wwPDB X-ray Structure Validation Summary Report (i)

Dec 17, 2023 – 01:07 PM EST

PDB ID	:	4U20
Title	:	Crystal structure of the E. coli ribosome bound to flopristin.
Authors	:	Noeske, J.; Huang, J.; Olivier, N.B.; Giacobbe, R.A.; Zambrowski, M.; Cate, J.H.D.
Deposited on	:	2014-07-16
Resolution	:	2.90 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

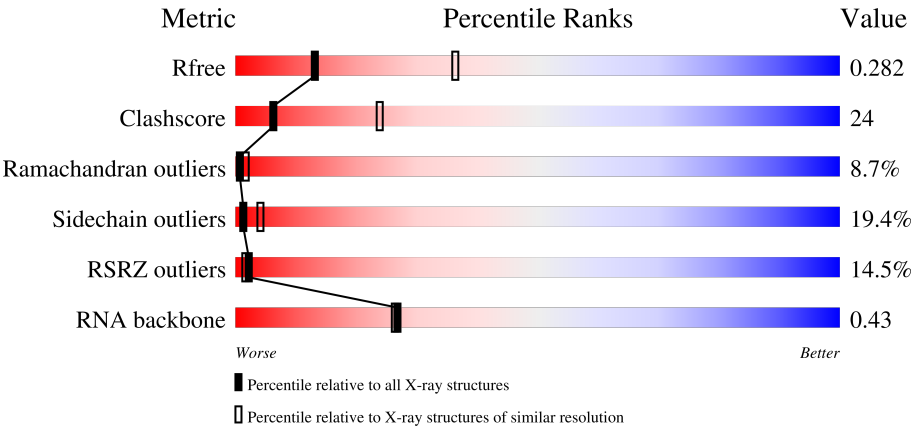
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	AA	1539	3% 30% 52% 17%
1	CA	1539	5% 31% 53% 16%
2	AB	218	19% 16% 46% 30% 7%
2	CB	218	29% 24% 48% 25% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	AC	206	4% 41% 45% 13%
3	CC	206	23% 36% 49% 14%
4	AD	205	6% 32% 47% 20%
4	CD	205	4% 42% 42% 14%
5	AE	150	4% 35% 46% 17%
5	CE	150	6% 36% 39% 23%
6	AF	100	% 29% 42% 26%
6	CF	100	8% 31% 44% 20% 5%
7	AG	151	18% 36% 46% 17%
7	CG	151	58% 42% 44% 12%
8	AH	129	2% 41% 42% 17%
8	CH	129	9% 43% 42% 14%
9	AI	127	17% 26% 50% 23%
9	CI	127	36% 32% 50% 16%
10	AJ	98	15% 20% 47% 28% 5%
10	CJ	98	58% 42% 43% 12%
11	AK	117	13% 35% 43% 21%
11	CK	117	5% 32% 52% 14%
12	AL	123	4% 51% 34% 12%
12	CL	123	7% 41% 37% 19%
13	AM	114	9% 39% 44% 13%
13	CM	114	69% 39% 43% 18%
14	AN	100	17% 25% 52% 15%
14	CN	100	50% 33% 46% 16%
15	AO	88	6% 33% 48% 19%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	CO	88	6% 41% 44% 14%
16	AP	82	13% 26% 43% 26% 6%
16	CP	82	24% 49% 38% 12%
17	AQ	80	8% 35% 38% 24%
17	CQ	80	31% 32% 41% 24%
18	AR	55	7% 53% 38% 7%
18	CR	55	5% 29% 58% 11%
19	AS	79	22% 47% 38% 13%
19	CS	79	78% 46% 49%
20	AT	85	8% 40% 48% 12%
20	CT	85	40% 38% 41% 20%
21	AU	51	25% 27% 35% 33%
21	CU	51	16% 18% 43% 29% 10%
22	BA	2903	4% 32% 46% 19%
22	DA	2903	6% 31% 53% 16%
23	BB	119	50% 37% 13%
23	DB	119	3% 34% 52% 13%
24	BC	271	47% 42% 11%
24	DC	271	15% 40% 48% 11%
25	BD	209	47% 46% 6%
25	DD	209	19% 56% 37% 6%
26	BE	201	% 54% 37% 9%
26	DE	201	40% 42% 43% 13%
27	BF	177	6% 50% 37% 11%
27	DF	177	78% 43% 48% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	BG	176	3% 55% 37% 7%
28	DG	176	56% 50% 41% 9%
29	BH	149	64% 27% 50% 19%
29	DH	149	42% 36% 51% 11%
30	BI	141	67% 30% 45% 25%
30	DI	141	94% 41% 42% 16%
31	BJ	142	61% 31% 7%
31	DJ	142	21% 49% 44% 6%
32	BK	122	50% 37% 11%
32	DK	122	20% 56% 38% 6%
33	BL	143	52% 34% 15%
33	DL	143	45% 45% 43% 11%
34	BM	136	54% 40%
34	DM	136	24% 63% 31% 5%
35	BN	120	45% 43% 11%
35	DN	120	24% 40% 44% 14%
36	BO	116	% 49% 41% 9%
36	DO	116	67% 46% 44% 10%
37	BP	114	56% 39%
37	DP	114	18% 46% 47% 5%
38	BQ	117	53% 37% 10%
38	DQ	117	18% 53% 42% 5%
39	BR	103	% 38% 50% 11%
39	DR	103	34% 50% 42% 7%
40	BS	110	% 50% 36% 12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
40	DS	110	45% 44% 48% 8%
41	BT	93	2% 46% 41% 12%
41	DT	93	69% 32% 51% 15%
42	BU	102	2% 54% 34% 11%
42	DU	102	63% 30% 50% 17%
43	BV	94	51% 38% 11%
43	DV	94	23% 56% 41%
44	BW	76	55% 42%
44	DW	76	46% 64% 26% 8%
45	BX	77	53% 36% 10%
45	DX	77	18% 25% 62% 13%
46	BY	63	8% 37% 49% 14%
46	DY	63	48% 24% 63% 11%
47	BZ	58	59% 34% 7%
47	DZ	58	21% 48% 38% 14%
48	B0	56	45% 43% 12%
48	D0	56	30% 55% 36% 9%
49	B1	50	2% 58% 32% 8%
49	D1	50	26% 46% 38% 16%
50	B2	46	2% 59% 33% 9%
50	D2	46	37% 41% 48% 9%
51	B3	64	64% 28% 8%
51	D3	64	25% 44% 50% 6%
52	B4	38	55% 42%
52	D4	38	55% 45% 32% 24%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	B5	228	

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
54	MG	AA	1645	-	-	-	X
54	MG	AA	1658	-	-	-	X
54	MG	BA	3193	-	-	-	X
54	MG	CA	1641	-	-	-	X
54	MG	DA	3005	-	-	-	X
54	MG	DA	3008	-	-	-	X
54	MG	DA	3027	-	-	-	X
54	MG	DA	3073	-	-	-	X
54	MG	DA	3093	-	-	-	X
54	MG	DA	3100	-	-	-	X
54	MG	DA	3120	-	-	-	X
54	MG	DA	3125	-	-	-	X
54	MG	DA	3132	-	-	-	X
54	MG	DA	3134	-	-	-	X
54	MG	DA	3144	-	-	-	X
54	MG	DA	3154	-	-	-	X
56	ZN	B4	101	-	-	X	-

2 Entry composition (i)

There are 57 unique types of molecules in this entry. The entry contains 288258 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 RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1538	Total	C	N	O	P	0	0	0
			32995	14716	6050	10691	1538			
1	CA	1539	Total	C	N	O	P	0	0	0
			33015	14725	6052	10699	1539			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0	0
			710	437	143	129	1			
15	CO	88	Total	C	N	O	S	0	0	0
			710	437	143	129	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	BA	2897	Total	C	N	O	P	0	0	0
			62195	27745	11446	20107	2897			
22	DA	2897	Total	C	N	O	P	0	0	0
			62195	27745	11446	20107	2897			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	BB	119	Total	C	N	O	P	0	0	0
			2549	1135	466	829	119			
23	DB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BH	149	Total	C	N	O	S	0	0	0
			1110	699	197	213	1			
29	DH	149	Total	C	N	O	S	0	0	0
			1110	699	197	213	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BW	76	Total 580	C 359	N 117	O 103	S 1	0	0	0
44	DW	75	Total 569	C 353	N 113	O 102	S 1	0	0	0

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	B1	50	Total	C	N	O	0	0	0
			410	263	75	72			
49	D1	50	Total	C	N	O	0	0	0
			410	263	75	72			

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

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

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

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

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

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

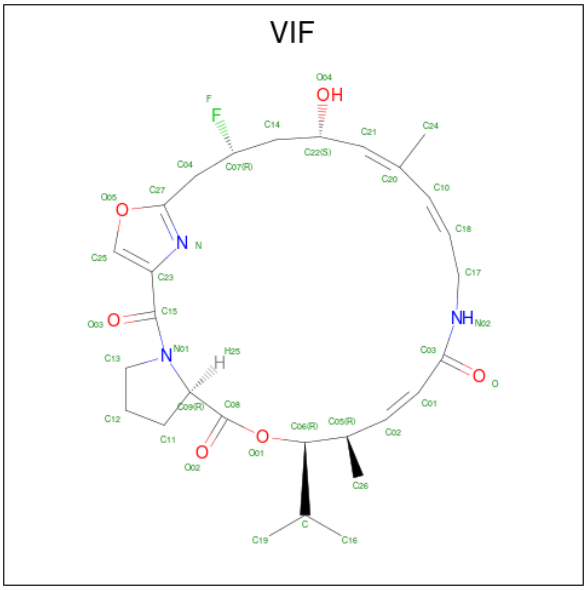
- Molecule 53 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
53	B5	191	Total	C	N	O	0	0	1
			1142	691	221	230			

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	AA	72	Total	Mg	0	0
			72	72		
54	BA	194	Total	Mg	0	0
			194	194		
54	BB	4	Total	Mg	0	0
			4	4		
54	BN	1	Total	Mg	0	0
			1	1		
54	CA	55	Total	Mg	0	0
			55	55		
54	CM	1	Total	Mg	0	0
			1	1		
54	DA	166	Total	Mg	0	0
			166	166		
54	DB	3	Total	Mg	0	0
			3	3		
54	DQ	1	Total	Mg	0	0
			1	1		
54	D2	1	Total	Mg	0	0
			1	1		

- Molecule 55 is Flopristin (three-letter code: VIF) (formula: $C_{28}H_{38}FN_3O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
55	BA	1	Total 38	C 28	F 1	N 3	O 6	0	0
55	DA	1	Total 38	C 28	F 1	N 3	O 6	0	0

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

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

- Molecule 57 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	AA	195	Total 195	O 195	0	0
57	AL	1	Total 1	O 1	0	0
57	AN	5	Total 5	O 5	0	0
57	AT	1	Total 1	O 1	0	0
57	AU	1	Total 1	O 1	0	0
57	BA	620	Total 620	O 620	0	0
57	BB	13	Total 13	O 13	0	0
57	BC	6	Total 6	O 6	0	0
57	BD	3	Total 3	O 3	0	0
57	BE	4	Total 4	O 4	0	0
57	BF	1	Total 1	O 1	0	0
57	BG	1	Total 1	O 1	0	0
57	BL	8	Total 8	O 8	0	0
57	BN	4	Total 4	O 4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	BS	1	Total O 1 1	0	0
57	BV	1	Total O 1 1	0	0
57	B2	1	Total O 1 1	0	0
57	B3	2	Total O 2 2	0	0
57	B4	1	Total O 1 1	0	0
57	CA	189	Total O 189 189	0	0
57	CL	1	Total O 1 1	0	0
57	CN	3	Total O 3 3	0	0
57	CT	4	Total O 4 4	0	0
57	CU	1	Total O 1 1	0	0
57	DA	613	Total O 613 613	0	0
57	DB	13	Total O 13 13	0	0
57	DC	9	Total O 9 9	0	0
57	DD	4	Total O 4 4	0	0
57	DE	2	Total O 2 2	0	0
57	DJ	1	Total O 1 1	0	0
57	DL	3	Total O 3 3	0	0
57	DN	1	Total O 1 1	0	0
57	DT	2	Total O 2 2	0	0
57	DV	1	Total O 1 1	0	0
57	D0	1	Total O 1 1	0	0

Continued on next page...

Continued from previous page...

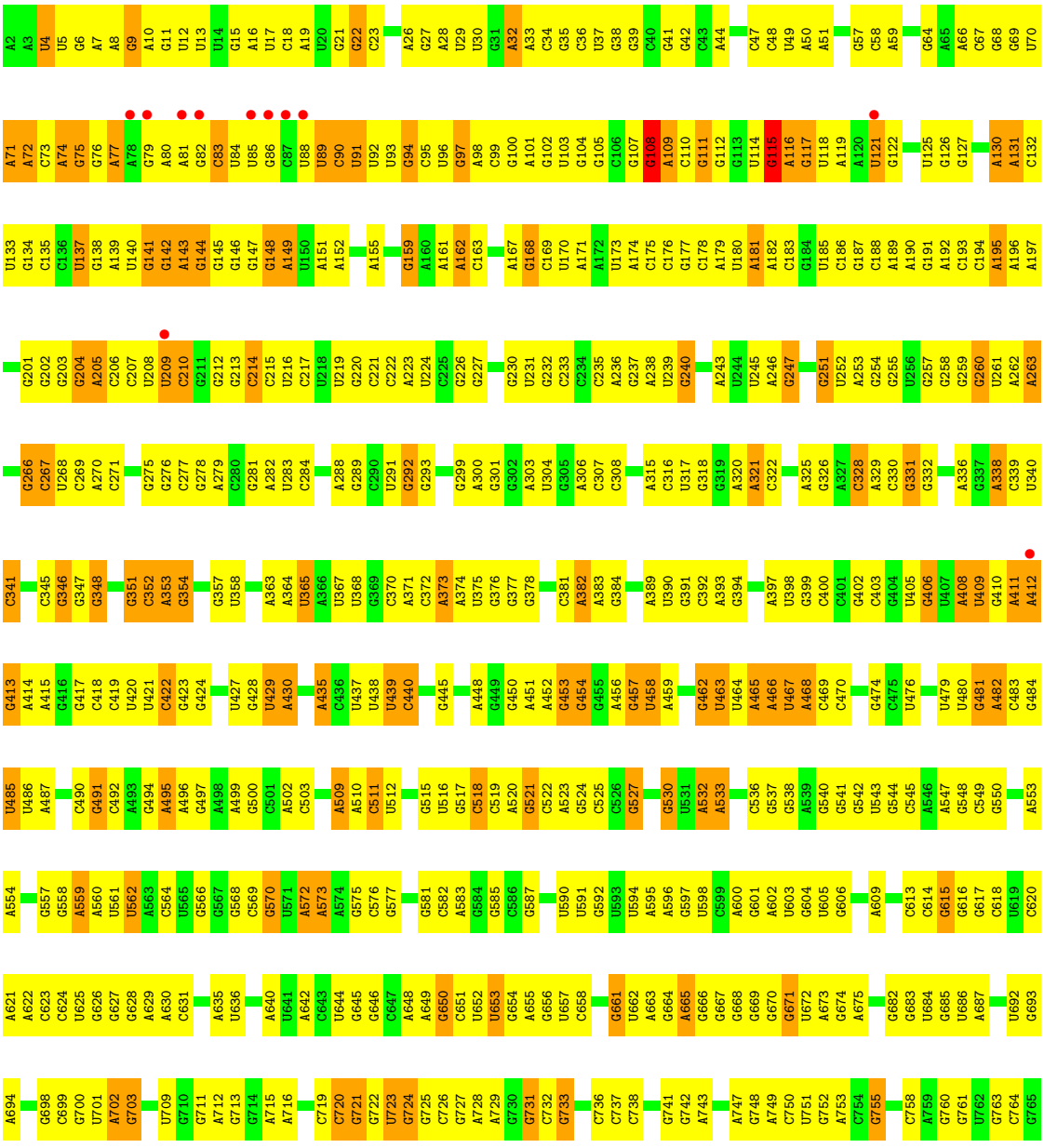
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	D2	3	Total O 3 3	0	0
57	D3	2	Total O 2 2	0	0
57	D4	1	Total O 1 1	0	0

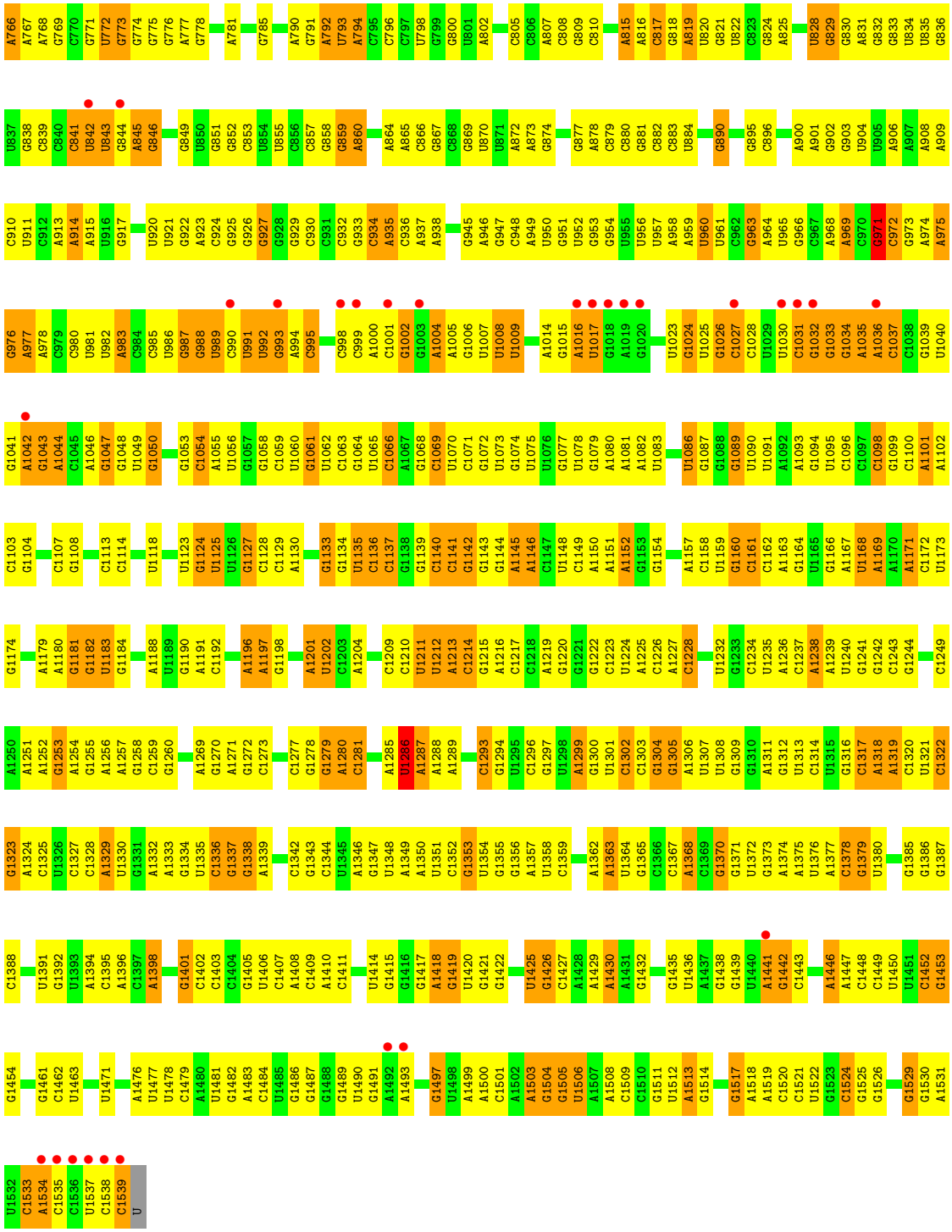
3 Residue-property plots (i)

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

- Molecule 1: 16S rRNA

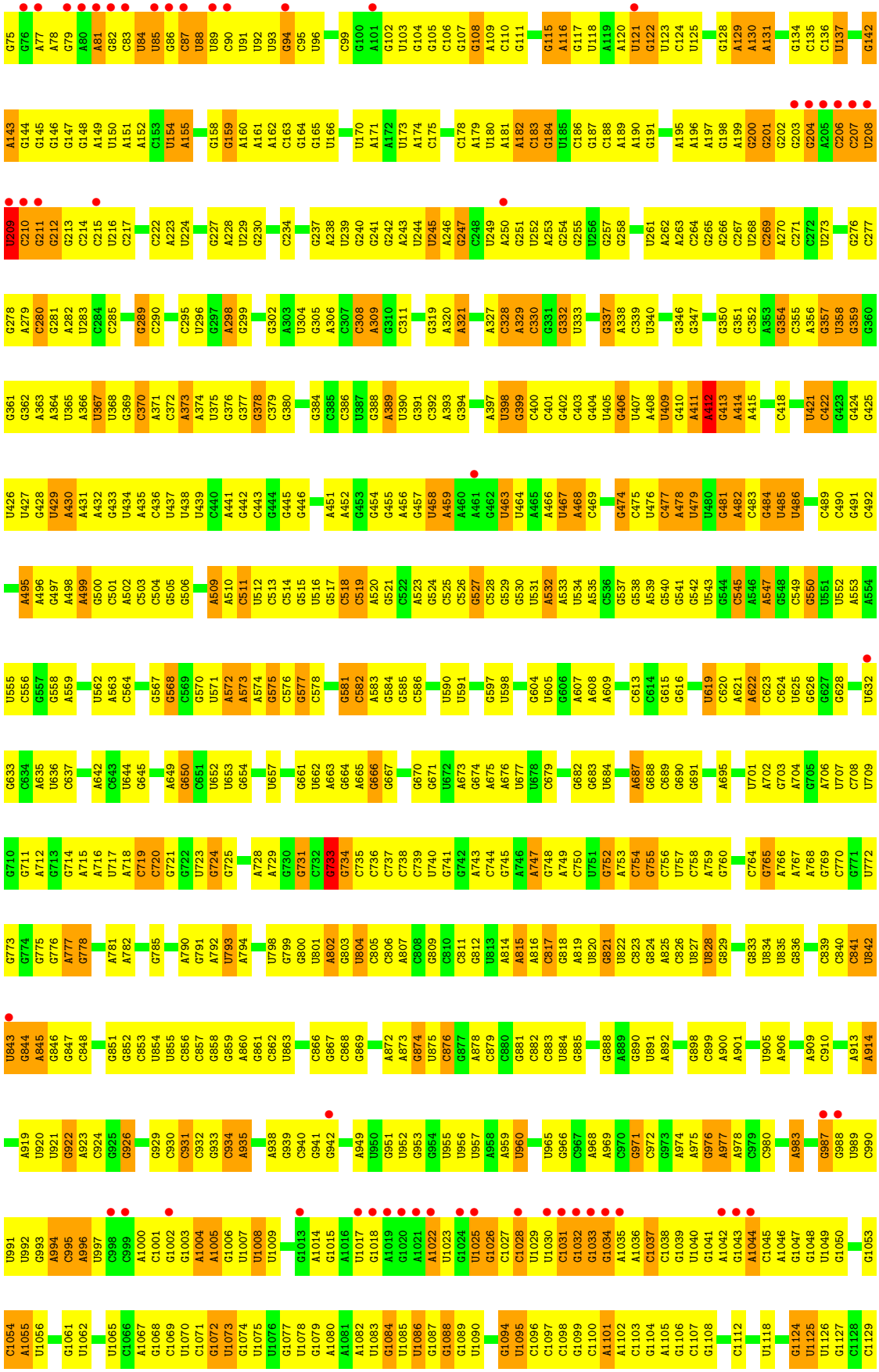
Chain AA: 

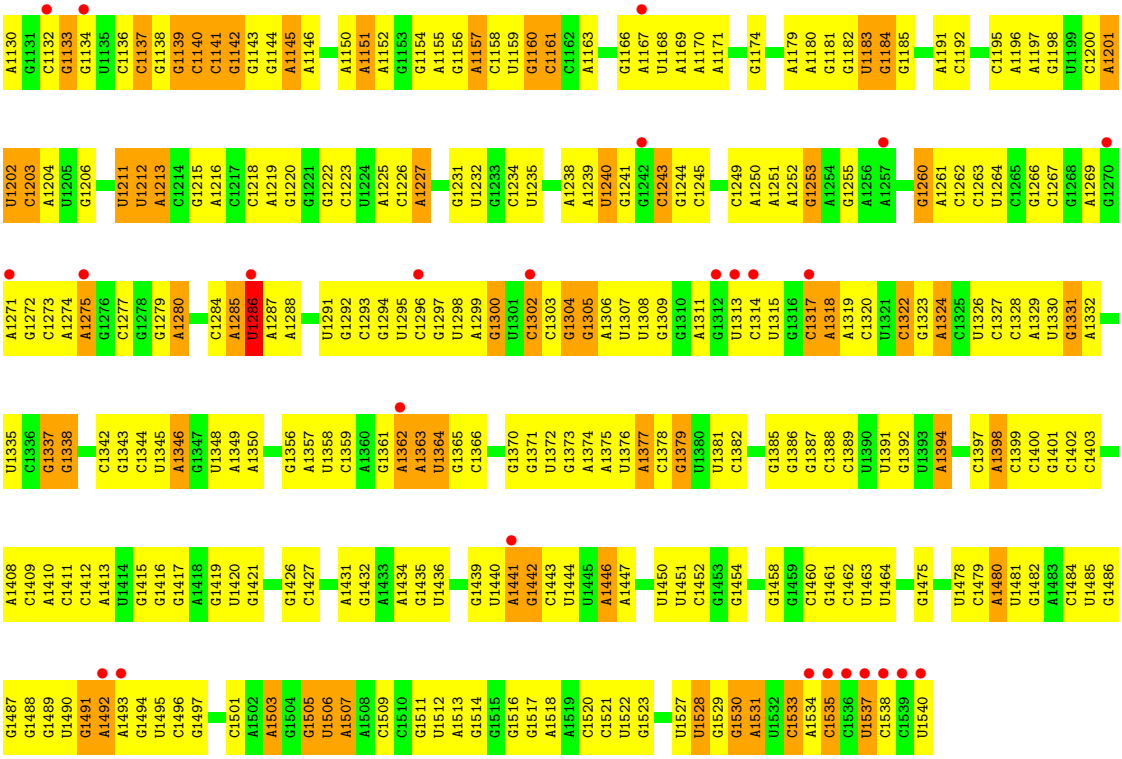




• Molecule 1: 16S rRNA

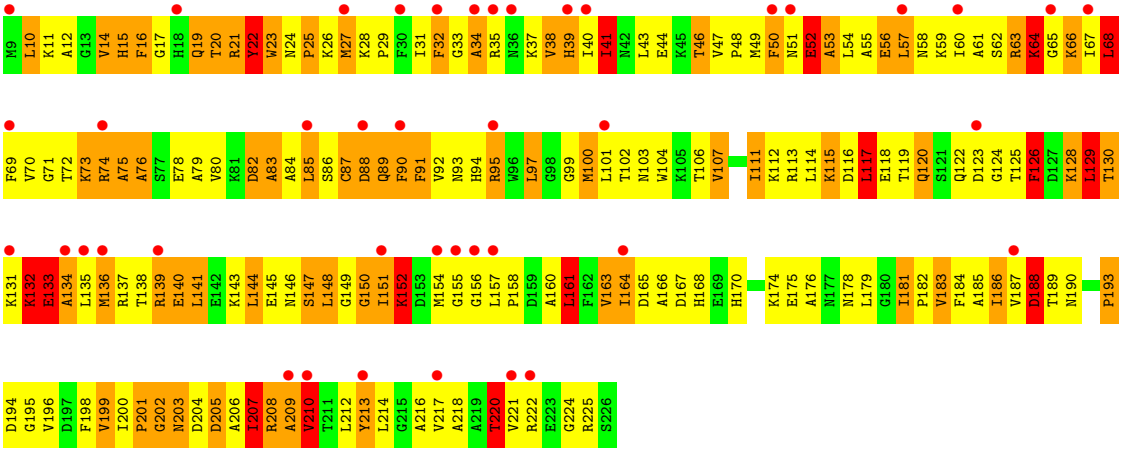
Chain CA:





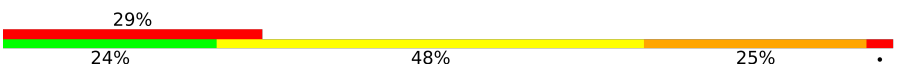
• Molecule 2: 30S ribosomal protein S2

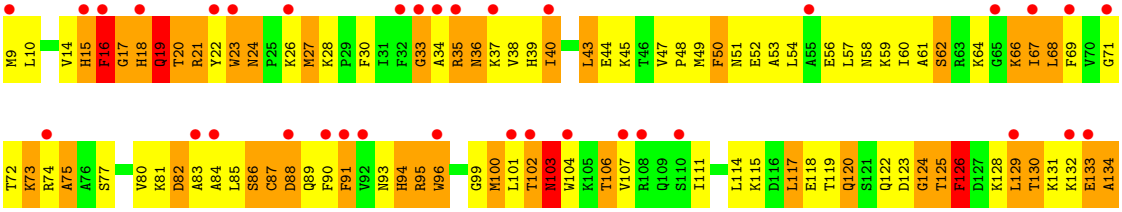
Chain AB:

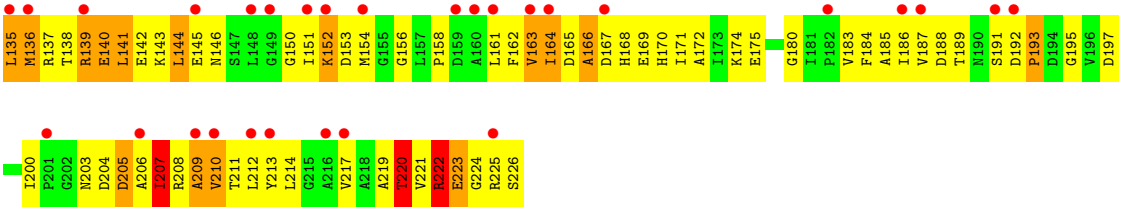


• Molecule 2: 30S ribosomal protein S2

Chain CB:

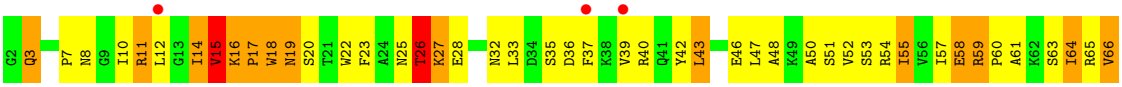


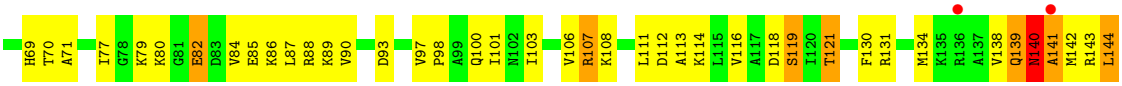


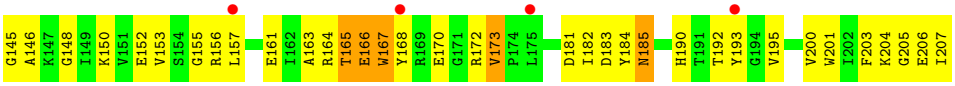


• Molecule 3: 30S ribosomal protein S3

Chain AC:

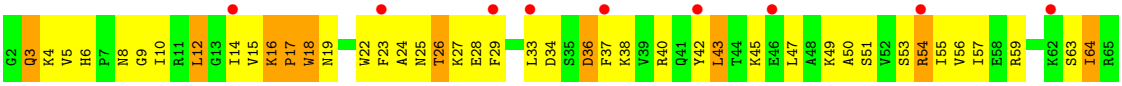


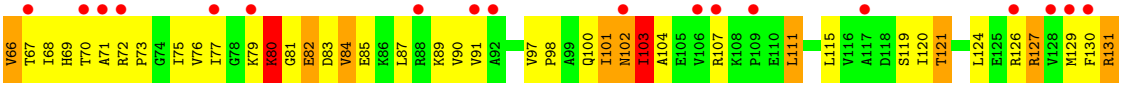


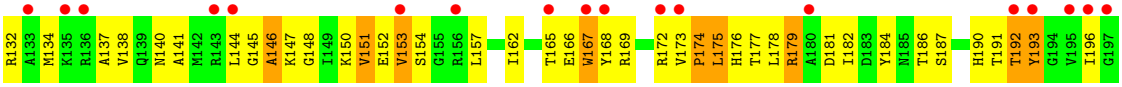


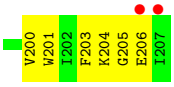
• Molecule 3: 30S ribosomal protein S3

Chain CC:



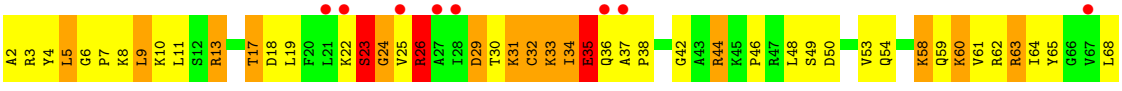


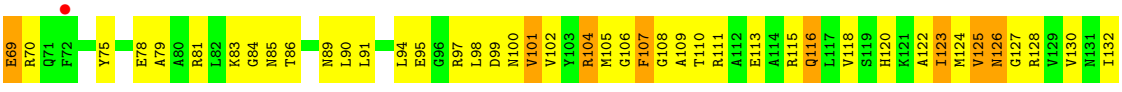


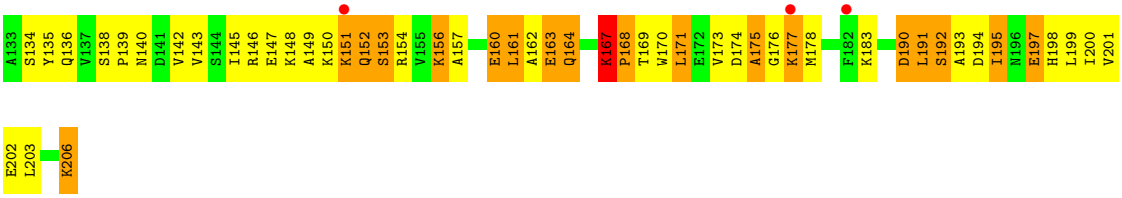


• Molecule 4: 30S ribosomal protein S4

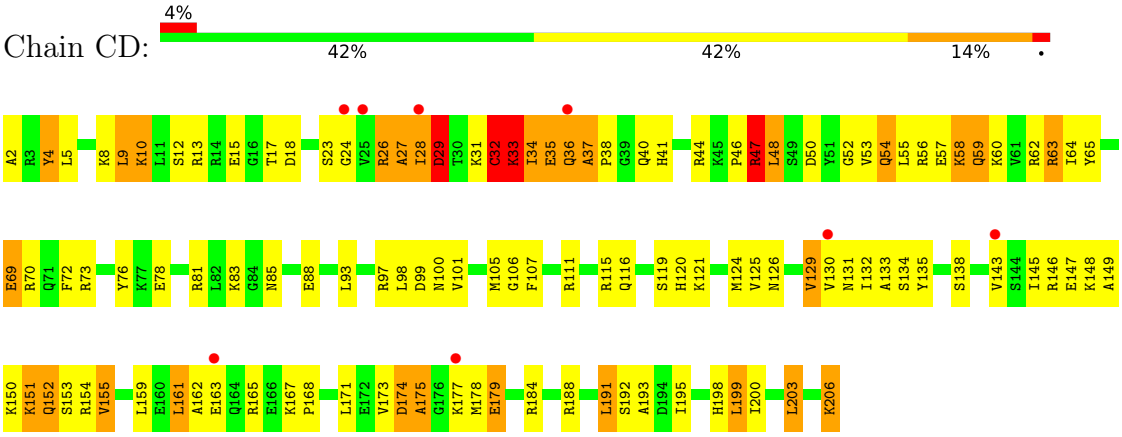
Chain AD:



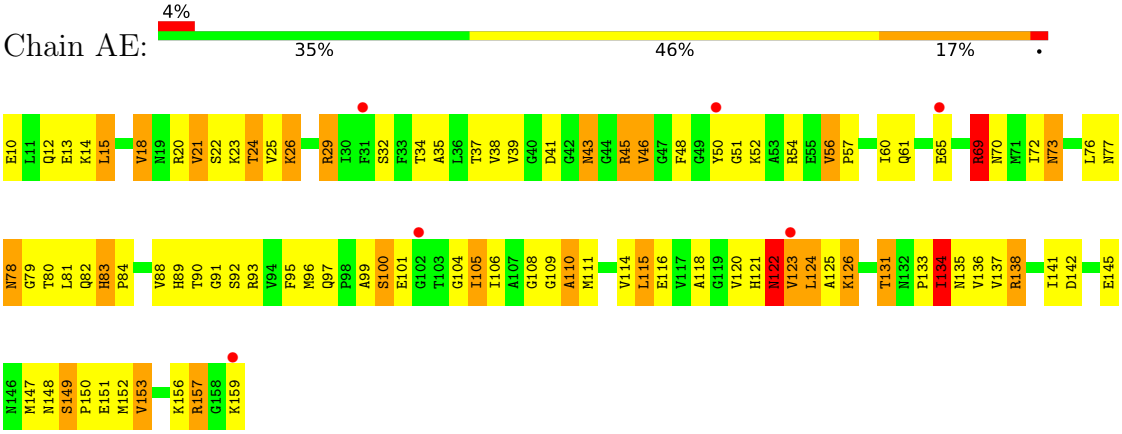




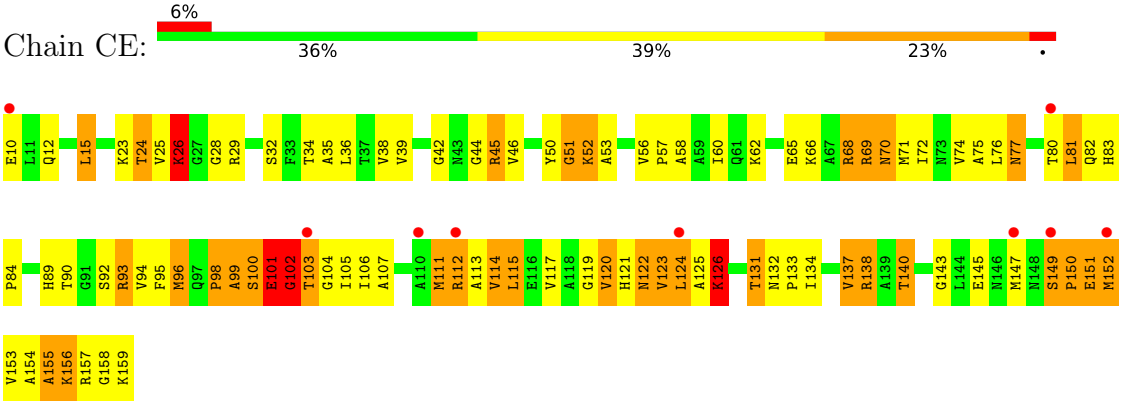
• Molecule 4: 30S ribosomal protein S4



• Molecule 5: 30S ribosomal protein S5

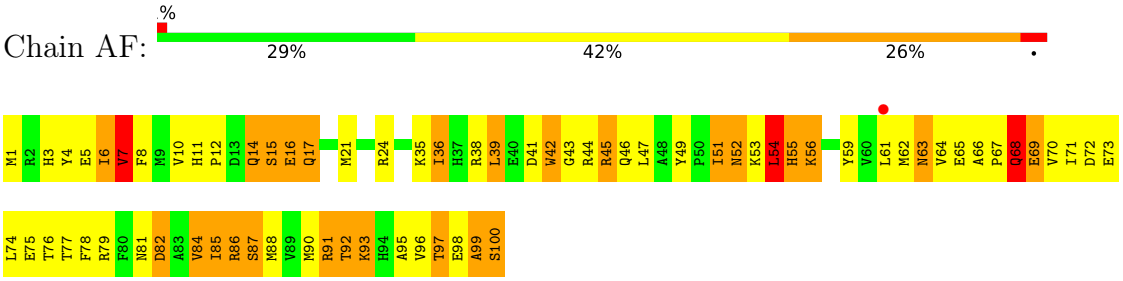


• Molecule 5: 30S ribosomal protein S5



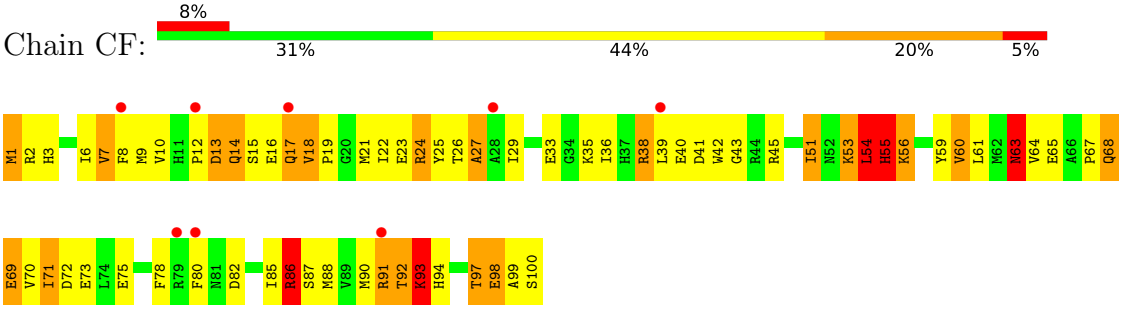
• Molecule 6: 30S ribosomal protein S6

Chain AF:



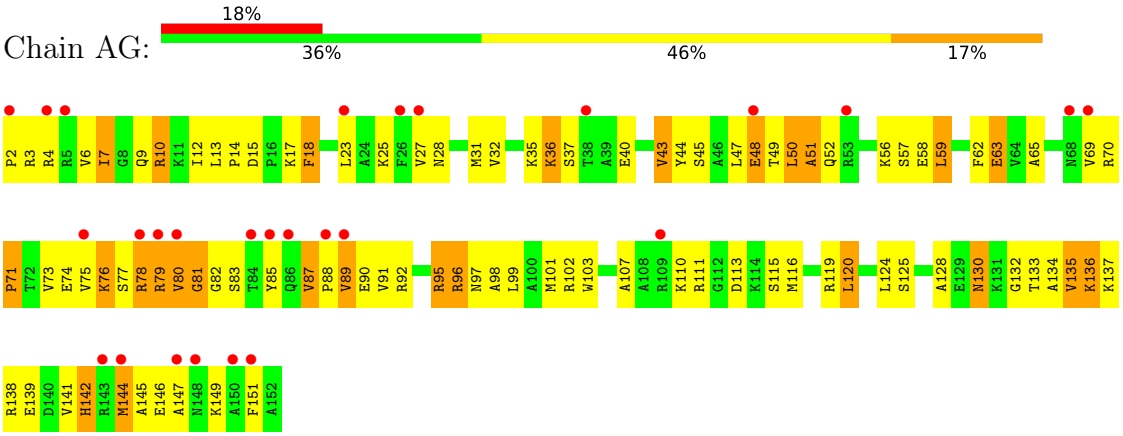
• Molecule 6: 30S ribosomal protein S6

Chain CF:



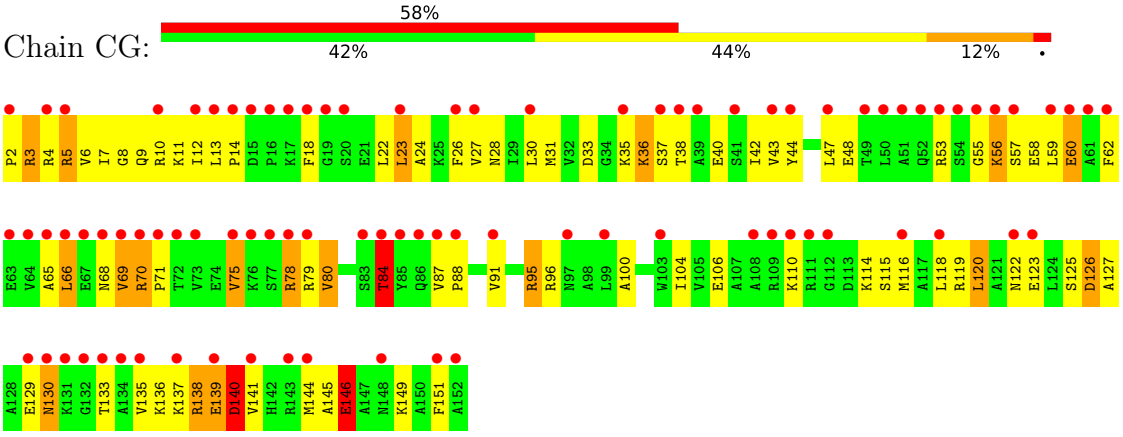
• Molecule 7: 30S ribosomal protein S7

Chain AG:



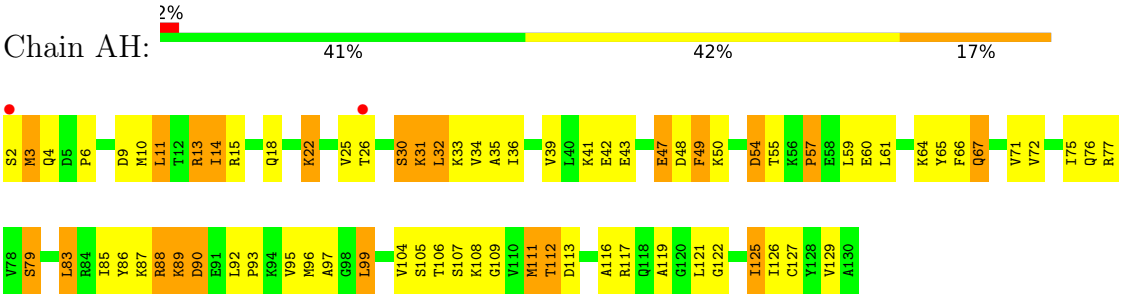
• Molecule 7: 30S ribosomal protein S7

Chain CG:



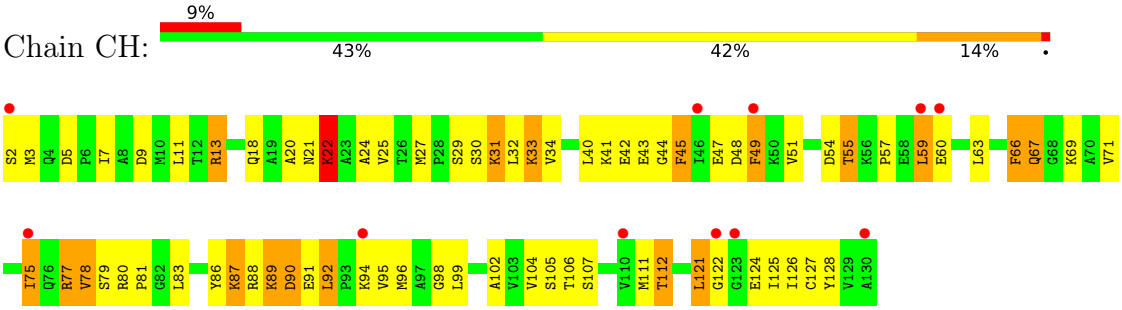
• Molecule 8: 30S ribosomal protein S8

Chain AH:



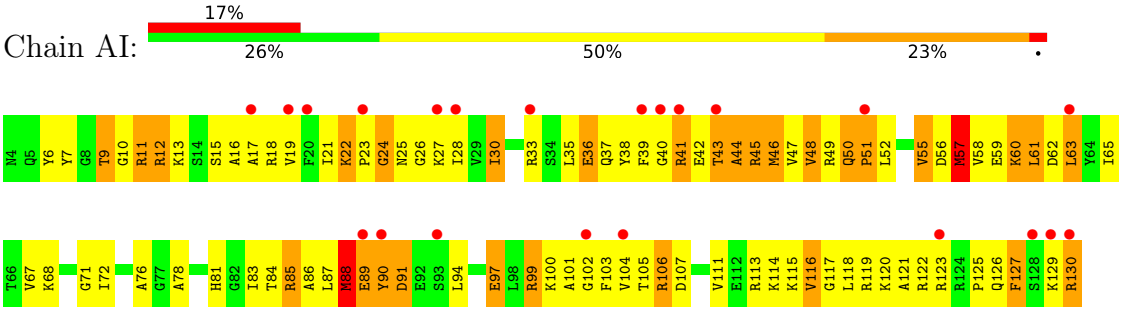
• Molecule 8: 30S ribosomal protein S8

Chain CH:



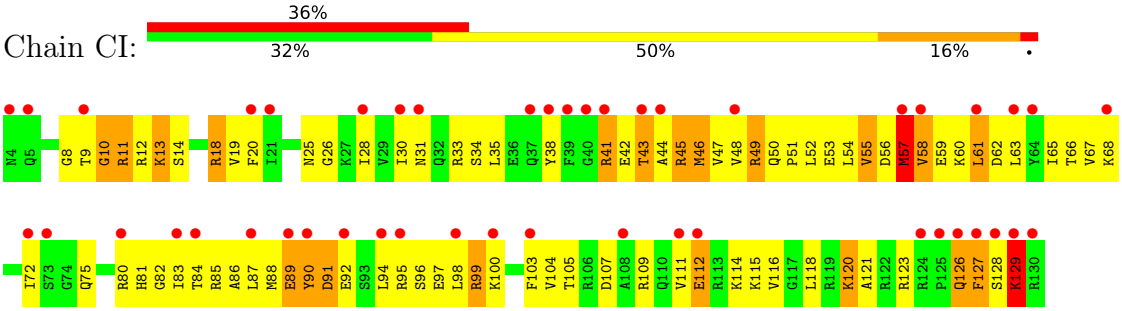
• Molecule 9: 30S ribosomal protein S9

Chain AI:



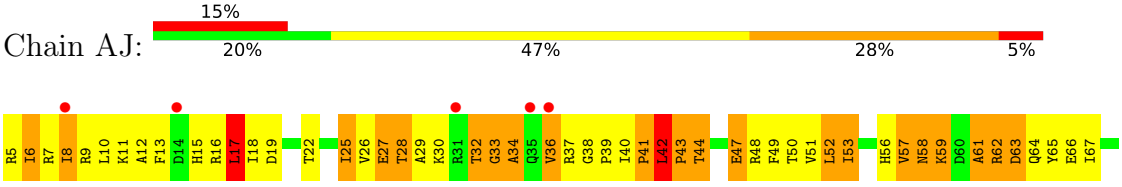
• Molecule 9: 30S ribosomal protein S9

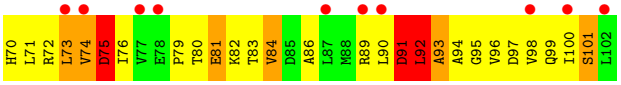
Chain CI:



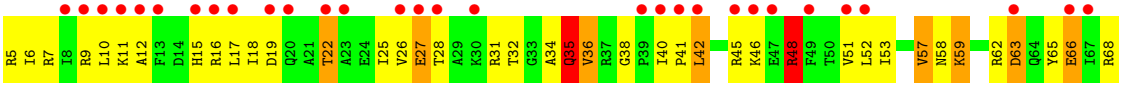
• Molecule 10: 30S ribosomal protein S10

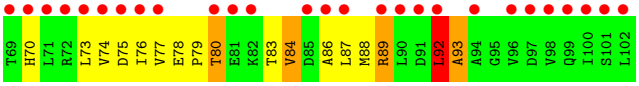
Chain AJ:



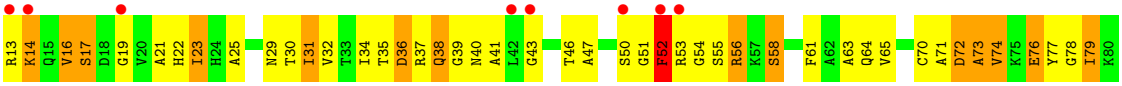


• Molecule 10: 30S ribosomal protein S10

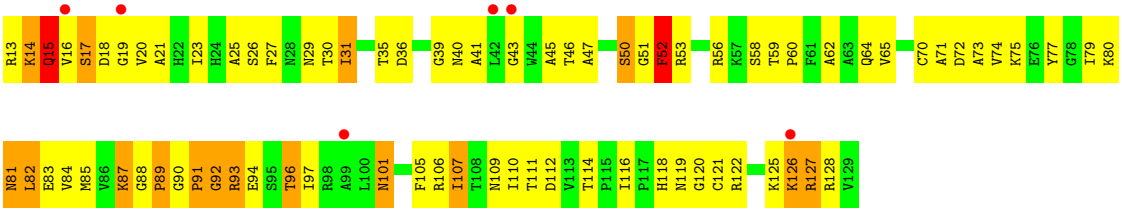




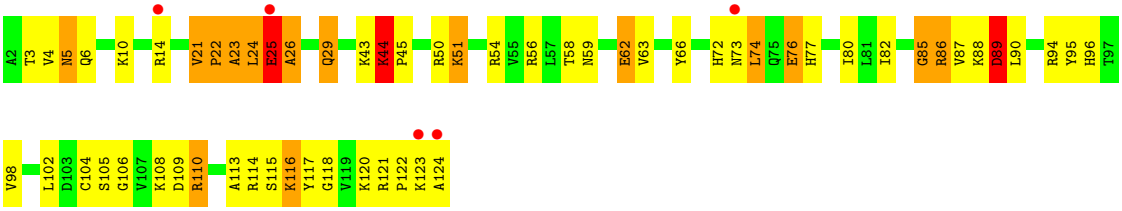
• Molecule 11: 30S ribosomal protein S11



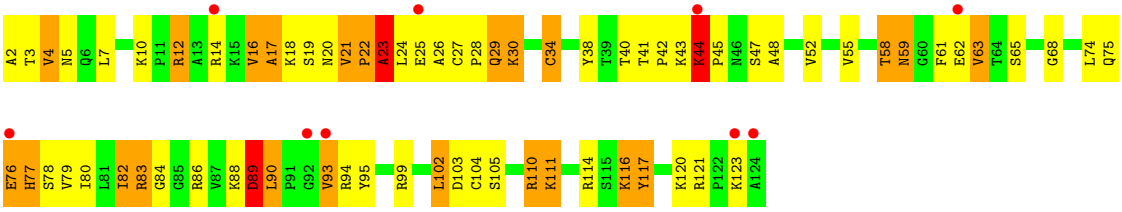
• Molecule 11: 30S ribosomal protein S11



• Molecule 12: 30S ribosomal protein S12

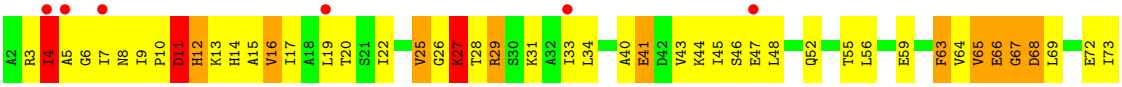


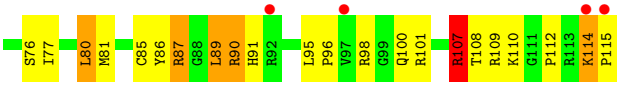
• Molecule 12: 30S ribosomal protein S12



• Molecule 13: 30S ribosomal protein S13

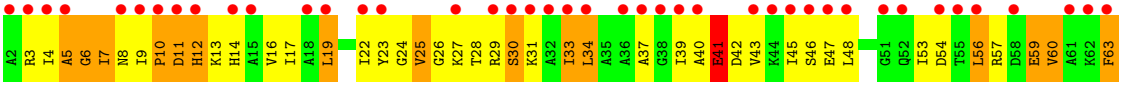
Chain AM:

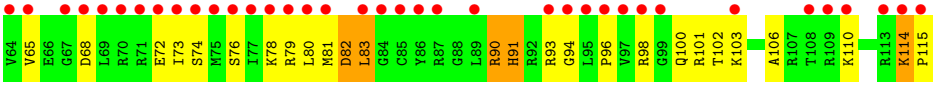




• Molecule 13: 30S ribosomal protein S13

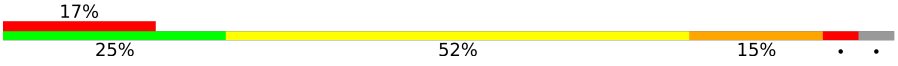
Chain CM:

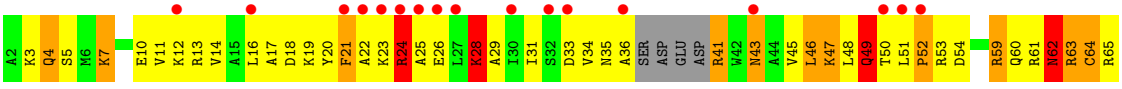




• Molecule 14: 30S ribosomal protein S14

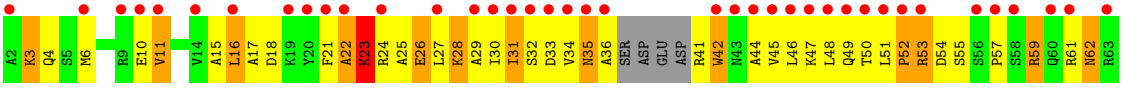
Chain AN:

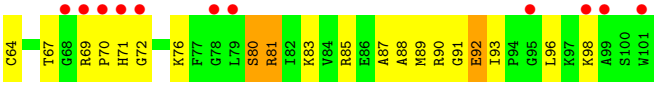




• Molecule 14: 30S ribosomal protein S14

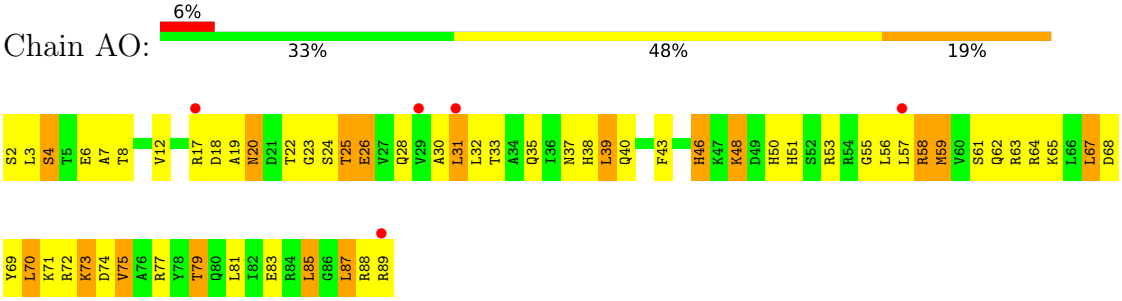
Chain CN:





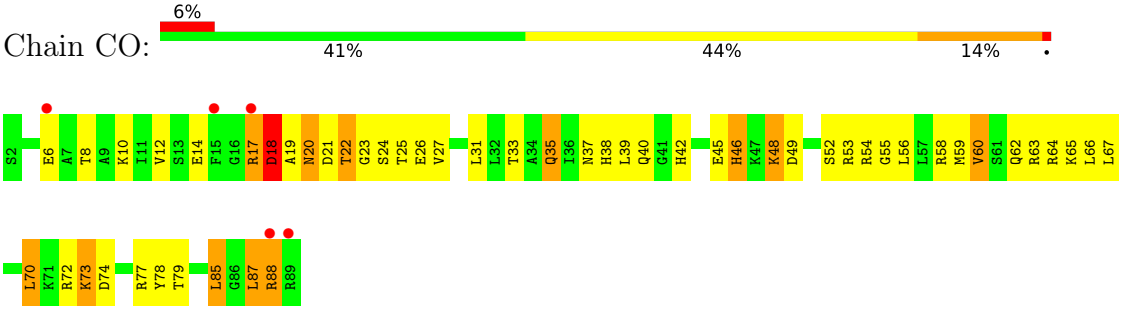
• Molecule 15: 30S ribosomal protein S15

Chain AO:



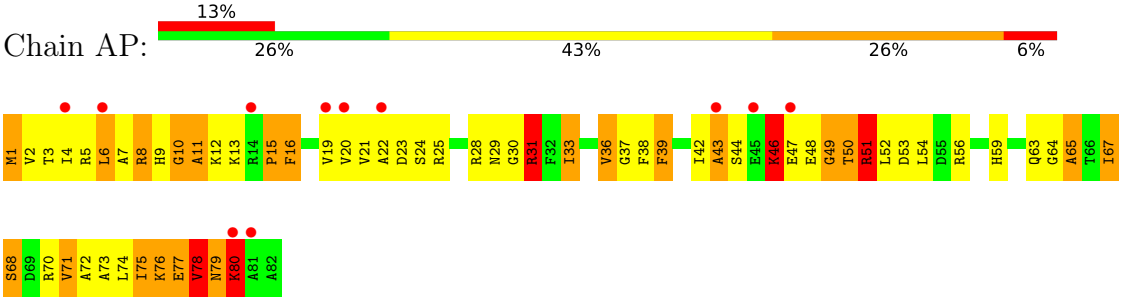
• Molecule 15: 30S ribosomal protein S15

Chain CO:



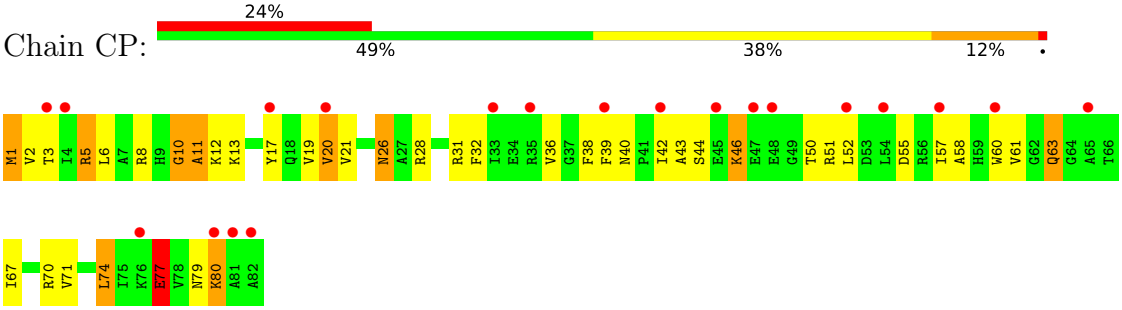
• Molecule 16: 30S ribosomal protein S16

Chain AP:



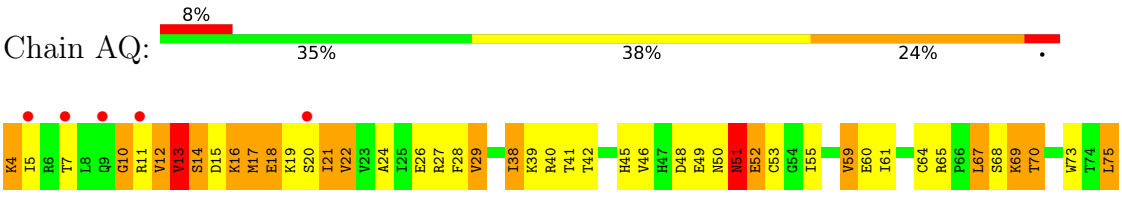
• Molecule 16: 30S ribosomal protein S16

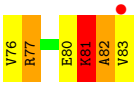
Chain CP:



• Molecule 17: 30S ribosomal protein S17

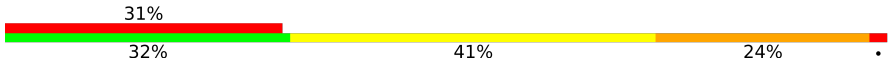
Chain AQ:

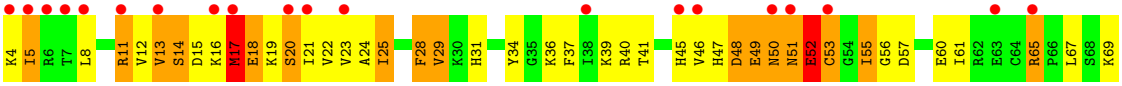


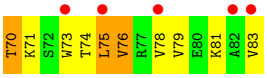


• Molecule 17: 30S ribosomal protein S17

Chain CQ:

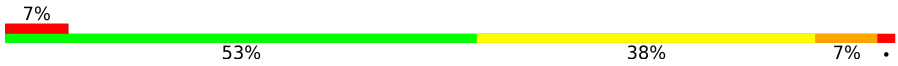


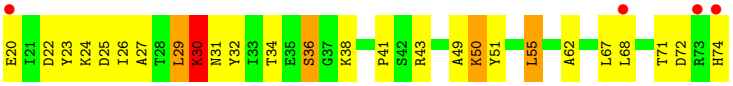




• Molecule 18: 30S ribosomal protein S18

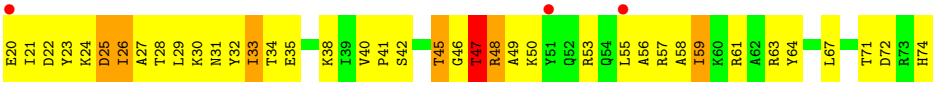
Chain AR:





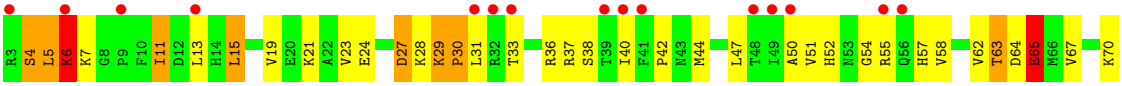
• Molecule 18: 30S ribosomal protein S18

Chain CR:



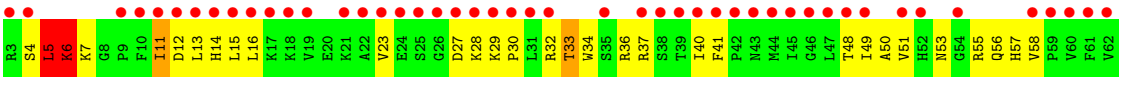
• Molecule 19: 30S ribosomal protein S19

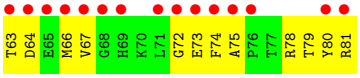
Chain AS:



• Molecule 19: 30S ribosomal protein S19

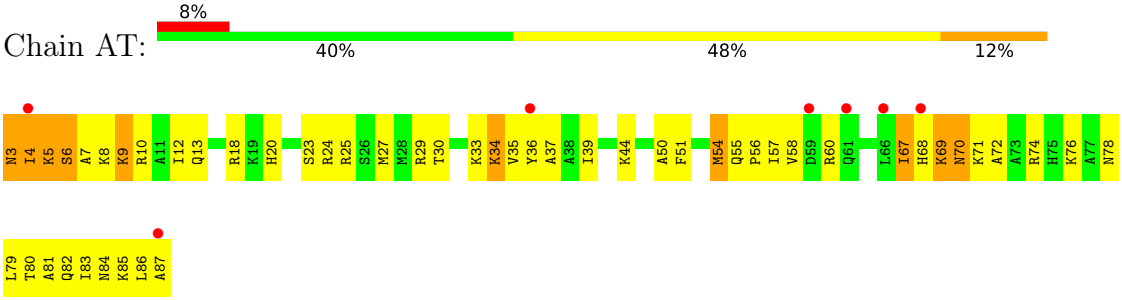
Chain CS:





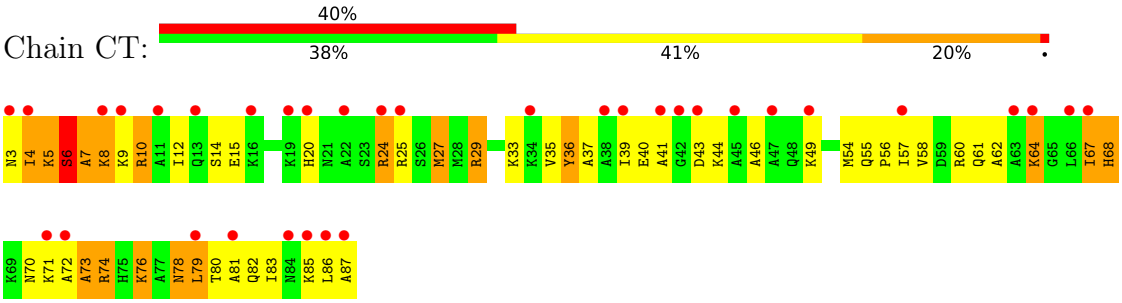
• Molecule 20: 30S ribosomal protein S20

Chain AT:



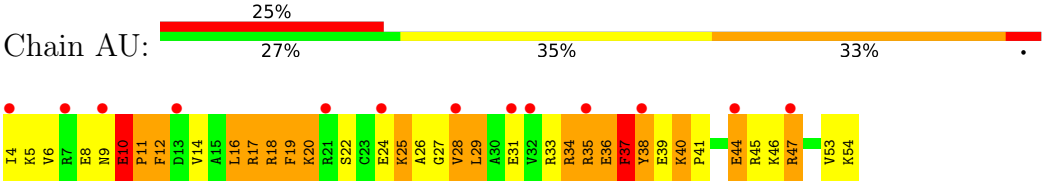
• Molecule 20: 30S ribosomal protein S20

Chain CT:



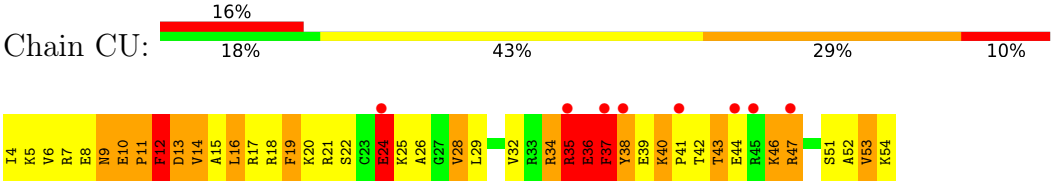
• Molecule 21: 30S ribosomal protein S21

Chain AU:



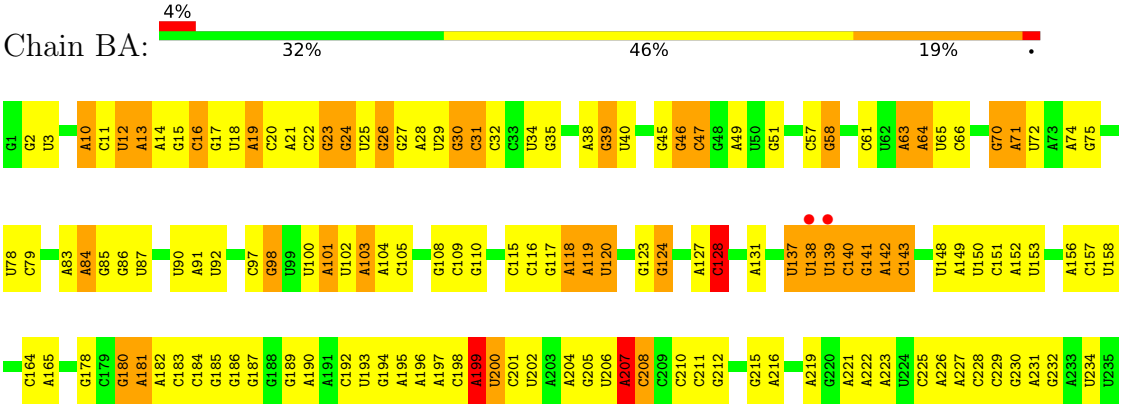
• Molecule 21: 30S ribosomal protein S21

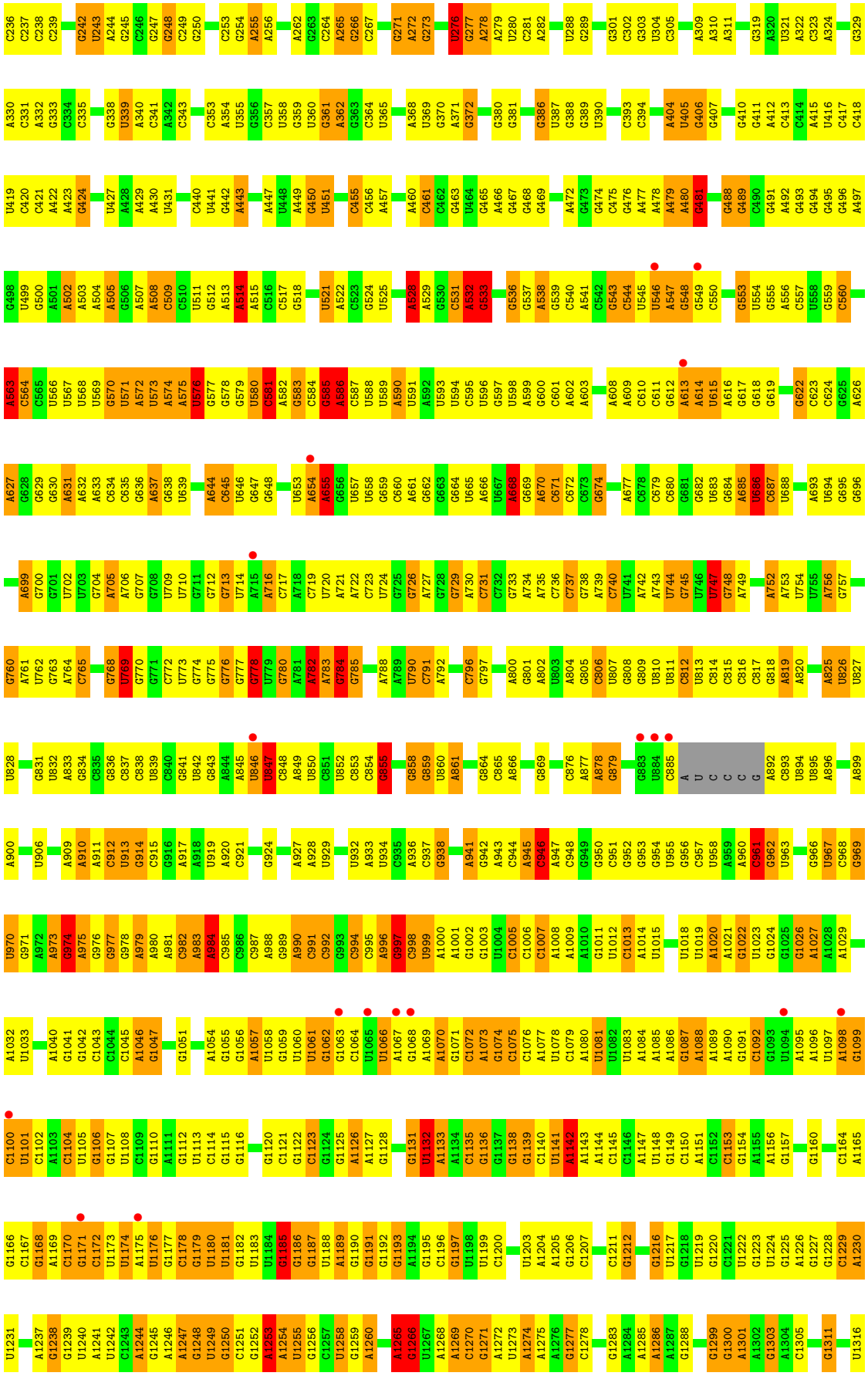
Chain CU:

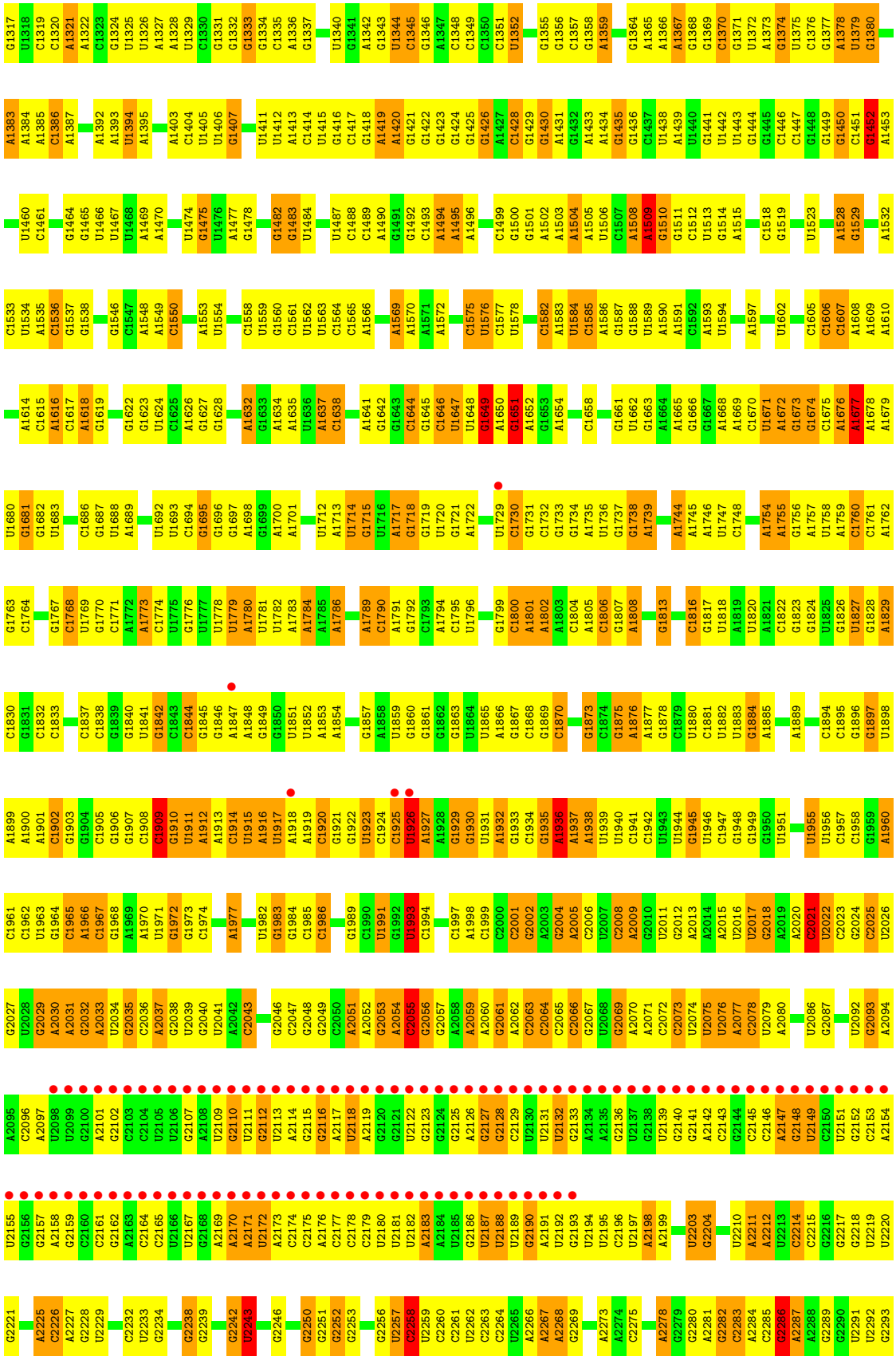


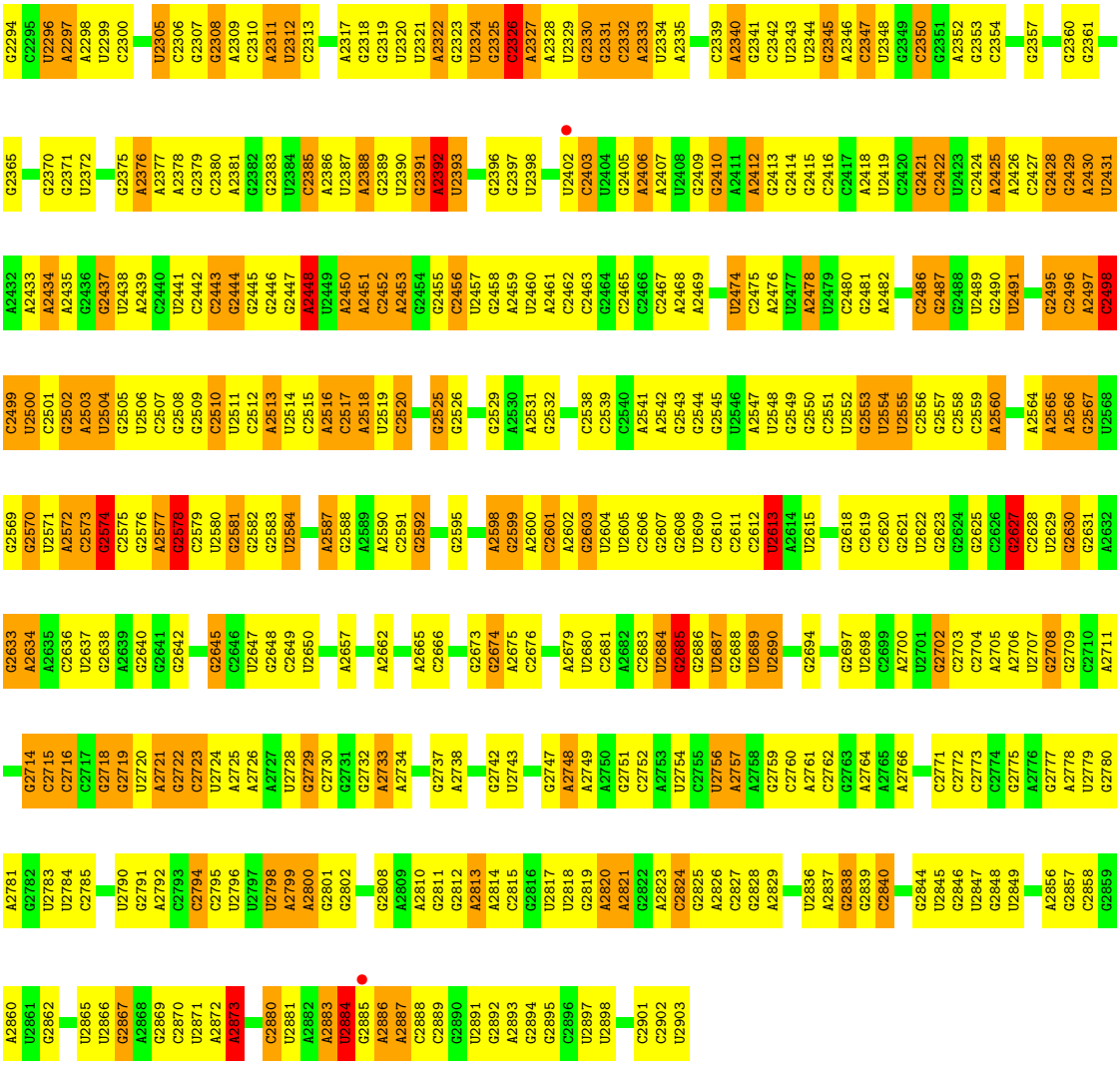
• Molecule 22: 23S rRNA

Chain BA:



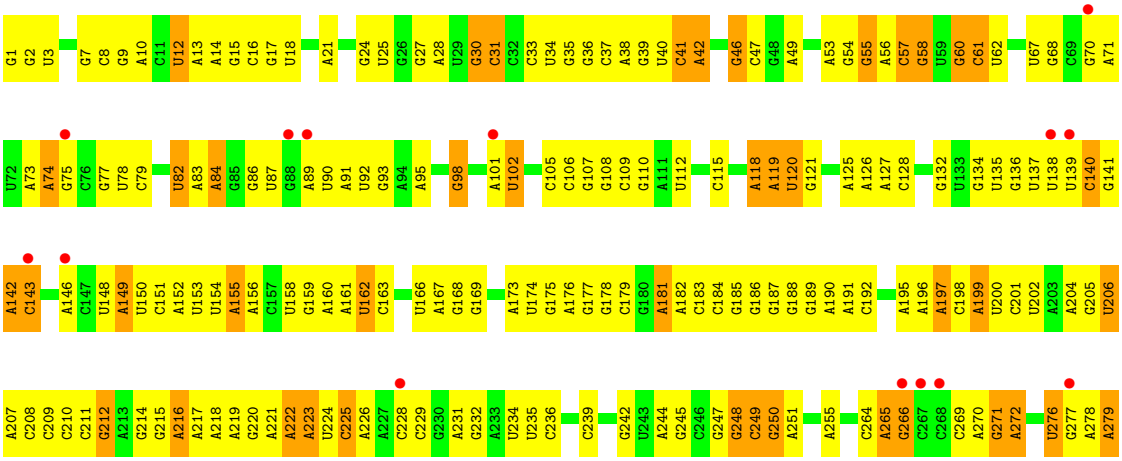


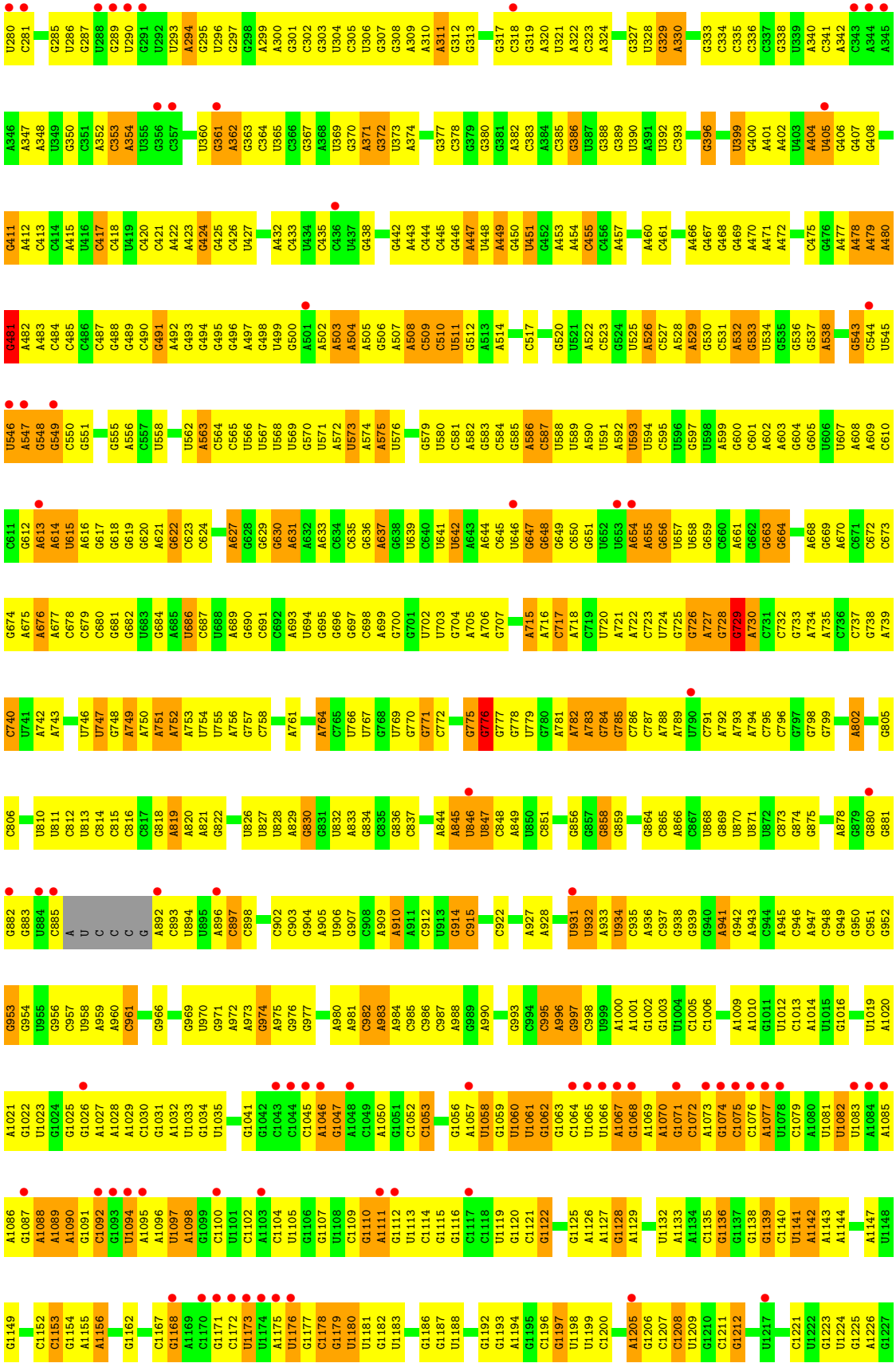


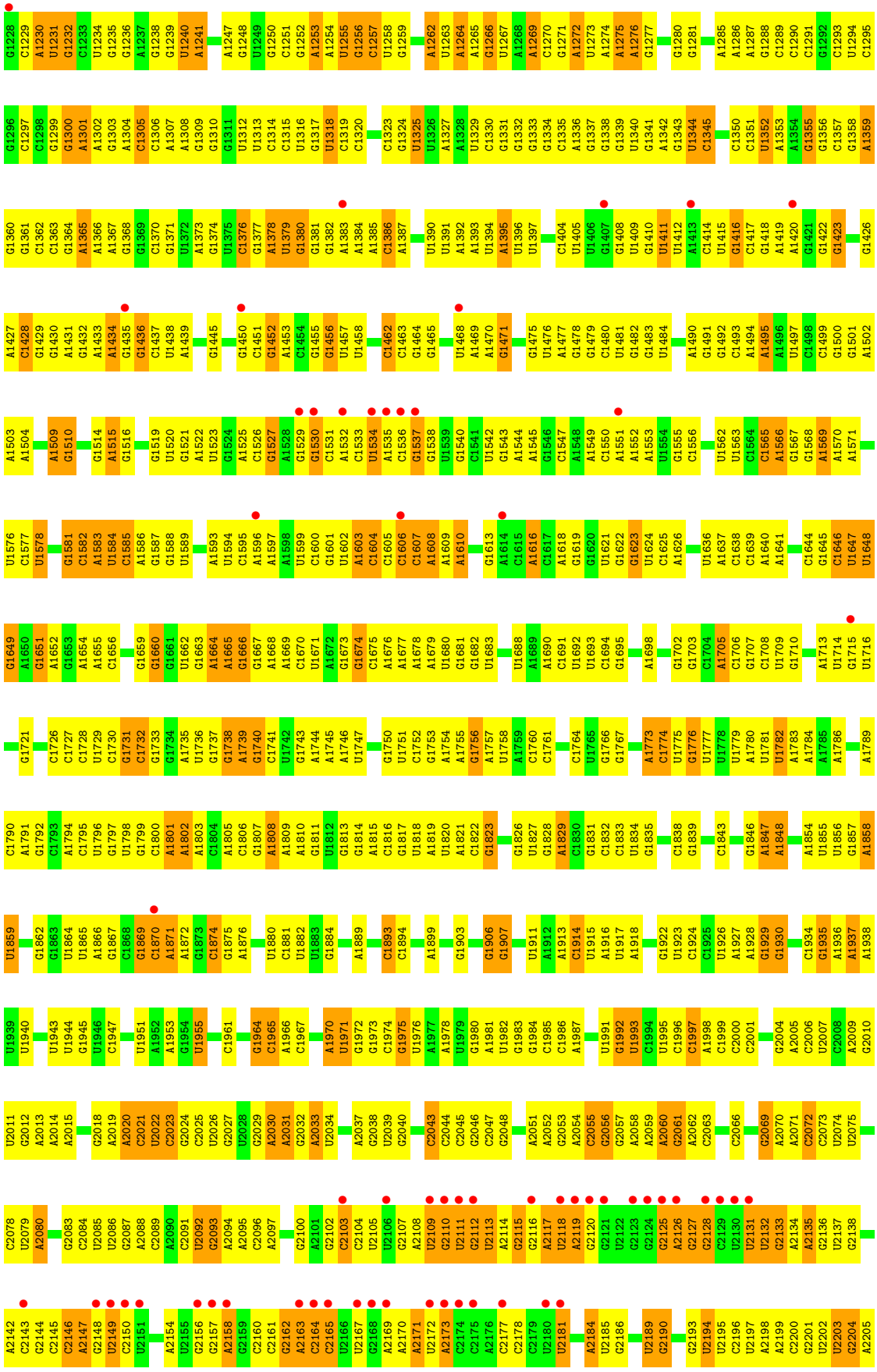


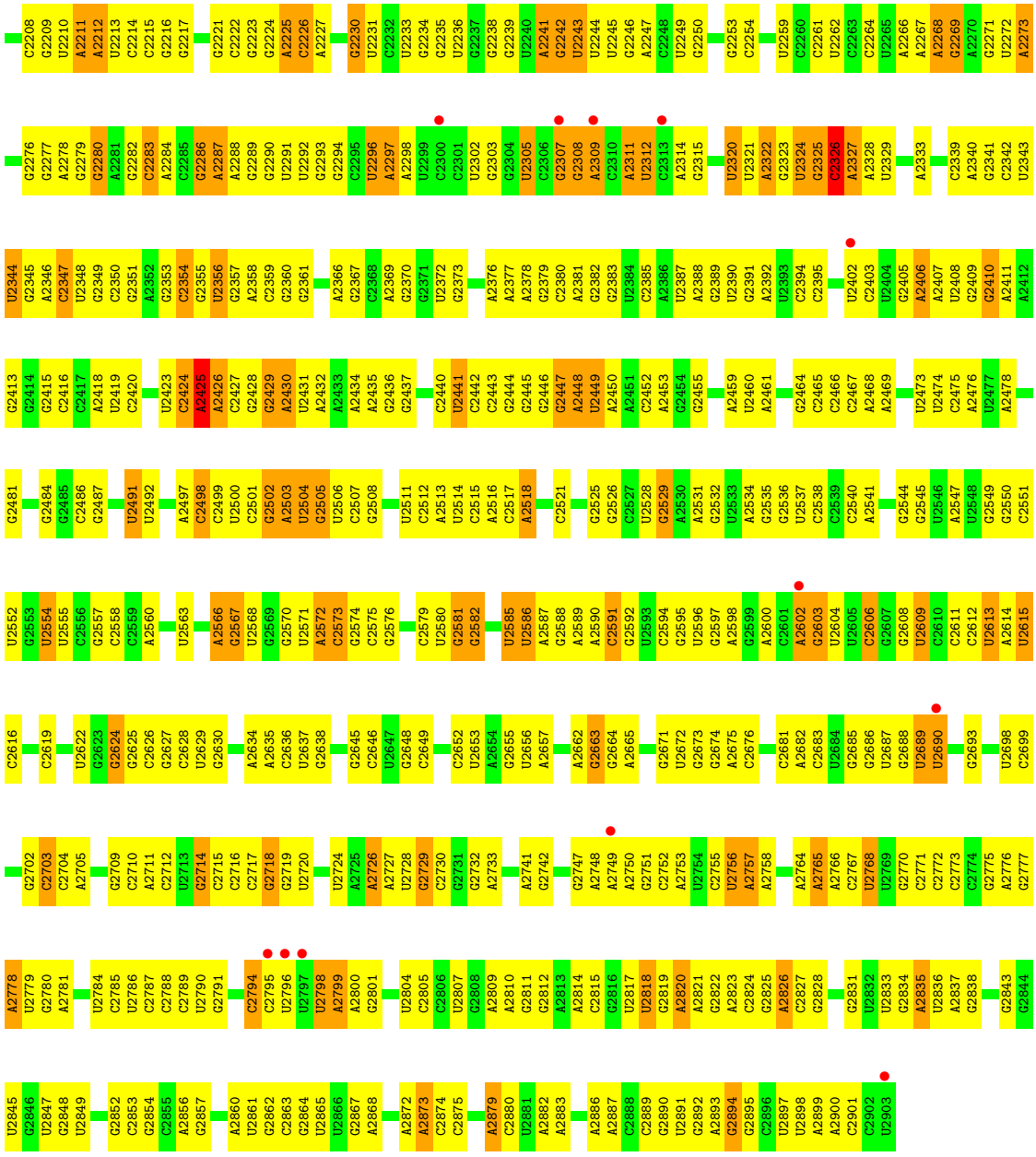
• Molecule 22: 23S rRNA

Chain DA:



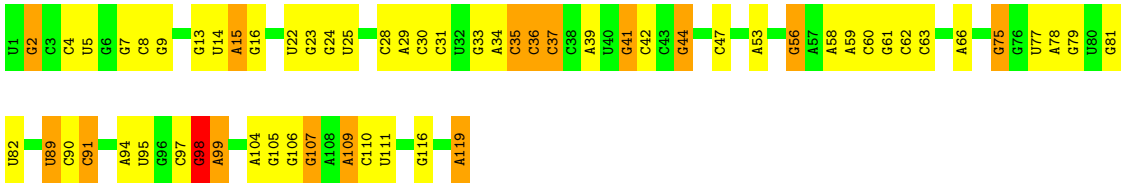






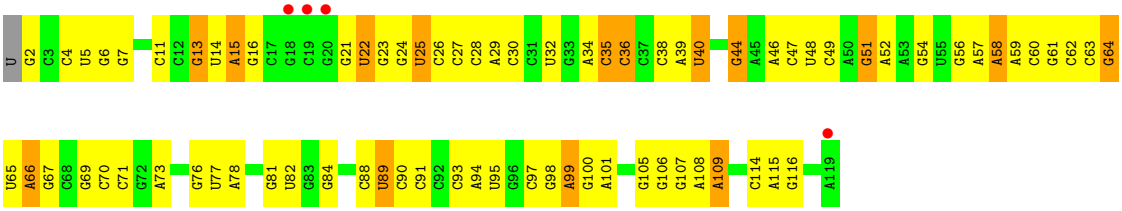
• Molecule 23: 5S rRNA

Chain BB:



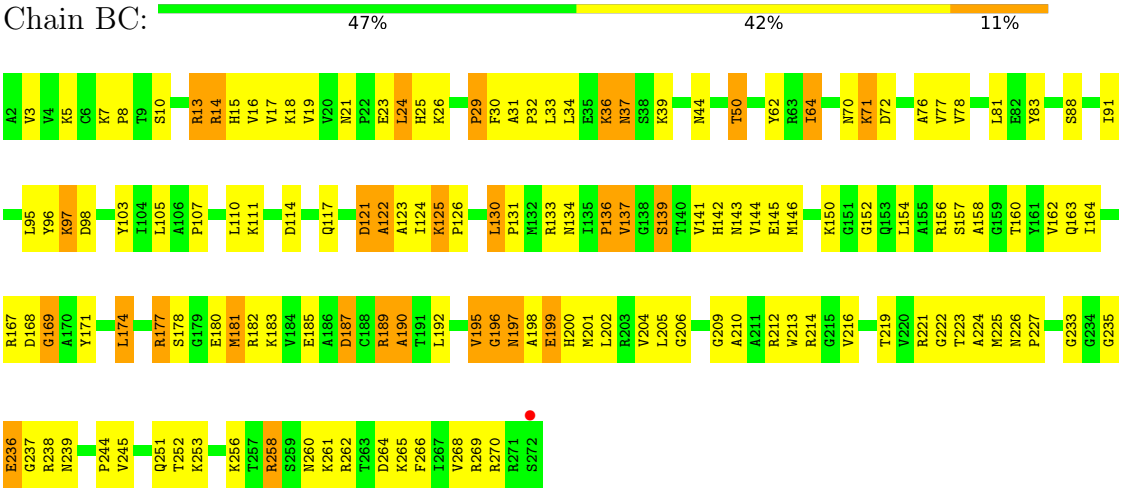
• Molecule 23: 5S rRNA

Chain DB:



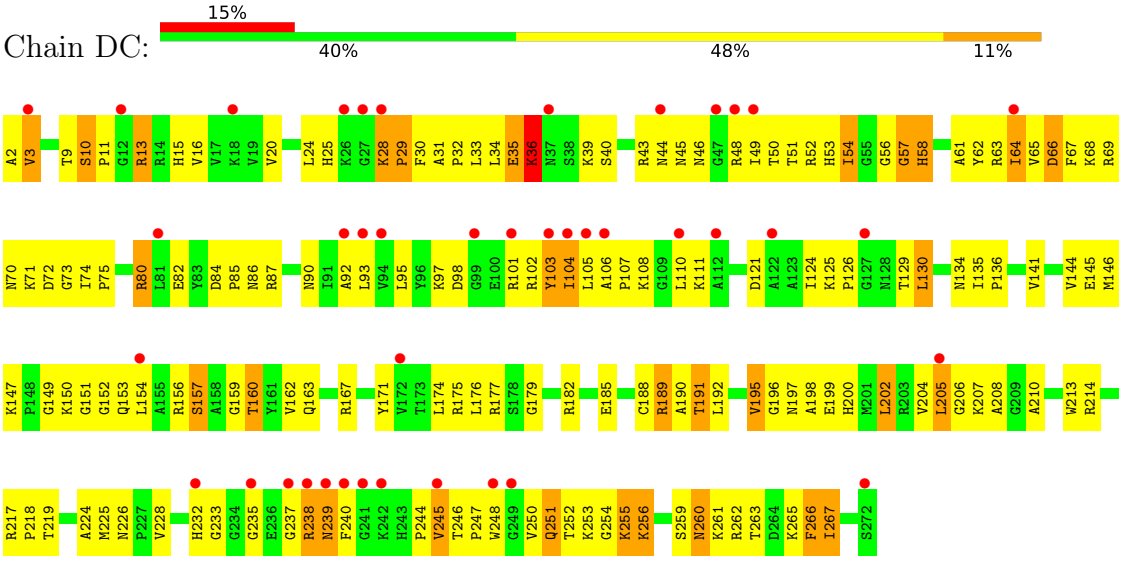
• Molecule 24: 50S ribosomal protein L2

Chain BC:



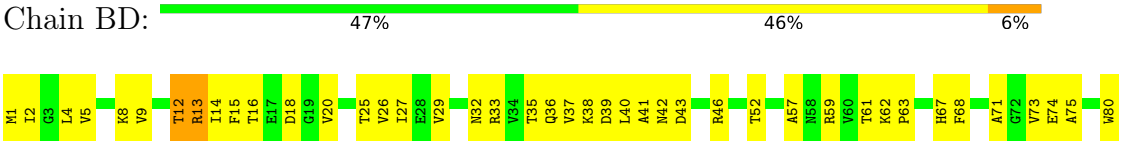
• Molecule 24: 50S ribosomal protein L2

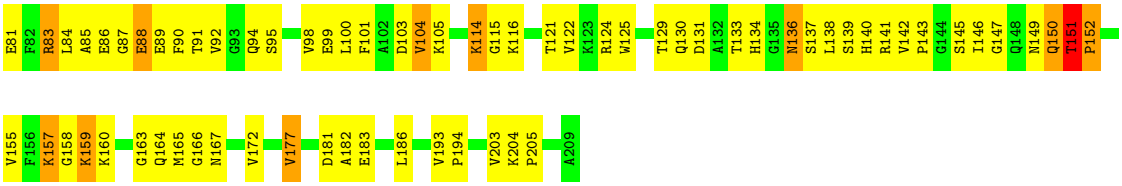
Chain DC:



• Molecule 25: 50S ribosomal protein L3

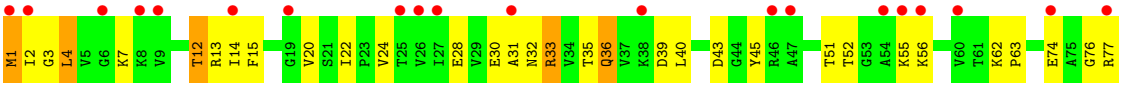
Chain BD:

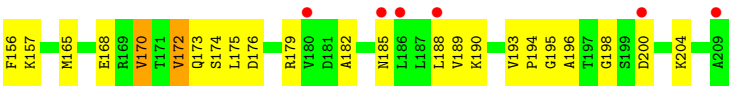




• Molecule 25: 50S ribosomal protein L3

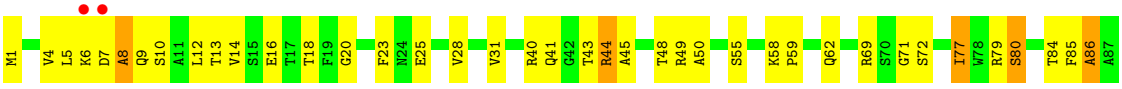
Chain DD:

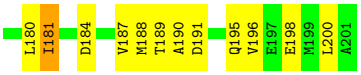




• Molecule 26: 50S ribosomal protein L4

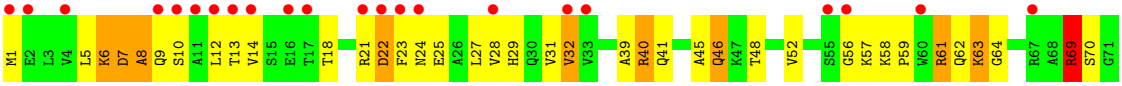
Chain BE:

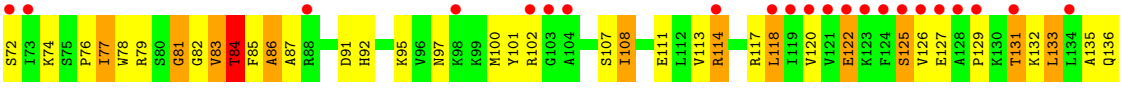


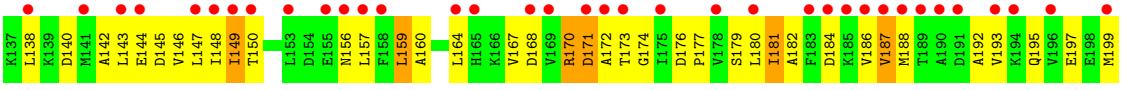


• Molecule 26: 50S ribosomal protein L4

Chain DE:

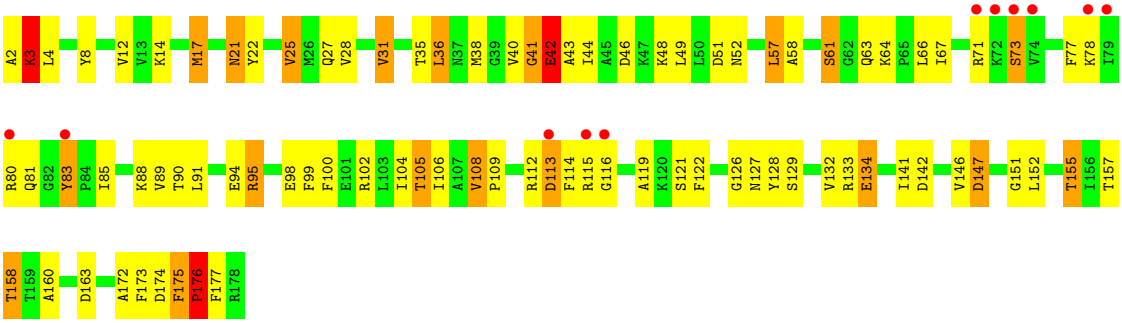






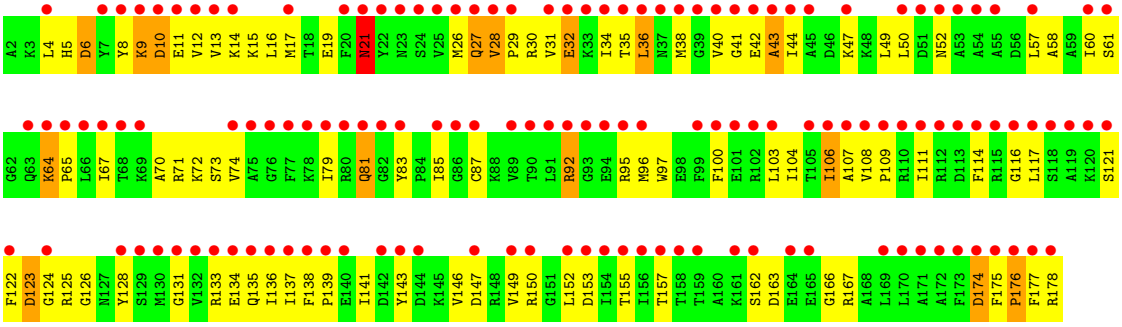
• Molecule 27: 50S ribosomal protein L5

Chain BF:



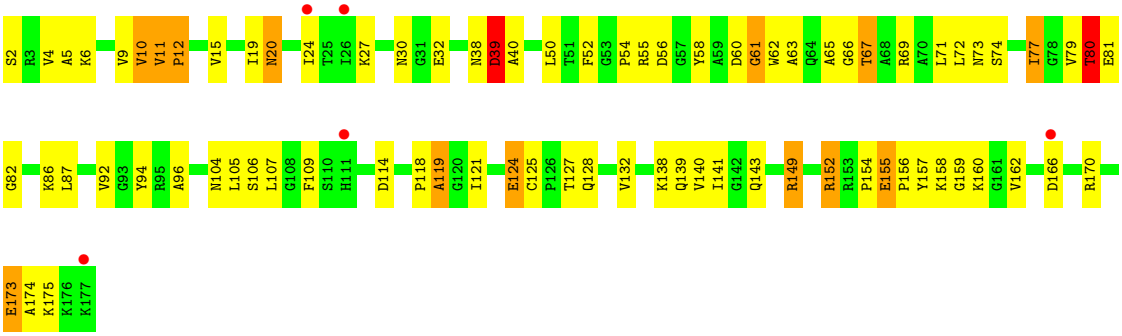
• Molecule 27: 50S ribosomal protein L5

Chain DF:



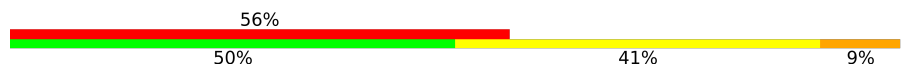
• Molecule 28: 50S ribosomal protein L6

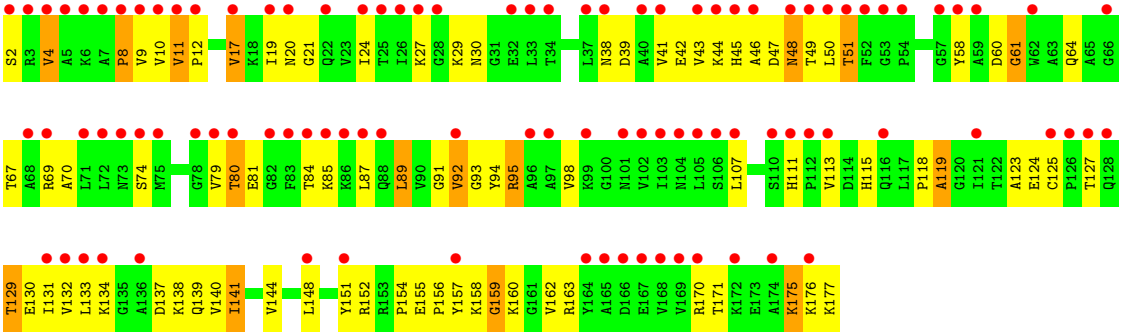
Chain BG:



• Molecule 28: 50S ribosomal protein L6

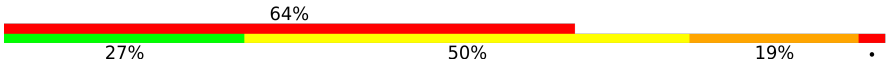
Chain DG:

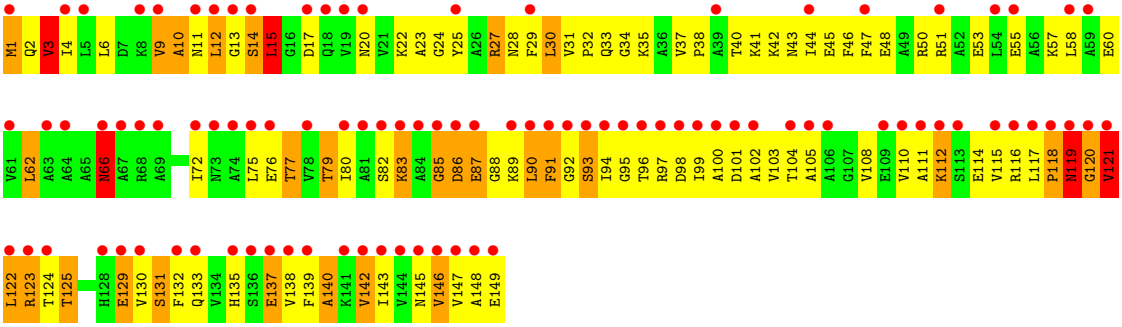




• Molecule 29: 50S ribosomal protein L9

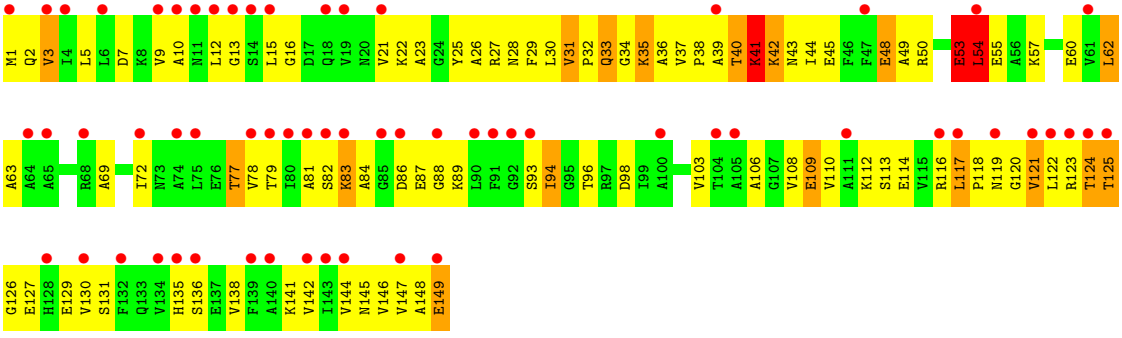
Chain BH:





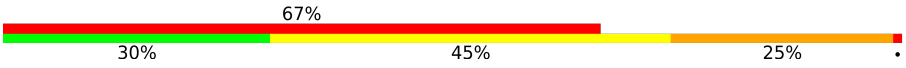
• Molecule 29: 50S ribosomal protein L9

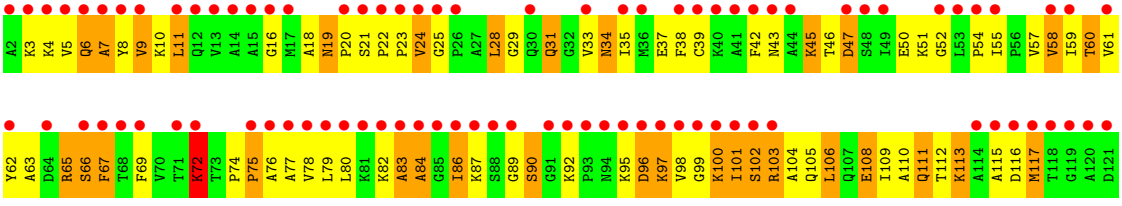
Chain DH:

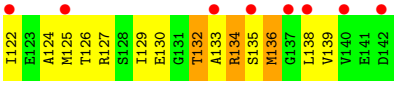


• Molecule 30: 50S ribosomal protein L11

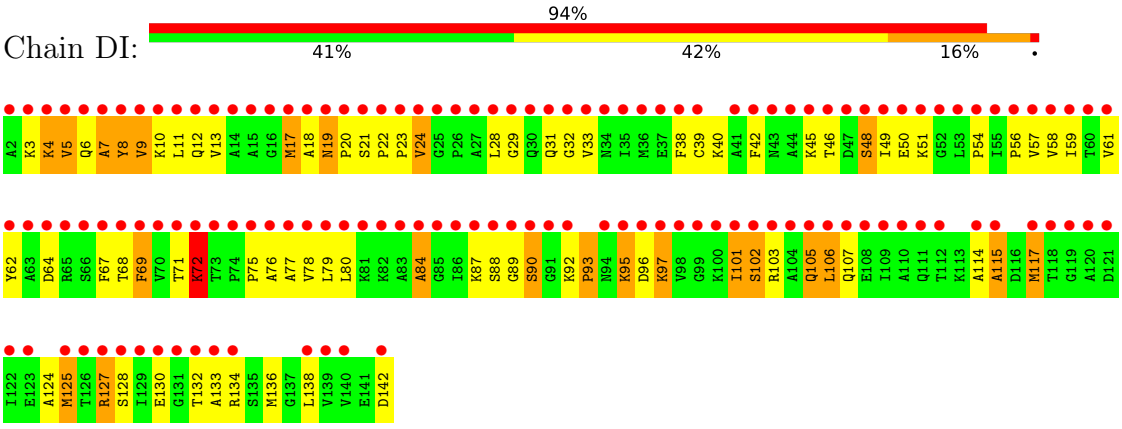
Chain BI:



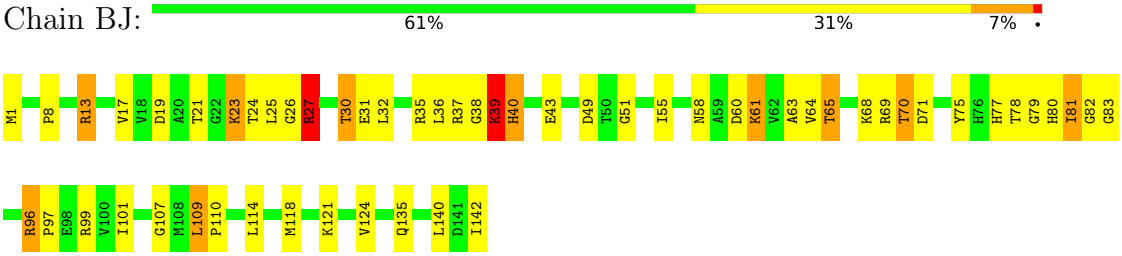




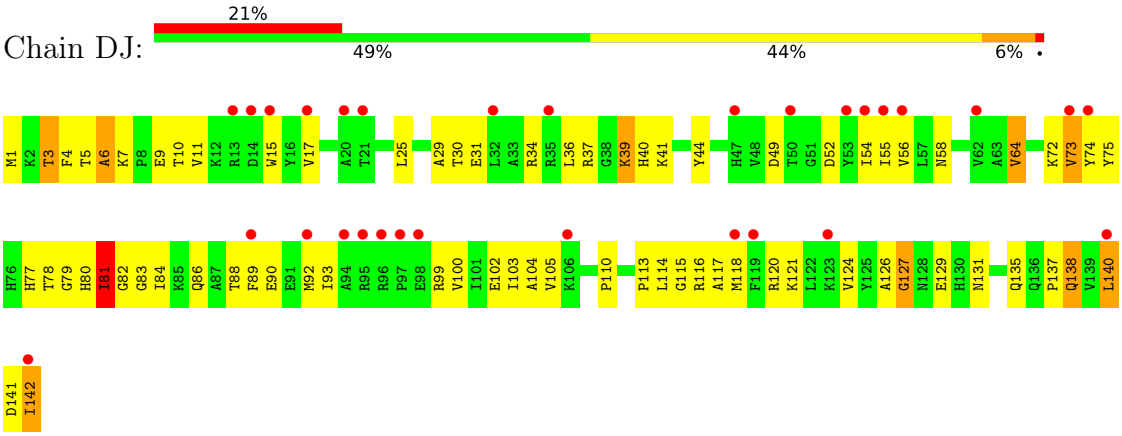
• Molecule 30: 50S ribosomal protein L11



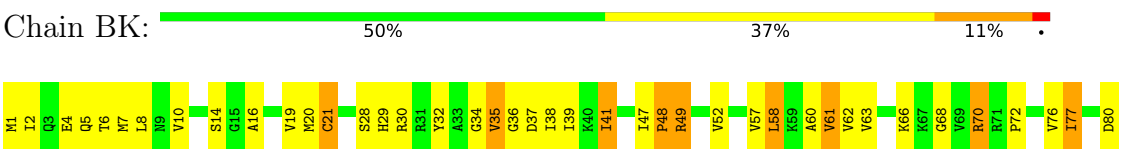
• Molecule 31: 50S ribosomal protein L13



• Molecule 31: 50S ribosomal protein L13

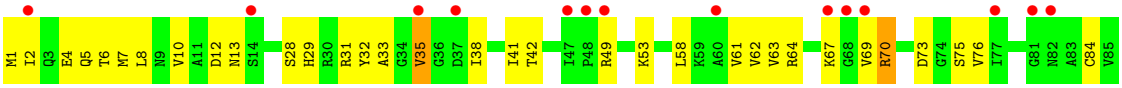


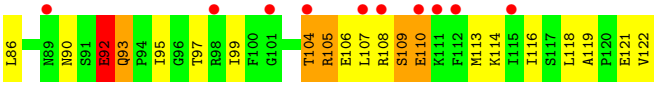
• Molecule 32: 50S ribosomal protein L14



• Molecule 32: 50S ribosomal protein L14

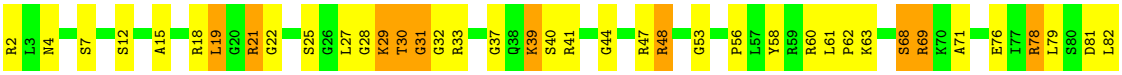
Chain DK:





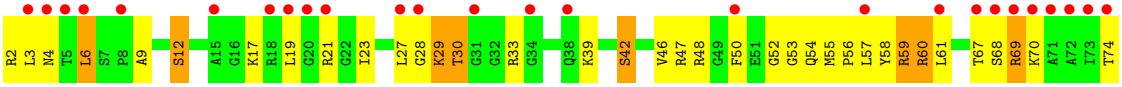
• Molecule 33: 50S ribosomal protein L15

Chain BL:



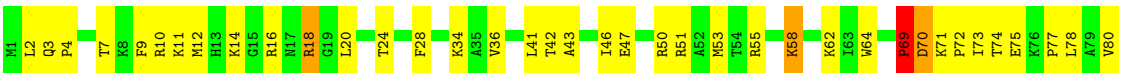
• Molecule 33: 50S ribosomal protein L15

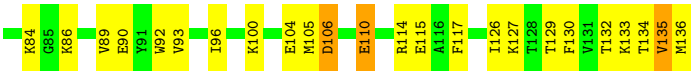
Chain DL:



• Molecule 34: 50S ribosomal protein L16

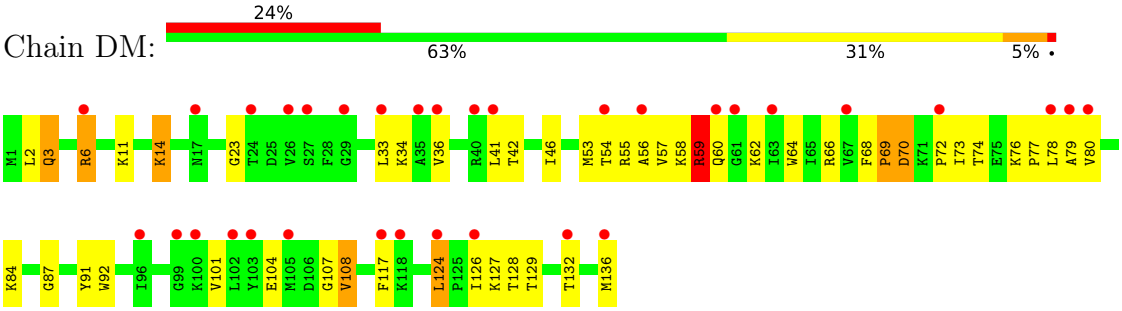
Chain BM:





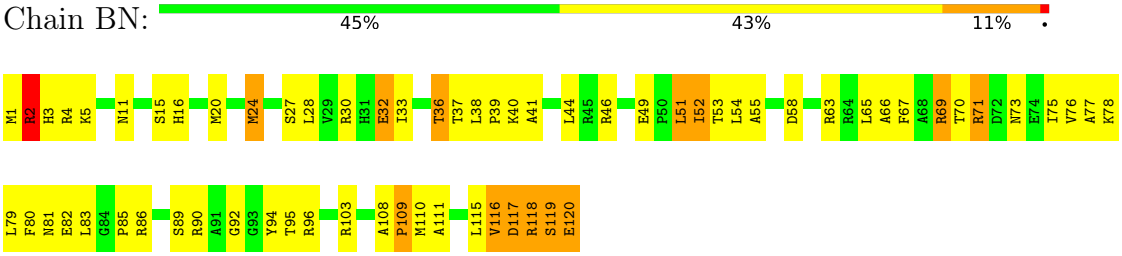
• Molecule 34: 50S ribosomal protein L16

Chain DM:



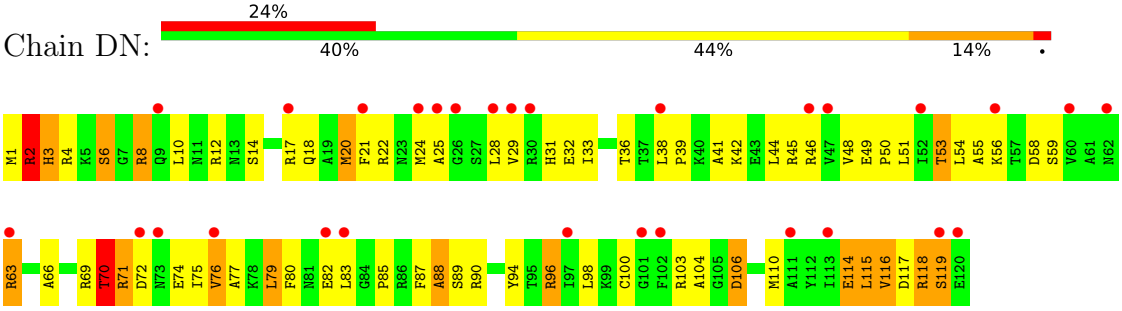
• Molecule 35: 50S ribosomal protein L17

Chain BN:



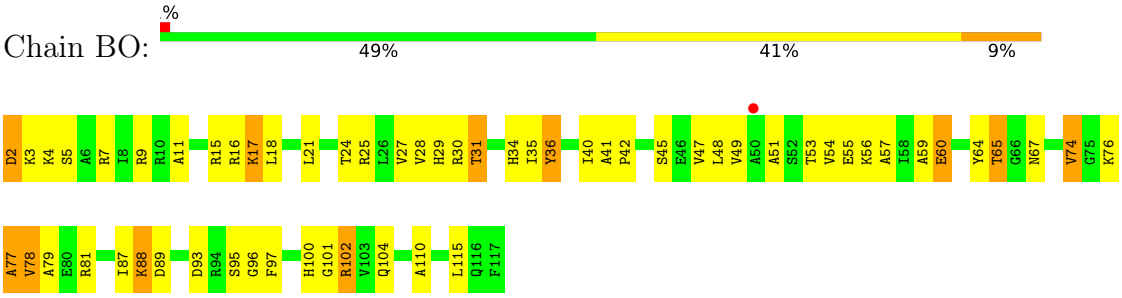
• Molecule 35: 50S ribosomal protein L17

Chain DN:



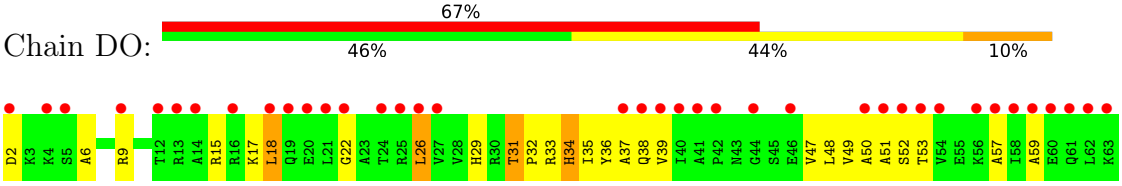
• Molecule 36: 50S ribosomal protein L18

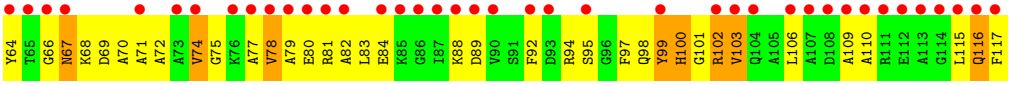
Chain BO:



• Molecule 36: 50S ribosomal protein L18

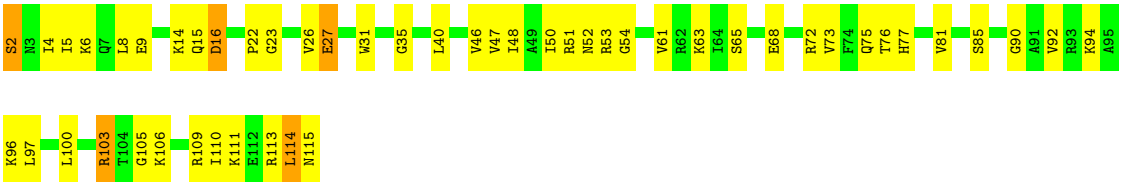
Chain DO:





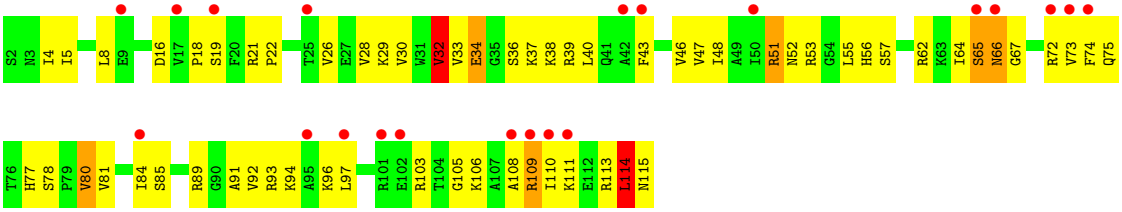
• Molecule 37: 50S ribosomal protein L19

Chain BP:



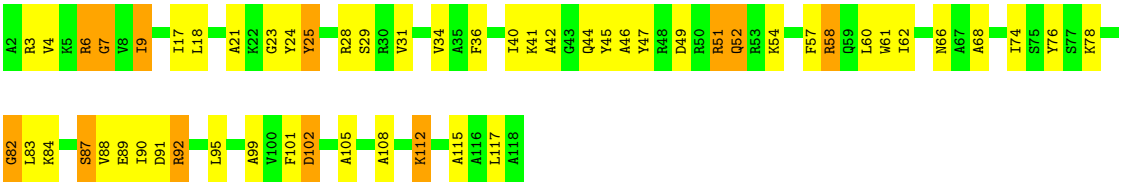
• Molecule 37: 50S ribosomal protein L19

Chain DP:



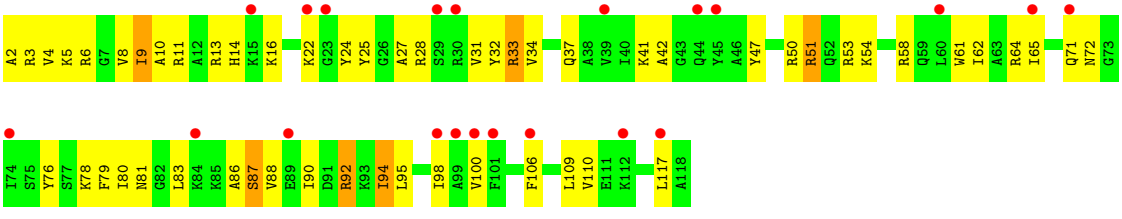
• Molecule 38: 50S ribosomal protein L20

Chain BQ:



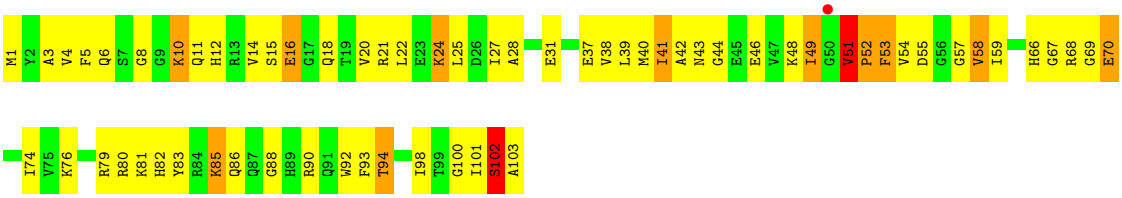
• Molecule 38: 50S ribosomal protein L20

Chain DQ:



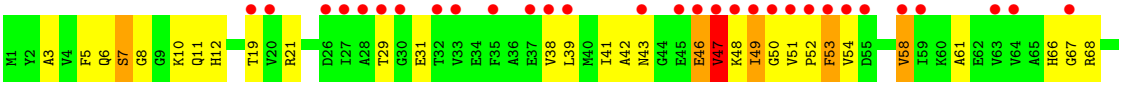
• Molecule 39: 50S ribosomal protein L21

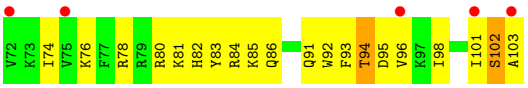
Chain BR:



• Molecule 39: 50S ribosomal protein L21

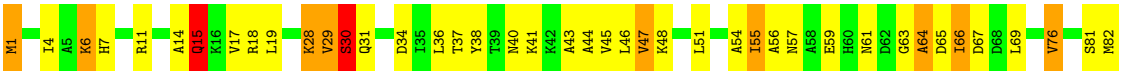
Chain DR:





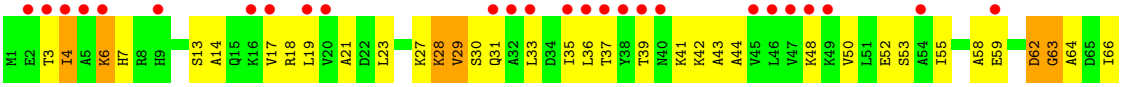
• Molecule 40: 50S ribosomal protein L22

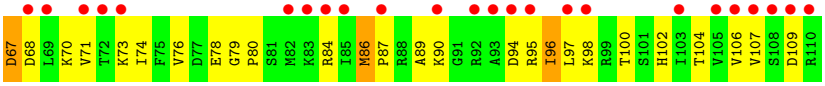
Chain BS:



• Molecule 40: 50S ribosomal protein L22

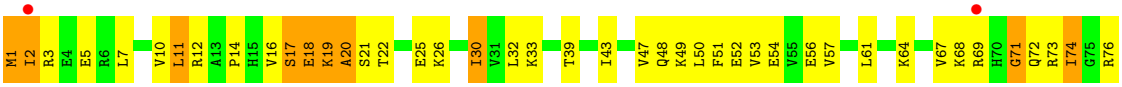
Chain DS:

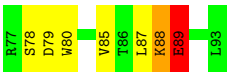




• Molecule 41: 50S ribosomal protein L23

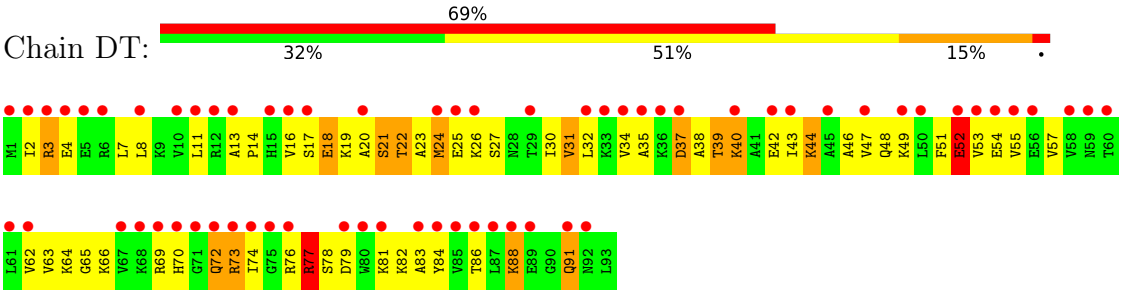
Chain BT:





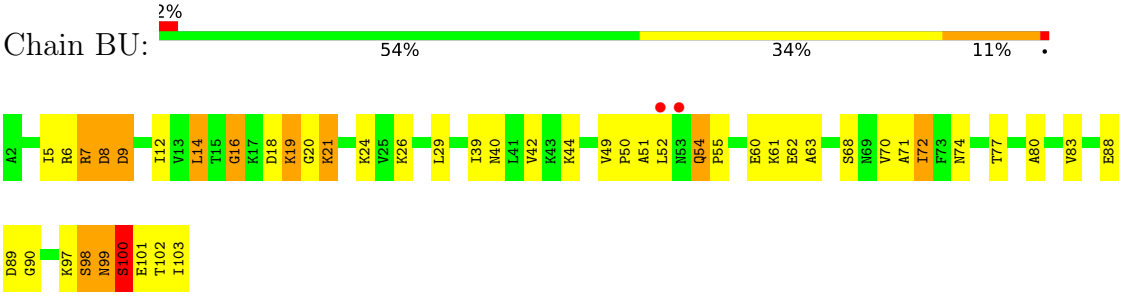
• Molecule 41: 50S ribosomal protein L23

Chain DT:



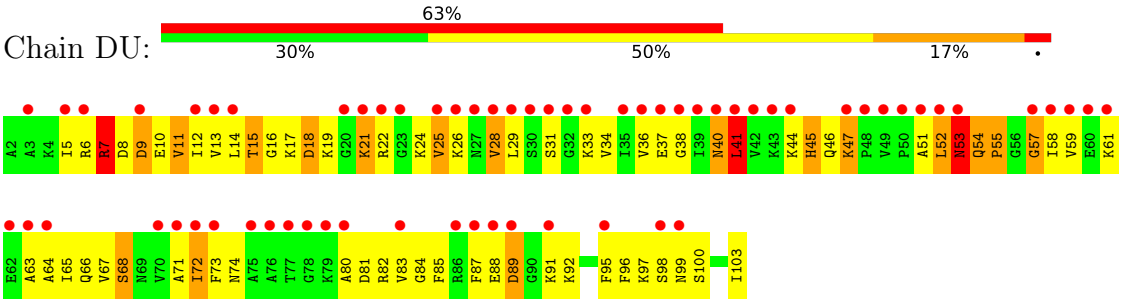
• Molecule 42: 50S ribosomal protein L24

Chain BU:



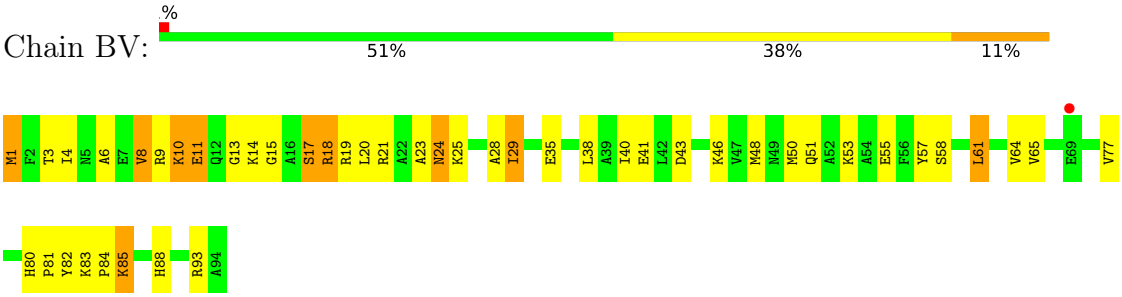
• Molecule 42: 50S ribosomal protein L24

Chain DU:



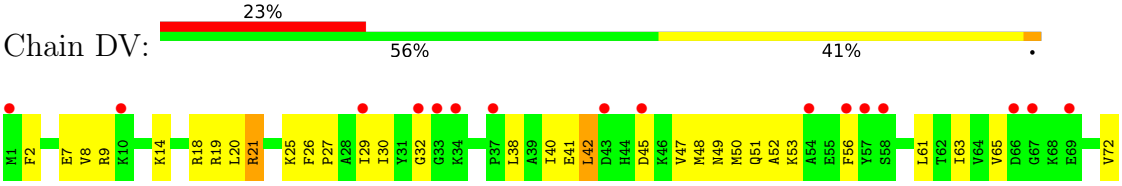
• Molecule 43: 50S ribosomal protein L25

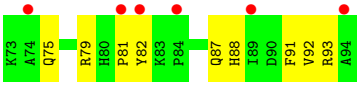
Chain BV:



• Molecule 43: 50S ribosomal protein L25

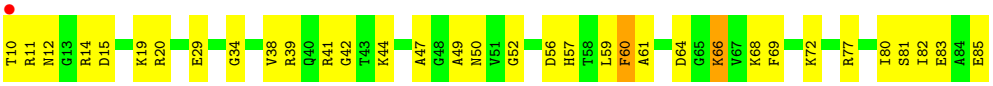
Chain DV:





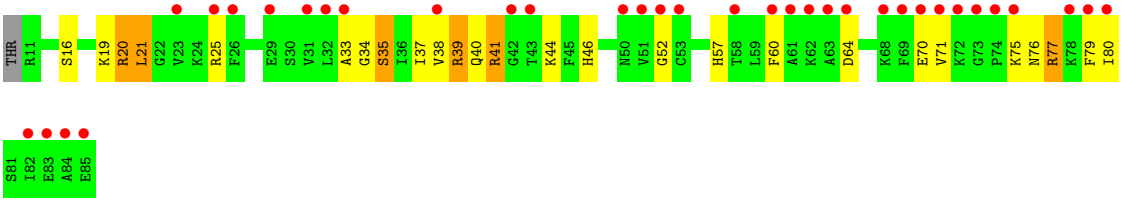
• Molecule 44: 50S ribosomal protein L27

Chain BW:



• Molecule 44: 50S ribosomal protein L27

Chain DW:

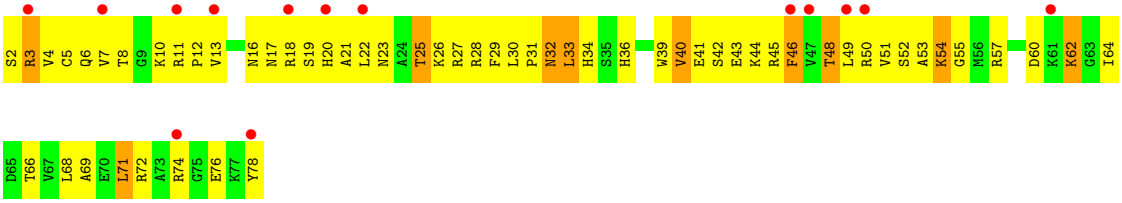


• Molecule 45: 50S ribosomal protein L28

Chain BX:

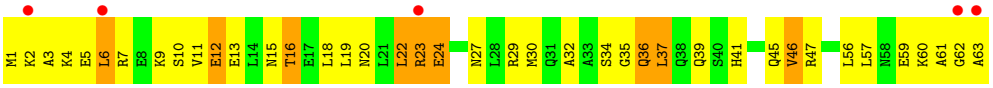
• Molecule 45: 50S ribosomal protein L28

Chain DX:



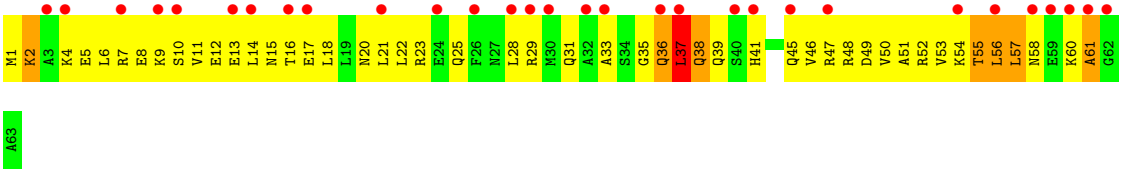
• Molecule 46: 50S ribosomal protein L29

Chain BY:

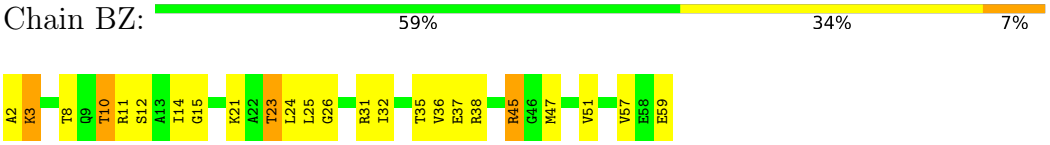


• Molecule 46: 50S ribosomal protein L29

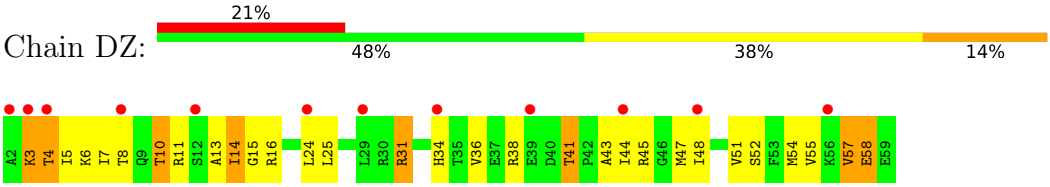
Chain DY:



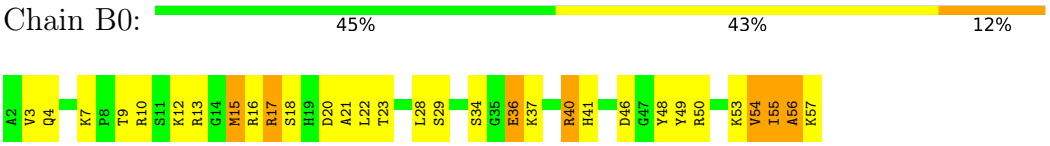
• Molecule 47: 50S ribosomal protein L30



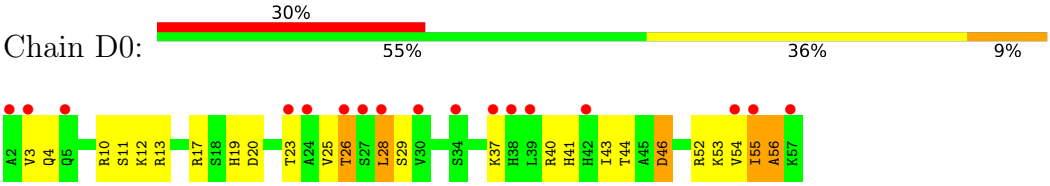
• Molecule 47: 50S ribosomal protein L30



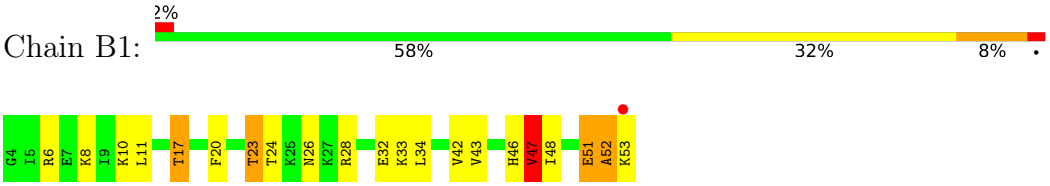
• Molecule 48: 50S ribosomal protein L32



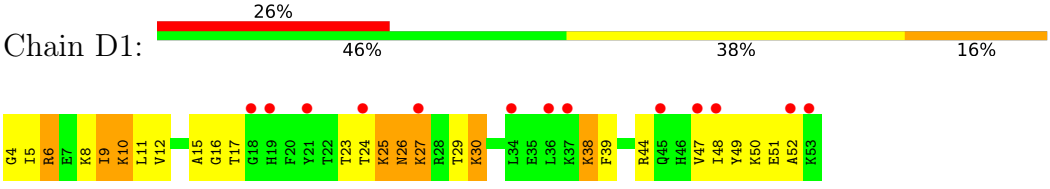
• Molecule 48: 50S ribosomal protein L32



• Molecule 49: 50S ribosomal protein L33

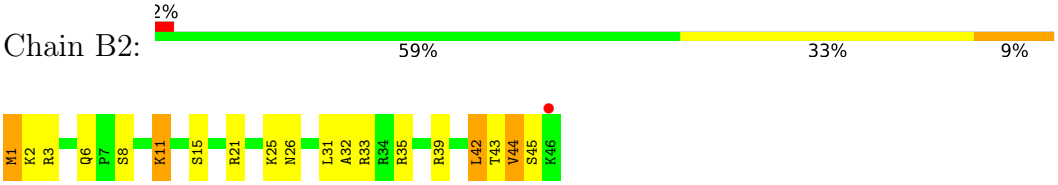


• Molecule 49: 50S ribosomal protein L33



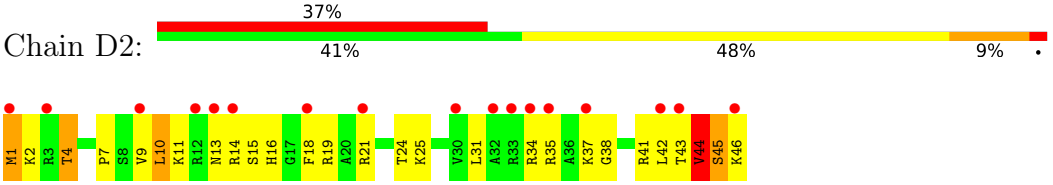
• Molecule 50: 50S ribosomal protein L34

Chain B2:



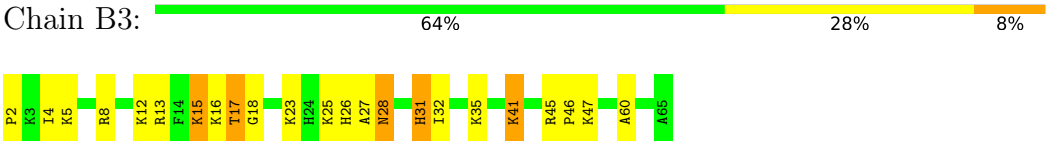
• Molecule 50: 50S ribosomal protein L34

Chain D2:



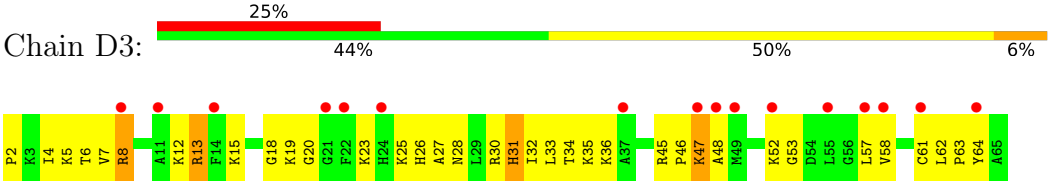
• Molecule 51: 50S ribosomal protein L35

Chain B3:



• Molecule 51: 50S ribosomal protein L35

Chain D3:

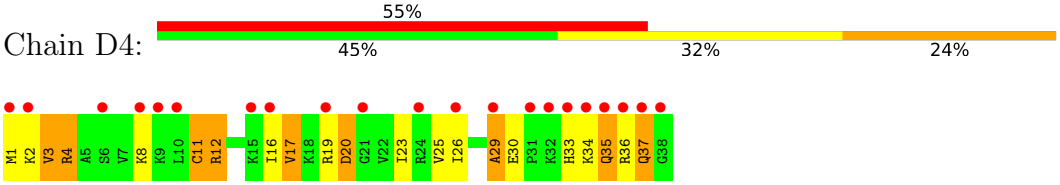


• Molecule 52: 50S ribosomal protein L36

Chain B4:

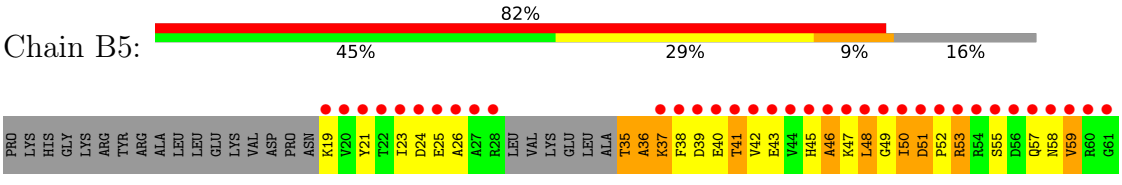
• Molecule 52: 50S ribosomal protein L36

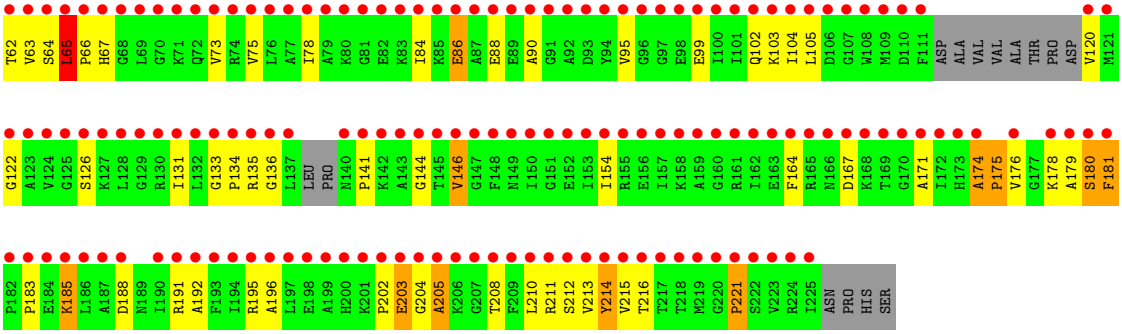
Chain D4:



• Molecule 53: 50S ribosomal protein L1

Chain B5:




T62 V63 S64 L65 P66 H67 G68 L69 G70 K71 Q72 V73 R74 V75 L76 A77 I78 A79 K80 G81 E82 K83 I84 K85 E86 A87 E88 E89 A90 G91 A92 D93 Y94 V95 G96 G97 E98 E99 I100 I101 Q102 K103 I104 L105 D106 G107 W108 M109 D110 F111 ASP ALA VAL VAL ALA THR PRO ASP V120 M121
G122 A123 V124 G125 S126 K127 L128 G129 R130 I131 L132 G133 P134 R135 G136 L137 LEU PRO N140 P141 K142 A143 G144 T145 V146 G147 F148 N149 I150 G151 E152 I153 I154 R155 E156 I157 K158 A159 G160 R161 I162 E163 F164 R165 N166 D167 K168 T169 G170 A171 I172 H173 A174 P175 V176 G177 K178 A179 S180 F181
P182 P183 E184 K185 L186 A187 D188 N189 I190 R191 A192 F193 I194 R195 A196 L197 E198 A199 H200 K201 P202 E203 G204 A205 K206 G207 T208 F209 L210 R211 S212 V213 Y214 V215 T216 T217 T218 M219 G220 P221 S222 V223 R224 I225 ASN PRO HIS SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	211.79Å 433.06Å 623.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.33 – 2.90 69.33 – 2.90	Depositor EDS
% Data completeness (in resolution range)	87.4 (69.33-2.90) 87.4 (69.33-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.235 , 0.279 0.240 , 0.282	Depositor DCC
R_{free} test set	4412 reflections (0.40%)	wwPDB-VP
Wilson B-factor (Å^2)	48.9	Xtriage
Anisotropy	0.742	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 56.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	288258	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.85% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: VIF, ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	AA	0.47	0/36944	0.95	29/57632 (0.1%)
1	CA	0.40	0/36966	0.90	9/57666 (0.0%)
2	AB	0.36	0/1736	0.64	0/2338
2	CB	0.33	0/1736	0.60	0/2338
3	AC	0.35	0/1652	0.61	0/2225
3	CC	0.31	0/1652	0.57	0/2225
4	AD	0.35	0/1665	0.63	0/2227
4	CD	0.40	0/1665	0.66	0/2227
5	AE	0.39	0/1119	0.70	0/1504
5	CE	0.36	0/1119	0.70	0/1504
6	AF	0.39	0/836	0.65	0/1128
6	CF	0.33	0/836	0.63	1/1128 (0.1%)
7	AG	0.34	0/1196	0.59	0/1602
7	CG	0.32	0/1196	0.55	0/1602
8	AH	0.34	0/989	0.58	0/1326
8	CH	0.32	0/989	0.59	0/1326
9	AI	0.33	0/1034	0.62	0/1375
9	CI	0.32	0/1034	0.62	0/1375
10	AJ	0.34	0/797	0.61	0/1077
10	CJ	0.31	0/797	0.62	1/1077 (0.1%)
11	AK	0.35	0/893	0.60	0/1205
11	CK	0.34	0/893	0.60	0/1205
12	AL	0.39	0/969	0.65	0/1300
12	CL	0.36	0/969	0.70	0/1300
13	AM	0.33	0/893	0.71	1/1193 (0.1%)
13	CM	0.34	0/893	0.59	0/1193
14	AN	0.34	0/785	0.63	0/1043
14	CN	0.30	0/785	0.54	0/1043
15	AO	0.33	0/718	0.60	0/959
15	CO	0.32	0/718	0.56	0/959
16	AP	0.36	0/659	0.70	1/884 (0.1%)
16	CP	0.35	0/659	0.58	0/884

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	AQ	0.37	0/658	0.66	1/881 (0.1%)
17	CQ	0.36	0/658	0.61	0/881
18	AR	0.33	0/463	0.57	0/621
18	CR	0.32	0/463	0.58	0/621
19	AS	0.34	0/653	0.63	0/877
19	CS	0.33	0/653	0.54	0/877
20	AT	0.34	0/671	0.60	0/888
20	CT	0.32	0/671	0.57	0/888
21	AU	0.45	0/431	0.72	0/570
21	CU	0.45	0/431	0.73	0/570
22	BA	0.80	22/69659 (0.0%)	1.31	570/108672 (0.5%)
22	DA	0.40	0/69659	0.90	13/108672 (0.0%)
23	BB	0.68	0/2850	1.17	9/4444 (0.2%)
23	DB	0.35	0/2828	0.85	0/4410
24	BC	0.48	0/2122	0.72	0/2852
24	DC	0.34	0/2122	0.60	0/2852
25	BD	0.54	0/1586	0.78	1/2134 (0.0%)
25	DD	0.33	0/1586	0.57	0/2134
26	BE	0.46	0/1571	0.66	0/2113
26	DE	0.35	0/1571	0.59	0/2113
27	BF	0.37	0/1435	0.59	0/1926
27	DF	0.32	0/1435	0.52	0/1926
28	BG	0.37	0/1343	0.65	0/1816
28	DG	0.32	0/1343	0.53	0/1816
29	BH	0.36	0/1121	0.66	1/1515 (0.1%)
29	DH	0.35	0/1121	0.56	0/1515
30	BI	0.37	0/1046	0.59	0/1410
30	DI	0.37	0/1046	0.61	0/1410
31	BJ	0.53	0/1152	0.74	1/1551 (0.1%)
31	DJ	0.32	0/1152	0.59	0/1551
32	BK	0.52	0/948	0.77	0/1268
32	DK	0.34	0/948	0.56	0/1268
33	BL	0.50	0/1054	0.81	1/1403 (0.1%)
33	DL	0.34	0/1054	0.61	0/1403
34	BM	0.53	0/1093	0.72	0/1460
34	DM	0.31	0/1093	0.54	0/1460
35	BN	0.54	0/974	0.75	0/1301
35	DN	0.35	0/974	0.58	0/1301
36	BO	0.40	0/902	0.64	0/1209
36	DO	0.30	0/902	0.51	0/1209
37	BP	0.49	0/929	0.72	1/1242 (0.1%)
37	DP	0.35	0/929	0.58	0/1242
38	BQ	0.65	0/960	0.83	0/1278

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	DQ	0.33	0/960	0.53	0/1278
39	BR	0.60	0/829	0.79	1/1107 (0.1%)
39	DR	0.34	0/829	0.58	0/1107
40	BS	0.63	0/864	0.82	0/1156
40	DS	0.34	0/864	0.59	0/1156
41	BT	0.43	0/745	0.62	0/994
41	DT	0.35	0/745	0.60	0/994
42	BU	0.43	0/788	0.66	0/1051
42	DU	0.37	0/788	0.59	0/1051
43	BV	0.44	0/766	0.65	0/1025
43	DV	0.30	0/766	0.50	0/1025
44	BW	0.55	0/587	0.73	0/776
44	DW	0.31	0/576	0.49	0/762
45	BX	0.43	0/635	0.72	0/848
45	DX	0.34	0/635	0.60	0/848
46	BY	0.40	0/510	0.69	0/677
46	DY	0.34	0/510	0.58	0/677
47	BZ	0.55	0/453	0.82	0/605
47	DZ	0.31	0/453	0.55	0/605
48	B0	0.55	0/450	0.76	0/599
48	D0	0.35	0/450	0.61	0/599
49	B1	0.40	0/417	0.62	0/554
49	D1	0.34	0/417	0.56	0/554
50	B2	0.50	0/380	0.77	0/498
50	D2	0.36	0/380	0.59	0/498
51	B3	0.48	0/513	0.67	0/676
51	D3	0.31	0/513	0.54	0/676
52	B4	0.56	0/303	0.68	0/397
52	D4	0.46	0/303	0.64	0/397
53	B5	0.33	0/1145	0.55	0/1556
All	All	0.52	22/310626 (0.0%)	0.97	641/464366 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	CB	0	1
5	CE	0	1
6	CF	0	1
11	AK	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
11	CK	0	1
12	CL	0	1
21	AU	0	2
21	CU	0	1
25	BD	0	1
25	DD	0	1
33	BL	0	1
47	BZ	0	1
All	All	0	13

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	984	A	N9-C4	-9.47	1.32	1.37
22	BA	1977	A	N9-C4	-7.26	1.33	1.37
22	BA	1142	A	N9-C4	-7.11	1.33	1.37
22	BA	528	A	N7-C5	-7.06	1.35	1.39
22	BA	2071	A	N9-C4	-6.99	1.33	1.37

The worst 5 of 641 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	528	A	N1-C6-N6	13.66	126.80	118.60
25	BD	151	THR	C-N-CD	-12.30	93.53	120.60
22	BA	984	A	C2-N3-C4	-11.24	104.98	110.60
22	BA	532	A	O5'-P-OP1	-10.12	96.59	105.70
22	BA	528	A	C6-C5-N7	-9.92	125.36	132.30

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	AK	126	LYS	Peptide
21	AU	39	GLU	Peptide
21	AU	8	GLU	Peptide
25	BD	151	THR	Peptide
33	BL	110	VAL	Peptide

5.2 Too-close contacts (i)

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	AA	32995	0	16607	1173	4
1	CA	33015	0	16617	1168	1
2	AB	1705	0	1732	198	0
2	CB	1705	0	1732	149	0
3	AC	1625	0	1696	88	0
3	CC	1625	0	1696	94	0
4	AD	1643	0	1707	143	0
4	CD	1643	0	1707	130	0
5	AE	1106	0	1148	82	0
5	CE	1106	0	1148	115	0
6	AF	818	0	808	60	0
6	CF	818	0	808	65	0
7	AG	1182	0	1238	78	0
7	CG	1182	0	1238	57	0
8	AH	979	0	1031	64	0
8	CH	979	0	1031	54	0
9	AI	1022	0	1070	91	0
9	CI	1022	0	1070	67	0
10	AJ	787	0	828	97	0
10	CJ	787	0	828	48	0
11	AK	877	0	887	87	0
11	CK	877	0	887	74	0
12	AL	955	0	1016	54	0
12	CL	955	0	1016	61	0
13	AM	884	0	941	70	0
13	CM	884	0	941	56	0
14	AN	774	0	824	74	0
14	CN	774	0	824	55	0
15	AO	710	0	728	45	0
15	CO	710	0	728	46	0
16	AP	649	0	666	64	0
16	CP	649	0	666	30	0
17	AQ	649	0	691	59	0
17	CQ	649	0	691	55	0
18	AR	456	0	478	22	0
18	CR	456	0	478	39	0
19	AS	638	0	665	40	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	CS	638	0	665	30	0
20	AT	665	0	714	53	0
20	CT	665	0	714	48	0
21	AU	426	0	449	57	0
21	CU	426	0	449	54	0
22	BA	62195	0	31280	1960	0
22	DA	62195	0	31280	2094	1
23	BB	2549	0	1291	47	0
23	DB	2529	0	1281	64	0
24	BC	2083	0	2154	131	0
24	DC	2083	0	2154	140	0
25	BD	1565	0	1616	108	0
25	DD	1565	0	1616	85	0
26	BE	1552	0	1619	71	0
26	DE	1552	0	1619	108	0
27	BF	1411	0	1444	84	0
27	DF	1411	0	1444	53	0
28	BG	1323	0	1371	62	0
28	DG	1323	0	1371	62	0
29	BH	1110	0	1147	167	0
29	DH	1110	0	1148	93	4
30	BI	1032	0	1085	89	0
30	DI	1032	0	1085	76	0
31	BJ	1129	0	1162	45	0
31	DJ	1129	0	1162	55	0
32	BK	939	0	1012	48	0
32	DK	939	0	1012	35	0
33	BL	1045	0	1117	54	0
33	DL	1045	0	1117	71	0
34	BM	1074	0	1157	49	0
34	DM	1074	0	1157	31	0
35	BN	961	0	1000	68	0
35	DN	961	0	1000	69	0
36	BO	892	0	923	41	0
36	DO	892	0	923	48	0
37	BP	917	0	962	43	0
37	DP	917	0	962	49	0
38	BQ	947	0	1019	62	0
38	DQ	947	0	1019	56	0
39	BR	816	0	839	84	0
39	DR	816	0	839	52	0
40	BS	857	0	922	58	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	DS	857	0	922	43	0
41	BT	739	0	807	34	0
41	DT	739	0	807	54	0
42	BU	780	0	831	35	0
42	DU	780	0	831	71	0
43	BV	753	0	780	35	0
43	DV	753	0	780	24	0
44	BW	580	0	594	21	0
44	DW	569	0	581	20	0
45	BX	625	0	652	26	0
45	DX	625	0	652	67	0
46	BY	509	0	543	36	0
46	DY	509	0	543	45	0
47	BZ	449	0	488	20	0
47	DZ	449	0	488	16	0
48	B0	444	0	458	35	0
48	D0	444	0	458	26	0
49	B1	410	0	440	17	0
49	D1	410	0	440	19	0
50	B2	377	0	418	14	0
50	D2	377	0	418	28	0
51	B3	504	0	572	25	0
51	D3	504	0	572	31	0
52	B4	302	0	340	18	0
52	D4	302	0	342	21	0
53	B5	1142	0	865	58	0
54	AA	72	0	0	0	0
54	BA	194	0	0	0	0
54	BB	4	0	0	0	0
54	BN	1	0	0	0	0
54	CA	55	0	0	0	0
54	CM	1	0	0	0	0
54	D2	1	0	0	0	0
54	DA	166	0	0	0	0
54	DB	3	0	0	0	0
54	DQ	1	0	0	0	0
55	BA	38	0	38	5	0
55	DA	38	0	37	11	0
56	B4	1	0	0	2	0
56	D4	1	0	0	0	0
57	AA	195	0	0	29	0
57	AL	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	AN	5	0	0	0	0
57	AT	1	0	0	0	0
57	AU	1	0	0	1	0
57	B2	1	0	0	1	0
57	B3	2	0	0	0	0
57	B4	1	0	0	0	0
57	BA	620	0	0	101	0
57	BB	13	0	0	0	0
57	BC	6	0	0	4	0
57	BD	3	0	0	3	0
57	BE	4	0	0	0	0
57	BF	1	0	0	1	0
57	BG	1	0	0	0	0
57	BL	8	0	0	0	0
57	BN	4	0	0	0	0
57	BS	1	0	0	0	0
57	BV	1	0	0	0	0
57	CA	189	0	0	19	0
57	CL	1	0	0	0	0
57	CN	3	0	0	0	0
57	CT	4	0	0	0	0
57	CU	1	0	0	0	0
57	D0	1	0	0	0	0
57	D2	3	0	0	0	0
57	D3	2	0	0	0	0
57	D4	1	0	0	0	0
57	DA	613	0	0	87	0
57	DB	13	0	0	1	0
57	DC	9	0	0	1	0
57	DD	4	0	0	2	0
57	DE	2	0	0	0	0
57	DJ	1	0	0	0	0
57	DL	3	0	0	1	0
57	DN	1	0	0	0	0
57	DT	2	0	0	0	0
57	DV	1	0	0	0	0
All	All	288258	0	192864	11506	5

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 24.

The worst 5 of 11506 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)
29:BH:123:ARG:NH2	1:CA:367:U:OP2	1.64	1.27
29:BH:117:LEU:O	29:BH:121:VAL:HG23	1.34	1.22
15:AO:89:ARG:NH1	22:BA:716:A:OP2	1.75	1.19
22:BA:1153:C:OP2	57:BA:3357:HOH:O	1.59	1.19
22:BA:2574:G:OP1	57:BA:3713:HOH:O	1.61	1.18

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:368:U:OP2	29:DH:123:ARG:NE[4_455]	1.71	0.49
1:AA:368:U:OP2	29:DH:123:ARG:CZ[4_455]	1.89	0.31
1:AA:368:U:OP2	29:DH:123:ARG:NH2[4_455]	2.04	0.16
1:AA:368:U:OP1	29:DH:93:SER:OG[4_455]	2.10	0.10
1:CA:204:G:OP1	22:DA:289:G:O2'[3_545]	2.12	0.08

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	
2	AB	216/218 (99%)	125 (58%)	36 (17%)	55 (26%)	0	0
2	CB	216/218 (99%)	126 (58%)	54 (25%)	36 (17%)	0	0
3	AC	204/206 (99%)	144 (71%)	48 (24%)	12 (6%)	1	5
3	CC	204/206 (99%)	146 (72%)	41 (20%)	17 (8%)	1	2
4	AD	203/205 (99%)	140 (69%)	38 (19%)	25 (12%)	0	1
4	CD	203/205 (99%)	148 (73%)	35 (17%)	20 (10%)	0	1
5	AE	148/150 (99%)	107 (72%)	24 (16%)	17 (12%)	0	1
5	CE	148/150 (99%)	100 (68%)	25 (17%)	23 (16%)	0	0
6	AF	98/100 (98%)	67 (68%)	17 (17%)	14 (14%)	0	0
6	CF	98/100 (98%)	65 (66%)	16 (16%)	17 (17%)	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
7	AG	149/151 (99%)	101 (68%)	33 (22%)	15 (10%)	0 1
7	CG	149/151 (99%)	120 (80%)	19 (13%)	10 (7%)	1 3
8	AH	127/129 (98%)	88 (69%)	29 (23%)	10 (8%)	1 2
8	CH	127/129 (98%)	101 (80%)	19 (15%)	7 (6%)	2 5
9	AI	125/127 (98%)	87 (70%)	23 (18%)	15 (12%)	0 1
9	CI	125/127 (98%)	91 (73%)	25 (20%)	9 (7%)	1 3
10	AJ	96/98 (98%)	63 (66%)	12 (12%)	21 (22%)	0 0
10	CJ	96/98 (98%)	72 (75%)	15 (16%)	9 (9%)	0 1
11	AK	115/117 (98%)	85 (74%)	17 (15%)	13 (11%)	0 1
11	CK	115/117 (98%)	83 (72%)	23 (20%)	9 (8%)	1 2
12	AL	121/123 (98%)	96 (79%)	15 (12%)	10 (8%)	1 2
12	CL	121/123 (98%)	92 (76%)	17 (14%)	12 (10%)	0 1
13	AM	112/114 (98%)	83 (74%)	17 (15%)	12 (11%)	0 1
13	CM	112/114 (98%)	80 (71%)	21 (19%)	11 (10%)	0 1
14	AN	92/100 (92%)	55 (60%)	25 (27%)	12 (13%)	0 0
14	CN	92/100 (92%)	57 (62%)	20 (22%)	15 (16%)	0 0
15	AO	86/88 (98%)	63 (73%)	18 (21%)	5 (6%)	1 5
15	CO	86/88 (98%)	63 (73%)	19 (22%)	4 (5%)	2 8
16	AP	80/82 (98%)	44 (55%)	17 (21%)	19 (24%)	0 0
16	CP	80/82 (98%)	57 (71%)	18 (22%)	5 (6%)	1 4
17	AQ	78/80 (98%)	53 (68%)	16 (20%)	9 (12%)	0 1
17	CQ	78/80 (98%)	55 (70%)	14 (18%)	9 (12%)	0 1
18	AR	53/55 (96%)	44 (83%)	7 (13%)	2 (4%)	3 13
18	CR	53/55 (96%)	42 (79%)	7 (13%)	4 (8%)	1 2
19	AS	77/79 (98%)	53 (69%)	16 (21%)	8 (10%)	0 1
19	CS	77/79 (98%)	61 (79%)	13 (17%)	3 (4%)	3 12
20	AT	83/85 (98%)	57 (69%)	20 (24%)	6 (7%)	1 3
20	CT	83/85 (98%)	62 (75%)	13 (16%)	8 (10%)	0 1
21	AU	49/51 (96%)	27 (55%)	10 (20%)	12 (24%)	0 0
21	CU	49/51 (96%)	24 (49%)	12 (24%)	13 (26%)	0 0
24	BC	269/271 (99%)	213 (79%)	39 (14%)	17 (6%)	1 4

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
24	DC	269/271 (99%)	200 (74%)	49 (18%)	20 (7%)	1 2
25	BD	207/209 (99%)	167 (81%)	33 (16%)	7 (3%)	3 15
25	DD	207/209 (99%)	165 (80%)	33 (16%)	9 (4%)	2 10
26	BE	199/201 (99%)	153 (77%)	39 (20%)	7 (4%)	3 14
26	DE	199/201 (99%)	146 (73%)	40 (20%)	13 (6%)	1 3
27	BF	175/177 (99%)	136 (78%)	30 (17%)	9 (5%)	2 7
27	DF	175/177 (99%)	136 (78%)	26 (15%)	13 (7%)	1 2
28	BG	174/176 (99%)	145 (83%)	19 (11%)	10 (6%)	1 5
28	DG	174/176 (99%)	129 (74%)	30 (17%)	15 (9%)	1 2
29	BH	147/149 (99%)	89 (60%)	37 (25%)	21 (14%)	0 0
29	DH	147/149 (99%)	100 (68%)	32 (22%)	15 (10%)	0 1
30	BI	139/141 (99%)	71 (51%)	44 (32%)	24 (17%)	0 0
30	DI	139/141 (99%)	75 (54%)	49 (35%)	15 (11%)	0 1
31	BJ	140/142 (99%)	124 (89%)	12 (9%)	4 (3%)	4 18
31	DJ	140/142 (99%)	123 (88%)	12 (9%)	5 (4%)	3 14
32	BK	120/122 (98%)	96 (80%)	16 (13%)	8 (7%)	1 3
32	DK	120/122 (98%)	97 (81%)	16 (13%)	7 (6%)	1 5
33	BL	141/143 (99%)	106 (75%)	20 (14%)	15 (11%)	0 1
33	DL	141/143 (99%)	104 (74%)	27 (19%)	10 (7%)	1 3
34	BM	134/136 (98%)	117 (87%)	15 (11%)	2 (2%)	10 34
34	DM	134/136 (98%)	111 (83%)	17 (13%)	6 (4%)	2 9
35	BN	118/120 (98%)	92 (78%)	19 (16%)	7 (6%)	1 5
35	DN	118/120 (98%)	91 (77%)	19 (16%)	8 (7%)	1 3
36	BO	114/116 (98%)	91 (80%)	19 (17%)	4 (4%)	3 14
36	DO	114/116 (98%)	97 (85%)	11 (10%)	6 (5%)	2 6
37	BP	112/114 (98%)	101 (90%)	6 (5%)	5 (4%)	2 9
37	DP	112/114 (98%)	89 (80%)	16 (14%)	7 (6%)	1 4
38	BQ	115/117 (98%)	93 (81%)	16 (14%)	6 (5%)	2 6
38	DQ	115/117 (98%)	104 (90%)	10 (9%)	1 (1%)	17 48
39	BR	101/103 (98%)	83 (82%)	9 (9%)	9 (9%)	1 1
39	DR	101/103 (98%)	80 (79%)	14 (14%)	7 (7%)	1 3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
40	BS	108/110 (98%)	83 (77%)	18 (17%)	7 (6%)	1 3
40	DS	108/110 (98%)	88 (82%)	13 (12%)	7 (6%)	1 3
41	BT	91/93 (98%)	69 (76%)	8 (9%)	14 (15%)	0 0
41	DT	91/93 (98%)	65 (71%)	14 (15%)	12 (13%)	0 0
42	BU	100/102 (98%)	75 (75%)	16 (16%)	9 (9%)	1 1
42	DU	100/102 (98%)	70 (70%)	19 (19%)	11 (11%)	0 1
43	BV	92/94 (98%)	85 (92%)	6 (6%)	1 (1%)	14 42
43	DV	92/94 (98%)	76 (83%)	14 (15%)	2 (2%)	6 24
44	BW	74/76 (97%)	70 (95%)	4 (5%)	0	100 100
44	DW	73/76 (96%)	59 (81%)	11 (15%)	3 (4%)	3 11
45	BX	75/77 (97%)	66 (88%)	6 (8%)	3 (4%)	3 11
45	DX	75/77 (97%)	57 (76%)	14 (19%)	4 (5%)	2 6
46	BY	61/63 (97%)	35 (57%)	19 (31%)	7 (12%)	0 1
46	DY	61/63 (97%)	42 (69%)	14 (23%)	5 (8%)	1 2
47	BZ	56/58 (97%)	47 (84%)	9 (16%)	0	100 100
47	DZ	56/58 (97%)	53 (95%)	1 (2%)	2 (4%)	3 14
48	B0	54/56 (96%)	44 (82%)	7 (13%)	3 (6%)	2 5
48	D0	54/56 (96%)	38 (70%)	12 (22%)	4 (7%)	1 2
49	B1	48/50 (96%)	39 (81%)	5 (10%)	4 (8%)	1 2
49	D1	48/50 (96%)	40 (83%)	5 (10%)	3 (6%)	1 4
50	B2	44/46 (96%)	36 (82%)	7 (16%)	1 (2%)	6 23
50	D2	44/46 (96%)	36 (82%)	6 (14%)	2 (4%)	2 9
51	B3	62/64 (97%)	54 (87%)	7 (11%)	1 (2%)	9 32
51	D3	62/64 (97%)	49 (79%)	10 (16%)	3 (5%)	2 8
52	B4	36/38 (95%)	31 (86%)	5 (14%)	0	100 100
52	D4	36/38 (95%)	28 (78%)	4 (11%)	4 (11%)	0 1
53	B5	183/228 (80%)	100 (55%)	49 (27%)	34 (19%)	0 0
All	All	11418/11672 (98%)	8486 (74%)	1941 (17%)	991 (9%)	1 2

5 of 991 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	12	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	AB	16	PHE
2	AB	22	TYR
2	AB	34	ALA
2	AB	64	LYS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	180/180 (100%)	117 (65%)	63 (35%)	0	0
2	CB	180/180 (100%)	130 (72%)	50 (28%)	0	1
3	AC	170/170 (100%)	134 (79%)	36 (21%)	1	3
3	CC	170/170 (100%)	134 (79%)	36 (21%)	1	3
4	AD	172/172 (100%)	135 (78%)	37 (22%)	1	3
4	CD	172/172 (100%)	136 (79%)	36 (21%)	1	3
5	AE	113/113 (100%)	86 (76%)	27 (24%)	0	2
5	CE	113/113 (100%)	85 (75%)	28 (25%)	0	2
6	AF	87/87 (100%)	60 (69%)	27 (31%)	0	1
6	CF	87/87 (100%)	61 (70%)	26 (30%)	0	1
7	AG	124/124 (100%)	94 (76%)	30 (24%)	0	2
7	CG	124/124 (100%)	91 (73%)	33 (27%)	0	1
8	AH	104/104 (100%)	81 (78%)	23 (22%)	1	3
8	CH	104/104 (100%)	81 (78%)	23 (22%)	1	3
9	AI	105/105 (100%)	75 (71%)	30 (29%)	0	1
9	CI	105/105 (100%)	76 (72%)	29 (28%)	0	1
10	AJ	86/86 (100%)	63 (73%)	23 (27%)	0	1
10	CJ	86/86 (100%)	68 (79%)	18 (21%)	1	3
11	AK	90/90 (100%)	67 (74%)	23 (26%)	0	1
11	CK	90/90 (100%)	71 (79%)	19 (21%)	1	3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
12	AL	103/103 (100%)	81 (79%)	22 (21%)	1 3
12	CL	103/103 (100%)	76 (74%)	27 (26%)	0 1
13	AM	92/92 (100%)	73 (79%)	19 (21%)	1 3
13	CM	92/92 (100%)	71 (77%)	21 (23%)	1 2
14	AN	79/83 (95%)	62 (78%)	17 (22%)	1 3
14	CN	79/83 (95%)	69 (87%)	10 (13%)	4 13
15	AO	75/76 (99%)	58 (77%)	17 (23%)	1 2
15	CO	75/76 (99%)	59 (79%)	16 (21%)	1 3
16	AP	65/65 (100%)	47 (72%)	18 (28%)	0 1
16	CP	65/65 (100%)	52 (80%)	13 (20%)	1 4
17	AQ	74/74 (100%)	49 (66%)	25 (34%)	0 0
17	CQ	74/74 (100%)	52 (70%)	22 (30%)	0 1
18	AR	48/48 (100%)	42 (88%)	6 (12%)	4 14
18	CR	48/48 (100%)	39 (81%)	9 (19%)	1 4
19	AS	70/70 (100%)	61 (87%)	9 (13%)	4 13
19	CS	70/70 (100%)	57 (81%)	13 (19%)	1 5
20	AT	65/65 (100%)	52 (80%)	13 (20%)	1 4
20	CT	65/65 (100%)	49 (75%)	16 (25%)	0 2
21	AU	44/44 (100%)	25 (57%)	19 (43%)	0 0
21	CU	44/44 (100%)	29 (66%)	15 (34%)	0 0
24	BC	216/216 (100%)	187 (87%)	29 (13%)	4 11
24	DC	216/216 (100%)	185 (86%)	31 (14%)	3 9
25	BD	164/164 (100%)	150 (92%)	14 (8%)	10 31
25	DD	164/164 (100%)	148 (90%)	16 (10%)	8 24
26	BE	165/165 (100%)	134 (81%)	31 (19%)	1 4
26	DE	165/165 (100%)	134 (81%)	31 (19%)	1 4
27	BF	148/148 (100%)	122 (82%)	26 (18%)	2 5
27	DF	148/148 (100%)	120 (81%)	28 (19%)	1 4
28	BG	137/137 (100%)	120 (88%)	17 (12%)	4 14
28	DG	137/137 (100%)	123 (90%)	14 (10%)	7 22
29	BH	114/114 (100%)	88 (77%)	26 (23%)	1 2

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
29	DH	114/114 (100%)	88 (77%)	26 (23%)	1 2
30	BI	109/109 (100%)	81 (74%)	28 (26%)	0 1
30	DI	109/109 (100%)	86 (79%)	23 (21%)	1 3
31	BJ	116/116 (100%)	97 (84%)	19 (16%)	2 7
31	DJ	116/116 (100%)	100 (86%)	16 (14%)	3 10
32	BK	103/103 (100%)	86 (84%)	17 (16%)	2 7
32	DK	103/103 (100%)	91 (88%)	12 (12%)	5 16
33	BL	102/102 (100%)	83 (81%)	19 (19%)	1 5
33	DL	102/102 (100%)	78 (76%)	24 (24%)	1 2
34	BM	109/109 (100%)	96 (88%)	13 (12%)	5 15
34	DM	109/109 (100%)	98 (90%)	11 (10%)	7 23
35	BN	100/100 (100%)	85 (85%)	15 (15%)	3 9
35	DN	100/100 (100%)	82 (82%)	18 (18%)	1 5
36	BO	86/86 (100%)	68 (79%)	18 (21%)	1 3
36	DO	86/86 (100%)	70 (81%)	16 (19%)	1 5
37	BP	99/99 (100%)	91 (92%)	8 (8%)	11 33
37	DP	99/99 (100%)	82 (83%)	17 (17%)	2 6
38	BQ	89/89 (100%)	77 (86%)	12 (14%)	4 11
38	DQ	89/89 (100%)	74 (83%)	15 (17%)	2 6
39	BR	84/84 (100%)	71 (84%)	13 (16%)	2 8
39	DR	84/84 (100%)	74 (88%)	10 (12%)	5 15
40	BS	93/93 (100%)	75 (81%)	18 (19%)	1 4
40	DS	93/93 (100%)	80 (86%)	13 (14%)	3 10
41	BT	80/80 (100%)	70 (88%)	10 (12%)	4 14
41	DT	80/80 (100%)	67 (84%)	13 (16%)	2 7
42	BU	83/83 (100%)	71 (86%)	12 (14%)	3 9
42	DU	83/83 (100%)	63 (76%)	20 (24%)	0 2
43	BV	78/78 (100%)	63 (81%)	15 (19%)	1 4
43	DV	78/78 (100%)	68 (87%)	10 (13%)	4 13
44	BW	57/58 (98%)	49 (86%)	8 (14%)	3 10
44	DW	56/58 (97%)	51 (91%)	5 (9%)	9 29

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
45	BX	67/67 (100%)	57 (85%)	10 (15%)	3 9
45	DX	67/67 (100%)	55 (82%)	12 (18%)	2 5
46	BY	55/55 (100%)	48 (87%)	7 (13%)	4 13
46	DY	55/55 (100%)	43 (78%)	12 (22%)	1 3
47	BZ	48/48 (100%)	38 (79%)	10 (21%)	1 3
47	DZ	48/48 (100%)	37 (77%)	11 (23%)	1 2
48	B0	47/47 (100%)	40 (85%)	7 (15%)	3 9
48	D0	47/47 (100%)	41 (87%)	6 (13%)	4 13
49	B1	45/45 (100%)	41 (91%)	4 (9%)	9 29
49	D1	45/45 (100%)	37 (82%)	8 (18%)	2 5
50	B2	38/38 (100%)	31 (82%)	7 (18%)	1 5
50	D2	38/38 (100%)	31 (82%)	7 (18%)	1 5
51	B3	51/51 (100%)	45 (88%)	6 (12%)	5 16
51	D3	51/51 (100%)	45 (88%)	6 (12%)	5 16
52	B4	34/34 (100%)	31 (91%)	3 (9%)	10 30
52	D4	34/34 (100%)	26 (76%)	8 (24%)	1 2
53	B5	61/180 (34%)	48 (79%)	13 (21%)	1 3
All	All	9386/9518 (99%)	7568 (81%)	1818 (19%)	1 4

5 of 1818 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	CB	23	TRP
47	DZ	10	THR
8	CH	104	VAL
45	DX	46	PHE
33	DL	143	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
28	DG	139	GLN
42	DU	74	ASN
28	DG	143	GLN
38	DQ	37	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	D1	19	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1537/1539 (99%)	349 (22%)	15 (0%)
1	CA	1538/1539 (99%)	331 (21%)	9 (0%)
22	BA	2895/2903 (99%)	643 (22%)	30 (1%)
22	DA	2895/2903 (99%)	637 (22%)	29 (1%)
23	BB	118/119 (99%)	21 (17%)	0
23	DB	117/119 (98%)	25 (21%)	0
All	All	9100/9122 (99%)	2006 (22%)	83 (0%)

5 of 2006 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	5	U
1	AA	6	G
1	AA	9	G
1	AA	13	U

5 of 83 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	DA	479	A
22	DA	2162	G
22	DA	614	A
22	DA	1378	A
22	DA	2296	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 502 ligands modelled in this entry, 500 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
55	VIF	BA	3001	-	35,40,40	2.30	13 (37%)	43,55,55	1.99	11 (25%)
55	VIF	DA	3001	-	35,40,40	2.26	12 (34%)	43,55,55	2.24	15 (34%)

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
55	VIF	BA	3001	-	-	9/42/58/58	0/2/3/3
55	VIF	DA	3001	-	-	9/42/58/58	0/2/3/3

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	BA	3001	VIF	O01-C06	-4.92	1.37	1.44
55	BA	3001	VIF	C11-C09	-4.46	1.43	1.53
55	DA	3001	VIF	C15-N01	4.39	1.44	1.34
55	BA	3001	VIF	O01-C08	-4.38	1.24	1.34
55	DA	3001	VIF	O01-C06	-4.29	1.38	1.44

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	DA	3001	VIF	C02-C01-C03	-7.56	103.77	122.69
55	BA	3001	VIF	C02-C01-C03	-5.72	108.38	122.69
55	BA	3001	VIF	C18-C10-C20	-4.96	118.40	125.89
55	DA	3001	VIF	C06-O01-C08	4.67	125.80	117.78
55	DA	3001	VIF	C18-C10-C20	-4.50	119.09	125.89

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	BA	3001	VIF	C19-C-C06-O01
55	BA	3001	VIF	C27-C04-C07-C14
55	BA	3001	VIF	C27-C04-C07-F
55	DA	3001	VIF	C18-C10-C20-C24
55	DA	3001	VIF	C27-C04-C07-F

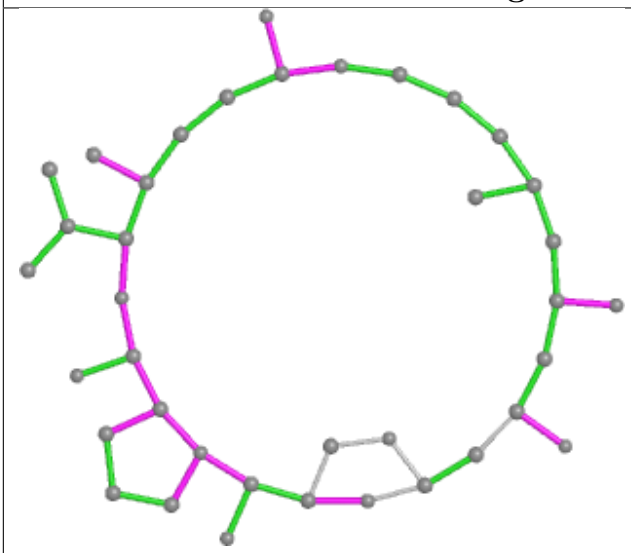
There are no ring outliers.

2 monomers are involved in 16 short contacts:

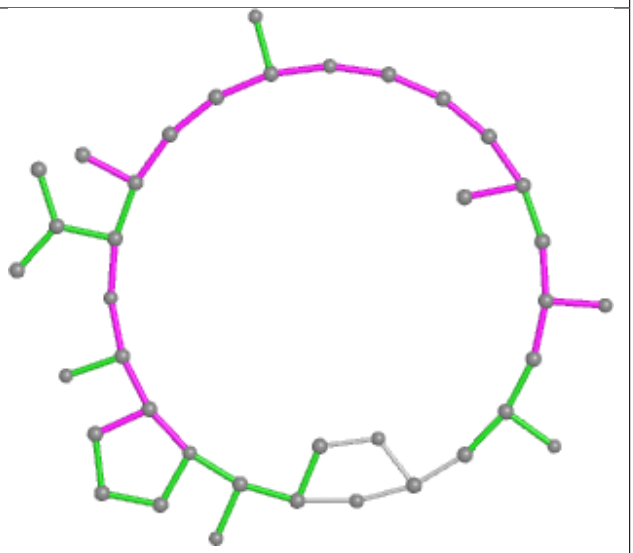
Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	BA	3001	VIF	5	0
55	DA	3001	VIF	11	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

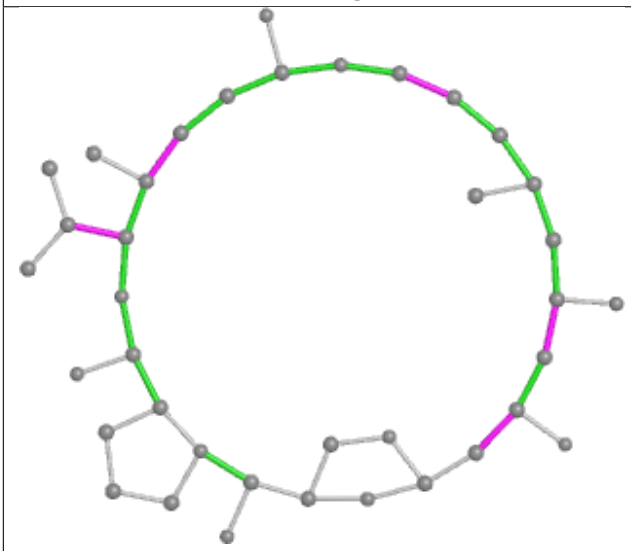
Ligand VIF BA 3001



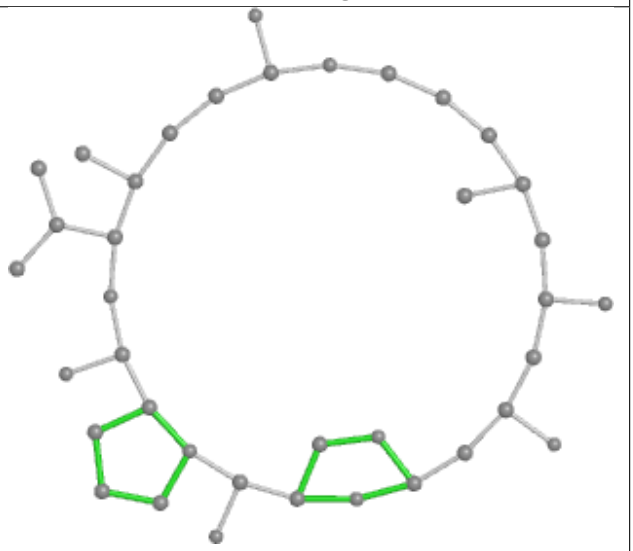
Bond lengths



Bond angles

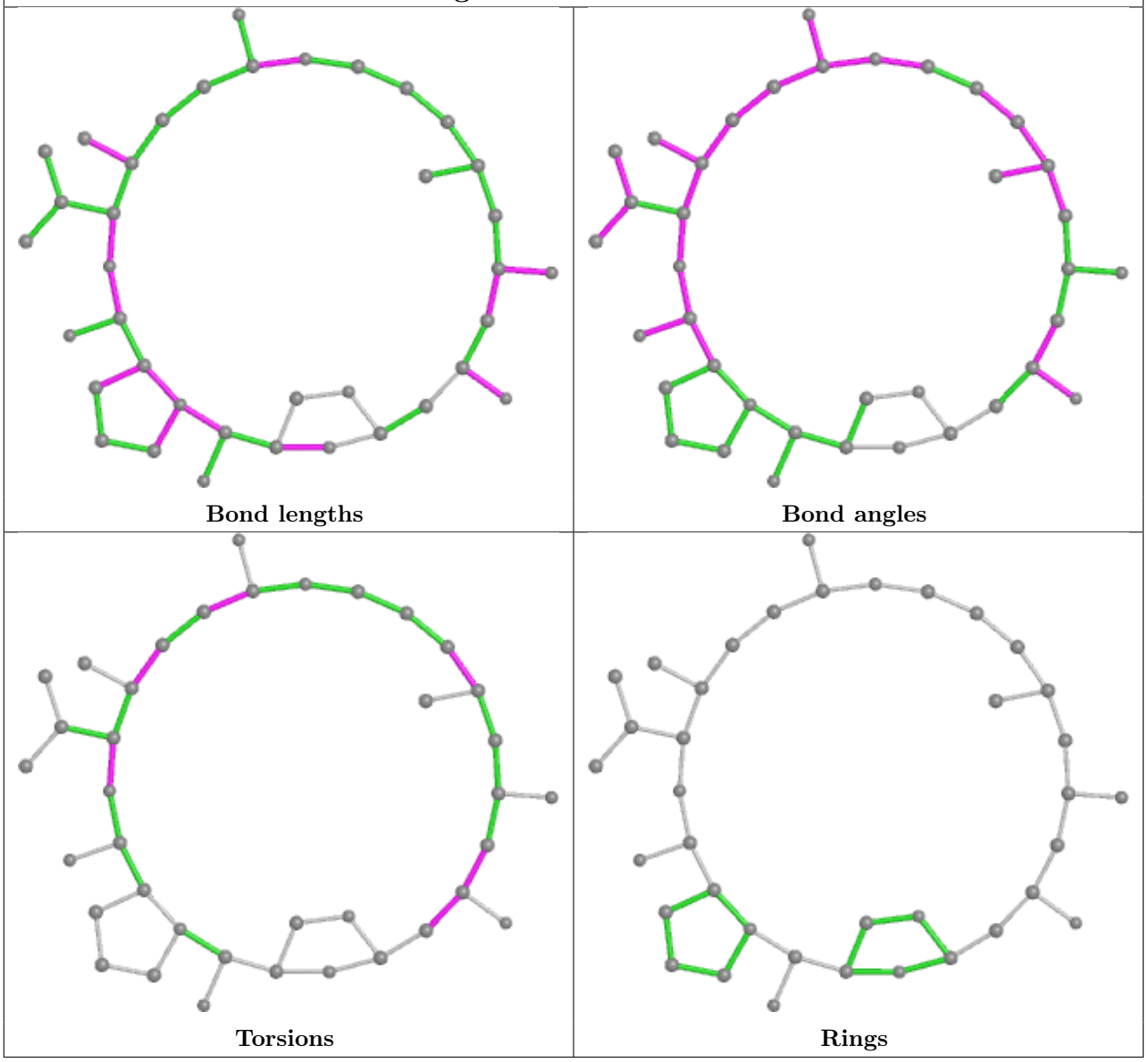


Torsions



Rings

Ligand VIF DA 3001



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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	AA	1538/1539 (99%)	-0.04	39 (2%) 57 55	13, 51, 135, 177	0
1	CA	1539/1539 (100%)	0.25	82 (5%) 26 22	27, 71, 143, 176	0
2	AB	218/218 (100%)	1.03	42 (19%) 1 0	40, 71, 99, 129	0
2	CB	218/218 (100%)	1.42	64 (29%) 0 0	57, 81, 107, 126	0
3	AC	206/206 (100%)	0.22	9 (4%) 34 30	36, 57, 81, 94	0
3	CC	206/206 (100%)	1.34	47 (22%) 0 0	53, 75, 93, 113	0
4	AD	205/205 (100%)	0.36	12 (5%) 22 18	33, 55, 79, 108	0
4	CD	205/205 (100%)	0.17	8 (3%) 39 35	21, 40, 74, 90	0
5	AE	150/150 (100%)	0.24	6 (4%) 38 33	28, 50, 82, 111	0
5	CE	150/150 (100%)	0.49	9 (6%) 21 18	33, 57, 84, 105	0
6	AF	100/100 (100%)	0.02	1 (1%) 82 82	33, 56, 75, 84	0
6	CF	100/100 (100%)	0.53	8 (8%) 12 9	47, 72, 95, 105	0
7	AG	151/151 (100%)	0.84	27 (17%) 1 1	49, 74, 98, 107	0
7	CG	151/151 (100%)	2.55	88 (58%) 0 0	77, 94, 106, 113	0
8	AH	129/129 (100%)	0.20	2 (1%) 72 71	29, 48, 71, 80	0
8	CH	129/129 (100%)	0.60	11 (8%) 10 8	47, 63, 82, 88	0
9	AI	127/127 (100%)	1.00	22 (17%) 1 1	45, 70, 95, 115	0
9	CI	127/127 (100%)	1.74	46 (36%) 0 0	68, 88, 106, 130	0
10	AJ	98/98 (100%)	0.88	15 (15%) 2 1	44, 64, 93, 121	0
10	CJ	98/98 (100%)	2.65	57 (58%) 0 0	68, 90, 109, 123	0
11	AK	117/117 (100%)	0.68	15 (12%) 3 2	27, 61, 87, 107	0
11	CK	117/117 (100%)	0.44	6 (5%) 28 24	37, 65, 83, 90	0
12	AL	123/123 (100%)	0.28	5 (4%) 37 32	24, 37, 71, 101	0
12	CL	123/123 (100%)	0.53	9 (7%) 15 11	38, 51, 79, 102	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	AM	114/114 (100%)	0.51	10 (8%) 10 7	46, 67, 90, 104	0
13	CM	114/114 (100%)	3.11	79 (69%) 0 0	84, 100, 114, 118	0
14	AN	96/100 (96%)	0.79	17 (17%) 1 1	41, 58, 92, 107	0
14	CN	96/100 (96%)	2.30	50 (52%) 0 0	64, 88, 107, 118	0
15	AO	88/88 (100%)	0.16	5 (5%) 23 19	31, 50, 66, 98	0
15	CO	88/88 (100%)	0.39	5 (5%) 23 19	39, 62, 84, 105	0
16	AP	82/82 (100%)	0.78	11 (13%) 3 2	33, 45, 80, 103	0
16	CP	82/82 (100%)	1.34	20 (24%) 0 0	44, 62, 89, 105	0
17	AQ	80/80 (100%)	0.54	6 (7%) 14 11	29, 54, 83, 123	0
17	CQ	80/80 (100%)	1.43	25 (31%) 0 0	41, 70, 96, 108	0
18	AR	55/55 (100%)	0.03	4 (7%) 15 11	37, 51, 76, 113	0
18	CR	55/55 (100%)	0.46	3 (5%) 25 21	39, 54, 82, 112	0
19	AS	79/79 (100%)	1.07	17 (21%) 0 0	46, 67, 92, 97	0
19	CS	79/79 (100%)	4.26	62 (78%) 0 0	82, 100, 113, 125	0
20	AT	85/85 (100%)	0.69	7 (8%) 11 9	33, 48, 72, 115	0
20	CT	85/85 (100%)	1.99	34 (40%) 0 0	53, 69, 91, 97	0
21	AU	51/51 (100%)	1.27	13 (25%) 0 0	45, 71, 92, 105	0
21	CU	51/51 (100%)	0.70	8 (15%) 2 1	42, 69, 92, 107	0
22	BA	2897/2903 (99%)	0.23	123 (4%) 36 32	2, 18, 128, 195	0
22	DA	2897/2903 (99%)	0.43	162 (5%) 24 20	44, 82, 142, 183	0
23	BB	119/119 (100%)	-0.30	0 100 100	5, 27, 53, 94	0
23	DB	118/119 (99%)	0.22	4 (3%) 45 40	68, 110, 132, 142	0
24	BC	271/271 (100%)	-0.04	1 (0%) 92 93	6, 24, 44, 62	0
24	DC	271/271 (100%)	0.93	41 (15%) 2 1	40, 61, 75, 83	0
25	BD	209/209 (100%)	-0.15	0 100 100	2, 14, 42, 69	0
25	DD	209/209 (100%)	1.04	39 (18%) 1 0	47, 65, 84, 98	0
26	BE	201/201 (100%)	-0.15	2 (0%) 82 82	4, 27, 55, 94	0
26	DE	201/201 (100%)	1.89	80 (39%) 0 0	38, 78, 97, 108	0
27	BF	177/177 (100%)	0.31	11 (6%) 20 16	23, 45, 85, 101	0
27	DF	177/177 (100%)	3.49	138 (77%) 0 0	80, 99, 114, 125	0
28	BG	176/176 (100%)	0.16	5 (2%) 53 49	21, 40, 66, 93	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	DG	176/176 (100%)	2.40	99 (56%) 0 0	68, 87, 103, 118	0
29	BH	149/149 (100%)	3.55	95 (63%) 0 0	25, 102, 121, 129	0
29	DH	149/149 (100%)	1.82	62 (41%) 0 0	25, 92, 107, 115	0
30	BI	141/141 (100%)	3.64	95 (67%) 0 0	82, 105, 120, 135	0
30	DI	141/141 (100%)	5.32	132 (93%) 0 0	95, 111, 121, 124	0
31	BJ	142/142 (100%)	-0.19	0 100 100	2, 11, 33, 52	0
31	DJ	142/142 (100%)	1.06	30 (21%) 1 0	50, 65, 81, 97	0
32	BK	122/122 (100%)	-0.27	0 100 100	6, 18, 37, 68	0
32	DK	122/122 (100%)	1.02	24 (19%) 1 0	46, 61, 80, 94	0
33	BL	143/143 (100%)	-0.07	0 100 100	3, 24, 50, 81	0
33	DL	143/143 (100%)	2.10	65 (45%) 0 0	45, 74, 91, 111	0
34	BM	136/136 (100%)	-0.23	0 100 100	3, 14, 33, 93	0
34	DM	136/136 (100%)	1.19	33 (24%) 0 0	44, 66, 82, 109	0
35	BN	120/120 (100%)	-0.23	0 100 100	6, 13, 25, 68	0
35	DN	120/120 (100%)	1.42	29 (24%) 0 0	53, 71, 88, 111	0
36	BO	116/116 (100%)	-0.03	1 (0%) 84 84	19, 29, 51, 57	0
36	DO	116/116 (100%)	3.08	78 (67%) 0 0	70, 88, 102, 113	0
37	BP	114/114 (100%)	-0.10	0 100 100	11, 21, 49, 73	0
37	DP	114/114 (100%)	1.06	21 (18%) 1 0	54, 67, 84, 91	0
38	BQ	117/117 (100%)	-0.18	0 100 100	3, 8, 19, 51	0
38	DQ	117/117 (100%)	0.91	21 (17%) 1 1	51, 65, 79, 82	0
39	BR	103/103 (100%)	-0.14	1 (0%) 82 82	3, 17, 36, 65	0
39	DR	103/103 (100%)	1.67	35 (33%) 0 0	52, 73, 87, 96	0
40	BS	110/110 (100%)	-0.12	1 (0%) 84 84	3, 8, 28, 88	0
40	DS	110/110 (100%)	2.03	50 (45%) 0 0	56, 70, 88, 96	0
41	BT	93/93 (100%)	0.32	2 (2%) 62 59	13, 30, 83, 101	0
41	DT	93/93 (100%)	2.96	64 (68%) 0 0	62, 81, 103, 109	0
42	BU	102/102 (100%)	-0.09	2 (1%) 65 63	13, 31, 60, 95	0
42	DU	102/102 (100%)	3.54	64 (62%) 0 0	66, 84, 105, 111	0
43	BV	94/94 (100%)	-0.13	1 (1%) 80 80	10, 24, 47, 58	0
43	DV	94/94 (100%)	1.12	22 (23%) 0 0	65, 79, 94, 97	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	BW	76/76 (100%)	-0.08	1 (1%) 77 77	9, 16, 38, 57	0
44	DW	75/76 (98%)	2.17	35 (46%) 0 0	51, 77, 88, 108	0
45	BX	77/77 (100%)	-0.20	1 (1%) 77 77	10, 26, 52, 79	0
45	DX	77/77 (100%)	0.99	14 (18%) 1 1	47, 67, 84, 89	0
46	BY	63/63 (100%)	0.40	5 (7%) 12 10	20, 44, 71, 96	0
46	DY	63/63 (100%)	2.07	30 (47%) 0 0	68, 88, 96, 103	0
47	BZ	58/58 (100%)	-0.14	0 100 100	6, 11, 36, 41	0
47	DZ	58/58 (100%)	0.97	12 (20%) 1 0	52, 70, 83, 88	0
48	B0	56/56 (100%)	-0.19	0 100 100	3, 14, 40, 75	0
48	D0	56/56 (100%)	1.38	17 (30%) 0 0	51, 71, 91, 105	0
49	B1	50/50 (100%)	-0.08	1 (2%) 65 63	20, 32, 58, 92	0
49	D1	50/50 (100%)	1.67	13 (26%) 0 0	64, 80, 92, 104	0
50	B2	46/46 (100%)	0.01	1 (2%) 62 59	7, 13, 20, 95	0
50	D2	46/46 (100%)	1.83	17 (36%) 0 0	51, 66, 79, 99	0
51	B3	64/64 (100%)	-0.09	0 100 100	9, 15, 25, 33	0
51	D3	64/64 (100%)	1.48	16 (25%) 0 0	54, 68, 79, 83	0
52	B4	38/38 (100%)	0.06	0 100 100	15, 22, 37, 55	0
52	D4	38/38 (100%)	2.21	21 (55%) 0 0	59, 72, 84, 97	0
53	B5	191/228 (83%)	6.51	186 (97%) 0 0	78, 108, 120, 133	0
All	All	20734/20794 (99%)	0.73	3009 (14%) 2 1	2, 62, 117, 195	0

The worst 5 of 3009 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
30	DI	2	ALA	21.5
30	DI	3	LYS	18.8
22	BA	2184	A	18.5
22	BA	2104	C	17.8
30	BI	53	LEU	17.4

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 monosaccharides 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. The B-factors column lists the minimum, median, 95^{th} 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	B-factors(Å^2)	Q<0.9
54	MG	DA	3134	1/1	0.12	0.63	75,75,75,75	0
54	MG	CA	1611	1/1	0.21	0.21	68,68,68,68	0
54	MG	CA	1635	1/1	0.23	0.15	91,91,91,91	0
54	MG	DA	3136	1/1	0.30	0.25	67,67,67,67	0
54	MG	DA	3132	1/1	0.34	0.91	83,83,83,83	0
54	MG	DA	3137	1/1	0.34	0.14	69,69,69,69	0
54	MG	DA	3007	1/1	0.36	0.20	84,84,84,84	0
54	MG	DA	3029	1/1	0.39	0.32	63,63,63,63	0
54	MG	DA	3094	1/1	0.48	0.40	78,78,78,78	0
54	MG	DA	3093	1/1	0.49	0.46	79,79,79,79	0
54	MG	AA	1627	1/1	0.49	0.22	50,50,50,50	0
54	MG	DA	3049	1/1	0.56	0.35	84,84,84,84	0
54	MG	DA	3006	1/1	0.57	0.12	76,76,76,76	0
54	MG	DA	3014	1/1	0.58	0.16	59,59,59,59	0
54	MG	DA	3035	1/1	0.58	0.20	52,52,52,52	0
54	MG	DA	3042	1/1	0.58	0.27	67,67,67,67	0
54	MG	DA	3125	1/1	0.58	0.43	76,76,76,76	0
54	MG	DA	3073	1/1	0.61	0.46	76,76,76,76	0
54	MG	DA	3072	1/1	0.61	0.23	63,63,63,63	0
54	MG	CA	1604	1/1	0.62	0.22	80,80,80,80	0
54	MG	DA	3105	1/1	0.63	0.09	57,57,57,57	0
54	MG	DA	3043	1/1	0.63	0.34	68,68,68,68	0
54	MG	DA	3025	1/1	0.64	0.10	40,40,40,40	0
54	MG	DA	3015	1/1	0.65	0.12	57,57,57,57	0
54	MG	DA	3017	1/1	0.65	0.35	65,65,65,65	0
54	MG	DA	3120	1/1	0.66	0.56	80,80,80,80	0
54	MG	DA	3089	1/1	0.66	0.10	57,57,57,57	0
54	MG	DA	3047	1/1	0.66	0.12	60,60,60,60	0
54	MG	DA	3048	1/1	0.69	0.17	59,59,59,59	0
54	MG	DA	3135	1/1	0.69	0.12	41,41,41,41	0
54	MG	DA	3027	1/1	0.70	0.44	60,60,60,60	0
54	MG	DA	3085	1/1	0.70	0.20	72,72,72,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	CA	1631	1/1	0.70	0.17	76,76,76,76	0
54	MG	AA	1658	1/1	0.70	0.49	47,47,47,47	0
54	MG	DA	3129	1/1	0.70	0.10	65,65,65,65	0
54	MG	D2	101	1/1	0.70	0.15	63,63,63,63	0
54	MG	AA	1638	1/1	0.71	0.13	57,57,57,57	0
54	MG	DA	3045	1/1	0.71	0.19	68,68,68,68	0
54	MG	BA	3169	1/1	0.71	0.33	25,25,25,25	0
54	MG	BA	3015	1/1	0.72	0.15	22,22,22,22	0
54	MG	CA	1615	1/1	0.72	0.19	38,38,38,38	0
54	MG	CA	1628	1/1	0.72	0.29	70,70,70,70	0
54	MG	AA	1645	1/1	0.73	0.48	41,41,41,41	0
54	MG	DA	3058	1/1	0.73	0.31	65,65,65,65	0
54	MG	CA	1602	1/1	0.73	0.10	69,69,69,69	0
54	MG	BA	3193	1/1	0.74	0.51	10,10,10,10	0
54	MG	DA	3095	1/1	0.74	0.13	75,75,75,75	0
54	MG	BA	3171	1/1	0.74	0.32	34,34,34,34	0
54	MG	CA	1636	1/1	0.74	0.27	92,92,92,92	0
54	MG	DA	3041	1/1	0.75	0.13	62,62,62,62	0
54	MG	DA	3102	1/1	0.75	0.08	49,49,49,49	0
54	MG	DA	3148	1/1	0.75	0.20	47,47,47,47	0
54	MG	CA	1630	1/1	0.75	0.36	81,81,81,81	0
54	MG	DA	3028	1/1	0.76	0.08	62,62,62,62	0
54	MG	DA	3005	1/1	0.76	0.43	76,76,76,76	0
54	MG	CA	1626	1/1	0.76	0.08	48,48,48,48	0
54	MG	DA	3019	1/1	0.76	0.20	66,66,66,66	0
54	MG	DA	3144	1/1	0.76	1.42	57,57,57,57	0
54	MG	BA	3154	1/1	0.76	0.28	11,11,11,11	0
54	MG	DA	3154	1/1	0.76	0.58	63,63,63,63	0
54	MG	AA	1672	1/1	0.76	0.33	40,40,40,40	0
54	MG	CA	1641	1/1	0.77	0.49	59,59,59,59	0
54	MG	DA	3100	1/1	0.77	0.53	68,68,68,68	0
54	MG	BA	3031	1/1	0.77	0.13	10,10,10,10	0
54	MG	DA	3163	1/1	0.77	0.35	49,49,49,49	0
54	MG	CA	1605	1/1	0.77	0.16	57,57,57,57	0
54	MG	BA	3016	1/1	0.78	0.38	67,67,67,67	0
54	MG	DA	3079	1/1	0.78	0.12	74,74,74,74	0
54	MG	DA	3080	1/1	0.78	0.11	79,79,79,79	0
54	MG	DA	3104	1/1	0.78	0.34	59,59,59,59	0
54	MG	BA	3191	1/1	0.78	0.23	43,43,43,43	0
54	MG	DA	3088	1/1	0.78	0.07	53,53,53,53	0
54	MG	CA	1638	1/1	0.78	0.10	54,54,54,54	0
54	MG	BA	3050	1/1	0.78	0.08	15,15,15,15	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	DA	3046	1/1	0.78	0.12	72,72,72,72	0
54	MG	DA	3008	1/1	0.79	0.46	70,70,70,70	0
54	MG	DA	3092	1/1	0.79	0.09	60,60,60,60	0
54	MG	DA	3106	1/1	0.79	0.21	61,61,61,61	0
54	MG	DA	3011	1/1	0.79	0.08	65,65,65,65	0
54	MG	AA	1623	1/1	0.79	0.06	42,42,42,42	0
54	MG	AA	1617	1/1	0.79	0.18	55,55,55,55	0
54	MG	CA	1649	1/1	0.79	0.28	48,48,48,48	0
54	MG	DA	3070	1/1	0.79	0.27	69,69,69,69	0
54	MG	DA	3030	1/1	0.80	0.26	61,61,61,61	0
54	MG	CA	1650	1/1	0.80	0.31	45,45,45,45	0
54	MG	DA	3038	1/1	0.80	0.16	74,74,74,74	0
54	MG	CA	1653	1/1	0.80	0.25	48,48,48,48	0
54	MG	CA	1627	1/1	0.80	0.29	69,69,69,69	0
54	MG	AA	1647	1/1	0.80	0.30	40,40,40,40	0
54	MG	AA	1614	1/1	0.80	0.18	52,52,52,52	0
54	MG	DA	3003	1/1	0.81	0.40	65,65,65,65	0
54	MG	BA	3047	1/1	0.81	0.15	19,19,19,19	0
54	MG	CA	1617	1/1	0.81	0.08	33,33,33,33	0
54	MG	CA	1621	1/1	0.81	0.12	63,63,63,63	0
54	MG	DA	3145	1/1	0.81	0.07	60,60,60,60	0
54	MG	DA	3078	1/1	0.81	0.17	64,64,64,64	0
54	MG	BA	3195	1/1	0.81	0.16	31,31,31,31	0
54	MG	DA	3039	1/1	0.81	0.13	54,54,54,54	0
54	MG	AA	1631	1/1	0.81	0.08	39,39,39,39	0
54	MG	DA	3059	1/1	0.82	0.48	63,63,63,63	0
54	MG	BA	3107	1/1	0.82	0.15	1,1,1,1	0
54	MG	BA	3145	1/1	0.82	0.37	37,37,37,37	0
54	MG	DA	3107	1/1	0.82	0.12	47,47,47,47	0
54	MG	BA	3049	1/1	0.82	0.10	37,37,37,37	0
54	MG	AA	1604	1/1	0.82	0.07	43,43,43,43	0
54	MG	DA	3152	1/1	0.82	0.36	54,54,54,54	0
54	MG	CA	1618	1/1	0.82	0.16	38,38,38,38	0
54	MG	BA	3104	1/1	0.82	0.14	16,16,16,16	0
54	MG	DA	3012	1/1	0.82	0.24	54,54,54,54	0
54	MG	BA	3174	1/1	0.83	0.22	24,24,24,24	0
54	MG	CA	1644	1/1	0.83	0.17	38,38,38,38	0
54	MG	DA	3020	1/1	0.83	0.24	75,75,75,75	0
54	MG	DA	3022	1/1	0.83	0.18	50,50,50,50	0
54	MG	BA	3075	1/1	0.83	0.19	3,3,3,3	0
54	MG	DA	3009	1/1	0.83	0.19	62,62,62,62	0
54	MG	CA	1633	1/1	0.83	0.48	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	BA	3100	1/1	0.83	0.18	52,52,52,52	0
54	MG	DA	3147	1/1	0.83	0.17	45,45,45,45	0
54	MG	BA	3035	1/1	0.83	0.14	4,4,4,4	0
54	MG	DA	3114	1/1	0.83	0.13	57,57,57,57	0
54	MG	DA	3033	1/1	0.83	0.15	53,53,53,53	0
54	MG	DA	3157	1/1	0.83	0.21	42,42,42,42	0
54	MG	BA	3027	1/1	0.83	0.15	47,47,47,47	0
54	MG	DA	3127	1/1	0.83	0.13	59,59,59,59	0
54	MG	BA	3092	1/1	0.84	0.11	20,20,20,20	0
54	MG	AA	1612	1/1	0.84	0.13	33,33,33,33	0
54	MG	BA	3057	1/1	0.84	0.39	37,37,37,37	0
54	MG	AA	1663	1/1	0.84	0.15	51,51,51,51	0
54	MG	BA	3116	1/1	0.84	0.17	29,29,29,29	0
54	MG	DA	3002	1/1	0.84	0.09	52,52,52,52	0
54	MG	DB	201	1/1	0.84	0.12	83,83,83,83	0
54	MG	BA	3080	1/1	0.84	0.06	50,50,50,50	0
54	MG	AA	1602	1/1	0.85	0.14	40,40,40,40	0
54	MG	DA	3061	1/1	0.85	0.34	69,69,69,69	0
54	MG	CA	1614	1/1	0.85	0.08	45,45,45,45	0
54	MG	AA	1628	1/1	0.85	0.10	45,45,45,45	0
54	MG	BA	3085	1/1	0.85	0.17	29,29,29,29	0
54	MG	DA	3074	1/1	0.85	0.11	49,49,49,49	0
54	MG	BA	3127	1/1	0.85	0.17	7,7,7,7	0
54	MG	DA	3146	1/1	0.85	0.17	54,54,54,54	0
54	MG	BA	3134	1/1	0.85	0.11	32,32,32,32	0
54	MG	BA	3135	1/1	0.85	0.21	46,46,46,46	0
54	MG	DA	3149	1/1	0.85	0.22	53,53,53,53	0
54	MG	AA	1601	1/1	0.85	0.15	53,53,53,53	0
54	MG	DA	3153	1/1	0.85	0.11	56,56,56,56	0
54	MG	DA	3119	1/1	0.85	0.09	52,52,52,52	0
54	MG	AA	1656	1/1	0.85	0.26	43,43,43,43	0
54	MG	BA	3167	1/1	0.85	0.27	35,35,35,35	0
54	MG	DA	3090	1/1	0.85	0.42	66,66,66,66	0
54	MG	CA	1654	1/1	0.85	0.23	40,40,40,40	0
54	MG	BA	3126	1/1	0.86	0.26	25,25,25,25	0
54	MG	AA	1670	1/1	0.86	0.31	50,50,50,50	0
54	MG	DA	3116	1/1	0.86	0.24	64,64,64,64	0
54	MG	BA	3101	1/1	0.86	0.10	8,8,8,8	0
54	MG	DA	3062	1/1	0.86	1.27	73,73,73,73	0
54	MG	CA	1655	1/1	0.86	0.31	53,53,53,53	0
54	MG	CA	1622	1/1	0.86	0.06	53,53,53,53	0
54	MG	BA	3173	1/1	0.86	0.27	24,24,24,24	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	BA	3082	1/1	0.86	0.10	12,12,12,12	0
54	MG	AA	1616	1/1	0.86	0.10	57,57,57,57	0
54	MG	AA	1667	1/1	0.86	0.27	47,47,47,47	0
54	MG	DA	3050	1/1	0.86	0.23	58,58,58,58	0
54	MG	DB	203	1/1	0.86	0.05	70,70,70,70	0
54	MG	DA	3056	1/1	0.86	0.10	52,52,52,52	0
54	MG	CA	1646	1/1	0.87	0.17	40,40,40,40	0
54	MG	AA	1660	1/1	0.87	0.54	38,38,38,38	0
54	MG	BA	3181	1/1	0.87	0.24	8,8,8,8	0
54	MG	CA	1652	1/1	0.87	0.10	45,45,45,45	0
54	MG	DA	3115	1/1	0.87	0.14	45,45,45,45	0
54	MG	BA	3079	1/1	0.87	0.06	30,30,30,30	0
54	MG	BA	3018	1/1	0.87	0.15	4,4,4,4	0
54	MG	BA	3137	1/1	0.87	0.14	44,44,44,44	0
54	MG	CA	1616	1/1	0.87	0.12	31,31,31,31	0
54	MG	AA	1630	1/1	0.87	0.11	53,53,53,53	0
54	MG	DA	3091	1/1	0.88	0.07	55,55,55,55	0
54	MG	BA	3120	1/1	0.88	0.08	24,24,24,24	0
54	MG	BA	3073	1/1	0.88	0.16	30,30,30,30	0
54	MG	DA	3076	1/1	0.88	0.10	55,55,55,55	0
54	MG	AA	1626	1/1	0.88	0.11	24,24,24,24	0
54	MG	AA	1668	1/1	0.88	0.20	41,41,41,41	0
54	MG	DA	3004	1/1	0.88	0.08	58,58,58,58	0
54	MG	CA	1624	1/1	0.88	0.11	33,33,33,33	0
54	MG	DA	3156	1/1	0.88	0.31	44,44,44,44	0
54	MG	DA	3086	1/1	0.88	0.12	61,61,61,61	0
54	MG	DA	3161	1/1	0.88	0.22	39,39,39,39	0
54	MG	DA	3016	1/1	0.88	0.76	65,65,65,65	0
54	MG	BB	204	1/1	0.88	0.35	15,15,15,15	0
54	MG	DA	3109	1/1	0.88	0.11	54,54,54,54	0
54	MG	BA	3163	1/1	0.88	0.18	31,31,31,31	0
54	MG	DA	3083	1/1	0.89	0.11	52,52,52,52	0
54	MG	AA	1618	1/1	0.89	0.08	41,41,41,41	0
54	MG	DA	3067	1/1	0.89	0.08	48,48,48,48	0
54	MG	DA	3150	1/1	0.89	0.27	41,41,41,41	0
54	MG	BA	3046	1/1	0.89	0.13	13,13,13,13	0
54	MG	DA	3036	1/1	0.89	0.18	65,65,65,65	0
54	MG	DA	3133	1/1	0.89	0.13	51,51,51,51	0
54	MG	DA	3024	1/1	0.89	0.08	63,63,63,63	0
54	MG	CA	1610	1/1	0.89	0.10	57,57,57,57	0
54	MG	DA	3111	1/1	0.89	0.23	45,45,45,45	0
54	MG	CA	1639	1/1	0.89	0.12	32,32,32,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	BB	203	1/1	0.89	0.07	6,6,6,6	0
54	MG	BA	3170	1/1	0.89	0.16	29,29,29,29	0
54	MG	BA	3025	1/1	0.89	0.11	4,4,4,4	0
54	MG	BA	3093	1/1	0.90	0.06	43,43,43,43	0
54	MG	CA	1613	1/1	0.90	0.14	16,16,16,16	0
54	MG	AA	1655	1/1	0.90	0.22	50,50,50,50	0
54	MG	AA	1641	1/1	0.90	0.11	16,16,16,16	0
54	MG	DA	3101	1/1	0.90	0.18	54,54,54,54	0
54	MG	DA	3138	1/1	0.90	0.29	42,42,42,42	0
54	MG	AA	1603	1/1	0.90	0.18	48,48,48,48	0
54	MG	DA	3103	1/1	0.90	0.09	45,45,45,45	0
54	MG	BA	3062	1/1	0.90	0.43	36,36,36,36	0
54	MG	BA	3065	1/1	0.90	0.19	2,2,2,2	0
54	MG	DA	3075	1/1	0.90	0.05	47,47,47,47	0
54	MG	BA	3068	1/1	0.90	0.14	8,8,8,8	0
54	MG	BA	3029	1/1	0.90	0.26	38,38,38,38	0
54	MG	DA	3151	1/1	0.90	0.33	53,53,53,53	0
54	MG	DA	3044	1/1	0.90	0.10	54,54,54,54	0
54	MG	BA	3074	1/1	0.90	0.14	3,3,3,3	0
54	MG	BA	3129	1/1	0.90	0.09	7,7,7,7	0
54	MG	AA	1625	1/1	0.90	0.06	35,35,35,35	0
54	MG	BA	3009	1/1	0.90	0.16	10,10,10,10	0
54	MG	BA	3038	1/1	0.90	0.13	30,30,30,30	0
54	MG	DA	3026	1/1	0.90	0.09	43,43,43,43	0
54	MG	DA	3164	1/1	0.90	0.23	50,50,50,50	0
54	MG	BA	3042	1/1	0.90	0.35	7,7,7,7	0
54	MG	AA	1661	1/1	0.90	0.16	49,49,49,49	0
54	MG	AA	1653	1/1	0.90	0.15	40,40,40,40	0
54	MG	BA	3146	1/1	0.91	0.23	12,12,12,12	0
54	MG	DA	3142	1/1	0.91	0.19	30,30,30,30	0
54	MG	BA	3151	1/1	0.91	0.32	44,44,44,44	0
54	MG	AA	1605	1/1	0.91	0.19	36,36,36,36	0
54	MG	DA	3113	1/1	0.91	0.27	56,56,56,56	0
54	MG	BA	3155	1/1	0.91	0.18	37,37,37,37	0
54	MG	DA	3065	1/1	0.91	0.23	46,46,46,46	0
54	MG	DA	3066	1/1	0.91	0.11	40,40,40,40	0
54	MG	DA	3118	1/1	0.91	0.06	56,56,56,56	0
54	MG	BA	3161	1/1	0.91	0.18	19,19,19,19	0
54	MG	BA	3059	1/1	0.91	0.30	23,23,23,23	0
54	MG	BA	3110	1/1	0.91	0.24	4,4,4,4	0
54	MG	DA	3126	1/1	0.91	0.17	51,51,51,51	0
54	MG	BA	3113	1/1	0.91	0.14	30,30,30,30	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	CA	1642	1/1	0.91	0.19	31,31,31,31	0
54	MG	AA	1664	1/1	0.91	0.19	30,30,30,30	0
54	MG	CA	1625	1/1	0.91	0.15	26,26,26,26	0
54	MG	AA	1650	1/1	0.91	0.15	31,31,31,31	0
54	MG	BA	3172	1/1	0.91	0.14	22,22,22,22	0
54	MG	DA	3031	1/1	0.91	0.26	49,49,49,49	0
54	MG	BA	3121	1/1	0.91	0.23	50,50,50,50	0
54	MG	BA	3048	1/1	0.92	0.09	25,25,25,25	0
54	MG	DA	3032	1/1	0.92	0.12	46,46,46,46	0
54	MG	BA	3177	1/1	0.92	0.14	13,13,13,13	0
54	MG	BA	3180	1/1	0.92	0.17	10,10,10,10	0
54	MG	CA	1640	1/1	0.92	0.17	22,22,22,22	0
54	MG	BA	3004	1/1	0.92	0.11	24,24,24,24	0
54	MG	BA	3188	1/1	0.92	0.21	19,19,19,19	0
54	MG	DA	3040	1/1	0.92	0.16	39,39,39,39	0
54	MG	CA	1643	1/1	0.92	0.39	54,54,54,54	0
54	MG	CA	1619	1/1	0.92	0.07	30,30,30,30	0
54	MG	BA	3078	1/1	0.92	0.21	26,26,26,26	0
54	MG	CA	1648	1/1	0.92	0.20	45,45,45,45	0
54	MG	BA	3007	1/1	0.92	0.15	17,17,17,17	0
54	MG	AA	1608	1/1	0.92	0.15	20,20,20,20	0
54	MG	DA	3021	1/1	0.92	0.16	50,50,50,50	0
54	MG	AA	1624	1/1	0.92	0.05	30,30,30,30	0
54	MG	AA	1669	1/1	0.92	0.15	28,28,28,28	0
54	MG	DA	3155	1/1	0.92	0.17	43,43,43,43	0
54	MG	DA	3124	1/1	0.92	0.12	52,52,52,52	0
54	MG	AA	1635	1/1	0.92	0.14	49,49,49,49	0
54	MG	DA	3159	1/1	0.92	0.14	57,57,57,57	0
54	MG	BA	3067	1/1	0.92	0.11	4,4,4,4	0
54	MG	BA	3021	1/1	0.92	0.21	0,0,0,0	0
54	MG	DA	3128	1/1	0.92	0.10	61,61,61,61	0
54	MG	DA	3167	1/1	0.92	0.12	39,39,39,39	0
54	MG	BA	3072	1/1	0.92	0.08	6,6,6,6	0
54	MG	AA	1620	1/1	0.92	0.04	51,51,51,51	0
54	MG	BA	3139	1/1	0.92	0.34	0,0,0,0	0
55	VIF	DA	3001	38/38	0.92	0.26	40,51,59,60	0
54	MG	AA	1606	1/1	0.93	0.08	36,36,36,36	0
54	MG	BA	3102	1/1	0.93	0.12	10,10,10,10	0
54	MG	DA	3131	1/1	0.93	0.12	58,58,58,58	0
54	MG	BA	3076	1/1	0.93	0.06	29,29,29,29	0
54	MG	DA	3018	1/1	0.93	0.14	53,53,53,53	0
54	MG	BA	3143	1/1	0.93	0.21	7,7,7,7	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	AA	1640	1/1	0.93	0.08	41,41,41,41	0
54	MG	BA	3064	1/1	0.93	0.17	0,0,0,0	0
54	MG	BA	3186	1/1	0.93	0.15	10,10,10,10	0
54	MG	DA	3097	1/1	0.93	0.06	49,49,49,49	0
54	MG	DA	3099	1/1	0.93	0.09	37,37,37,37	0
54	MG	BA	3187	1/1	0.93	0.27	16,16,16,16	0
54	MG	AA	1621	1/1	0.93	0.06	30,30,30,30	0
54	MG	BA	3190	1/1	0.93	0.20	19,19,19,19	0
54	MG	BA	3152	1/1	0.93	0.15	27,27,27,27	0
54	MG	BA	3002	1/1	0.93	0.08	15,15,15,15	0
54	MG	AA	1629	1/1	0.93	0.12	42,42,42,42	0
54	MG	CM	201	1/1	0.93	0.30	50,50,50,50	0
54	MG	BA	3087	1/1	0.93	0.14	0,0,0,0	0
54	MG	DA	3108	1/1	0.93	0.07	60,60,60,60	0
54	MG	BA	3088	1/1	0.93	0.21	8,8,8,8	0
54	MG	AA	1665	1/1	0.93	0.14	48,48,48,48	0
54	MG	DA	3034	1/1	0.93	0.06	54,54,54,54	0
54	MG	CA	1632	1/1	0.93	0.14	66,66,66,66	0
54	MG	BA	3168	1/1	0.93	0.17	32,32,32,32	0
54	MG	CA	1634	1/1	0.93	0.12	55,55,55,55	0
54	MG	AA	1636	1/1	0.93	0.12	31,31,31,31	0
54	MG	CA	1608	1/1	0.93	0.26	56,56,56,56	0
54	MG	DA	3081	1/1	0.93	0.09	67,67,67,67	0
54	MG	DA	3121	1/1	0.93	0.07	54,54,54,54	0
54	MG	DA	3082	1/1	0.93	0.09	42,42,42,42	0
54	MG	CA	1637	1/1	0.93	0.26	52,52,52,52	0
54	MG	BA	3133	1/1	0.93	0.30	48,48,48,48	0
54	MG	AA	1659	1/1	0.93	0.15	43,43,43,43	0
54	MG	AA	1644	1/1	0.94	0.29	41,41,41,41	0
54	MG	DA	3122	1/1	0.94	0.07	42,42,42,42	0
54	MG	BA	3117	1/1	0.94	0.28	40,40,40,40	0
54	MG	BA	3012	1/1	0.94	0.06	17,17,17,17	0
54	MG	BA	3014	1/1	0.94	0.18	0,0,0,0	0
54	MG	AA	1615	1/1	0.94	0.07	43,43,43,43	0
54	MG	AA	1632	1/1	0.94	0.11	41,41,41,41	0
54	MG	BA	3017	1/1	0.94	0.10	9,9,9,9	0
54	MG	BA	3081	1/1	0.94	0.14	28,28,28,28	0
54	MG	DA	3087	1/1	0.94	0.13	48,48,48,48	0
54	MG	AA	1639	1/1	0.94	0.06	56,56,56,56	0
54	MG	AA	1671	1/1	0.94	0.32	37,37,37,37	0
54	MG	BA	3184	1/1	0.94	0.20	21,21,21,21	0
54	MG	AA	1662	1/1	0.94	0.14	25,25,25,25	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	BA	3061	1/1	0.94	0.20	22,22,22,22	0
54	MG	BA	3141	1/1	0.94	0.17	8,8,8,8	0
54	MG	DA	3139	1/1	0.94	0.46	35,35,35,35	0
54	MG	DA	3010	1/1	0.94	0.13	57,57,57,57	0
54	MG	AA	1634	1/1	0.94	0.11	40,40,40,40	0
54	MG	DA	3096	1/1	0.94	0.22	62,62,62,62	0
54	MG	BA	3144	1/1	0.94	0.27	14,14,14,14	0
54	MG	BA	3192	1/1	0.94	0.17	22,22,22,22	0
54	MG	AA	1607	1/1	0.94	0.10	47,47,47,47	0
54	MG	BA	3097	1/1	0.94	0.06	18,18,18,18	0
54	MG	BA	3030	1/1	0.94	0.11	4,4,4,4	0
54	MG	BA	3066	1/1	0.94	0.12	6,6,6,6	0
54	MG	DA	3060	1/1	0.94	0.10	43,43,43,43	0
54	MG	AA	1642	1/1	0.94	0.10	21,21,21,21	0
54	MG	BA	3034	1/1	0.94	0.14	20,20,20,20	0
54	MG	BA	3069	1/1	0.94	0.17	2,2,2,2	0
54	MG	CA	1606	1/1	0.94	0.08	49,49,49,49	0
54	MG	CA	1607	1/1	0.94	0.10	46,46,46,46	0
54	MG	DA	3158	1/1	0.94	0.22	46,46,46,46	0
54	MG	DA	3068	1/1	0.94	0.10	43,43,43,43	0
54	MG	DA	3112	1/1	0.94	0.18	67,67,67,67	0
54	MG	BA	3162	1/1	0.94	0.23	17,17,17,17	0
54	MG	DA	3071	1/1	0.94	0.13	75,75,75,75	0
54	MG	BA	3008	1/1	0.94	0.09	29,29,29,29	0
54	MG	CA	1645	1/1	0.94	0.12	50,50,50,50	0
54	MG	DB	202	1/1	0.94	0.08	49,49,49,49	0
54	MG	BA	3166	1/1	0.94	0.09	6,6,6,6	0
54	MG	CA	1612	1/1	0.94	0.12	43,43,43,43	0
54	MG	BA	3036	1/1	0.94	0.18	9,9,9,9	0
54	MG	DA	3052	1/1	0.95	0.08	32,32,32,32	0
54	MG	DA	3053	1/1	0.95	0.07	44,44,44,44	0
54	MG	DA	3054	1/1	0.95	0.16	40,40,40,40	0
54	MG	BA	3124	1/1	0.95	0.22	0,0,0,0	0
54	MG	DA	3023	1/1	0.95	0.14	36,36,36,36	0
54	MG	CA	1651	1/1	0.95	0.05	54,54,54,54	0
54	MG	CA	1601	1/1	0.95	0.09	34,34,34,34	0
54	MG	BA	3147	1/1	0.95	0.23	25,25,25,25	0
54	MG	CA	1603	1/1	0.95	0.12	43,43,43,43	0
54	MG	DA	3141	1/1	0.95	0.40	39,39,39,39	0
54	MG	CA	1629	1/1	0.95	0.07	67,67,67,67	0
54	MG	AA	1649	1/1	0.95	0.12	34,34,34,34	0
54	MG	BA	3089	1/1	0.95	0.07	13,13,13,13	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	BA	3178	1/1	0.95	0.09	27,27,27,27	0
54	MG	BA	3040	1/1	0.95	0.14	3,3,3,3	0
54	MG	BA	3132	1/1	0.95	0.18	2,2,2,2	0
54	MG	BA	3182	1/1	0.95	0.12	26,26,26,26	0
54	MG	BA	3112	1/1	0.95	0.08	16,16,16,16	0
54	MG	AA	1613	1/1	0.95	0.08	25,25,25,25	0
54	MG	DA	3037	1/1	0.95	0.12	46,46,46,46	0
54	MG	BA	3115	1/1	0.95	0.16	11,11,11,11	0
54	MG	BA	3164	1/1	0.95	0.14	27,27,27,27	0
54	MG	BA	3189	1/1	0.95	0.09	25,25,25,25	0
54	MG	BA	3044	1/1	0.95	0.14	4,4,4,4	0
54	MG	DA	3117	1/1	0.95	0.14	54,54,54,54	0
54	MG	DA	3013	1/1	0.95	0.20	40,40,40,40	0
54	MG	BA	3054	1/1	0.95	0.15	6,6,6,6	0
54	MG	DA	3160	1/1	0.95	0.15	47,47,47,47	0
54	MG	BA	3119	1/1	0.95	0.07	9,9,9,9	0
54	MG	DA	3084	1/1	0.95	0.06	50,50,50,50	0
54	MG	BA	3020	1/1	0.95	0.09	24,24,24,24	0
54	MG	DA	3166	1/1	0.95	0.32	41,41,41,41	0
54	MG	CA	1620	1/1	0.95	0.07	49,49,49,49	0
54	MG	BA	3058	1/1	0.95	0.11	11,11,11,11	0
54	MG	CA	1647	1/1	0.95	0.20	19,19,19,19	0
54	MG	BB	202	1/1	0.95	0.09	12,12,12,12	0
54	MG	BA	3122	1/1	0.95	0.11	10,10,10,10	0
54	MG	DA	3051	1/1	0.95	0.19	43,43,43,43	0
54	MG	DA	3130	1/1	0.96	0.18	35,35,35,35	0
54	MG	BA	3157	1/1	0.96	0.14	7,7,7,7	0
54	MG	AA	1651	1/1	0.96	0.44	36,36,36,36	0
54	MG	AA	1652	1/1	0.96	0.24	28,28,28,28	0
54	MG	BA	3039	1/1	0.96	0.20	2,2,2,2	0
54	MG	BA	3094	1/1	0.96	0.23	23,23,23,23	0
54	MG	BA	3095	1/1	0.96	0.07	26,26,26,26	0
54	MG	BA	3026	1/1	0.96	0.11	9,9,9,9	0
54	MG	AA	1611	1/1	0.96	0.09	25,25,25,25	0
54	MG	DA	3098	1/1	0.96	0.08	46,46,46,46	0
54	MG	BA	3077	1/1	0.96	0.18	11,11,11,11	0
54	MG	AA	1654	1/1	0.96	0.21	25,25,25,25	0
54	MG	DA	3143	1/1	0.96	0.18	28,28,28,28	0
54	MG	BA	3103	1/1	0.96	0.15	0,0,0,0	0
54	MG	CA	1609	1/1	0.96	0.04	57,57,57,57	0
54	MG	DA	3063	1/1	0.96	0.46	52,52,52,52	0
54	MG	DA	3064	1/1	0.96	0.15	43,43,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	BA	3063	1/1	0.96	0.20	41,41,41,41	0
54	MG	BA	3136	1/1	0.96	0.14	1,1,1,1	0
54	MG	BA	3105	1/1	0.96	0.11	9,9,9,9	0
54	MG	BA	3175	1/1	0.96	0.12	11,11,11,11	0
54	MG	BA	3176	1/1	0.96	0.30	15,15,15,15	0
54	MG	BA	3138	1/1	0.96	0.39	8,8,8,8	0
54	MG	BA	3106	1/1	0.96	0.18	3,3,3,3	0
54	MG	BA	3140	1/1	0.96	0.27	0,0,0,0	0
54	MG	BA	3005	1/1	0.96	0.05	32,32,32,32	0
54	MG	BA	3006	1/1	0.96	0.13	46,46,46,46	0
54	MG	BA	3111	1/1	0.96	0.13	0,0,0,0	0
54	MG	BA	3185	1/1	0.96	0.14	16,16,16,16	0
54	MG	BA	3033	1/1	0.96	0.10	15,15,15,15	0
54	MG	BA	3084	1/1	0.96	0.06	10,10,10,10	0
54	MG	DA	3162	1/1	0.96	0.09	56,56,56,56	0
54	MG	AA	1609	1/1	0.96	0.06	28,28,28,28	0
54	MG	BA	3148	1/1	0.96	0.23	0,0,0,0	0
54	MG	BA	3086	1/1	0.96	0.10	10,10,10,10	0
54	MG	AA	1610	1/1	0.96	0.18	53,53,53,53	0
54	MG	BA	3118	1/1	0.96	0.19	7,7,7,7	0
54	MG	BA	3052	1/1	0.96	0.07	8,8,8,8	0
54	MG	BA	3194	1/1	0.96	0.15	4,4,4,4	0
54	MG	DQ	201	1/1	0.96	0.34	36,36,36,36	0
54	MG	BA	3156	1/1	0.96	0.10	17,17,17,17	0
55	VIF	BA	3001	38/38	0.96	0.21	3,9,14,18	0
54	MG	BB	201	1/1	0.96	0.09	20,20,20,20	0
54	MG	AA	1633	1/1	0.97	0.14	29,29,29,29	0
54	MG	BN	201	1/1	0.97	0.06	6,6,6,6	0
54	MG	BA	3051	1/1	0.97	0.22	11,11,11,11	0
54	MG	AA	1619	1/1	0.97	0.19	44,44,44,44	0
54	MG	BA	3098	1/1	0.97	0.15	5,5,5,5	0
54	MG	BA	3142	1/1	0.97	0.30	1,1,1,1	0
54	MG	BA	3099	1/1	0.97	0.15	5,5,5,5	0
54	MG	BA	3022	1/1	0.97	0.12	3,3,3,3	0
54	MG	BA	3056	1/1	0.97	0.12	7,7,7,7	0
54	MG	BA	3043	1/1	0.97	0.14	11,11,11,11	0
54	MG	BA	3123	1/1	0.97	0.10	17,17,17,17	0
54	MG	BA	3070	1/1	0.97	0.16	0,0,0,0	0
54	MG	BA	3149	1/1	0.97	0.15	26,26,26,26	0
54	MG	BA	3125	1/1	0.97	0.21	6,6,6,6	0
54	MG	BA	3183	1/1	0.97	0.13	20,20,20,20	0
54	MG	BA	3023	1/1	0.97	0.15	0,0,0,0	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	BA	3153	1/1	0.97	0.13	15,15,15,15	0
54	MG	BA	3010	1/1	0.97	0.12	3,3,3,3	0
54	MG	DA	3055	1/1	0.97	0.10	48,48,48,48	0
54	MG	BA	3128	1/1	0.97	0.15	5,5,5,5	0
54	MG	DA	3057	1/1	0.97	0.31	62,62,62,62	0
54	MG	BA	3060	1/1	0.97	0.06	16,16,16,16	0
54	MG	BA	3130	1/1	0.97	0.20	4,4,4,4	0
54	MG	BA	3159	1/1	0.97	0.15	25,25,25,25	0
54	MG	DA	3165	1/1	0.97	0.05	46,46,46,46	0
54	MG	BA	3131	1/1	0.97	0.14	0,0,0,0	0
54	MG	AA	1622	1/1	0.97	0.22	17,17,17,17	0
54	MG	CA	1623	1/1	0.97	0.15	42,42,42,42	0
54	MG	BA	3108	1/1	0.97	0.16	0,0,0,0	0
54	MG	BA	3090	1/1	0.97	0.12	28,28,28,28	0
54	MG	BA	3165	1/1	0.97	0.23	9,9,9,9	0
54	MG	BA	3091	1/1	0.97	0.10	4,4,4,4	0
54	MG	BA	3013	1/1	0.97	0.16	3,3,3,3	0
54	MG	BA	3028	1/1	0.97	0.11	4,4,4,4	0
54	MG	BA	3071	1/1	0.98	0.11	45,45,45,45	0
54	MG	BA	3179	1/1	0.98	0.21	7,7,7,7	0
54	MG	DA	3069	1/1	0.98	0.08	56,56,56,56	0
54	MG	DA	3110	1/1	0.98	0.19	36,36,36,36	0
54	MG	AA	1666	1/1	0.98	0.37	25,25,25,25	0
54	MG	BA	3037	1/1	0.98	0.14	1,1,1,1	0
54	MG	AA	1637	1/1	0.98	0.10	17,17,17,17	0
54	MG	AA	1648	1/1	0.98	0.16	54,54,54,54	0
54	MG	BA	3024	1/1	0.98	0.13	5,5,5,5	0
54	MG	BA	3150	1/1	0.98	0.27	0,0,0,0	0
54	MG	BA	3041	1/1	0.98	0.16	7,7,7,7	0
54	MG	DA	3140	1/1	0.98	0.30	36,36,36,36	0
54	MG	DA	3077	1/1	0.98	0.13	56,56,56,56	0
54	MG	BA	3053	1/1	0.98	0.15	6,6,6,6	0
54	MG	BA	3032	1/1	0.98	0.25	6,6,6,6	0
54	MG	BA	3055	1/1	0.98	0.14	5,5,5,5	0
54	MG	AA	1643	1/1	0.98	0.13	12,12,12,12	0
54	MG	DA	3123	1/1	0.98	0.16	35,35,35,35	0
54	MG	BA	3019	1/1	0.98	0.10	17,17,17,17	0
54	MG	BA	3083	1/1	0.98	0.15	0,0,0,0	0
54	MG	BA	3158	1/1	0.98	0.25	17,17,17,17	0
54	MG	BA	3003	1/1	0.98	0.04	19,19,19,19	0
54	MG	BA	3160	1/1	0.98	0.18	16,16,16,16	0
56	ZN	B4	101	1/1	0.98	0.14	102,102,102,102	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	ZN	D4	101	1/1	0.98	0.10	78,78,78,78	0
54	MG	AA	1646	1/1	0.99	0.10	39,39,39,39	0
54	MG	AA	1657	1/1	0.99	0.07	28,28,28,28	0
54	MG	BA	3096	1/1	0.99	0.06	17,17,17,17	0
54	MG	BA	3011	1/1	0.99	0.11	3,3,3,3	0
54	MG	BA	3114	1/1	0.99	0.06	18,18,18,18	0
54	MG	BA	3045	1/1	0.99	0.07	14,14,14,14	0
54	MG	BA	3109	1/1	0.99	0.12	20,20,20,20	0

6.5 Other polymers (i)

There are no such residues in this entry.