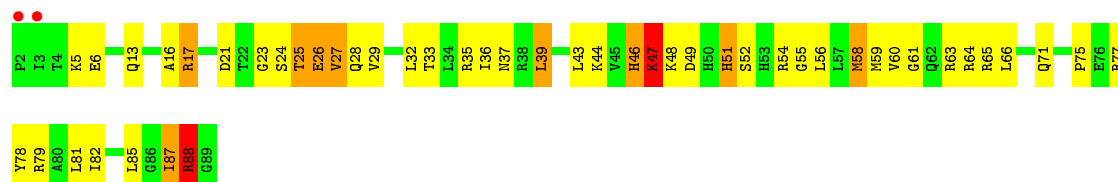
- Molecule 13: 30S ribosomal protein S14 type Z



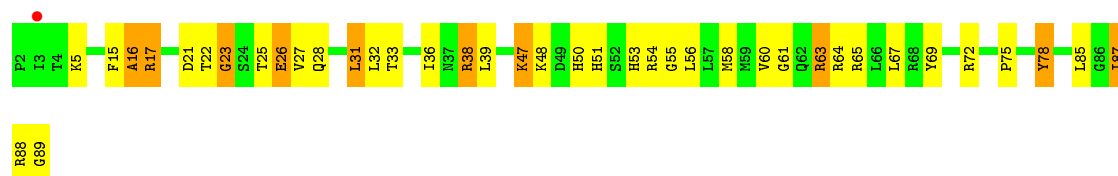
- Molecule 13: 30S ribosomal protein S14 type Z



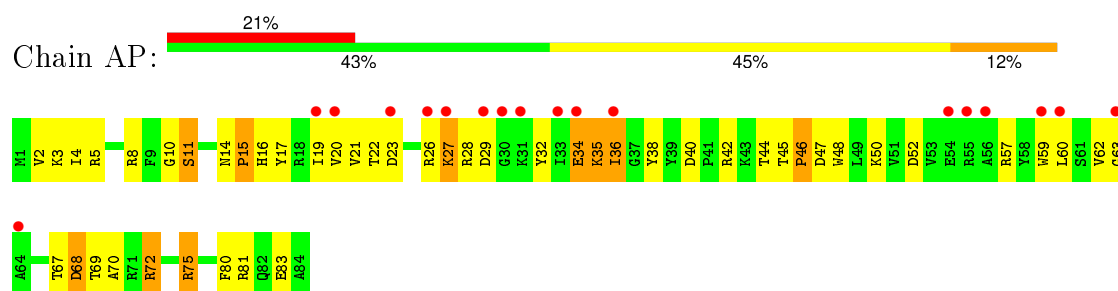
- Molecule 14: 30S ribosomal protein S15



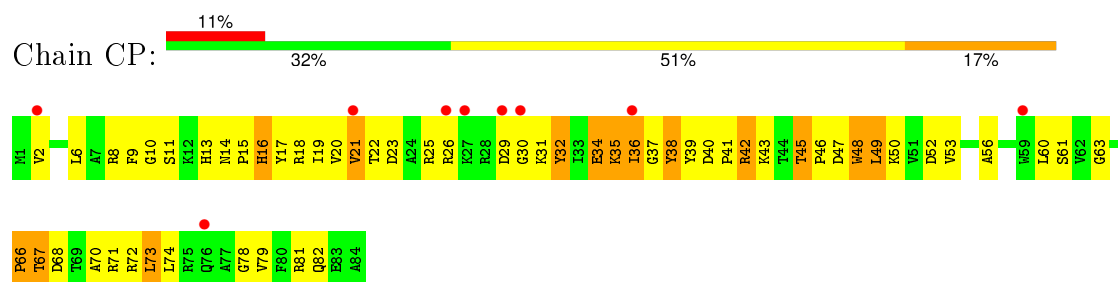
- Molecule 14: 30S ribosomal protein S15



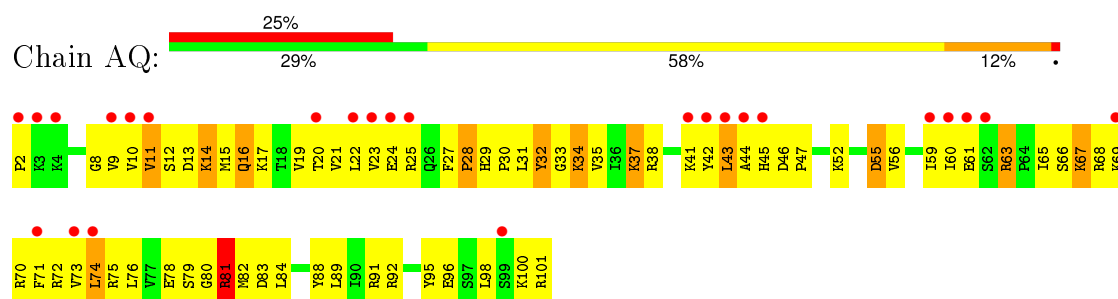
- Molecule 15: 30S ribosomal protein S16



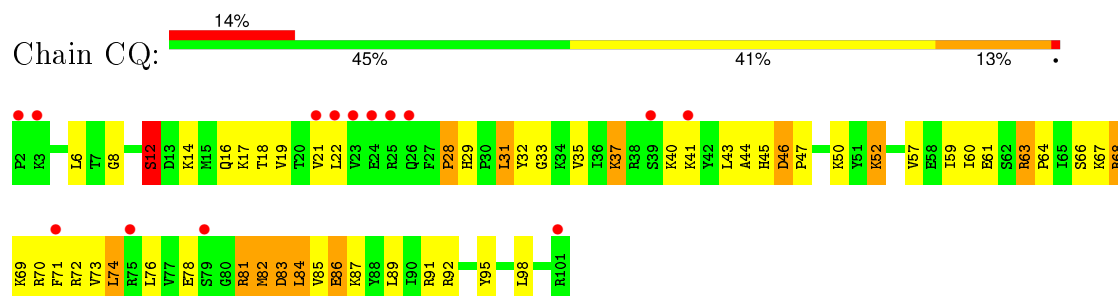
- Molecule 15: 30S ribosomal protein S16



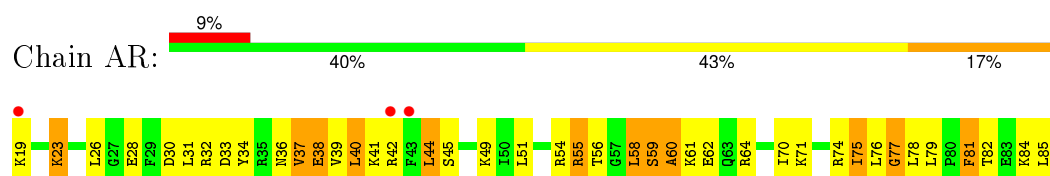
- Molecule 16: 30S ribosomal protein S17



- Molecule 16: 30S ribosomal protein S17

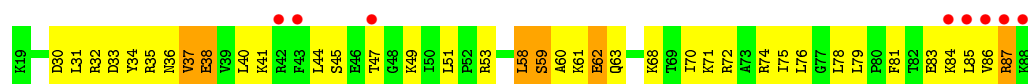


- Molecule 17: 30S ribosomal protein S18

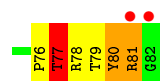
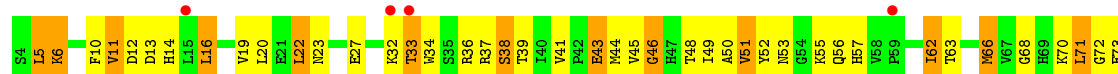


- Molecule 17: 30S ribosomal protein S18

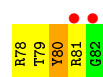
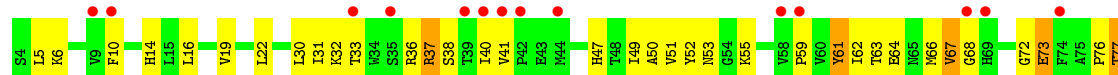




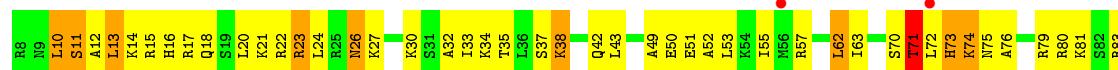
- Molecule 18: 30S ribosomal protein S19



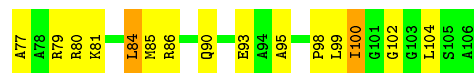
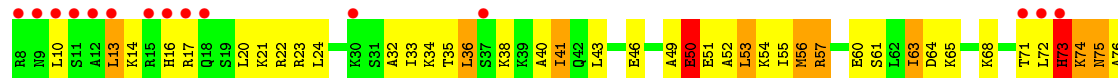
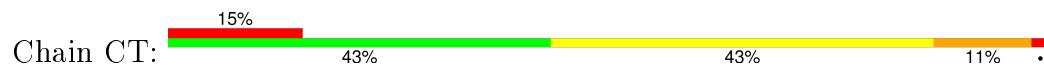
- Molecule 18: 30S ribosomal protein S19



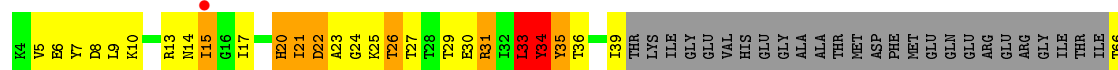
- Molecule 19: 30S ribosomal protein S20

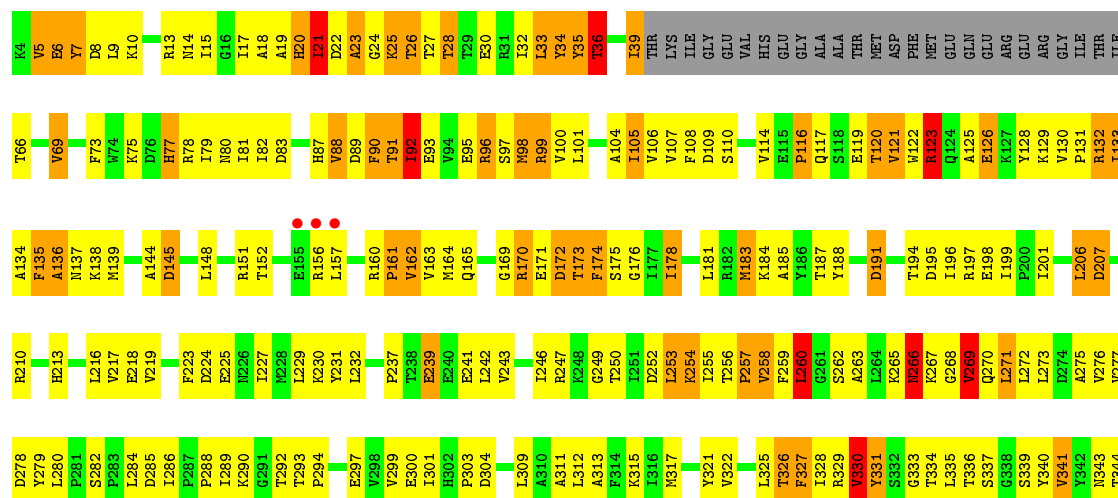


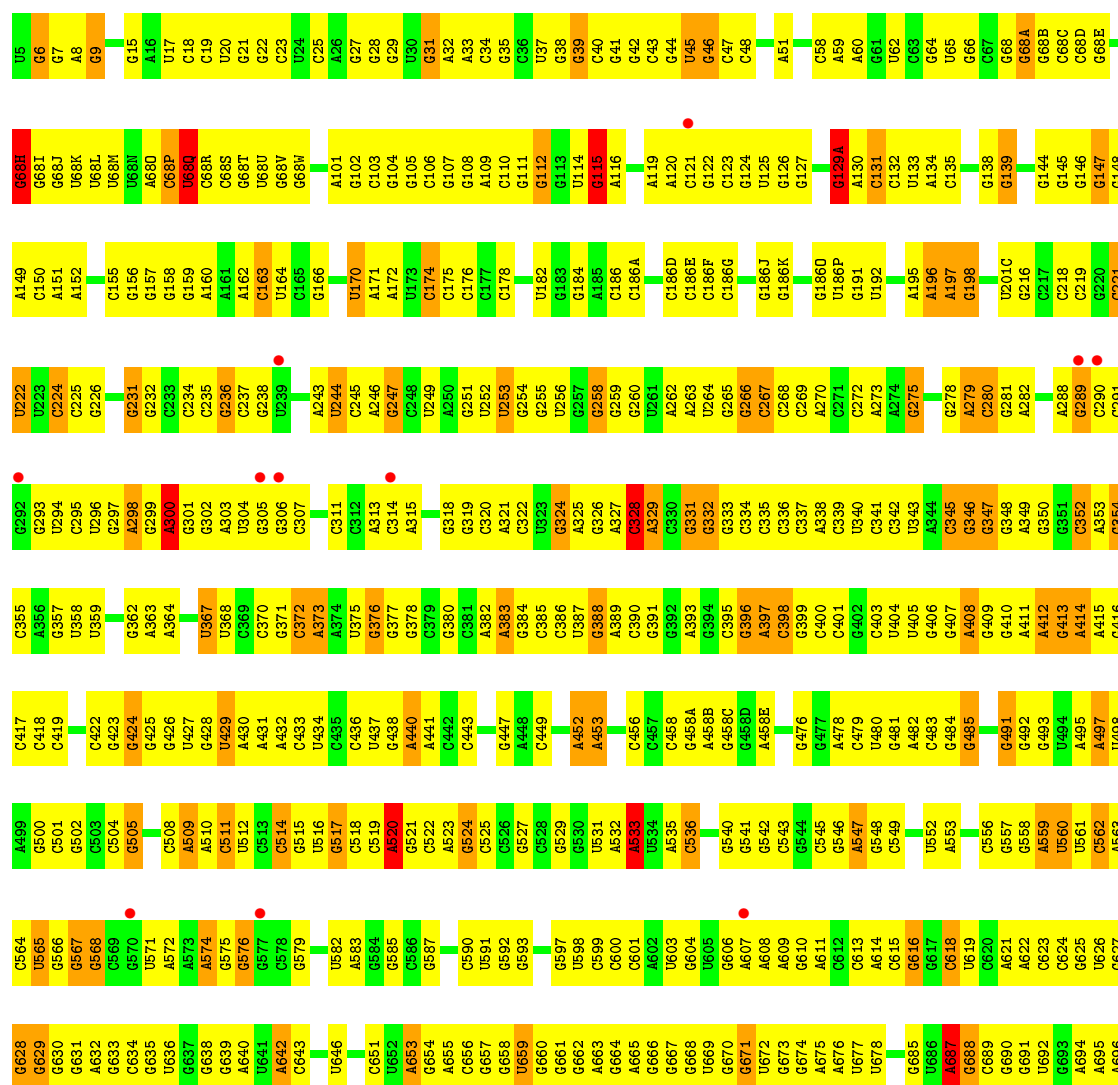
- Molecule 19: 30S ribosomal protein S20

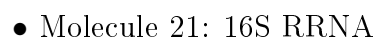


- Molecule 20: Elongation factor G



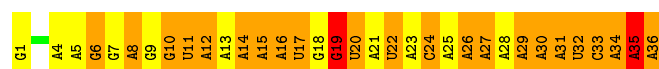








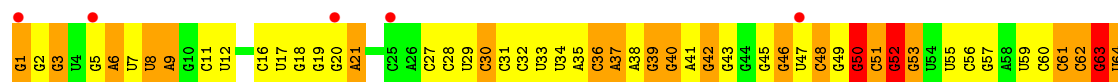
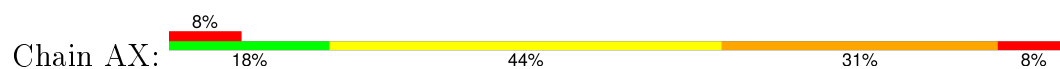




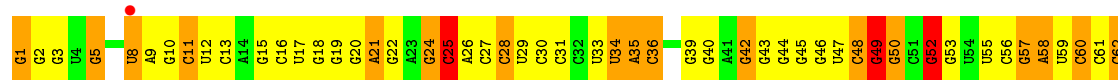
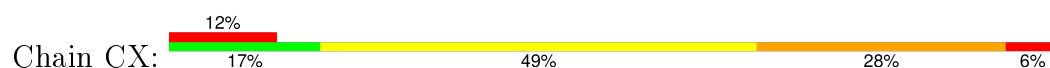
• Molecule 23: mRNA



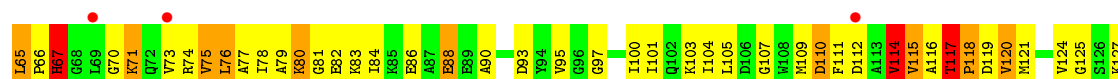
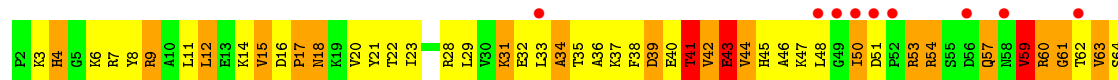
• Molecule 24: tRNA

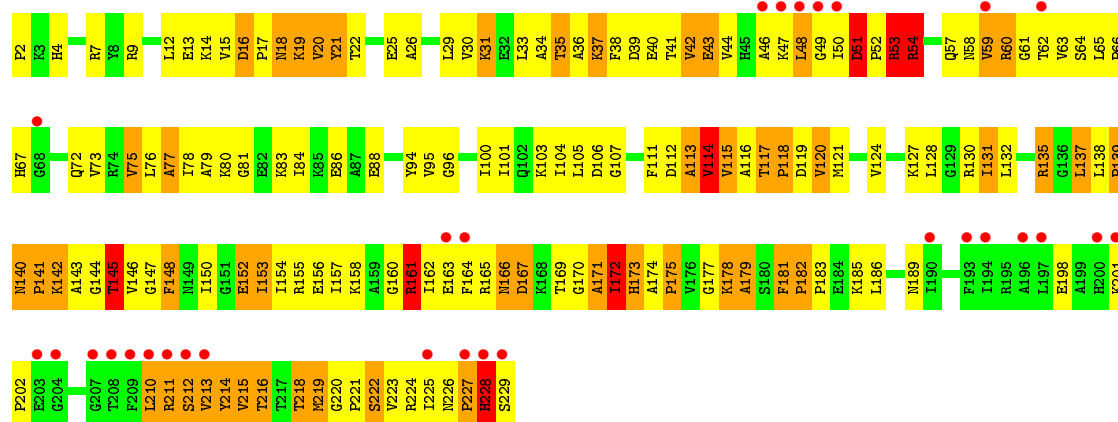


• Molecule 24: tRNA

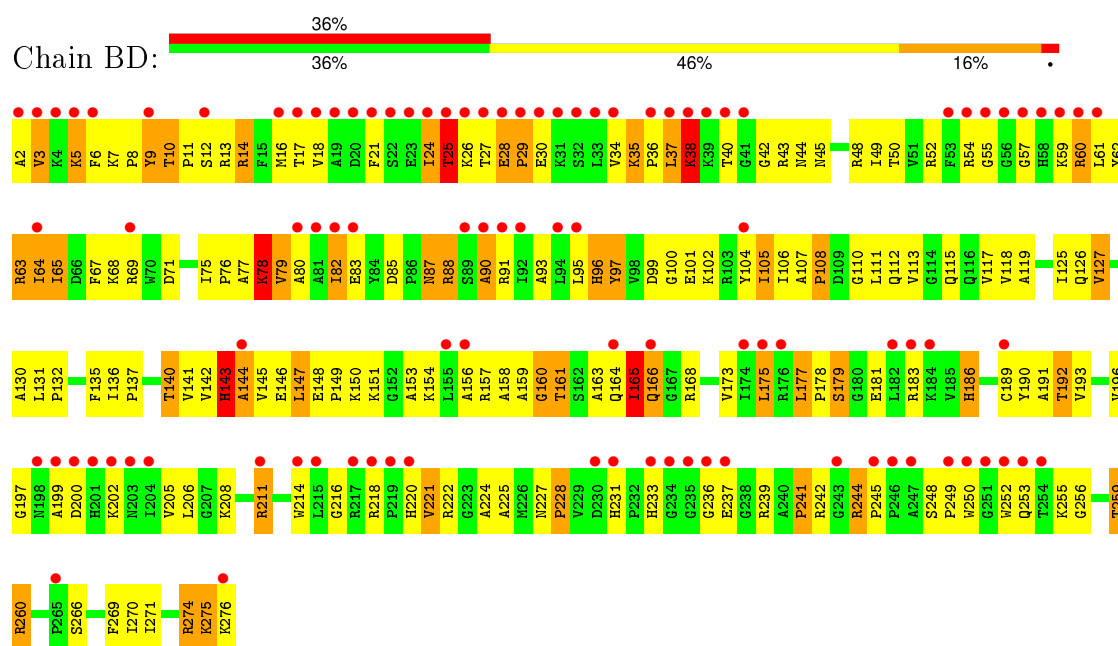


• Molecule 25: 50S ribosomal protein L1

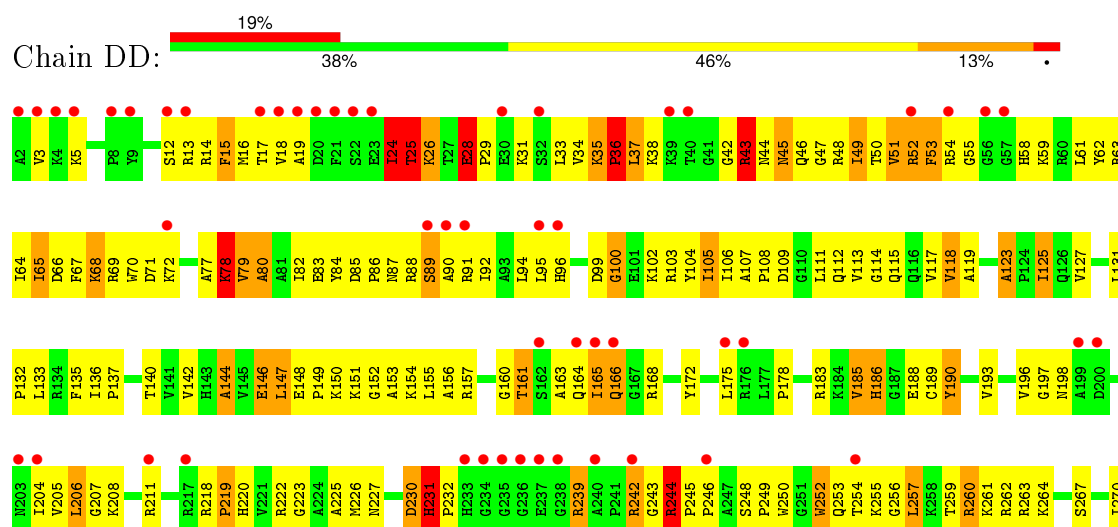




• Molecule 26: 50S ribosomal protein L2

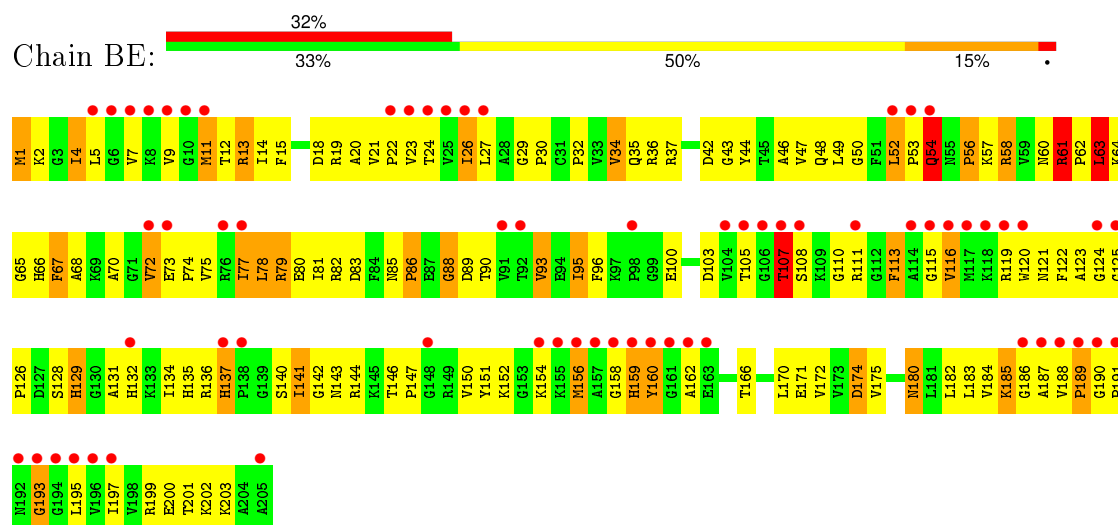


• Molecule 26: 50S ribosomal protein L2

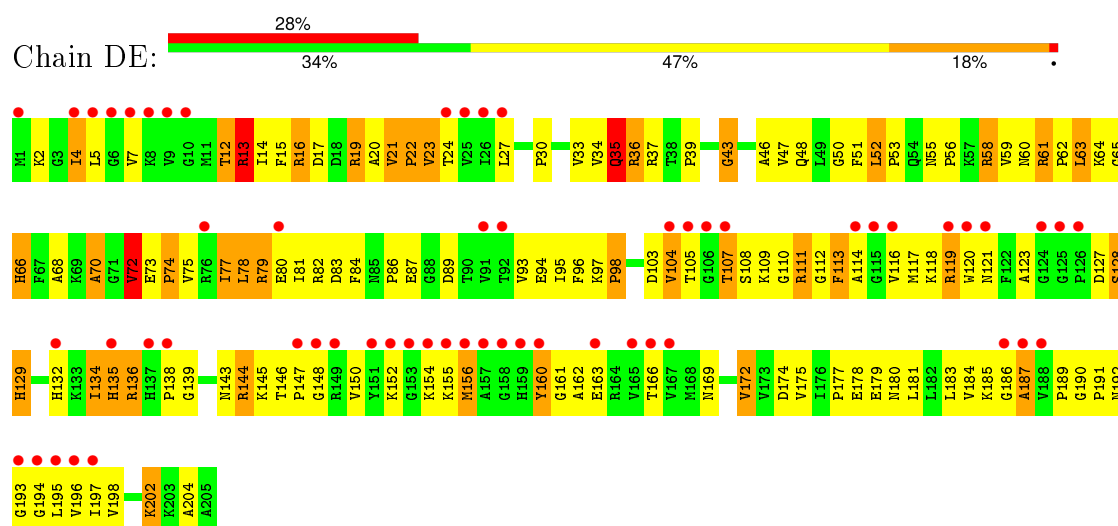




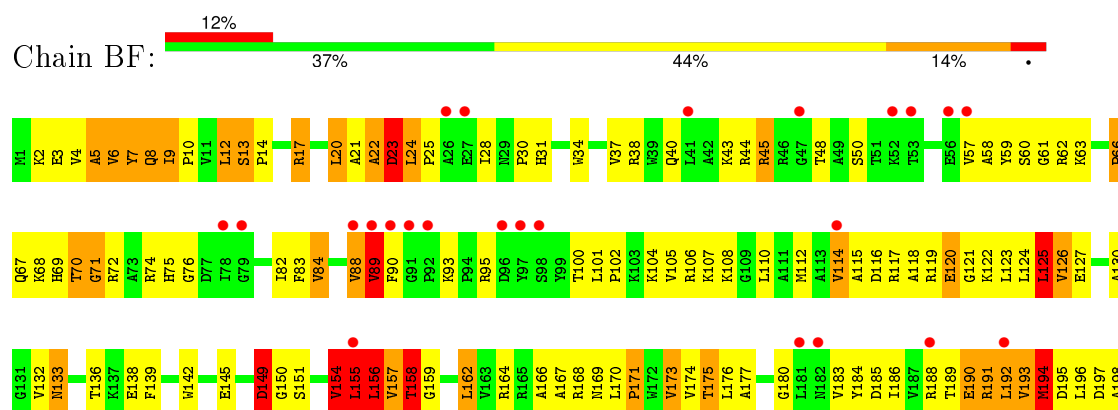
• Molecule 27: 50S ribosomal protein L3

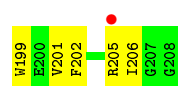


• Molecule 27: 50S ribosomal protein L3

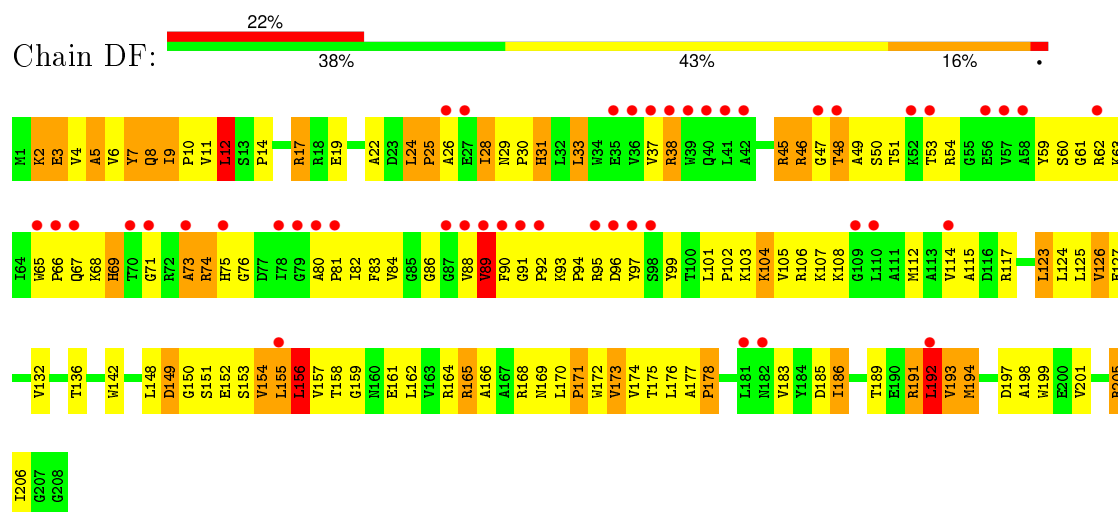


• Molecule 28: 50S ribosomal protein L4

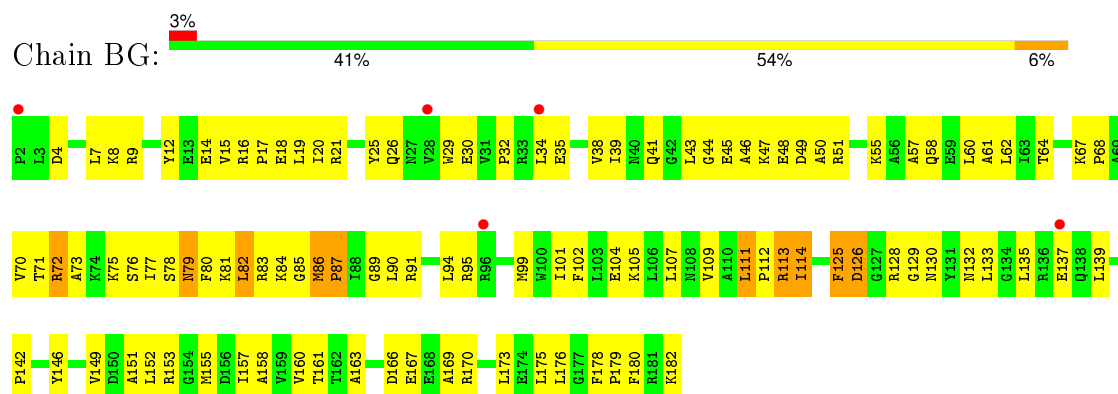




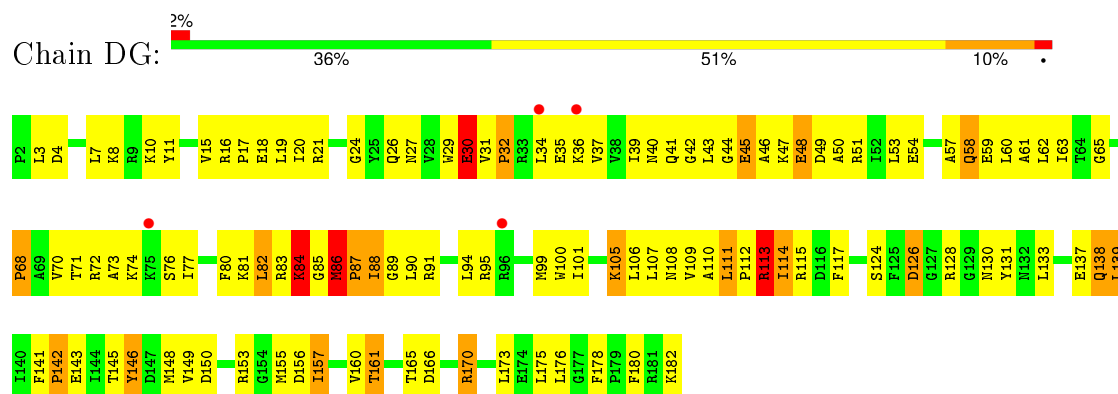
- Molecule 28: 50S ribosomal protein L4



- Molecule 29: 50S ribosomal protein L5

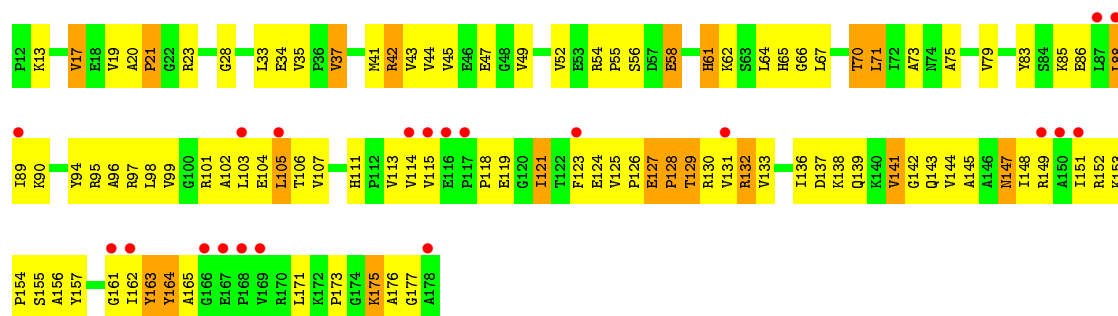


- Molecule 29: 50S ribosomal protein L5

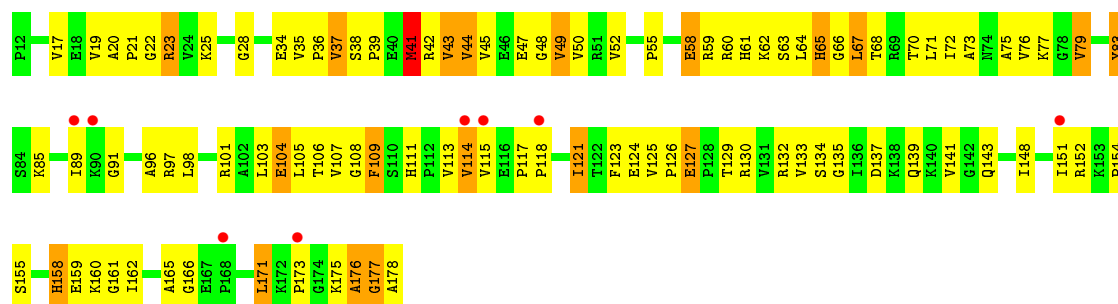
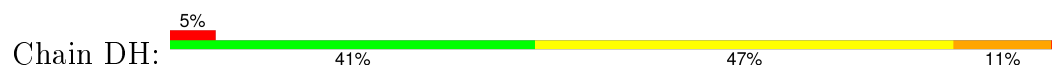


- Molecule 30: 50S ribosomal protein L6

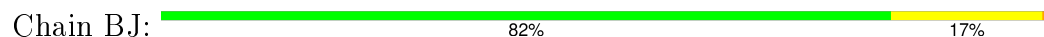




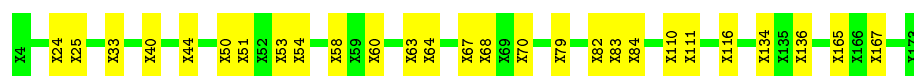
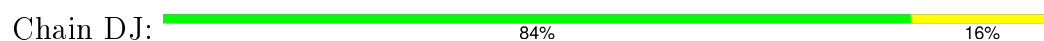
- Molecule 30: 50S ribosomal protein L6



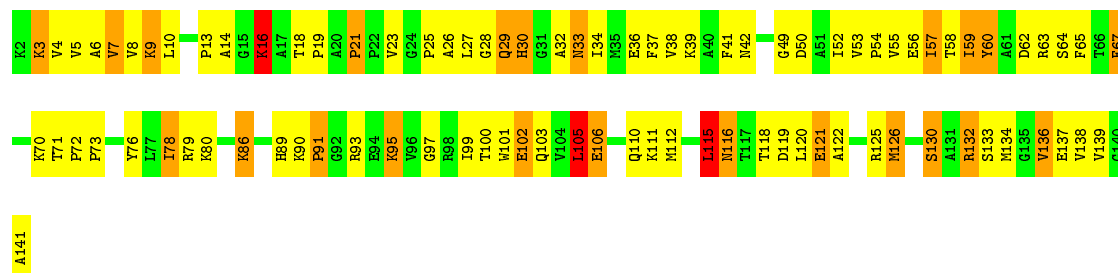
- Molecule 31: 50S ribosomal protein L10



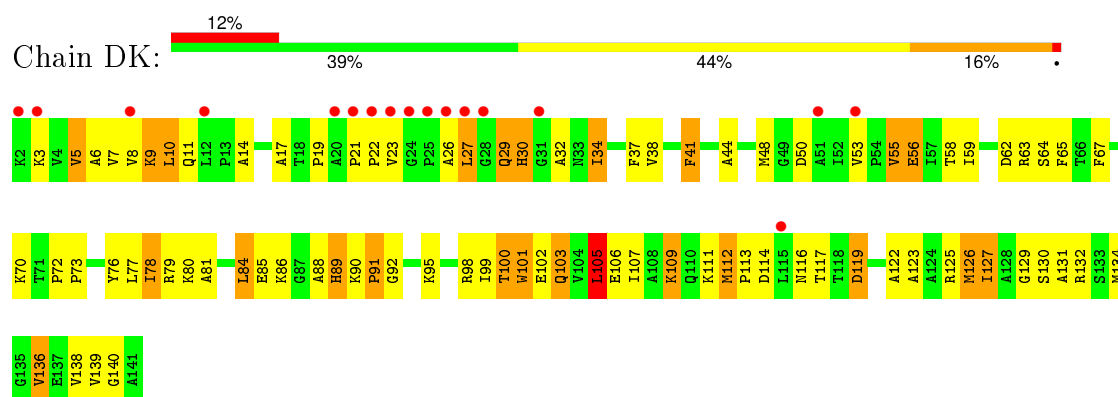
- Molecule 31: 50S ribosomal protein L10



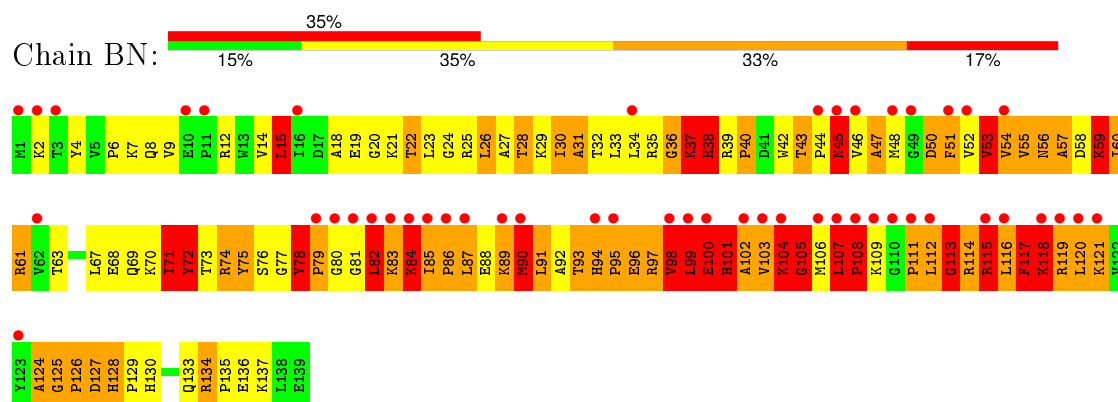
- Molecule 32: 50S ribosomal protein L11



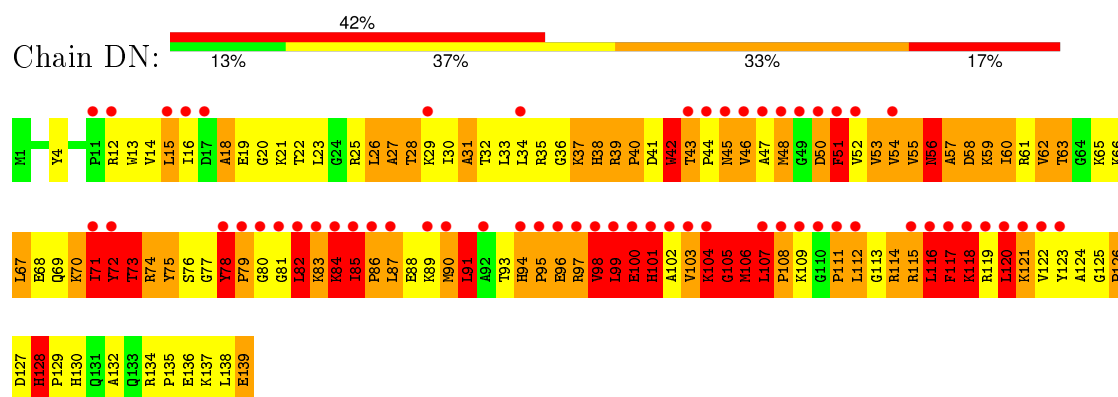
- Molecule 32: 50S ribosomal protein L11



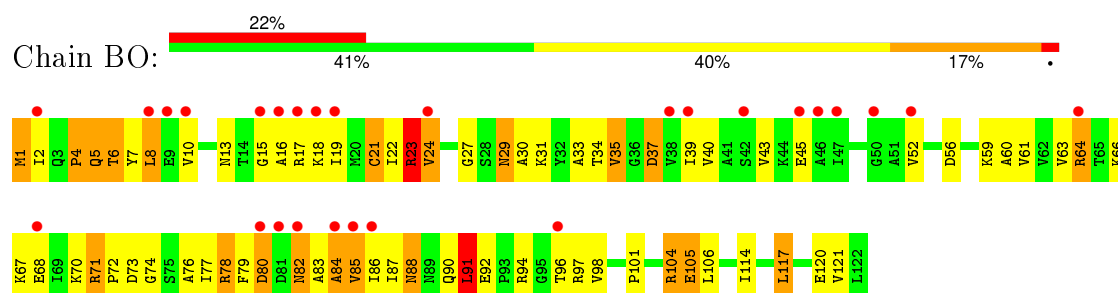
• Molecule 33: 50S ribosomal protein L13



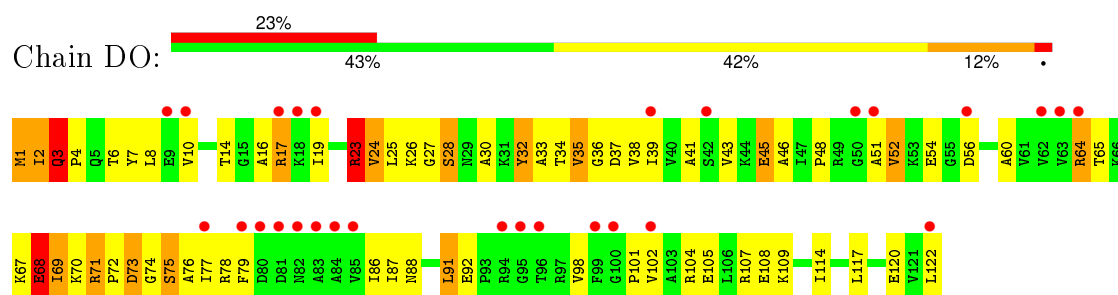
• Molecule 33: 50S ribosomal protein L13



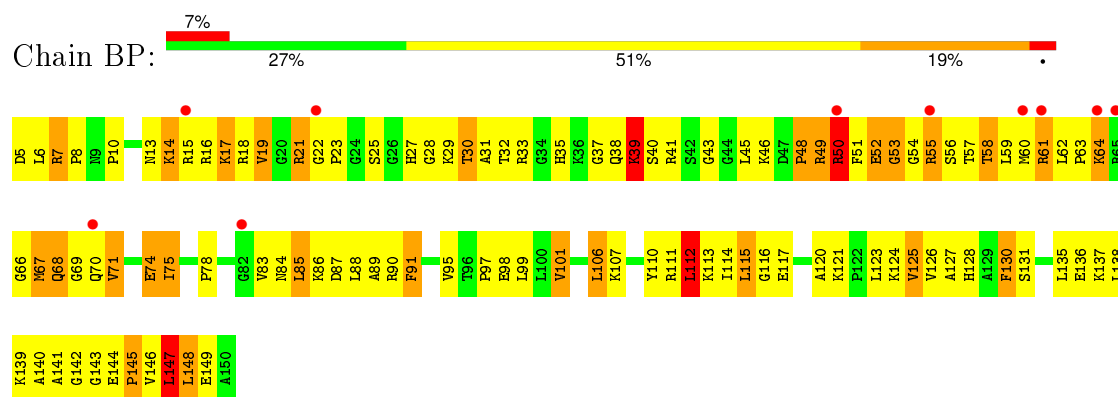
• Molecule 34: 50S ribosomal protein L14



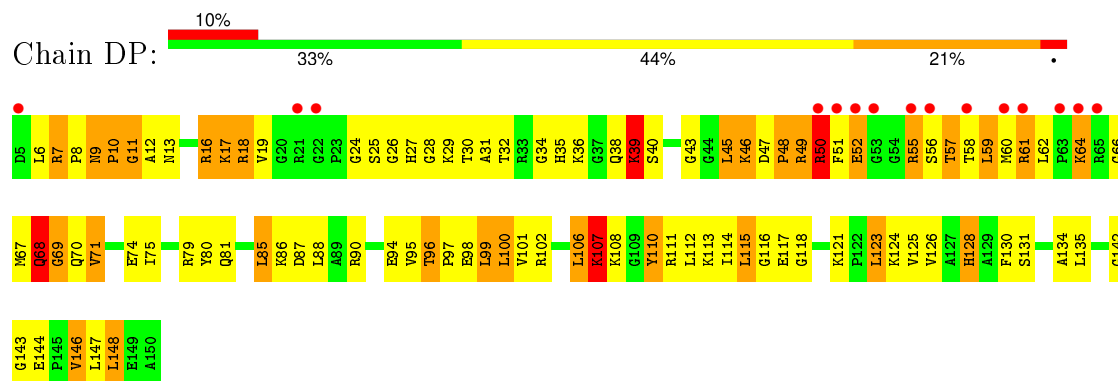
• Molecule 34: 50S ribosomal protein L14



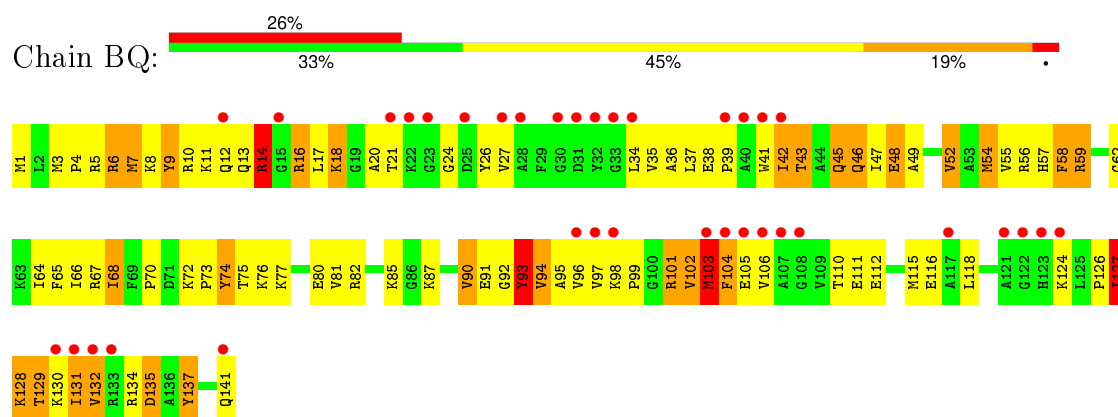
- Molecule 35: 50S ribosomal protein L15



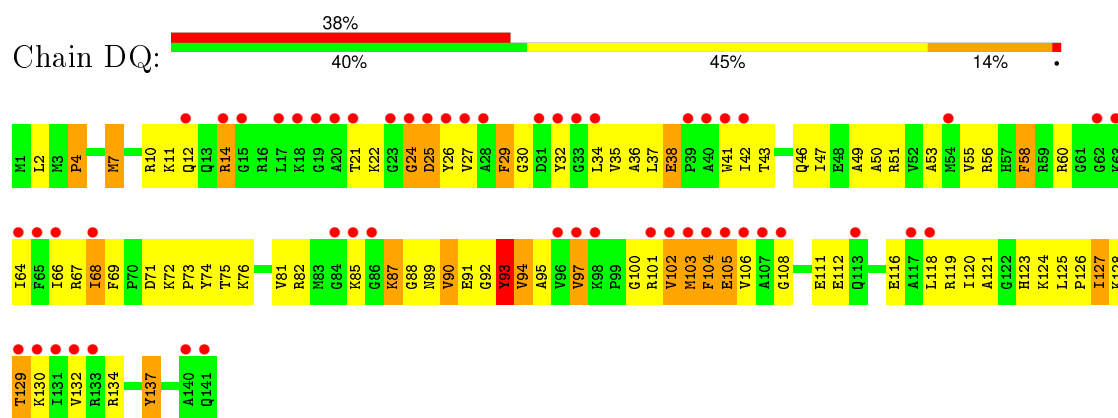
- Molecule 35: 50S ribosomal protein L15



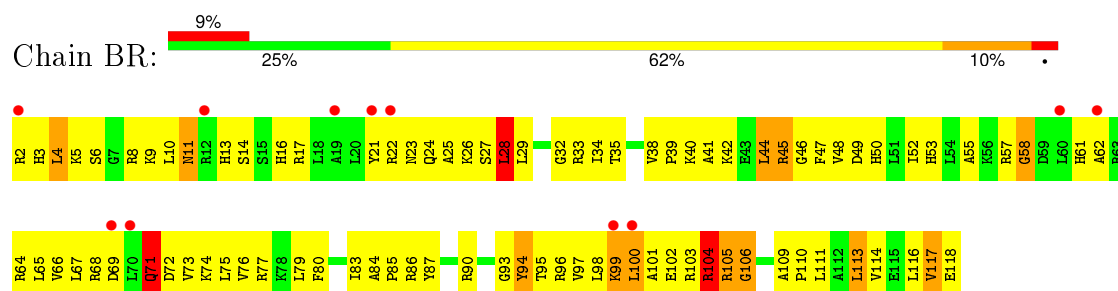
- Molecule 36: 50S ribosomal protein L16



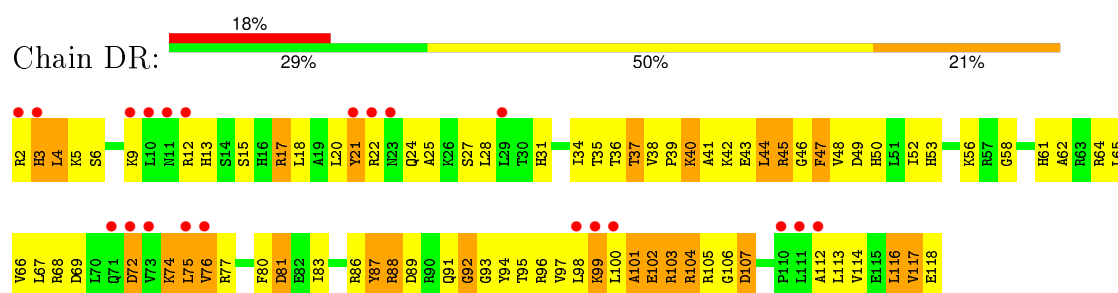
- Molecule 36: 50S ribosomal protein L16



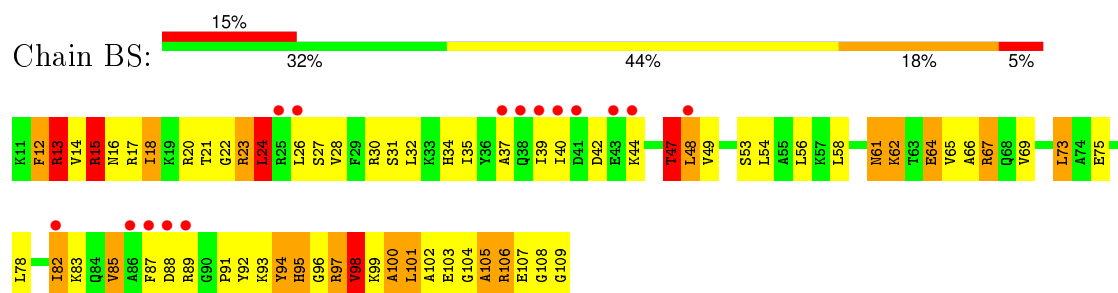
- Molecule 37: 50S ribosomal protein L17



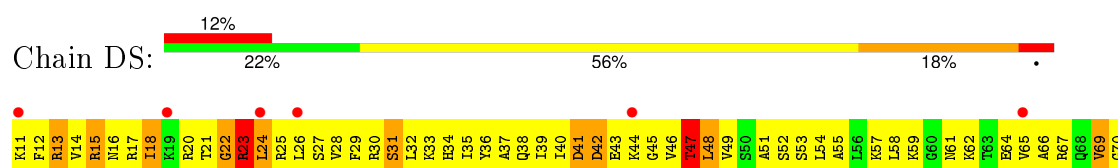
- Molecule 37: 50S ribosomal protein L17

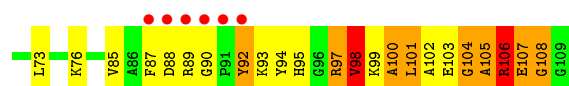


- Molecule 38: 50S ribosomal protein L18

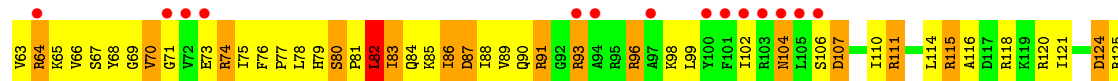
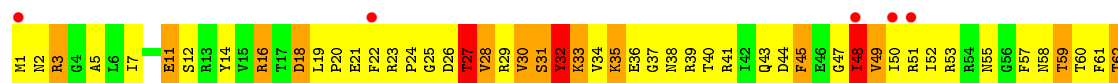


- Molecule 38: 50S ribosomal protein L18

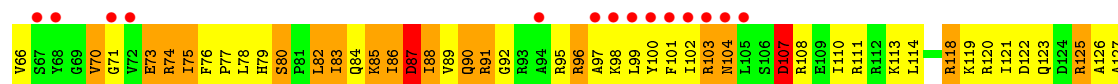
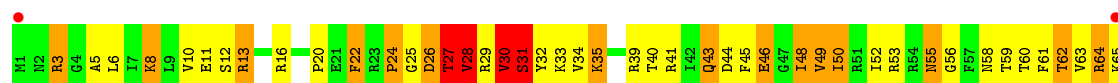




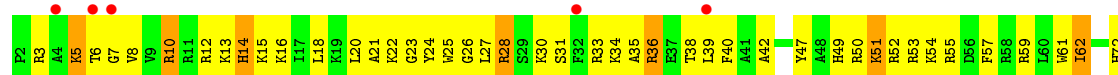
• Molecule 39: 50S ribosomal protein L19



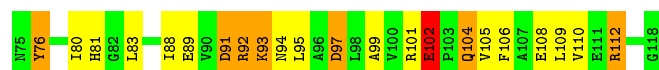
• Molecule 39: 50S ribosomal protein L19



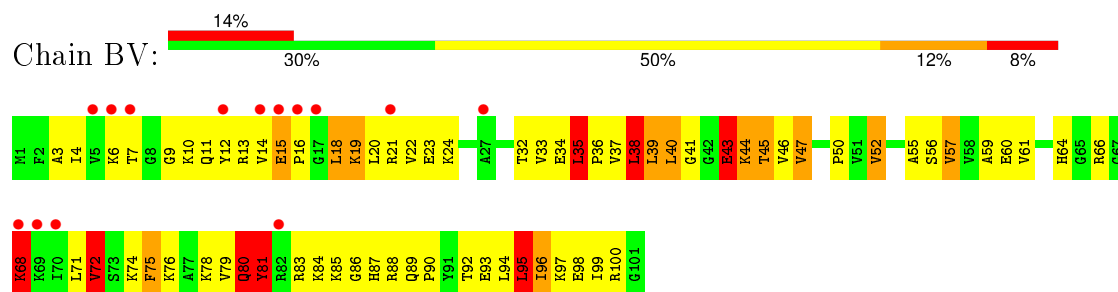
• Molecule 40: 50S ribosomal protein L20



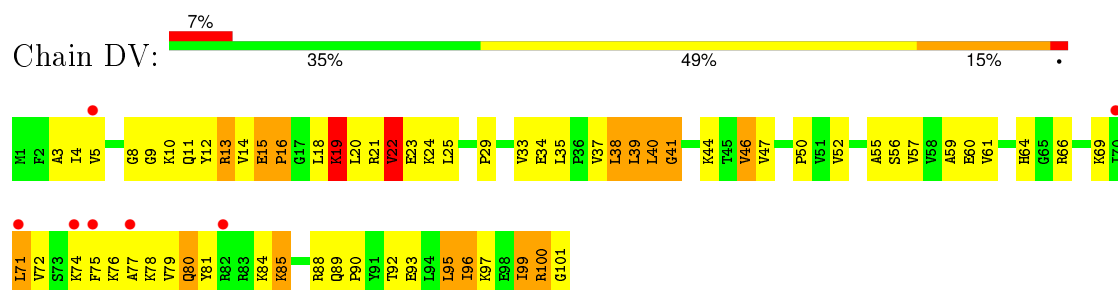
• Molecule 40: 50S ribosomal protein L20



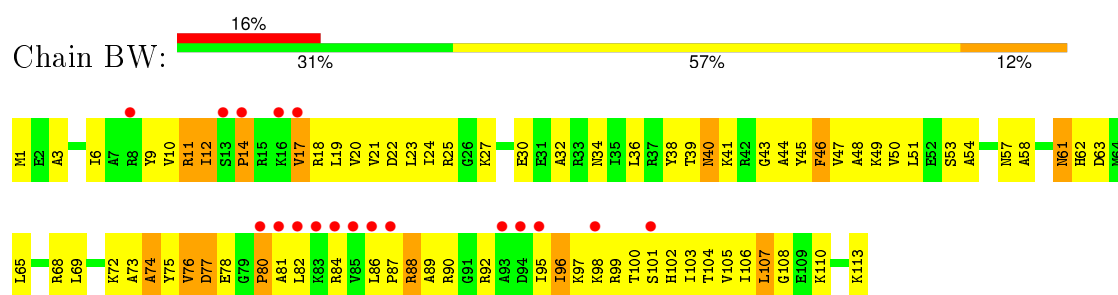
- Molecule 41: 50S ribosomal protein L21



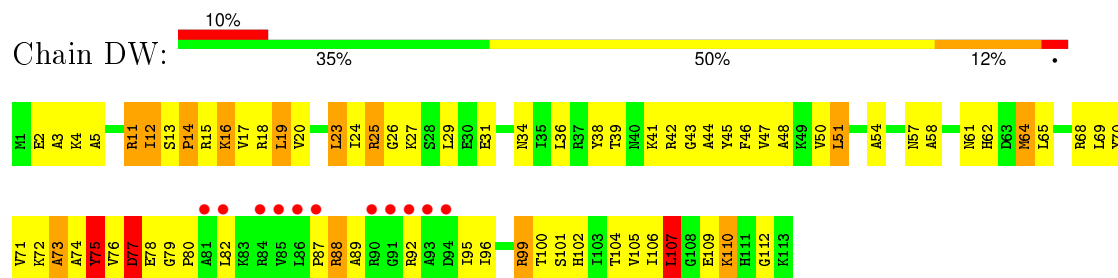
- Molecule 41: 50S ribosomal protein L21



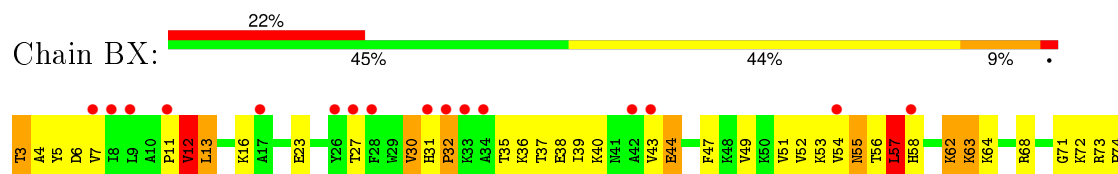
- Molecule 42: 50S ribosomal protein L22

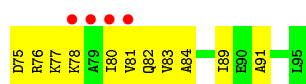


- Molecule 42: 50S ribosomal protein L22

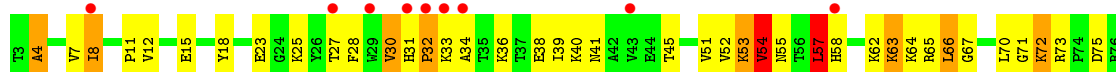


- Molecule 43: 50S ribosomal protein L23

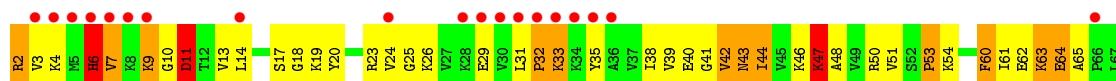




- Molecule 43: 50S ribosomal protein L23



- Molecule 44: 50S ribosomal protein L24



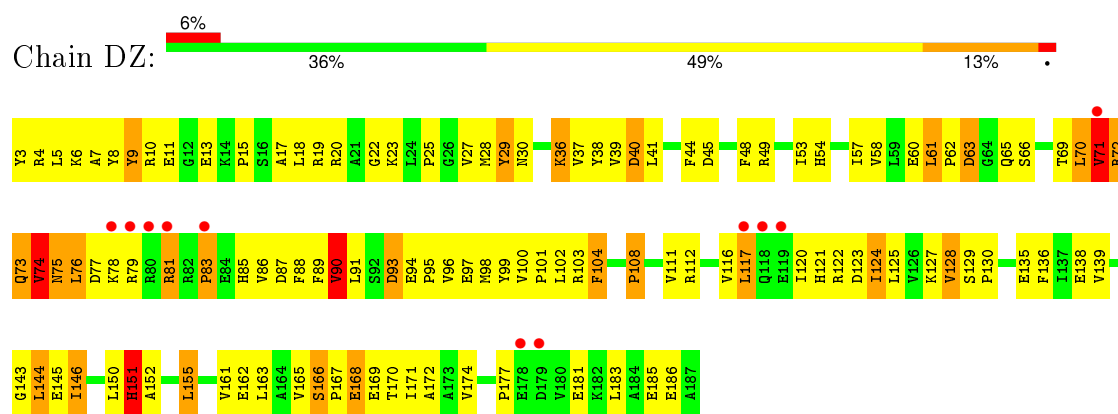
- Molecule 44: 50S ribosomal protein L24



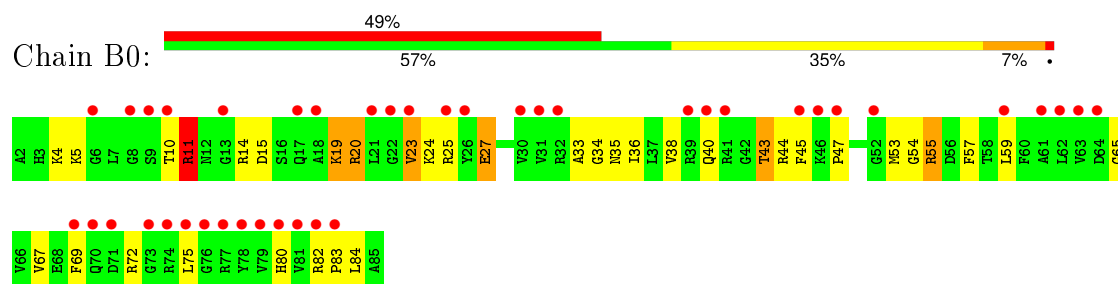
- Molecule 45: 50S ribosomal protein L25



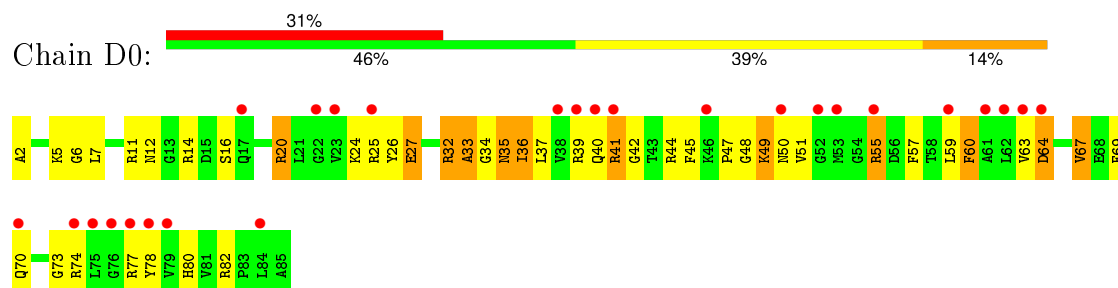
- Molecule 45: 50S ribosomal protein L25



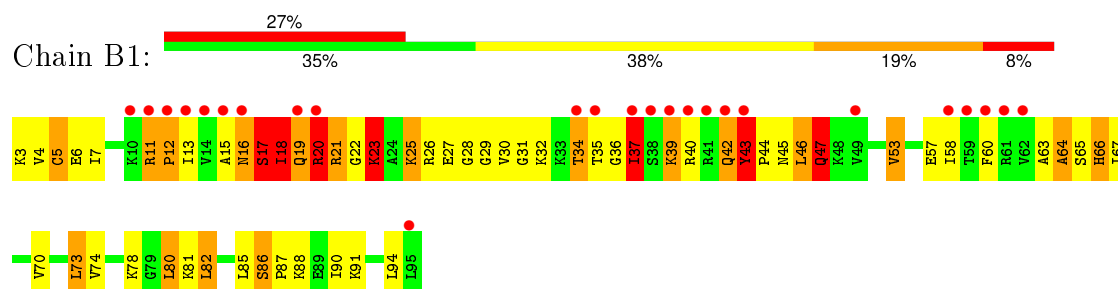
• Molecule 46: 50S ribosomal protein L27



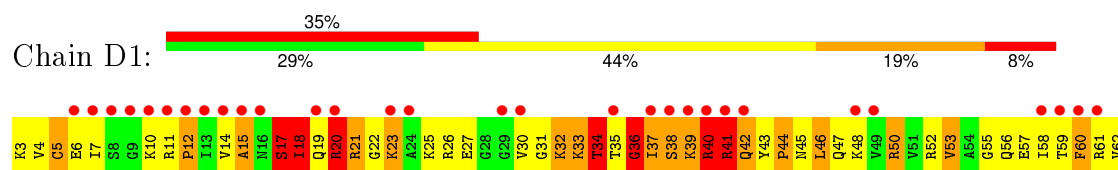
• Molecule 46: 50S ribosomal protein L27

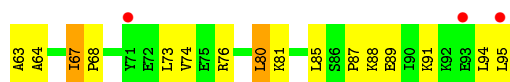


• Molecule 47: 50S ribosomal protein L28

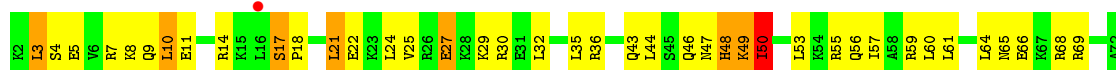
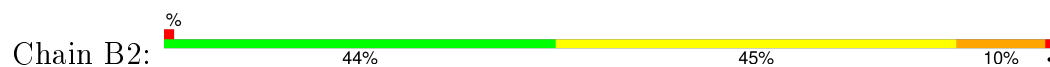


• Molecule 47: 50S ribosomal protein L28





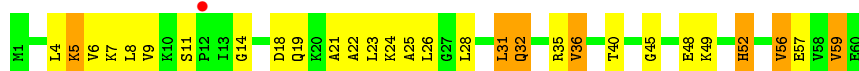
- Molecule 48: 50S ribosomal protein L29



- Molecule 48: 50S ribosomal protein L29



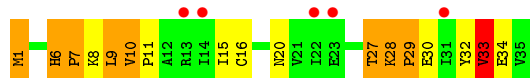
- Molecule 49: 50S ribosomal protein L30



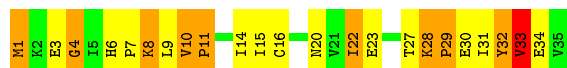
- Molecule 49: 50S ribosomal protein L30



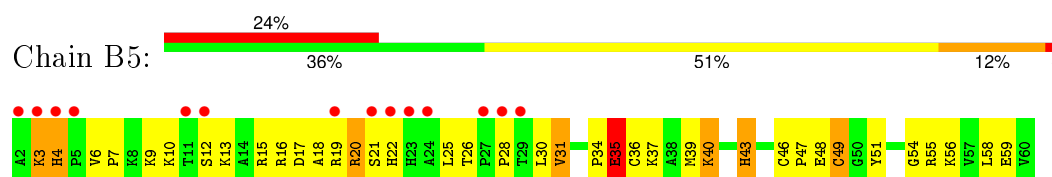
- Molecule 50: 50S ribosomal protein L31



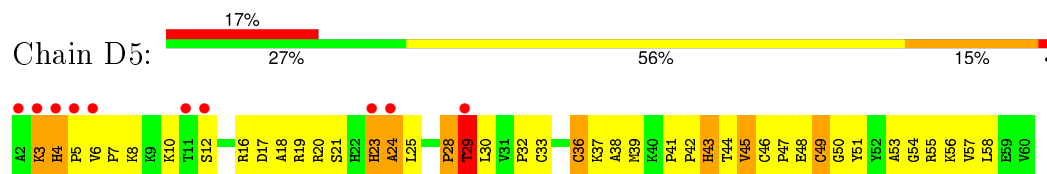
- Molecule 50: 50S ribosomal protein L31



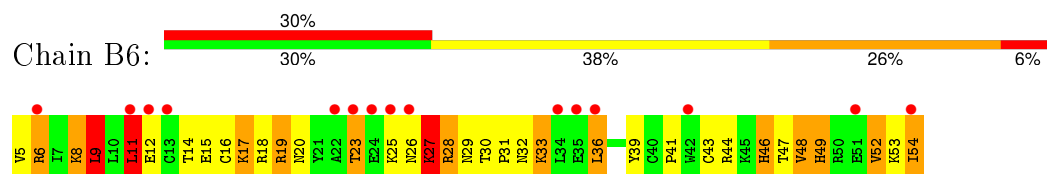
- Molecule 51: 50S ribosomal protein L32



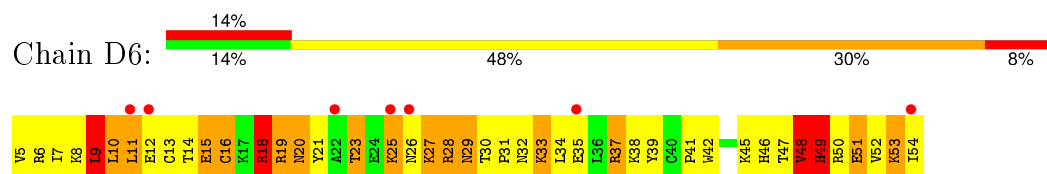
- Molecule 51: 50S ribosomal protein L32



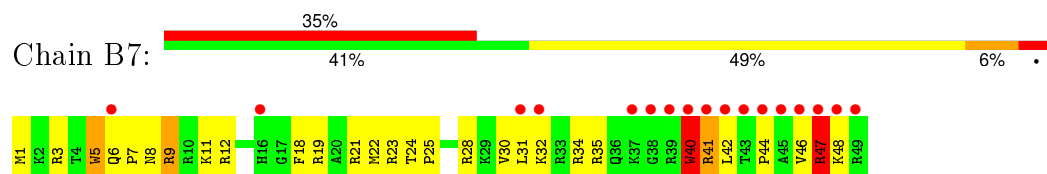
- Molecule 52: 50S ribosomal protein L33



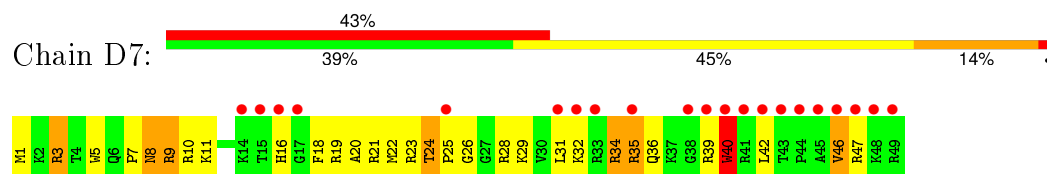
- Molecule 52: 50S ribosomal protein L33



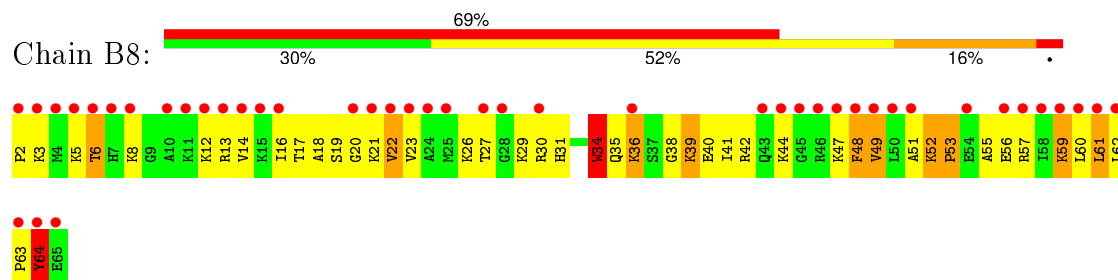
- Molecule 53: 50S ribosomal protein L34



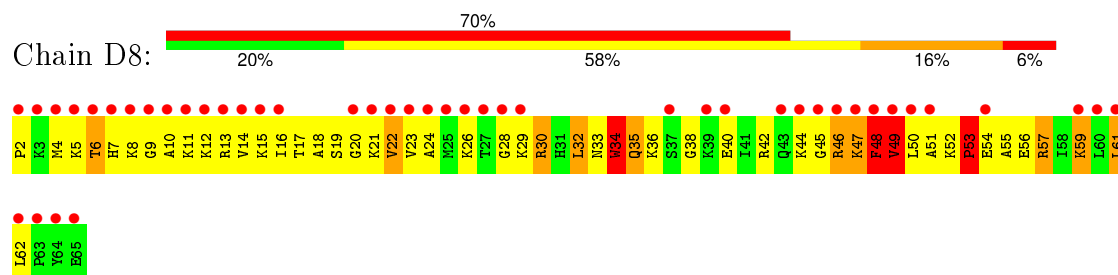
- Molecule 53: 50S ribosomal protein L34



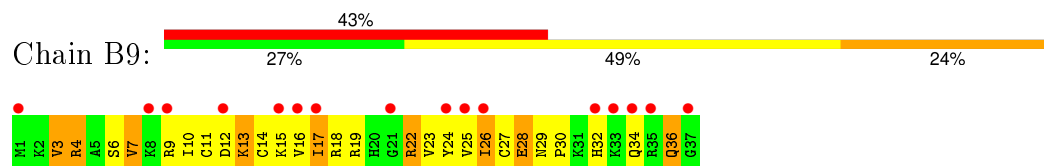
- Molecule 54: 50S ribosomal protein L35



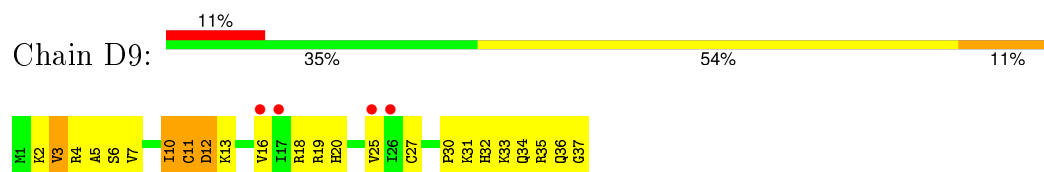
- Molecule 54: 50S ribosomal protein L35



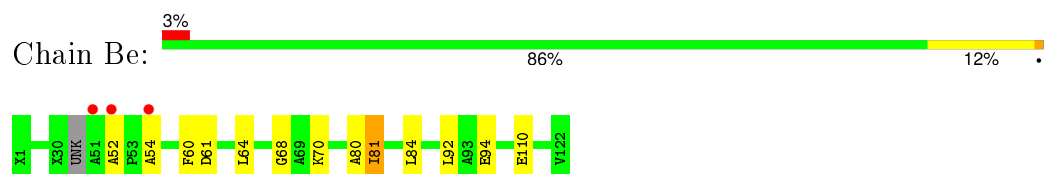
- Molecule 55: 50S ribosomal protein L36



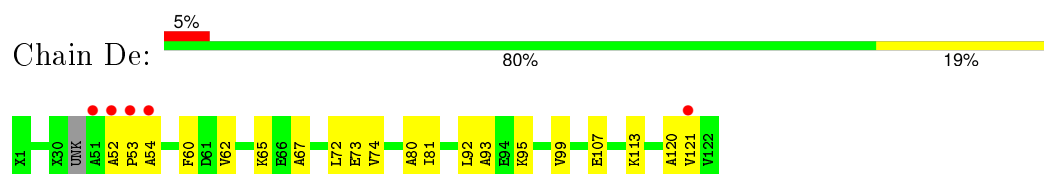
- Molecule 55: 50S ribosomal protein L36



- Molecule 56: 50S ribosomal protein L7/L12



- Molecule 56: 50S ribosomal protein L7/L12



- Molecule 57: 50S ribosomal protein L7/L12



There are no outlier residues recorded for this chain.

- Molecule 57: 50S ribosomal protein L7/L12



There are no outlier residues recorded for this chain.

- Molecule 57: 50S ribosomal protein L7/L12

Chain Df:  100%

There are no outlier residues recorded for this chain.

- Molecule 57: 50S ribosomal protein L7/L12

Chain Dg:  100%

There are no outlier residues recorded for this chain.

- Molecule 58: 50S ribosomal protein L7/L12

Chain Bh:  100%

There are no outlier residues recorded for this chain.

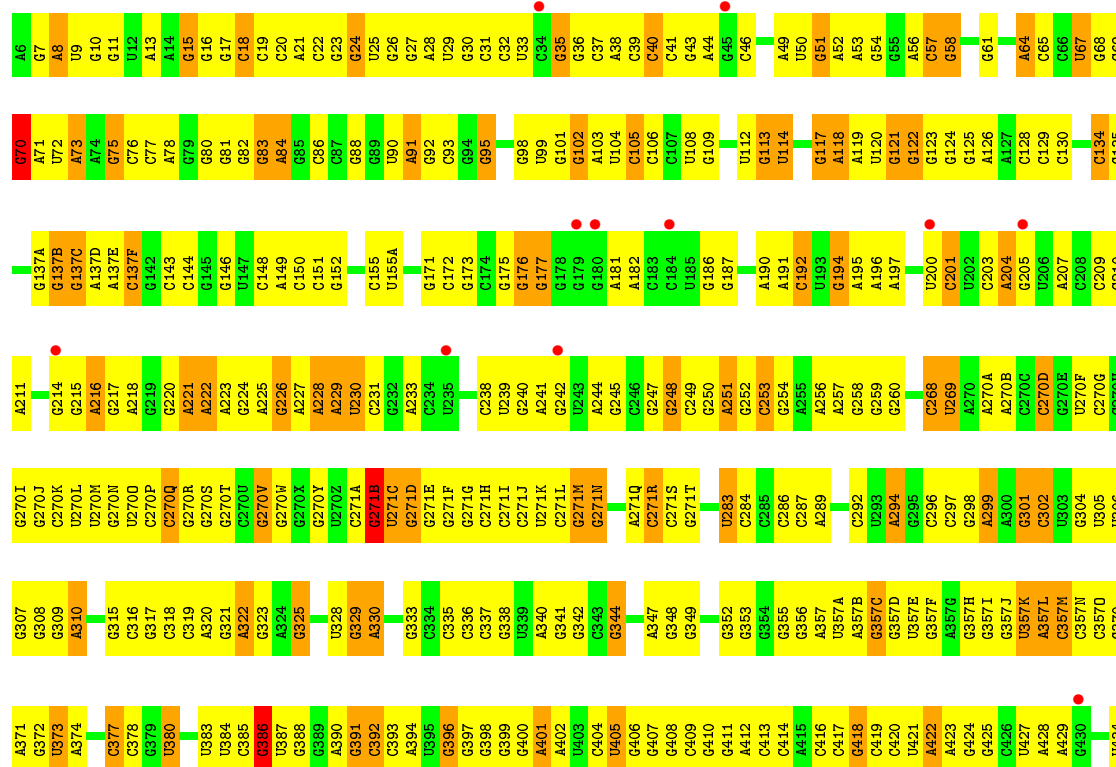
- Molecule 58: 50S ribosomal protein L7/L12

Chain Dh:  100%

There are no outlier residues recorded for this chain.

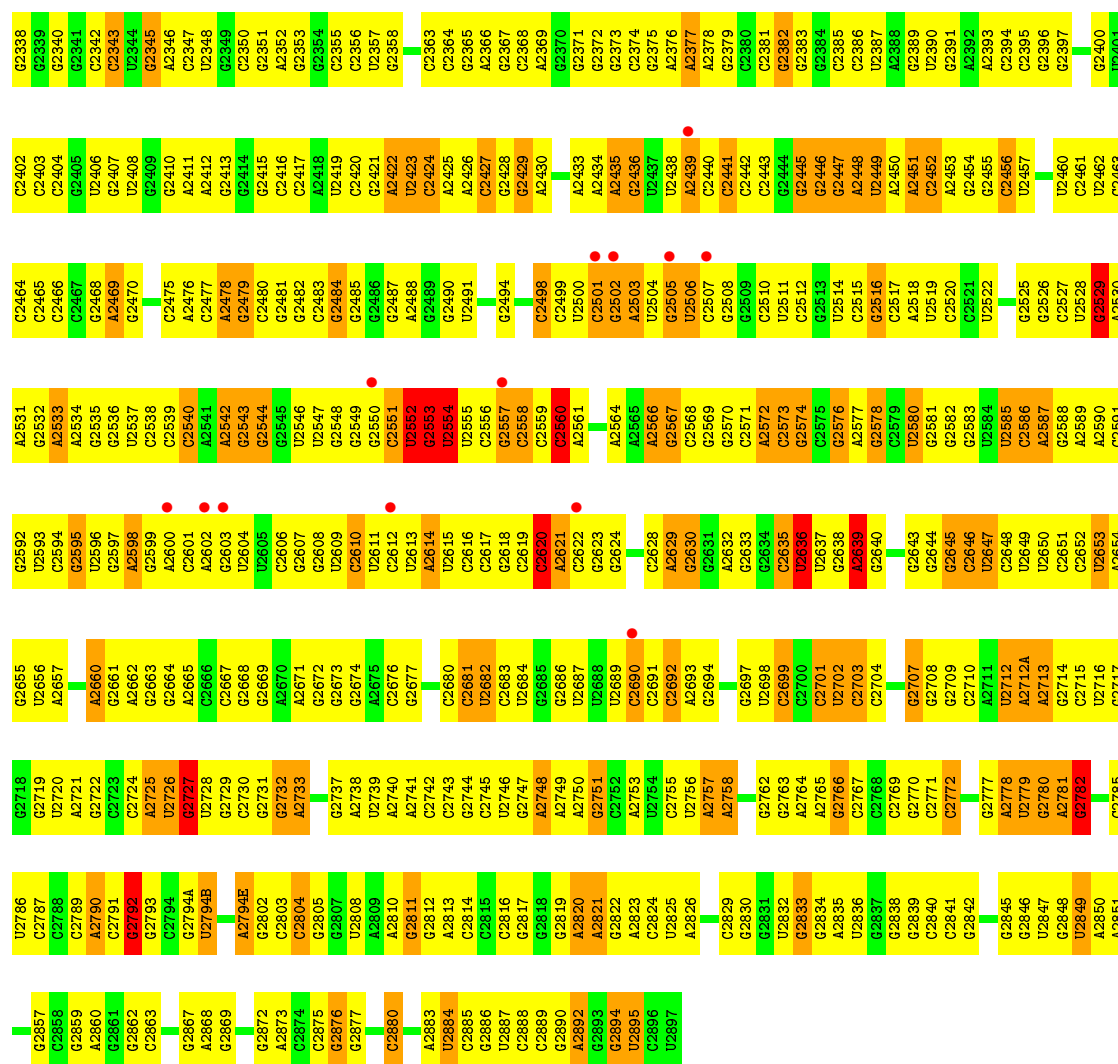
- Molecule 59: 23S RRNA

Chain BA:  4% 23% 57% 19%

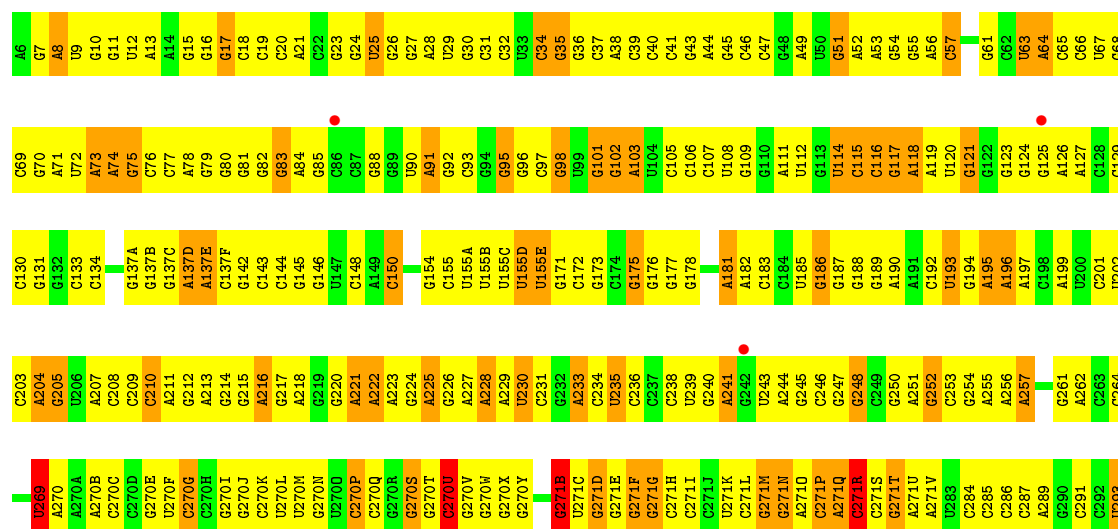


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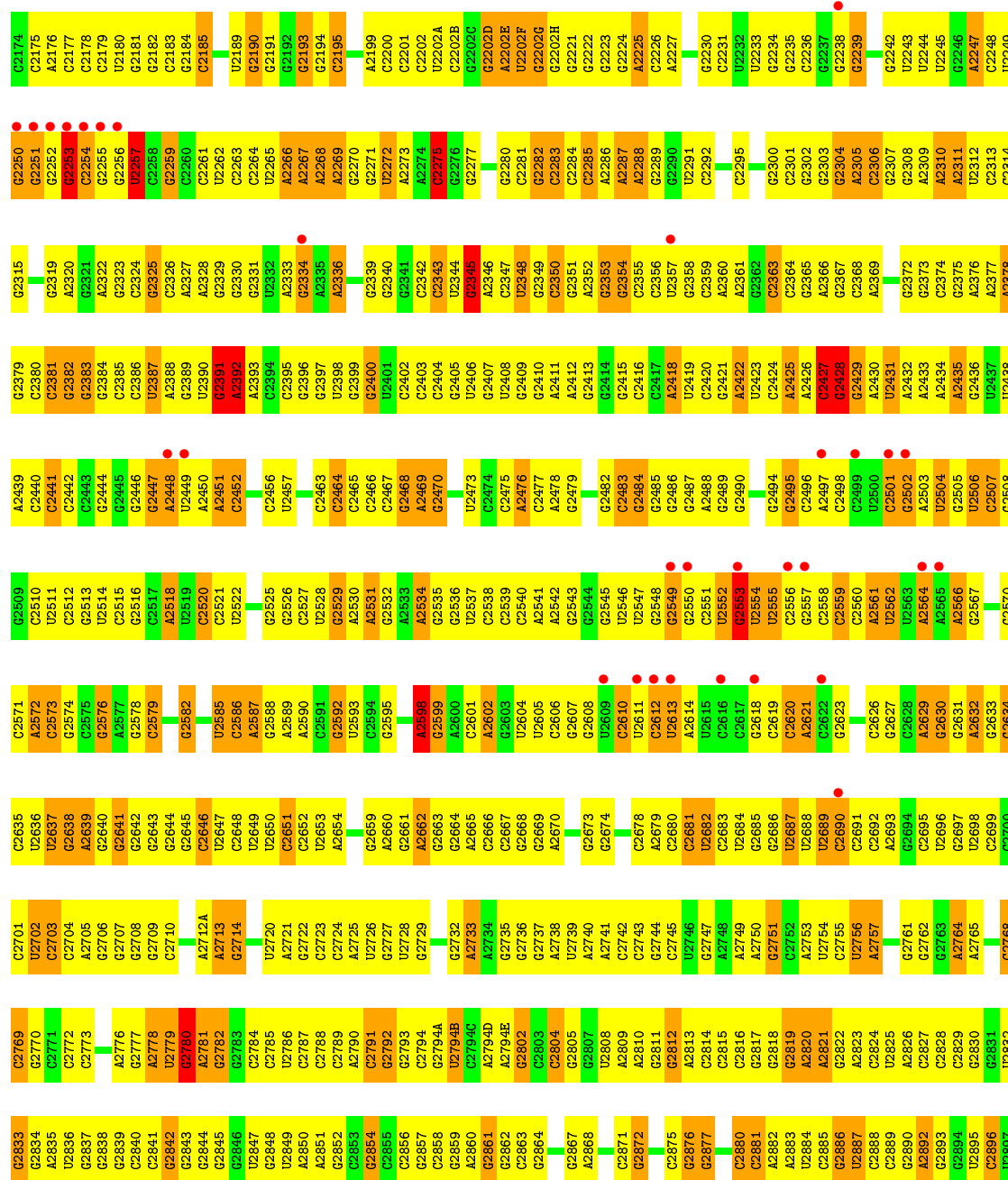


• Molecule 59: 23S RRNA



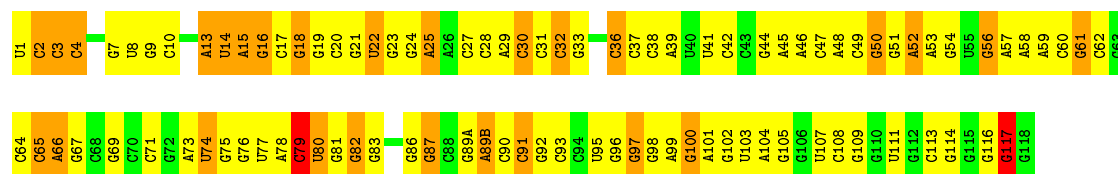
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G1232	G1172	G1106	C1043	G977	G916	G852	C791	G730	C665	G600		U475	G406	G349
C1233	A1173	G1107	G1044		G917	G853	G792	C731	G666	C501	G538	A476	G407	
U1234	U1174	U1108	A1045	A980	A917	G854	A793	G732	U667	G602	G539	A477	G408	
G1235	G1175	C1109	A1046		A918	G855	G794	G733	G668	A803	C540	A478	C409	G352
	A1177	G1110	G1047	A983	G919	C856	C795	A734	G669	G604	C541	A479	G410	G353
G1238	U1178	A1111	A1048	A984	G920	C857	C796	A735	G669	C605	C542	A480	G411	G354
G1239	C1179	G1112	C985	G985	G921	U858	G797	C736	A670	C543	C543	G481	A412	G355
U1240	C1180	U1113	G986	C986	U922	G859	G798	C737	C671	U607	G343A	A482	C413	G356
A1241	C1181	G1114	G987	G987	C923	U860	G799	G738	C672	A608	C543B	A483	C414	G357
A1242	A1182	G1115	C1052	A988	C924	A861	A800	G739	C673	A609	A543C	C484	A415	U357A
G1243	G1183	C1116	C1053	G989	C925	G862	G801	U740	G674	G610	A543D	C485	C416	A357B
G1244	C1184	U1055	A1054	G989	A926	A863	A802	G741	A675	C511	G550	C486	C417	G357C
G1245	C1185	G1056	G1056	C991	G928	G864	U803	G742	A676	C511A	G551	C487	G418	G357D
A1246	G1186	A1057	C992	C992	G929	C865	A804	G744	A677		G552	G488	C419	U357E

U2109	U2110	U2047	G1985	G1920	G1946	A1784	G1702	G1636	A1569	A1506A	C1437	G1374	G1310	A1247
G2110	G2111	G2048	A1986	G1921	A1947	A1785	G1703	C1635	A1570	A1506B	U1438	C1375	G1311	G1248
C2111	C2112	G2049	G1987	G1922	A1948	A1786	G1704	A1637	A1571	A1506C	G1441	C1376	U1312	U1250
G2112	G2113	C2050	G1988	G1923	G1949	A1787	G1705	C1638	A1572	A1506D	G1442	G1377	U1313	U1251
A2114	A2115	G2052	G1989	G1924	G1950	A1788	G1706	A1641	G1575	C1506E	G1443	A1378	C1314	G1251
G2115	G2116	C2053	G1990	G1925	U1851	A1789	G1707	A1642	U1576	C1506F	G1444	A1379	C1315	G1252
U2118	U2119	C2055	U1991	A1927	A1854	C1790	G1708	G1643	U1577	C1506G	G1444	G1380	U1316	A1253
A2119	A2120	G2056	G1992	A1928	G1955	A1791	G1709	C1644	C1577	C1506H	A1444A	G1381	U1317	A1254
G2120	G2121	C2057	G1993	A1929	G1956	C1792	G1710	G1645	U1578	C1506I	C1446	G1382	G1322	U1255
G2121	G2122	A2058	G1994	G1930	G1957	A1793	G1711	G1646	A1579	C1506J	C1446	G1383	A1322	A1256
A2123	A2124	G2059	U1995	U1931	G1958	C1794	G1712	G1647	A1580	C1506K	C1446	G1384	U1323	C1257
U2122	U2123	A2060	G1996	A1932	A1859	C1795	U1712B	G1648	G1581	C1506L	C1450	G1385	G1324	G1258
G2123	G2124	G2061	G1997	G1933	G1860	U1796	G1712C	C1649	C1582	U1506M	C1452	G1386	G1325	G1259
G2125	A2126	C2062	G1998	C1934	G1861	C1797	G1712D	G1650	A1583	C1506N	U1453	C1387	U1326	G1260
U2130	U2131	C2063	G2002	G1935	G1864	U1798	G1712E	G1651	C1584	G1506O	U1454	G1388	C1327	C1261
G2132	G2133	C2064	A1936	A1936	C1864A	G1799	G1712F	A1652	A1586	G1506P	G1455	G1389	C1328	A1262
A2134	A2135	C2065	A1937	A1937	C1864B	C1800	G1712G	A1653	A1587	G1525	G1459	A1392	U1329	U1263
G2136	G2137	C2066	A1938	A1938	C1864C	G1801	G1712H	G1654	C1588	G1527	A1460	A1393	C1330	G1264
U2139	U2140	C2067	A1939	U1939	A1864D	A1802	U1712I	A1655	G1589	A1528	G1461	A1394	A1331	A1265
G2141	G2142	G2068	U1940	U1940	G1878	A1803	G1712J	A1656	U1590	G1530	G1462	U1395	G1332	G1266
A2143	A2144	C2069	G1941	G1941	C1879	A1804	G1712K	A1657	C1591	G1533	C1464	U1396	G1334	U1267
U2145	U2146	G2070	C1942	C1942	C1880	U1805	G1712L	C1657	G1595	G1534	G1465	U1397	G1335	A1268
G2147	G2148	A2071	U1943	U1943	C1881	C1806	G1712M	C1658	A1596	G1535	G1466	G1398	A1336	G1270
C2149	C2150	G2072	G1944	G1944	C1882	G1807	U1712N	U1659	A1597	U1535	C1467	G1399	G1337	G1271
U2151	U2152	C2073	G1945	G1945	C1883	U1808	G1712O	G1660	A1598	G1536	G1468	G1400	G1338	A1272
G2153	G2154	U2091	U1946	U1946	A1884	A1809	G1712P	G1661	C1599	U1536	C1468H	U1406	G1344	U1273
C2155	C2156	U2092	G1947	G1947	A1885	A1810	G1712Q	G1662	G1599	A1537	C1468I	U1407	C1345	A1274
U2157	U2158	C2093	A1948	A1948	C1886	G1811	G1712R	G1663	C1600	G1538	A1468D	U1408	G1346	A1275
G2159	G2160	G2094	G1949	G1949	C1887	A1812	G1712S	A1664	G1601	G1539	G1468E	C1403	U1341	U1276
C2161	C2162	U2095	G1950	G1950	C1888	G1813	U1712T	A1665	U1602	G1540	G1468F	C1404	G1342	G1277
U2167	U2168	C2096	U1951	U1951	A1889	G1814	G1712U	G1666	U1603	U1541	G1468G	U1405	G1343	G1278
A2169	A2170	G2101	A1890	A1890	C1890	G1815	G1712V	G1667	G1606	G1542	C1468J	U1406	C1344	A1279
G2171	G2172	C2102	G1952	G1952	G1891	G1817	C1751	G1668	C1607	A1543	G1468K	U1408	G1346	G1280
C2173	C2174	U2103	A1953	A1953	C1892	U1818	G1752	A1669	A1608	G1543A	G1468L	C1409	G1347	U1281
U2175	U2176	G2104	G1954	G1954	C1893	A1819	G1753	U1671	A1609	A1544	U1468M	G1410	G1348	U1282
G2177	G2178	C2105	U1955	U1955	C1894	U1820	G1756	G1674	A1610	A1545	C1468N	C1411	A1349	G1283
A2179	A2180	U2105	G1956	G1956	G1895	A1821	G1757	G1675	C1611	C1546	G1483	A1412	U1352	A1284
C2181	C2182	G2106	G1957	G1957	C1896	G1822	G1758	G1676	C1612	C1547	G1484	G1413	U1353	G1285
U2183	U2184	C2107	A1958	A1958	G1897	G1823	A1762	A1675	G1485	C1548	G1485	G1414	A1353	A1286
G2185	G2186	U2107	G1959	G1959	C1898	G1824	G1763	A1676	A1614	C1549	A1486	U1415	A1354	A1287
C2187	C2188	G2108	A1960	A1960	A1900	A1825	G1764	G1677	G1615	C1550	G1487	G1416	G1355	U1288
U2189	U2190	C2097	C1961	C1961	A1901	G1826	C1765	G1678	A1616	C1551	G1488	C1417	G1356	G1289
G2191	G2192	U2098	G1962	G1962	C1902	G1827	U1766	G1679	U1489	G1552	U1489	U1357	C1290	C1291
C2193	C2194	U2099	U1963	U1963	G1903	G1828	C1767	G1681	C1617	A1553	A1490	G1358	U1357	U1290
U2195	U2196	G2109	C1964	C1964	G1904	A1829	U1768	G1682	C1618	A1554	A1491	G1359	U1358	G1291
G2197	G2198	C2110	A1965	A1965	C1905	G1830	G1769	C1683	G1619	A1555	G1491	G1421	G1360	U1294
A2199	A2200	U2101	G1966	G1966	G1906	G1831	G1770	C1684	G1620	C1556	G1492	G1422	G1361	U1295
C2201	C2202	G2111	C1967	C1967	G1907	G1832	C1771	C1685	G1621	C1557	C1493	G1423	G1362	G1296
U2203	U2204	C2098	G1968	G1968	C1908	G1833	G1772	C1686	G1622	C1558	A1494	G1424	C1363	C1297
G2205	G2206	U2102	A1969	A1969	C1909	U1834	A1773	G1687	G1623	A1559	A1495	G1425	G1364	G1303
C2207	C2208	G2112	C1970	C1970	G1910	U1835	C1774	U1688	G1624	G1560	A1496	C1428	G1365	C1306
U2209	U2210	C2103	G1971	G1971	U1911	G1836	U1775	U1689	C1625	A1561	U1497	G1429	A1366	A1301
G2211	G2212	U2104	A1972	A1972	A1912	G1837	G1776	A1690	G1626	G1562	C1498	C1430	A1367	A1302
C2213	C2214	G2105	G1973	G1973	A1913	G1838	U1777	C1691	G1627	A1563	C1499	U1431	G1368	G1304
U2215	U2216	C2106	C1974	C1974	G1914	G1839	U1778	G1692	G1628	G1564	G1500	G1432	G1369	C1305
G2217	G2218	U2106	U1975	U1975	U1915	U1841	U1779	G1693	U1629	C1565	U1503	C1433	G1370	C1306
A2219	A2220	C2107	G1976	G1976	U1916	G1842	A1780	G1694	G1630	A1566	C1504	U1434	G1371	A1307
C2221	C2222	G2108	A1977	A1977	A1917	G1843	C1781	G1695	G1630A	A1567	C1505	G1435	U1372	A1308
U2223	U2224	C2109	U1978	U1978	A1918	G1844	C1782	A1698	G1631	G1568	C1506	G1436	G1373	G1309
G2225	G2226	U2110	G1979	G1979	A1919	G1845	A1783	A1701	A1634					



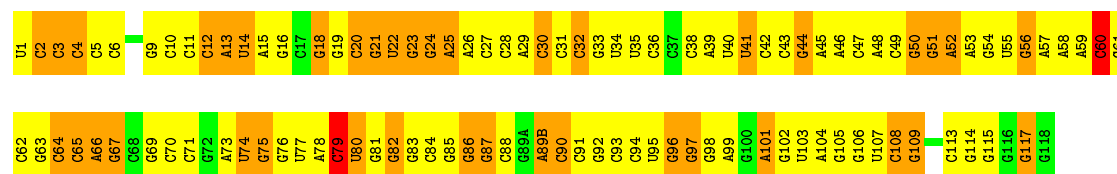
• Molecule 60: 5S rRNA

Chain BB: 19% 56% 23%



• Molecule 60: 5S rRNA

Category	Percentage
Fair	11%
Good	55%
Bad	33%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	306.92Å 677.00Å 356.78Å 90.00° 89.90° 90.00°	Depositor
Resolution (Å)	49.98 – 3.80 127.40 – 3.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (49.98-3.80) 60.2 (127.40-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 3.78Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.295 , 0.331 0.315 , 0.354	Depositor DCC
R_{free} test set	6492 reflections (1.51%)	DCC
Wilson B-factor (Å ²)	66.8	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.11 , -10.0	EDS
Estimated twinning fraction	0.340 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.17$, $\langle L^2 \rangle = 0.05$	Xtriage
Outliers	0 of 428645 reflections	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	312066	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.07% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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, FUA, ACE, NMY

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AB	0.41	0/1945	0.69	0/2621
1	CB	0.41	0/1945	0.69	1/2621 (0.0%)
2	AC	0.27	0/1645	0.55	0/2216
2	CC	0.29	0/1645	0.56	0/2216
3	AD	0.31	0/1733	0.59	0/2318
3	CD	0.29	0/1733	0.61	1/2318 (0.0%)
4	AE	0.30	0/1172	0.57	0/1576
4	CE	0.30	0/1172	0.61	1/1576 (0.1%)
5	AF	0.28	0/856	0.56	0/1154
5	CF	0.30	0/856	0.59	0/1154
6	AG	0.27	0/1276	0.51	0/1709
6	CG	0.28	0/1276	0.51	0/1709
7	AH	0.29	0/1136	0.60	0/1527
7	CH	0.28	0/1136	0.55	0/1527
8	AI	0.27	0/1029	0.56	0/1379
8	CI	0.27	0/1029	0.50	0/1379
9	AJ	0.27	0/815	0.54	0/1095
9	CJ	0.28	0/815	0.56	0/1095
10	AK	0.38	0/900	0.62	0/1213
10	CK	0.39	0/900	0.61	0/1213
11	AL	0.43	0/992	0.80	0/1327
11	CL	0.45	0/992	0.81	1/1327 (0.1%)
12	AM	0.27	0/1008	0.53	0/1347
12	CM	0.27	0/1008	0.58	0/1347
13	AN	0.29	0/501	0.51	0/664
13	CN	0.34	0/501	0.57	0/664
14	AO	0.34	0/745	0.61	0/992
14	CO	0.33	0/745	0.57	1/992 (0.1%)
15	AP	0.32	0/722	0.61	0/970
15	CP	0.32	0/722	0.60	0/970
16	AQ	0.35	0/848	0.67	1/1131 (0.1%)
16	CQ	0.36	0/848	0.68	0/1131

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AR	0.29	0/579	0.58	0/768
17	CR	0.29	0/579	0.57	0/768
18	AS	0.29	0/647	0.56	0/870
18	CS	0.26	0/647	0.53	0/870
19	AT	0.30	0/765	0.54	0/1007
19	CT	0.31	0/765	0.51	0/1007
20	AY	0.37	0/5270	0.66	1/7135 (0.0%)
20	CY	0.36	0/5270	0.67	3/7135 (0.0%)
21	AA	0.39	9/36351 (0.0%)	1.12	149/56736 (0.3%)
21	CA	0.42	6/36351 (0.0%)	1.17	239/56736 (0.4%)
22	AW	0.52	0/1827	1.42	41/2845 (1.4%)
22	CW	0.48	0/1827	1.36	23/2845 (0.8%)
23	AV	1.27	1/881 (0.1%)	1.42	12/1372 (0.9%)
23	CV	0.82	7/880 (0.8%)	2.11	42/1372 (3.1%)
24	AX	0.62	1/1815 (0.1%)	1.56	47/2826 (1.7%)
24	CX	0.60	3/1815 (0.2%)	1.54	43/2826 (1.5%)
25	BC	0.51	1/1774 (0.1%)	0.86	2/2391 (0.1%)
25	DC	0.51	0/1774	0.80	0/2391
26	BD	0.40	2/2195 (0.1%)	0.62	1/2955 (0.0%)
26	DD	0.31	0/2195	0.60	0/2955
27	BE	0.35	0/1602	0.69	2/2160 (0.1%)
27	DE	0.33	0/1602	0.67	0/2160
28	BF	0.39	0/1663	0.81	6/2249 (0.3%)
28	DF	0.38	0/1663	0.78	4/2249 (0.2%)
29	BG	0.27	0/1499	0.54	0/2016
29	DG	0.29	0/1499	0.58	0/2016
30	BH	0.28	0/1298	0.58	0/1751
30	DH	0.28	0/1298	0.55	0/1751
32	BK	0.28	0/1054	0.55	1/1427 (0.1%)
32	DK	0.31	0/1054	0.58	1/1427 (0.1%)
33	BN	0.81	3/1141 (0.3%)	1.39	16/1537 (1.0%)
33	DN	0.81	2/1141 (0.2%)	1.28	13/1537 (0.8%)
34	BO	0.32	0/943	0.63	2/1269 (0.2%)
34	DO	0.32	0/943	0.65	0/1269
35	BP	0.28	0/1131	0.64	2/1504 (0.1%)
35	DP	0.29	0/1131	0.63	0/1504
36	BQ	0.36	0/1143	0.67	0/1527
36	DQ	0.33	0/1143	0.63	0/1527
37	BR	0.33	0/974	0.64	1/1302 (0.1%)
37	DR	0.32	0/974	0.59	0/1302
38	BS	0.35	0/783	0.69	0/1041
38	DS	0.36	0/783	0.71	0/1041
39	BT	0.30	0/1161	0.63	0/1549

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	DT	0.30	0/1161	0.64	0/1549
40	BU	0.36	0/982	0.57	0/1306
40	DU	0.33	0/982	0.57	0/1306
41	BV	0.34	0/790	0.76	2/1057 (0.2%)
41	DV	0.31	0/790	0.65	1/1057 (0.1%)
42	BW	0.32	0/911	0.64	0/1220
42	DW	0.38	0/911	0.69	1/1220 (0.1%)
43	BX	0.28	0/748	0.56	1/1004 (0.1%)
43	DX	0.28	0/748	0.56	1/1004 (0.1%)
44	BY	0.28	0/831	0.54	0/1108
44	DY	0.27	0/831	0.57	1/1108 (0.1%)
45	BZ	0.28	0/1505	0.58	0/2042
45	DZ	0.29	0/1505	0.58	0/2042
46	B0	0.25	0/671	0.54	0/892
46	D0	0.25	0/671	0.50	0/892
47	B1	0.51	0/739	1.01	5/981 (0.5%)
47	D1	0.48	0/739	0.92	2/981 (0.2%)
48	B2	0.37	0/600	0.63	0/793
48	D2	0.34	0/600	0.65	0/793
49	B3	0.29	0/482	0.58	0/646
49	D3	0.26	0/482	0.58	0/646
50	B4	0.38	0/276	0.67	0/372
50	D4	0.37	0/276	0.68	0/372
51	B5	0.28	0/473	0.57	0/639
51	D5	0.32	0/473	0.62	0/639
52	B6	0.30	0/440	0.82	3/586 (0.5%)
52	D6	0.31	0/440	0.68	0/586
53	B7	1.14	6/438 (1.4%)	1.51	7/575 (1.2%)
53	D7	0.29	0/438	0.55	0/575
54	B8	0.31	0/525	0.58	0/691
54	D8	0.30	0/525	0.61	0/691
55	B9	0.28	0/310	0.55	0/407
55	D9	0.32	0/310	0.57	0/407
56	Be	0.25	0/538	0.53	0/715
56	De	0.27	0/538	0.51	0/715
59	BA	0.38	1/69437 (0.0%)	1.11	247/108401 (0.2%)
59	DA	0.40	2/69437 (0.0%)	1.14	333/108401 (0.3%)
60	BB	0.43	0/2853	1.28	29/4451 (0.7%)
60	DB	0.48	0/2853	1.34	49/4451 (1.1%)
All	All	0.40	44/334735 (0.0%)	1.04	1339/498724 (0.3%)

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	1
3	CD	0	1
10	AK	0	1
10	CK	0	1
15	AP	0	1
15	CP	0	1
20	AY	0	2
25	BC	0	6
25	DC	0	5
26	BD	0	1
26	DD	0	1
27	BE	0	1
28	BF	0	4
28	DF	0	2
29	DG	0	1
31	BJ	0	2
31	DJ	0	3
33	BN	0	17
33	DN	0	15
34	BO	0	1
34	DO	0	1
36	BQ	0	1
38	BS	0	1
38	DS	0	1
39	BT	0	1
39	DT	0	1
42	BW	0	1
42	DW	0	2
45	BZ	0	1
45	DZ	0	1
47	B1	0	4
47	D1	0	3
53	B7	0	1
All	All	0	86

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AV	1	G	P-O5'	35.77	1.95	1.59
53	B7	40	TRP	CD2-CE2	-12.82	1.25	1.41
21	AA	1126	U	C2-O2	-9.80	1.13	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	CA	1126	U	C2-O2	-9.32	1.14	1.22
53	B7	40	TRP	CE3-CZ3	8.92	1.53	1.38

The worst 5 of 1339 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	AV	1	G	O5'-P-OP2	24.05	139.56	110.70
23	CV	10	G	N1-C6-O6	-22.12	106.63	119.90
21	AA	1126	U	N1-C2-N3	18.77	126.16	114.90
53	B7	40	TRP	CE2-CD2-CG	18.75	122.30	107.30
21	CA	1126	U	N1-C2-N3	18.50	126.00	114.90

There are no chirality outliers.

5 of 86 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AB	163	PHE	Peptide
10	AK	43	SER	Peptide
15	AP	34	GLU	Peptide
20	AY	34	TYR	Peptide
20	AY	630	GLN	Peptide

5.2 Too-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 hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AB	1910	0	1957	118	0
1	CB	1910	0	1957	112	0
2	AC	1621	0	1688	90	0
2	CC	1621	0	1688	85	0
3	AD	1703	0	1767	109	0
3	CD	1703	0	1767	92	0
4	AE	1156	0	1213	55	0
4	CE	1156	0	1213	57	0
5	AF	843	0	857	33	0
5	CF	843	0	857	49	0
6	AG	1257	0	1296	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	CG	1257	0	1296	61	0
7	AH	1116	0	1177	78	0
7	CH	1116	0	1177	76	0
8	AI	1010	0	1037	62	0
8	CI	1010	0	1037	59	0
9	AJ	802	0	849	48	0
9	CJ	802	0	849	57	0
10	AK	885	0	904	62	0
10	CK	885	0	904	63	0
11	AL	976	0	1062	107	0
11	CL	976	0	1062	105	0
12	AM	997	0	1072	35	0
12	CM	997	0	1072	68	0
13	AN	492	0	533	36	0
13	CN	492	0	533	40	0
14	AO	734	0	771	49	0
14	CO	734	0	771	32	0
15	AP	706	0	725	44	0
15	CP	706	0	725	45	0
16	AQ	835	0	904	69	0
16	CQ	835	0	904	63	0
17	AR	574	0	644	34	0
17	CR	574	0	644	35	0
18	AS	634	0	655	40	0
18	CS	634	0	655	28	0
19	AT	763	0	861	50	0
19	CT	763	0	861	44	0
20	AY	5173	0	5239	335	0
20	CY	5173	0	5239	330	0
21	AA	32474	0	16393	1203	0
21	CA	32474	0	16392	1571	0
22	AW	1635	0	831	83	0
22	CW	1635	0	831	86	0
23	AV	783	0	391	43	0
23	CV	781	0	393	76	0
24	AX	1629	0	832	75	0
24	CX	1629	0	832	92	0
25	BC	1742	0	1798	155	0
25	DC	1742	0	1798	126	0
26	BD	2145	0	2234	174	0
26	DD	2145	0	2234	154	0
27	BE	1569	0	1634	135	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	DE	1569	0	1634	124	0
28	BF	1628	0	1680	156	0
28	DF	1628	0	1680	128	0
29	BG	1474	0	1535	78	0
29	DG	1474	0	1535	102	0
30	BH	1274	0	1342	65	0
30	DH	1274	0	1342	75	0
31	BJ	851	0	207	26	0
31	DJ	851	0	207	18	0
32	BK	1035	0	1082	63	0
32	DK	1035	0	1082	72	0
33	BN	1114	0	1185	281	0
33	DN	1114	0	1185	309	0
34	BO	933	0	996	71	0
34	DO	933	0	996	60	0
35	BP	1114	0	1187	105	0
35	DP	1114	0	1187	106	0
36	BQ	1122	0	1179	91	0
36	DQ	1122	0	1179	85	0
37	BR	960	0	1021	85	0
37	DR	960	0	1021	85	0
38	BS	775	0	835	74	0
38	DS	775	0	835	82	0
39	BT	1147	0	1207	89	0
39	DT	1147	0	1207	92	0
40	BU	964	0	1022	77	0
40	DU	964	0	1022	69	0
41	BV	779	0	852	70	0
41	DV	779	0	852	54	0
42	BW	900	0	964	71	0
42	DW	900	0	964	58	0
43	BX	734	0	789	31	0
43	DX	734	0	789	28	0
44	BY	818	0	908	54	0
44	DY	818	0	908	62	0
45	BZ	1473	0	1497	85	0
45	DZ	1473	0	1497	80	0
46	B0	662	0	688	31	0
46	D0	662	0	688	47	0
47	B1	732	0	808	58	0
47	D1	732	0	808	67	0
48	B2	598	0	653	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	D2	598	0	653	52	0
49	B3	477	0	529	25	0
49	D3	477	0	529	29	0
50	B4	271	0	284	11	0
50	D4	271	0	284	21	0
51	B5	459	0	480	28	0
51	D5	459	0	480	36	0
52	B6	433	0	461	34	0
52	D6	433	0	461	43	0
53	B7	430	0	480	29	0
53	D7	430	0	480	33	0
54	B8	517	0	582	44	0
54	D8	517	0	582	43	0
55	B9	307	0	338	31	0
55	D9	307	0	338	26	0
56	Be	686	0	620	0	0
56	De	686	0	621	0	0
57	Bf	156	0	47	0	0
57	Bg	156	0	47	0	0
57	Df	156	0	48	0	0
57	Dg	156	0	46	0	0
58	Bh	151	0	41	0	0
58	Dh	151	0	48	0	0
59	BA	61997	0	31250	2493	0
59	DA	61997	0	31250	2828	0
60	BB	2551	0	1295	143	0
60	DB	2551	0	1295	165	0
61	AY	28	0	12	8	0
61	CY	28	0	12	14	0
62	AY	37	0	47	21	0
62	CY	37	0	47	14	0
63	AA	42	0	46	26	0
63	BA	126	0	138	60	0
63	CA	42	0	46	34	0
63	DA	42	0	46	23	0
64	BA	1	0	0	0	0
64	CY	1	0	0	0	0
All	All	312066	0	215233	14871	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 29.

The worst 5 of 14871 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:DN:114:ARG:HH21	59:DA:527:C:C1'	1.22	1.51
24:CX:75:C:N4	59:DA:2553:G:H1	1.11	1.47
59:DA:2681:C:N4	59:DA:2725:A:H62	1.09	1.47
33:DN:114:ARG:NH2	59:DA:527:C:H1'	1.12	1.44
21:CA:1538:C:C2	23:CV:7:G:N2	1.88	1.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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%)	168 (72%)	45 (19%)	20 (9%)	1	17
1	CB	233/235 (99%)	171 (73%)	45 (19%)	17 (7%)	1	22
2	AC	205/207 (99%)	137 (67%)	39 (19%)	29 (14%)	0	6
2	CC	205/207 (99%)	150 (73%)	35 (17%)	20 (10%)	1	14
3	AD	206/208 (99%)	140 (68%)	41 (20%)	25 (12%)	0	8
3	CD	206/208 (99%)	152 (74%)	33 (16%)	21 (10%)	1	13
4	AE	149/151 (99%)	122 (82%)	20 (13%)	7 (5%)	3	33
4	CE	149/151 (99%)	115 (77%)	24 (16%)	10 (7%)	1	25
5	AF	99/101 (98%)	76 (77%)	15 (15%)	8 (8%)	1	18
5	CF	99/101 (98%)	74 (75%)	16 (16%)	9 (9%)	1	16
6	AG	153/155 (99%)	123 (80%)	22 (14%)	8 (5%)	2	30
6	CG	153/155 (99%)	118 (77%)	23 (15%)	12 (8%)	1	20
7	AH	136/138 (99%)	102 (75%)	23 (17%)	11 (8%)	1	18
7	CH	136/138 (99%)	96 (71%)	30 (22%)	10 (7%)	1	21
8	AI	125/127 (98%)	97 (78%)	22 (18%)	6 (5%)	3	32
8	CI	125/127 (98%)	98 (78%)	21 (17%)	6 (5%)	3	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	AJ	97/99 (98%)	71 (73%)	15 (16%)	11 (11%)	0	10
9	CJ	97/99 (98%)	74 (76%)	16 (16%)	7 (7%)	1	22
10	AK	117/119 (98%)	83 (71%)	21 (18%)	13 (11%)	0	10
10	CK	117/119 (98%)	79 (68%)	21 (18%)	17 (14%)	0	6
11	AL	123/125 (98%)	41 (33%)	44 (36%)	38 (31%)	0	0
11	CL	123/125 (98%)	49 (40%)	37 (30%)	37 (30%)	0	0
12	AM	123/125 (98%)	94 (76%)	19 (15%)	10 (8%)	1	18
12	CM	123/125 (98%)	95 (77%)	17 (14%)	11 (9%)	1	16
13	AN	58/60 (97%)	38 (66%)	17 (29%)	3 (5%)	2	30
13	CN	58/60 (97%)	35 (60%)	14 (24%)	9 (16%)	0	5
14	AO	86/88 (98%)	72 (84%)	12 (14%)	2 (2%)	8	51
14	CO	86/88 (98%)	65 (76%)	18 (21%)	3 (4%)	4	42
15	AP	82/84 (98%)	58 (71%)	16 (20%)	8 (10%)	1	14
15	CP	82/84 (98%)	62 (76%)	13 (16%)	7 (8%)	1	17
16	AQ	98/100 (98%)	70 (71%)	22 (22%)	6 (6%)	2	27
16	CQ	98/100 (98%)	76 (78%)	16 (16%)	6 (6%)	2	27
17	AR	68/70 (97%)	50 (74%)	9 (13%)	9 (13%)	0	6
17	CR	68/70 (97%)	56 (82%)	8 (12%)	4 (6%)	2	27
18	AS	77/79 (98%)	43 (56%)	23 (30%)	11 (14%)	0	6
18	CS	77/79 (98%)	47 (61%)	27 (35%)	3 (4%)	4	38
19	AT	97/99 (98%)	72 (74%)	17 (18%)	8 (8%)	1	18
19	CT	97/99 (98%)	82 (84%)	10 (10%)	5 (5%)	2	30
20	AY	657/687 (96%)	407 (62%)	174 (26%)	76 (12%)	0	9
20	CY	657/687 (96%)	437 (66%)	135 (20%)	85 (13%)	0	7
25	BC	226/228 (99%)	107 (47%)	63 (28%)	56 (25%)	0	1
25	DC	226/228 (99%)	114 (50%)	52 (23%)	60 (26%)	0	1
26	BD	273/275 (99%)	174 (64%)	60 (22%)	39 (14%)	0	6
26	DD	273/275 (99%)	180 (66%)	59 (22%)	34 (12%)	0	8
27	BE	203/205 (99%)	134 (66%)	41 (20%)	28 (14%)	0	6
27	DE	203/205 (99%)	124 (61%)	49 (24%)	30 (15%)	0	5
28	BF	206/208 (99%)	139 (68%)	43 (21%)	24 (12%)	0	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	DF	206/208 (99%)	127 (62%)	51 (25%)	28 (14%)	0	6
29	BG	179/181 (99%)	131 (73%)	37 (21%)	11 (6%)	2	27
29	DG	179/181 (99%)	127 (71%)	37 (21%)	15 (8%)	1	17
30	BH	165/167 (99%)	117 (71%)	31 (19%)	17 (10%)	1	12
30	DH	165/167 (99%)	116 (70%)	30 (18%)	19 (12%)	0	9
32	BK	138/140 (99%)	91 (66%)	32 (23%)	15 (11%)	0	11
32	DK	138/140 (99%)	77 (56%)	44 (32%)	17 (12%)	0	8
33	BN	137/139 (99%)	52 (38%)	32 (23%)	53 (39%)	0	0
33	DN	137/139 (99%)	55 (40%)	28 (20%)	54 (39%)	0	0
34	BO	120/122 (98%)	89 (74%)	21 (18%)	10 (8%)	1	18
34	DO	120/122 (98%)	86 (72%)	22 (18%)	12 (10%)	1	13
35	BP	144/146 (99%)	84 (58%)	36 (25%)	24 (17%)	0	4
35	DP	144/146 (99%)	82 (57%)	39 (27%)	23 (16%)	0	5
36	BQ	139/141 (99%)	84 (60%)	35 (25%)	20 (14%)	0	6
36	DQ	139/141 (99%)	94 (68%)	34 (24%)	11 (8%)	1	19
37	BR	115/117 (98%)	80 (70%)	20 (17%)	15 (13%)	0	7
37	DR	115/117 (98%)	80 (70%)	22 (19%)	13 (11%)	0	10
38	BS	97/99 (98%)	52 (54%)	26 (27%)	19 (20%)	0	3
38	DS	97/99 (98%)	51 (53%)	27 (28%)	19 (20%)	0	3
39	BT	136/138 (99%)	81 (60%)	27 (20%)	28 (21%)	0	2
39	DT	136/138 (99%)	79 (58%)	31 (23%)	26 (19%)	0	3
40	BU	115/117 (98%)	88 (76%)	17 (15%)	10 (9%)	1	16
40	DU	115/117 (98%)	90 (78%)	17 (15%)	8 (7%)	1	23
41	BV	99/101 (98%)	56 (57%)	28 (28%)	15 (15%)	0	5
41	DV	99/101 (98%)	64 (65%)	21 (21%)	14 (14%)	0	6
42	BW	111/113 (98%)	74 (67%)	25 (22%)	12 (11%)	0	11
42	DW	111/113 (98%)	76 (68%)	23 (21%)	12 (11%)	0	11
43	BX	91/93 (98%)	71 (78%)	13 (14%)	7 (8%)	1	20
43	DX	91/93 (98%)	67 (74%)	10 (11%)	14 (15%)	0	5
44	BY	105/107 (98%)	54 (51%)	31 (30%)	20 (19%)	0	3
44	DY	105/107 (98%)	59 (56%)	26 (25%)	20 (19%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	BZ	183/185 (99%)	121 (66%)	43 (24%)	19 (10%)	1	12
45	DZ	183/185 (99%)	109 (60%)	45 (25%)	29 (16%)	0	5
46	B0	82/84 (98%)	63 (77%)	14 (17%)	5 (6%)	2	27
46	D0	82/84 (98%)	59 (72%)	18 (22%)	5 (6%)	2	27
47	B1	91/93 (98%)	48 (53%)	24 (26%)	19 (21%)	0	2
47	D1	91/93 (98%)	52 (57%)	20 (22%)	19 (21%)	0	2
48	B2	69/71 (97%)	51 (74%)	12 (17%)	6 (9%)	1	16
48	D2	69/71 (97%)	53 (77%)	12 (17%)	4 (6%)	2	28
49	B3	58/60 (97%)	49 (84%)	7 (12%)	2 (3%)	5	43
49	D3	58/60 (97%)	47 (81%)	8 (14%)	3 (5%)	2	30
50	B4	33/35 (94%)	15 (46%)	13 (39%)	5 (15%)	0	5
50	D4	33/35 (94%)	17 (52%)	11 (33%)	5 (15%)	0	5
51	B5	57/59 (97%)	36 (63%)	14 (25%)	7 (12%)	0	8
51	D5	57/59 (97%)	38 (67%)	6 (10%)	13 (23%)	0	1
52	B6	48/50 (96%)	24 (50%)	15 (31%)	9 (19%)	0	3
52	D6	48/50 (96%)	20 (42%)	17 (35%)	11 (23%)	0	1
53	B7	47/49 (96%)	33 (70%)	11 (23%)	3 (6%)	2	26
53	D7	47/49 (96%)	26 (55%)	14 (30%)	7 (15%)	0	5
54	B8	62/64 (97%)	34 (55%)	16 (26%)	12 (19%)	0	3
54	D8	62/64 (97%)	35 (56%)	13 (21%)	14 (23%)	0	1
55	B9	35/37 (95%)	29 (83%)	5 (14%)	1 (3%)	6	46
55	D9	35/37 (95%)	25 (71%)	7 (20%)	3 (9%)	1	17
56	Be	70/103 (68%)	39 (56%)	23 (33%)	8 (11%)	0	9
56	De	70/103 (68%)	40 (57%)	17 (24%)	13 (19%)	0	3
All	All	13246/13568 (98%)	8764 (66%)	2800 (21%)	1682 (13%)	0	7

5 of 1682 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AB	76	GLN
1	AB	190	THR
2	AC	12	LEU
2	AC	110	ASN
2	AC	130	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AB	203/203 (100%)	163 (80%)	40 (20%)	1	13
1	CB	203/203 (100%)	158 (78%)	45 (22%)	1	9
2	AC	161/161 (100%)	129 (80%)	32 (20%)	1	12
2	CC	161/161 (100%)	128 (80%)	33 (20%)	1	11
3	AD	180/180 (100%)	142 (79%)	38 (21%)	1	10
3	CD	180/180 (100%)	148 (82%)	32 (18%)	2	17
4	AE	116/116 (100%)	92 (79%)	24 (21%)	1	11
4	CE	116/116 (100%)	89 (77%)	27 (23%)	1	8
5	AF	90/90 (100%)	73 (81%)	17 (19%)	2	14
5	CF	90/90 (100%)	77 (86%)	13 (14%)	4	28
6	AG	126/126 (100%)	111 (88%)	15 (12%)	6	35
6	CG	126/126 (100%)	110 (87%)	16 (13%)	5	32
7	AH	119/119 (100%)	98 (82%)	21 (18%)	2	17
7	CH	119/119 (100%)	94 (79%)	25 (21%)	1	10
8	AI	98/98 (100%)	83 (85%)	15 (15%)	3	25
8	CI	98/98 (100%)	78 (80%)	20 (20%)	1	11
9	AJ	89/89 (100%)	71 (80%)	18 (20%)	1	12
9	CJ	89/89 (100%)	68 (76%)	21 (24%)	1	7
10	AK	90/90 (100%)	80 (89%)	10 (11%)	8	39
10	CK	90/90 (100%)	79 (88%)	11 (12%)	6	34
11	AL	104/104 (100%)	82 (79%)	22 (21%)	1	10
11	CL	104/104 (100%)	82 (79%)	22 (21%)	1	10
12	AM	100/100 (100%)	84 (84%)	16 (16%)	3	22
12	CM	100/100 (100%)	79 (79%)	21 (21%)	1	10
13	AN	49/49 (100%)	40 (82%)	9 (18%)	2	15
13	CN	49/49 (100%)	38 (78%)	11 (22%)	1	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	AO	79/79 (100%)	61 (77%)	18 (23%)	1	8
14	CO	79/79 (100%)	68 (86%)	11 (14%)	4	30
15	AP	72/72 (100%)	68 (94%)	4 (6%)	26	67
15	CP	72/72 (100%)	60 (83%)	12 (17%)	3	20
16	AQ	95/95 (100%)	80 (84%)	15 (16%)	3	23
16	CQ	95/95 (100%)	81 (85%)	14 (15%)	4	27
17	AR	61/61 (100%)	49 (80%)	12 (20%)	1	13
17	CR	61/61 (100%)	54 (88%)	7 (12%)	7	37
18	AS	69/69 (100%)	52 (75%)	17 (25%)	1	7
18	CS	69/69 (100%)	53 (77%)	16 (23%)	1	8
19	AT	76/76 (100%)	64 (84%)	12 (16%)	3	23
19	CT	76/76 (100%)	58 (76%)	18 (24%)	1	7
20	AY	558/579 (96%)	450 (81%)	108 (19%)	2	13
20	CY	558/579 (96%)	446 (80%)	112 (20%)	1	12
25	BC	180/180 (100%)	130 (72%)	50 (28%)	0	4
25	DC	180/180 (100%)	146 (81%)	34 (19%)	2	14
26	BD	217/217 (100%)	182 (84%)	35 (16%)	3	22
26	DD	217/217 (100%)	173 (80%)	44 (20%)	1	11
27	BE	165/165 (100%)	134 (81%)	31 (19%)	2	14
27	DE	165/165 (100%)	127 (77%)	38 (23%)	1	8
28	BF	165/165 (100%)	129 (78%)	36 (22%)	1	9
28	DF	165/165 (100%)	132 (80%)	33 (20%)	1	12
29	BG	155/155 (100%)	140 (90%)	15 (10%)	10	45
29	DG	155/155 (100%)	131 (84%)	24 (16%)	3	24
30	BH	136/136 (100%)	111 (82%)	25 (18%)	2	15
30	DH	136/136 (100%)	117 (86%)	19 (14%)	4	29
32	BK	105/105 (100%)	77 (73%)	28 (27%)	0	5
32	DK	105/105 (100%)	81 (77%)	24 (23%)	1	8
33	BN	118/118 (100%)	88 (75%)	30 (25%)	1	6
33	DN	118/118 (100%)	84 (71%)	34 (29%)	0	4
34	BO	100/100 (100%)	79 (79%)	21 (21%)	1	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	DO	100/100 (100%)	82 (82%)	18 (18%)	2	16
35	BP	112/112 (100%)	84 (75%)	28 (25%)	1	6
35	DP	112/112 (100%)	88 (79%)	24 (21%)	1	10
36	BQ	111/111 (100%)	78 (70%)	33 (30%)	0	4
36	DQ	111/111 (100%)	91 (82%)	20 (18%)	2	16
37	BR	100/100 (100%)	82 (82%)	18 (18%)	2	16
37	DR	100/100 (100%)	78 (78%)	22 (22%)	1	9
38	BS	77/77 (100%)	64 (83%)	13 (17%)	2	19
38	DS	77/77 (100%)	58 (75%)	19 (25%)	1	7
39	BT	120/120 (100%)	93 (78%)	27 (22%)	1	9
39	DT	120/120 (100%)	91 (76%)	29 (24%)	1	7
40	BU	93/93 (100%)	78 (84%)	15 (16%)	3	22
40	DU	93/93 (100%)	76 (82%)	17 (18%)	2	15
41	BV	82/82 (100%)	59 (72%)	23 (28%)	0	4
41	DV	82/82 (100%)	68 (83%)	14 (17%)	2	19
42	BW	92/92 (100%)	79 (86%)	13 (14%)	4	29
42	DW	92/92 (100%)	72 (78%)	20 (22%)	1	9
43	BX	75/75 (100%)	58 (77%)	17 (23%)	1	8
43	DX	75/75 (100%)	59 (79%)	16 (21%)	1	10
44	BY	88/88 (100%)	65 (74%)	23 (26%)	0	5
44	DY	88/88 (100%)	74 (84%)	14 (16%)	3	23
45	BZ	162/162 (100%)	127 (78%)	35 (22%)	1	9
45	DZ	162/162 (100%)	135 (83%)	27 (17%)	3	20
46	B0	66/66 (100%)	59 (89%)	7 (11%)	8	41
46	D0	66/66 (100%)	53 (80%)	13 (20%)	1	13
47	B1	78/78 (100%)	56 (72%)	22 (28%)	0	4
47	D1	78/78 (100%)	57 (73%)	21 (27%)	0	5
48	B2	66/66 (100%)	56 (85%)	10 (15%)	3	25
48	D2	66/66 (100%)	57 (86%)	9 (14%)	5	30
49	B3	52/52 (100%)	44 (85%)	8 (15%)	3	24
49	D3	52/52 (100%)	45 (86%)	7 (14%)	5	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	B4	31/31 (100%)	23 (74%)	8 (26%)	0	6
50	D4	31/31 (100%)	22 (71%)	9 (29%)	0	4
51	B5	51/51 (100%)	38 (74%)	13 (26%)	1	6
51	D5	51/51 (100%)	45 (88%)	6 (12%)	6	35
52	B6	49/49 (100%)	35 (71%)	14 (29%)	0	4
52	D6	49/49 (100%)	31 (63%)	18 (37%)	0	1
53	B7	42/42 (100%)	35 (83%)	7 (17%)	3	20
53	D7	42/42 (100%)	36 (86%)	6 (14%)	4	28
54	B8	54/54 (100%)	45 (83%)	9 (17%)	3	20
54	D8	54/54 (100%)	42 (78%)	12 (22%)	1	9
55	B9	34/34 (100%)	26 (76%)	8 (24%)	1	7
55	D9	34/34 (100%)	31 (91%)	3 (9%)	12	50
56	Be	54/54 (100%)	48 (89%)	6 (11%)	8	39
56	De	54/54 (100%)	47 (87%)	7 (13%)	5	32
All	All	11130/11172 (100%)	8951 (80%)	2179 (20%)	1	13

5 of 2179 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
46	B0	80	HIS
4	CE	112	LEU
43	DX	23	GLU
48	B2	44	LEU
1	CB	121	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 79 such sidechains are listed below:

Mol	Chain	Res	Type
3	CD	125	HIS
12	CM	101	GLN
44	DY	68	HIS
5	CF	7	ASN
10	CK	116	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1510/1511 (99%)	358 (23%)	16 (1%)
21	CA	1511/1511 (100%)	377 (24%)	16 (1%)
22	AW	76/77 (98%)	37 (48%)	1 (1%)
22	CW	76/77 (98%)	42 (55%)	2 (2%)
23	AV	35/36 (97%)	24 (68%)	9 (25%)
23	CV	35/36 (97%)	27 (77%)	7 (20%)
24	AX	75/78 (96%)	29 (38%)	1 (1%)
24	CX	75/78 (96%)	30 (40%)	0
59	BA	2878/2879 (99%)	748 (25%)	28 (0%)
59	DA	2878/2879 (99%)	715 (24%)	29 (1%)
60	BB	118/119 (99%)	27 (22%)	0
60	DB	118/119 (99%)	32 (27%)	0
All	All	9385/9400 (99%)	2446 (26%)	109 (1%)

5 of 2446 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	6	G
21	AA	7	G
21	AA	9	G
21	AA	31	G
21	AA	32	A

5 of 109 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
59	BA	2250	G
21	CA	748	C
59	DA	2438	U
59	BA	2422	A
21	CA	5	U

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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
63	NMY	AA	1601	-	45,45,45	0.57	0	58,67,67	0.95	2 (3%)
61	GDP	AY	701	-	23,30,30	1.37	3 (13%)	30,47,47	2.34	10 (33%)
62	FUA	AY	702	-	37,40,40	1.69	6 (16%)	45,64,64	1.66	7 (15%)
63	NMY	BA	2902	-	45,45,45	0.57	0	58,67,67	0.95	2 (3%)
63	NMY	BA	2903	-	45,45,45	0.58	0	58,67,67	0.95	2 (3%)
63	NMY	BA	2904	-	45,45,45	0.57	0	58,67,67	0.95	3 (5%)
63	NMY	CA	1601	-	45,45,45	0.57	0	58,67,67	0.95	2 (3%)
61	GDP	CY	701	-	23,30,30	1.35	4 (17%)	30,47,47	1.89	8 (26%)
62	FUA	CY	702	-	37,40,40	1.70	6 (16%)	45,64,64	1.66	7 (15%)
63	NMY	DA	2901	-	45,45,45	0.57	0	58,67,67	0.95	2 (3%)

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
63	NMY	AA	1601	-	-	1/18/94/94	0/4/4/4
61	GDP	AY	701	-	-	0/12/32/32	0/3/3/3
62	FUA	AY	702	-	-	0/10/92/92	0/4/4/4
63	NMY	BA	2902	-	-	1/18/94/94	0/4/4/4
63	NMY	BA	2903	-	-	1/18/94/94	0/4/4/4
63	NMY	BA	2904	-	-	1/18/94/94	0/4/4/4
63	NMY	CA	1601	-	-	1/18/94/94	0/4/4/4
61	GDP	CY	701	-	-	0/12/32/32	0/3/3/3
62	FUA	CY	702	-	-	0/10/92/92	0/4/4/4
63	NMY	DA	2901	-	-	1/18/94/94	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	CY	702	FUA	C23-C22	-5.99	1.39	1.51
62	AY	702	FUA	C23-C22	-5.91	1.40	1.51
62	AY	702	FUA	C23-C24	-4.19	1.39	1.53
62	CY	702	FUA	C23-C24	-4.17	1.39	1.53
62	AY	702	FUA	C24-C25	-3.83	1.39	1.50

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	AY	701	GDP	N3-C2-N1	-5.36	119.28	127.44
61	CY	701	GDP	N3-C2-N1	-4.63	120.39	127.44
62	CY	702	FUA	C13-C12-C11	-4.51	105.84	111.95
62	AY	702	FUA	C13-C12-C11	-4.49	105.87	111.95
62	AY	702	FUA	C16-O2-C31	-3.73	111.13	117.14

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
63	BA	2903	NMY	C15-O18-C18-C19
63	CA	1601	NMY	C15-O18-C18-C19
63	AA	1601	NMY	C15-O18-C18-C19
63	BA	2902	NMY	C15-O18-C18-C19
63	DA	2901	NMY	C15-O18-C18-C19

There are no ring outliers.

10 monomers are involved in 199 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
63	AA	1601	NMY	26	0
61	AY	701	GDP	8	0
62	AY	702	FUA	21	0
63	BA	2902	NMY	13	0
63	BA	2903	NMY	15	0
63	BA	2904	NMY	32	0
63	CA	1601	NMY	34	0
61	CY	701	GDP	14	0
62	CY	702	FUA	14	0
63	DA	2901	NMY	23	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AB	235/235 (100%)	-0.00	11 (4%) 35 23	17, 55, 103, 129	0
1	CB	235/235 (100%)	0.01	14 (5%) 25 15	17, 63, 111, 140	0
2	AC	207/207 (100%)	0.67	38 (18%) 2 1	18, 52, 99, 118	0
2	CC	207/207 (100%)	0.04	13 (6%) 23 14	15, 58, 99, 132	0
3	AD	208/208 (100%)	0.02	10 (4%) 34 22	14, 59, 107, 137	0
3	CD	208/208 (100%)	0.88	38 (18%) 2 1	20, 52, 102, 136	0
4	AE	151/151 (100%)	0.60	27 (17%) 2 2	26, 62, 96, 129	0
4	CE	151/151 (100%)	1.13	41 (27%) 1 1	19, 56, 99, 143	0
5	AF	101/101 (100%)	-0.17	0 100 100	22, 57, 111, 128	0
5	CF	101/101 (100%)	-0.28	2 (1%) 68 53	19, 56, 106, 128	0
6	AG	155/155 (100%)	0.19	11 (7%) 19 11	26, 78, 122, 150	0
6	CG	155/155 (100%)	-0.28	5 (3%) 51 35	38, 85, 120, 147	0
7	AH	138/138 (100%)	0.17	10 (7%) 18 11	16, 43, 87, 109	0
7	CH	138/138 (100%)	0.17	7 (5%) 32 21	10, 49, 86, 102	0
8	AI	127/127 (100%)	0.55	15 (11%) 6 5	30, 64, 101, 127	0
8	CI	127/127 (100%)	0.67	21 (16%) 2 2	9, 77, 108, 134	0
9	AJ	99/99 (100%)	1.00	24 (24%) 1 1	34, 64, 104, 146	0
9	CJ	99/99 (100%)	0.98	23 (23%) 1 1	22, 57, 107, 115	0
10	AK	119/119 (100%)	0.82	20 (16%) 2 2	13, 74, 139, 160	0
10	CK	119/119 (100%)	1.59	43 (36%) 0 1	21, 71, 125, 161	0
11	AL	125/125 (100%)	0.91	20 (16%) 3 2	15, 73, 145, 164	0
11	CL	125/125 (100%)	0.83	20 (16%) 3 2	27, 85, 148, 170	0
12	AM	125/125 (100%)	0.79	16 (12%) 5 4	43, 86, 129, 159	0
12	CM	125/125 (100%)	0.78	26 (20%) 1 1	27, 63, 103, 139	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
13	AN	60/60 (100%)	2.27	34 (56%)	0 1	33, 70, 116, 128	0
13	CN	60/60 (100%)	1.54	20 (33%)	0 1	30, 58, 105, 128	0
14	AO	88/88 (100%)	-0.10	2 (2%)	64 48	26, 53, 99, 110	0
14	CO	88/88 (100%)	-0.10	1 (1%)	82 69	8, 44, 84, 109	0
15	AP	84/84 (100%)	1.02	18 (21%)	1 1	33, 71, 110, 143	0
15	CP	84/84 (100%)	0.49	9 (10%)	8 5	39, 69, 111, 165	0
16	AQ	100/100 (100%)	1.03	25 (25%)	1 1	27, 62, 107, 131	0
16	CQ	100/100 (100%)	0.72	14 (14%)	4 3	22, 66, 120, 135	0
17	AR	70/70 (100%)	0.44	6 (8%)	13 8	19, 61, 102, 130	0
17	CR	70/70 (100%)	0.36	8 (11%)	7 5	24, 56, 100, 125	0
18	AS	79/79 (100%)	0.27	6 (7%)	17 10	17, 69, 111, 124	0
18	CS	79/79 (100%)	1.03	16 (20%)	1 1	28, 65, 108, 130	0
19	AT	99/99 (100%)	0.35	2 (2%)	68 53	17, 51, 85, 128	0
19	CT	99/99 (100%)	0.63	15 (15%)	3 2	26, 69, 110, 139	0
20	AY	661/687 (96%)	-0.23	20 (3%)	54 37	19, 64, 113, 178	0
20	CY	661/687 (96%)	-0.26	11 (1%)	73 58	11, 66, 108, 152	0
21	AA	1511/1511 (100%)	0.11	39 (2%)	59 43	10, 90, 161, 248	0
21	CA	1511/1511 (100%)	0.04	23 (1%)	76 62	10, 88, 160, 242	0
22	AW	77/77 (100%)	-0.04	0	100 100	15, 71, 130, 150	0
22	CW	77/77 (100%)	-0.14	0	100 100	30, 88, 145, 178	0
23	AV	36/36 (100%)	0.37	0	100 100	32, 89, 137, 186	0
23	CV	36/36 (100%)	0.62	3 (8%)	14 9	23, 139, 232, 237	0
24	AX	77/78 (98%)	0.69	6 (7%)	16 9	3, 65, 233, 320	0
24	CX	77/78 (98%)	0.84	9 (11%)	6 5	37, 123, 185, 285	0
25	BC	228/228 (100%)	0.46	26 (11%)	7 5	55, 104, 139, 159	0
25	DC	228/228 (100%)	0.45	30 (13%)	4 4	37, 90, 130, 169	0
26	BD	275/275 (100%)	1.52	99 (36%)	0 1	10, 61, 103, 125	0
26	DD	275/275 (100%)	0.91	52 (18%)	2 1	16, 57, 100, 127	0
27	BE	205/205 (100%)	1.47	65 (31%)	1 1	21, 60, 107, 131	0
27	DE	205/205 (100%)	1.19	58 (28%)	1 1	22, 57, 97, 142	0
28	BF	208/208 (100%)	0.55	25 (12%)	6 5	20, 67, 108, 149	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9
28	DF	208/208 (100%)	0.77	46 (22%)	1 1	23, 75, 120, 140	0
29	BG	181/181 (100%)	-0.06	5 (2%)	56 40	28, 69, 113, 148	0
29	DG	181/181 (100%)	-0.19	4 (2%)	65 50	25, 71, 113, 148	0
30	BH	167/167 (100%)	0.37	21 (12%)	5 4	29, 65, 108, 121	0
30	DH	167/167 (100%)	0.11	8 (4%)	34 22	24, 59, 100, 132	0
31	BJ	0/170	-	-	-	-	-
31	DJ	0/170	-	-	-	-	-
32	BK	140/140 (100%)	-0.29	0	100 100	32, 71, 114, 126	0
32	DK	140/140 (100%)	0.26	17 (12%)	6 5	34, 77, 113, 138	0
33	BN	139/139 (100%)	1.86	49 (35%)	0 1	23, 105, 298, 334	0
33	DN	139/139 (100%)	2.97	59 (42%)	0 1	16, 116, 252, 312	0
34	BO	122/122 (100%)	1.00	27 (22%)	1 1	12, 50, 93, 111	0
34	DO	122/122 (100%)	1.19	28 (22%)	1 1	28, 59, 103, 132	0
35	BP	146/146 (100%)	0.18	10 (6%)	20 12	25, 63, 106, 123	0
35	DP	146/146 (100%)	0.31	15 (10%)	9 6	25, 67, 104, 131	0
36	BQ	141/141 (100%)	1.32	36 (25%)	1 1	5, 54, 93, 109	0
36	DQ	141/141 (100%)	1.82	53 (37%)	0 1	27, 70, 113, 141	0
37	BR	117/117 (100%)	0.64	11 (9%)	11 6	29, 65, 116, 145	0
37	DR	117/117 (100%)	0.90	21 (17%)	2 2	27, 62, 97, 126	0
38	BS	99/99 (100%)	0.70	15 (15%)	3 2	14, 70, 108, 117	0
38	DS	99/99 (100%)	0.75	12 (12%)	6 5	19, 52, 96, 120	0
39	BT	138/138 (100%)	0.37	19 (13%)	4 3	16, 59, 101, 123	0
39	DT	138/138 (100%)	0.14	16 (11%)	6 5	15, 51, 109, 140	0
40	BU	117/117 (100%)	0.33	5 (4%)	39 25	20, 56, 96, 121	0
40	DU	117/117 (100%)	0.16	0	100 100	13, 53, 94, 142	0
41	BV	101/101 (100%)	0.75	14 (13%)	4 3	21, 66, 108, 127	0
41	DV	101/101 (100%)	0.51	7 (6%)	20 12	15, 65, 101, 126	0
42	BW	113/113 (100%)	0.66	18 (15%)	3 2	13, 54, 99, 111	0
42	DW	113/113 (100%)	0.39	11 (9%)	10 6	15, 64, 116, 148	0
43	BX	93/93 (100%)	1.06	20 (21%)	1 1	20, 54, 96, 115	0
43	DX	93/93 (100%)	0.78	14 (15%)	3 2	13, 45, 87, 126	0
44	BY	107/107 (100%)	0.78	21 (19%)	1 1	29, 58, 109, 149	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	DY	107/107 (100%)	1.47	37 (34%) 0 1	25, 62, 97, 138	0
45	BZ	185/185 (100%)	-0.22	3 (1%) 74 60	17, 58, 97, 113	0
45	DZ	185/185 (100%)	-0.03	11 (5%) 26 15	33, 64, 101, 138	0
46	B0	84/84 (100%)	2.11	41 (48%) 0 1	26, 75, 117, 131	0
46	D0	84/84 (100%)	1.71	26 (30%) 1 1	19, 65, 108, 116	0
47	B1	93/93 (100%)	1.27	25 (26%) 1 1	21, 84, 140, 156	0
47	D1	93/93 (100%)	2.03	33 (35%) 0 1	31, 103, 148, 181	0
48	B2	71/71 (100%)	0.00	1 (1%) 78 63	23, 55, 95, 116	0
48	D2	71/71 (100%)	0.28	3 (4%) 40 26	35, 61, 103, 118	0
49	B3	60/60 (100%)	-0.05	1 (1%) 73 58	29, 60, 99, 112	0
49	D3	60/60 (100%)	0.16	5 (8%) 14 9	36, 68, 94, 110	0
50	B4	35/35 (100%)	0.44	5 (14%) 4 3	27, 71, 110, 122	0
50	D4	35/35 (100%)	-0.29	0 100 100	64, 109, 144, 185	0
51	B5	59/59 (100%)	0.77	14 (23%) 1 1	25, 63, 106, 123	0
51	D5	59/59 (100%)	0.57	10 (16%) 2 2	31, 68, 113, 138	0
52	B6	50/50 (100%)	0.78	15 (30%) 1 1	13, 57, 107, 154	0
52	D6	50/50 (100%)	0.30	7 (14%) 4 3	26, 65, 120, 154	0
53	B7	49/49 (100%)	1.87	17 (34%) 0 1	46, 91, 136, 164	0
53	D7	49/49 (100%)	1.99	21 (42%) 0 1	51, 73, 109, 134	0
54	B8	64/64 (100%)	2.65	44 (68%) 0 1	26, 58, 109, 132	0
54	D8	64/64 (100%)	2.99	45 (70%) 0 1	30, 64, 104, 118	0
55	B9	37/37 (100%)	1.78	16 (43%) 0 1	39, 64, 109, 116	0
55	D9	37/37 (100%)	0.73	4 (10%) 8 5	34, 65, 116, 134	0
56	Be	72/103 (69%)	-0.06	3 (4%) 40 26	15, 49, 122, 163	0
56	De	72/103 (69%)	0.03	5 (6%) 20 12	14, 57, 118, 157	0
57	Bf	0/31	-	-	-	-
57	Bg	0/31	-	-	-	-
57	Df	0/31	-	-	-	-
57	Dg	0/31	-	-	-	-
58	Bh	0/30	-	-	-	-
58	Dh	0/30	-	-	-	-
59	BA	2879/2879 (100%)	0.25	109 (3%) 44 30	11, 89, 164, 284	0
59	DA	2879/2879 (100%)	0.28	122 (4%) 40 26	9, 88, 171, 274	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
60	BB	119/119 (100%)	-0.33	0 100 100	18, 80, 158, 172	0
60	DB	119/119 (100%)	-0.23	0 100 100	30, 88, 150, 175	0
All	All	22852/23492 (97%)	0.42	2302 (10%) 9 6	3, 73, 146, 334	0

The worst 5 of 2302 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
33	DN	108	PRO	21.5
33	DN	81	GLY	18.6
33	DN	95	PRO	15.4
33	DN	86	PRO	14.7
33	DN	107	LEU	14.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
62	FUA	AY	702	37/37	0.74	0.63	4.35	198,199,200,201	0
62	FUA	CY	702	37/37	0.80	0.64	3.75	194,196,197,197	0
63	NMY	AA	1601	42/42	0.76	0.43	3.18	16,27,36,38	42
63	NMY	BA	2902	42/42	0.74	0.44	1.86	14,24,43,44	42
63	NMY	CA	1601	42/42	0.82	0.34	1.54	14,25,34,37	42
61	GDP	CY	701	28/28	0.77	0.21	1.41	104,108,109,110	0
63	NMY	DA	2901	42/42	0.77	0.37	1.29	31,42,51,53	42
61	GDP	AY	701	28/28	0.69	0.24	1.01	179,183,185,185	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
63	NMY	BA	2903	42/42	0.74	0.56	0.76	18,29,38,41	42
63	NMY	BA	2904	42/42	0.67	0.52	0.71	42,50,59,62	42
64	MG	CY	703	1/1	0.91	0.19	-0.08	6,6,6,6	0
64	MG	BA	2901	1/1	0.56	0.14	-1.28	2,2,2,2	0

6.5 Other polymers [i](#)

There are no such residues in this entry.