



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 09:27 AM UTC

PDB ID : 4U26 / pdb_00004u26
Title : Crystal structure of the E. coli ribosome bound to dalfopristin and quinupristin.
Authors : Noeske, J.; Huang, J.; Olivier, N.B.; Giacobbe, R.A.; Zambrowski, M.; Cate, J.H.D.
Deposited on : 2014-07-16
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

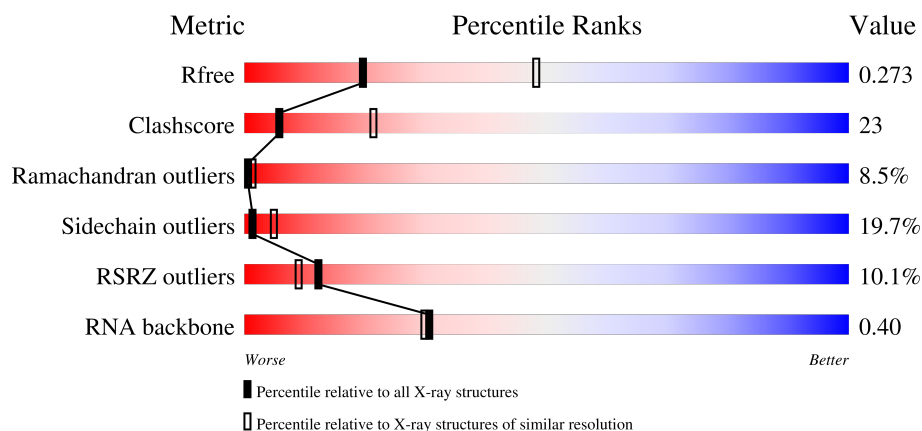
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)
RNA backbone	3983	1114 (3.00-2.60)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1539	34% 50% 15%
1	CA	1539	3% 30% 54% 16%
2	AB	218	6% 22% 48% 23% 6%

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Mol	Chain	Length	Quality of chain
2	CB	218	
3	AC	206	
3	CC	206	
4	AD	205	
4	CD	205	
5	AE	150	
5	CE	150	
6	AF	100	
6	CF	100	
7	AG	151	
7	CG	151	
8	AH	129	
8	CH	129	
9	AI	127	
9	CI	127	
10	AJ	98	
10	CJ	98	
11	AK	117	
11	CK	117	
12	AL	123	
12	CL	123	
13	AM	114	
13	CM	114	
14	AN	100	
14	CN	100	

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Mol	Chain	Length	Quality of chain
15	AO	88	
15	CO	88	
16	AP	82	
16	CP	82	
17	AQ	80	
17	CQ	80	
18	AR	55	
18	CR	55	
19	AS	79	
19	CS	79	
20	AT	85	
20	CT	85	
21	AU	51	
21	CU	51	
22	BA	2903	
22	DA	2903	
23	BB	119	
23	DB	119	
24	BC	271	
24	DC	271	
25	BD	209	
25	DD	209	
26	BE	201	
26	DE	201	
27	BF	177	

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Mol	Chain	Length	Quality of chain
27	DF	177	
28	BG	176	
28	DG	176	
29	BH	149	
29	DH	149	
30	BI	141	
30	DI	141	
31	BJ	142	
31	DJ	142	
32	BK	122	
32	DK	122	
33	BL	143	
33	DL	143	
34	BM	136	
34	DM	136	
35	BN	120	
35	DN	120	
36	BO	116	
36	DO	116	
37	BP	114	
37	DP	114	
38	BQ	117	
38	DQ	117	
39	BR	103	
39	DR	103	

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Mol	Chain	Length	Quality of chain
40	BS	110	
40	DS	110	
41	BT	93	
41	DT	93	
42	BU	102	
42	DU	102	
43	BV	94	
43	DV	94	
44	BW	76	
44	DW	76	
45	BX	77	
45	DX	77	
46	BY	63	
46	DY	63	
47	BZ	58	
47	DZ	58	
48	B0	56	
48	D0	56	
49	B1	50	
49	D1	50	
50	B2	46	
50	D2	46	
51	B3	64	
51	D3	64	
52	B4	38	

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Mol	Chain	Length	Quality of chain
52	D4	38	
53	B5	228	
54	B6	8	
54	D6	8	

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
55	MG	DA	3058	-	-	-	X
55	MG	DA	3061	-	-	-	X
55	MG	DA	3112	-	-	-	X
56	DOL	DA	3001	-	-	X	-

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 288423 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			

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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			

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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	S	0	0	0
			947	604	192	151				
38	DQ	117	Total	C	N	O	S	0	0	0
			947	604	192	151				

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BY	63	Total 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			

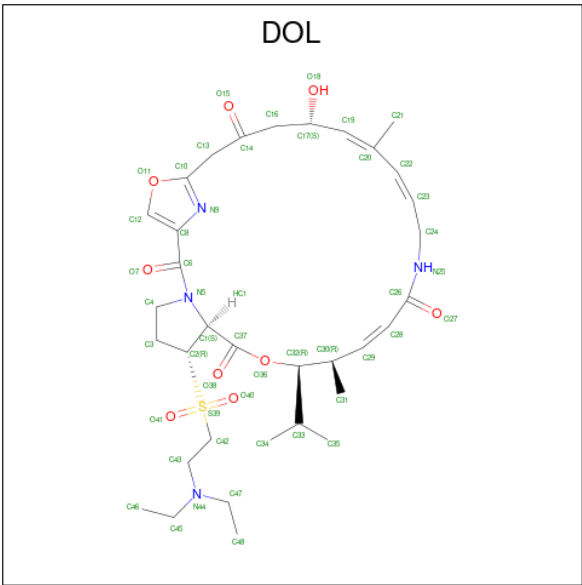
- Molecule 54 is a protein called Quinupristin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B6	8	Total	C	N	O	S	0	0	0
			73	53	9	10	1			
54	D6	8	Total	C	N	O	S	0	0	0
			73	53	9	10	1			

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	AA	71	Total	Mg	0	0
			71	71		
55	AM	1	Total	Mg	0	0
			1	1		
55	BA	194	Total	Mg	0	0
			194	194		
55	BB	4	Total	Mg	0	0
			4	4		
55	BQ	1	Total	Mg	0	0
			1	1		
55	CA	56	Total	Mg	0	0
			56	56		
55	DA	166	Total	Mg	0	0
			166	166		
55	DB	3	Total	Mg	0	0
			3	3		
55	DQ	1	Total	Mg	0	0
			1	1		
55	D2	1	Total	Mg	0	0
			1	1		

- Molecule 56 is 5-(2-DIETHYLAMINO-ETHANESULFONYL)-21-HYDROXY-10-ISOPROPYL-11,19-DIMETHYL-9,26-DIOXA-3,15,28-TRIAZA-TRICYCLO[23.2.1.00,255]OCTACOSA-1(27),12,17,19,25(28)-PENTAENE-2,8,14,23-TETRAONE (CCD ID: DOL) (formula: C₃₄H₅₀N₄O₉S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
56	BA	1	Total	C	N	O	S	0	0
			48	34	4	9	1		
56	DA	1	Total	C	N	O	S	0	0
			48	34	4	9	1		

- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 58 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	AA	194	Total	O	0	0
			194	194		
58	AE	2	Total	O	0	0
			2	2		
58	AL	1	Total	O	0	0
			1	1		
58	AN	3	Total	O	0	0
			3	3		
58	AT	2	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	AU	1	Total 1	O 1	0	0
58	BA	617	Total 617	O 617	0	0
58	BB	14	Total 14	O 14	0	0
58	BC	6	Total 6	O 6	0	0
58	BD	4	Total 4	O 4	0	0
58	BE	1	Total 1	O 1	0	0
58	BF	1	Total 1	O 1	0	0
58	BG	1	Total 1	O 1	0	0
58	BJ	1	Total 1	O 1	0	0
58	BL	7	Total 7	O 7	0	0
58	BN	5	Total 5	O 5	0	0
58	BQ	1	Total 1	O 1	0	0
58	BS	1	Total 1	O 1	0	0
58	BT	2	Total 2	O 2	0	0
58	B3	3	Total 3	O 3	0	0
58	B4	1	Total 1	O 1	0	0
58	CA	192	Total 192	O 192	0	0
58	CL	1	Total 1	O 1	0	0
58	CN	2	Total 2	O 2	0	0
58	CT	2	Total 2	O 2	0	0
58	CU	1	Total 1	O 1	0	0

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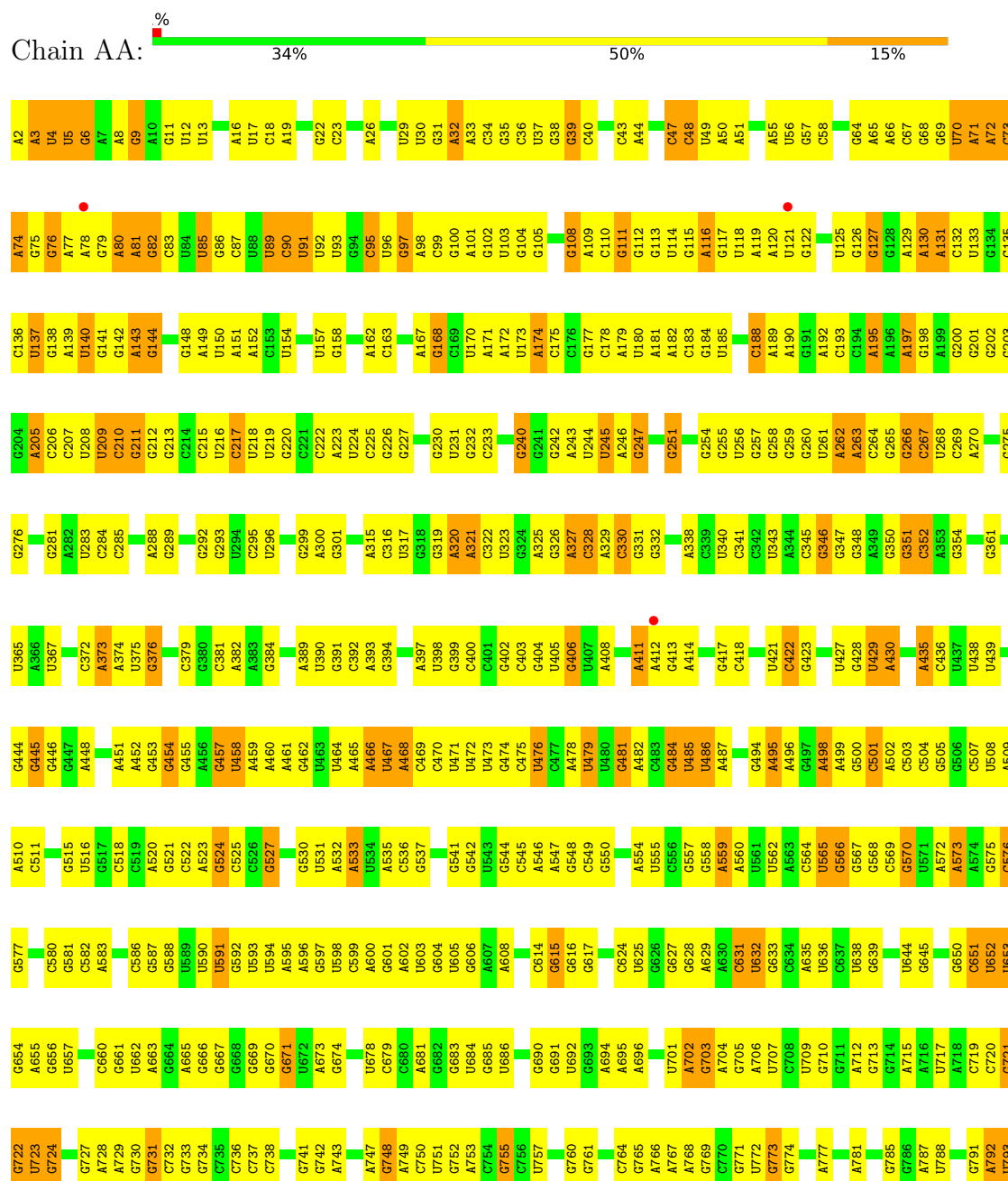
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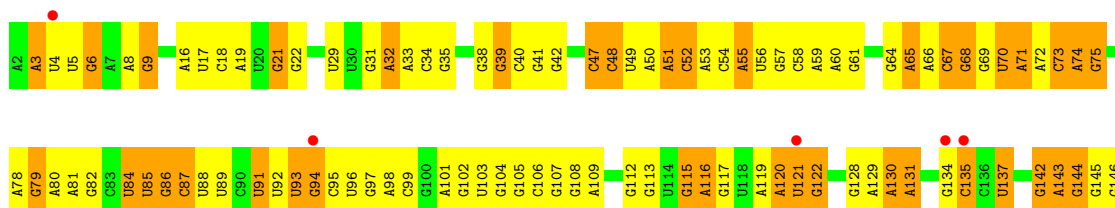
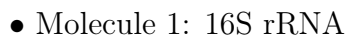
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	DA	610	Total 610	O 610	0	0
58	DB	13	Total 13	O 13	0	0
58	DC	8	Total 8	O 8	0	0
58	DD	4	Total 4	O 4	0	0
58	DE	4	Total 4	O 4	0	0
58	DJ	1	Total 1	O 1	0	0
58	DL	4	Total 4	O 4	0	0
58	DN	2	Total 2	O 2	0	0
58	DS	2	Total 2	O 2	0	0
58	DT	3	Total 3	O 3	0	0
58	DU	1	Total 1	O 1	0	0
58	DV	1	Total 1	O 1	0	0
58	D2	1	Total 1	O 1	0	0
58	D3	1	Total 1	O 1	0	0
58	D4	1	Total 1	O 1	0	0

3 Residue-property plots

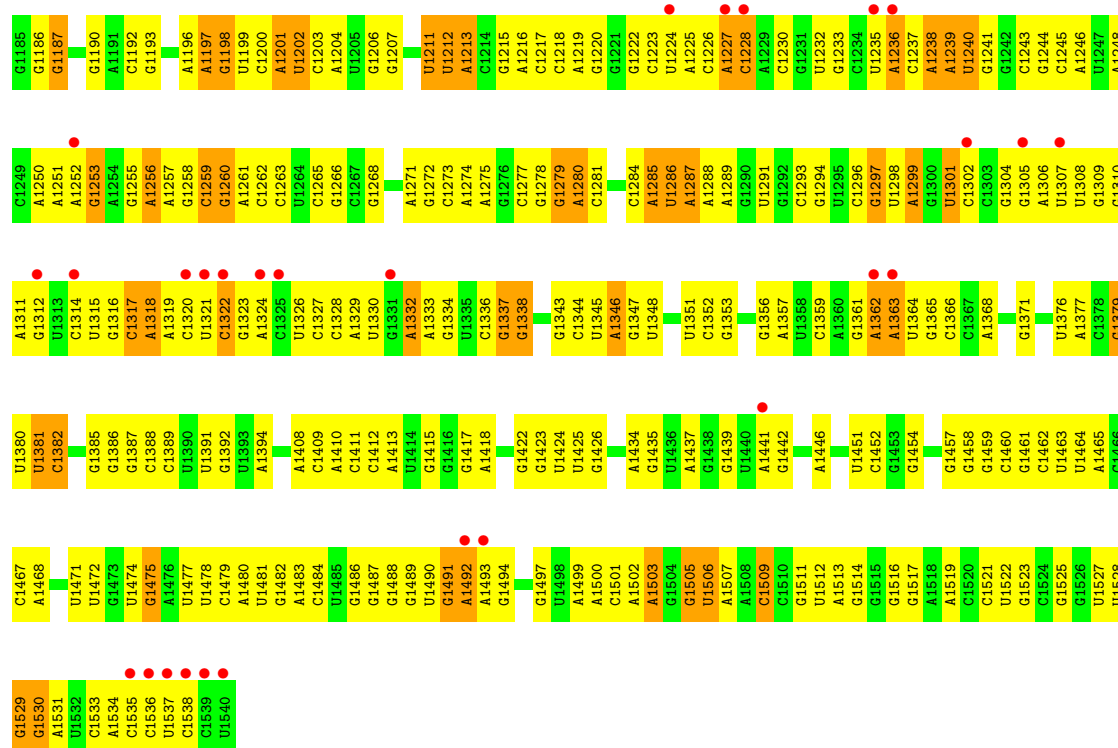
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

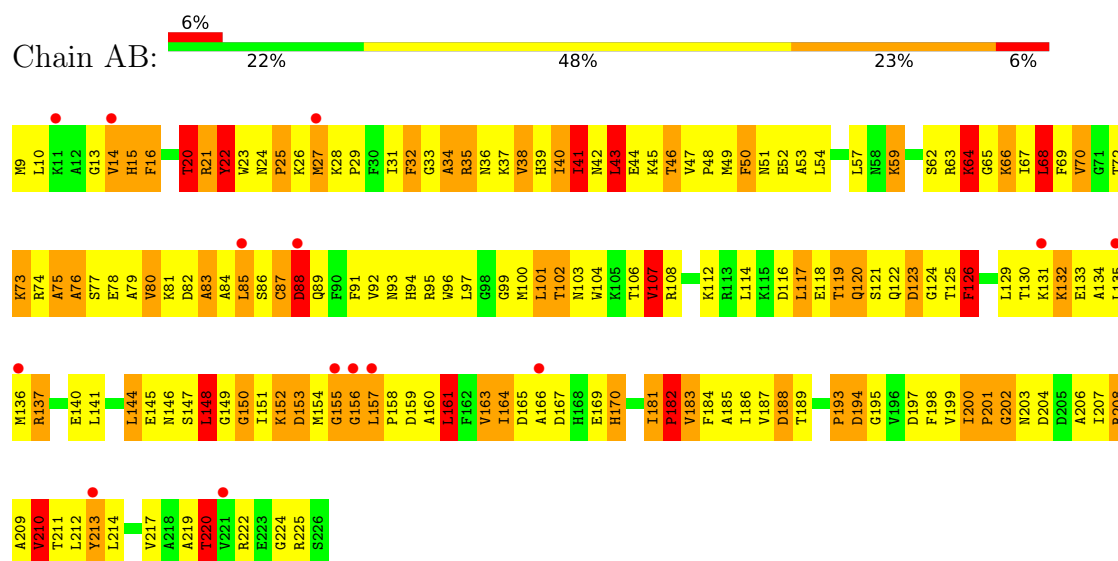




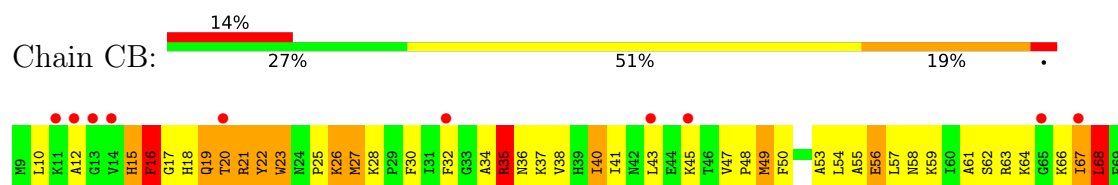
C1114	A1046	A978	A907	U837	U772	G710	U636	G566	A498	G425	A353	C271	U209	G147
G1047	G1047	C979	A908	G838	G773	G711	C837	G567	A499	U426	G354	C276	C210	G148
G1048	G1048	C980	A909	G839	G774	G712	A642	C568	A502	U427	C355	C277	G211	G149
U1049	U1049	A983	C910	C840	G775	A712	A643	C569	A503	G428	A356	C278	G212	U150
G1050	G1050	A983	C911	C841	G776	G713	U644	C570	C504	U429	G357	A279	G213	A151
G1051	G1051	A983	C912	U842	A777	G714	U645	U571	C505	A430	U358	C280	G214	A152
U1052	U1052	A991	A913	U843	G778	A715	G645	A572	G505	A431	G359	C281	C215	G153
G1053	G1053	U992	A914	U844	C779	A716	A649	A573	G506	A432	G360	G282	U216	U154
G993	G993	U992	A915	A845	A780	U717	A650	A574	A509	A435	C362	A283	C217	U155
A994	A994	A994	A919	G846	A781	A718	G650	G575	A510	A436	C363	U284	U218	C156
C995	C995	A996	A920	G847	A782	C719	C651	C576	C511	C437	C284	C285	U219	U157
A996	A996	A996	U921	C848	A783	G720	U652	G577	U512	U437	C286	C286	G220	G158
C999	C999	C999	G922	G849	A784	G721	U653	C578	C513	U438	G369	C289	C221	G159
A1000	A1000	A1000	A923	U850	G785	G722	G654	A579	C514	U439	C370	C290	C222	A160
C1001	C1001	C1001	C924	G851	A786	U723	G661	C580	G517	C440	C371	C291	A223	A161
G1002	G1002	G1002	G925	G852	A787	G724	U662	G581	G518	G445	C372	U291	U224	A162
G1003	G1003	G1003	G927	U854	A790	G725	A663	C582	C519	G446	C373	G227	G227	G163
A1004	A1004	A1004	C932	C857	A791	A728	G664	A584	A520	A451	A374	U294	A228	G164
A1005	A1005	A1005	G933	G858	A792	A729	A665	G585	A520	A452	U375	C295	U229	G165
G1006	G1006	G1006	C934	C859	A793	G730	G666	C586	G524	A453	G376	U296	G230	U166
C1007	C1007	C1007	A935	A860	A794	G731	G667	U590	G524	G454	G377	C297	U231	G168
U1008	U1008	U1008	C936	G861	C795	G732	G668	U591	G524	G455	G378	A298	G232	C169
G1009	G1009	G1009	A937	C862	C796	G733	G669	U591	G524	A456	C379	G299	C233	U170
U1010	U1010	U1010	A938	C863	C797	G734	G670	U591	G524	A457	A300	A300	C234	A171
C1011	C1011	C1011	G939	U866	U798	C735	G671	G597	G529	G457	G384	G301	G237	A172
A1012	A1012	A1012	C940	C866	G799	C736	U672	U598	G530	U458	C385	G302	G237	U173
G1013	G1013	G1013	G941	C867	G800	C737	A673	C599	G531	A459	C386	A303	A238	A174
A1014	A1014	A1014	G942	U867	A801	C738	G674	A532	A532	A460	U387	U239	U239	C175
U1015	U1015	U1015	G943	C868	G802	C739	A675	U603	U534	A461	A388	A306	G240	C176
A1016	A1016	A1016	A946	G869	U804	G741	A676	G604	A535	G462	A389	C307	G241	G177
U1017	U1017	U1017	G947	C870	U805	G742	U677	U605	A535	U463	U390	C308	G242	C178
G1018	G1018	G1018	C948	A872	G806	G743	U678	G606	C536	U464	G391	A309	A244	A179
A1019	A1019	A1019	A949	U874	C807	G744	U679	A607	G537	A465	C392	C312	U245	U180
U1020	U1020	U1020	G950	C873	G808	G745	C879	A608	G538	A466	A393	A313	A246	A181
G951	G951	G951	U952	U875	C810	A746	A681	A609	A539	U467	A397	C316	G247	A182
A1021	A1021	A1021	U952	C876	C811	A747	G882	U610	G540	A468	U398	C316	A248	C183
U1022	U1022	U1022	U952	U877	G812	G748	G883	C611	G541	C469	G399	C316	U249	G184
G1023	G1023	G1023	U955	A878	A815	A749	U684	C612	G542	C470	C400	G319	A250	U185
U1024	U1024	U1024	U956	C879	A816	C750	G885	C613	U543	U471	C401	A320	G251	C186
G1025	G1025	G1025	U957	C880	C817	G751	U686	C614	G544	U472	G402	A321	U252	G187
U1026	U1026	U1026	A958	G881	C818	U752	A687	G615	C545	U473	C403	A321	G252	C188
C1027	C1027	C1027	A959	C882	G819	A753	U688	C618	A546	G474	C404	A327	A253	A189
U1028	U1028	U1028	U959	C883	A819	C754	C689	C618	A547	C475	G404	C328	G254	A190
G1029	G1029	G1029	U960	U884	U820	G755	G890	U619	G550	U476	U405	C329	G255	G191
U1030	U1030	U1030	C963	G885	G821	C756	G891	C620	G551	C477	G406	C330	U256	A195
C1031	C1031	C1031	A964	U886	U822	U757	U692	A621	U552	A478	U407	G331	G257	A196
G1032	G1032	G1032	U965	C887	C823	C758	G893	A622	U553	U479	A408	G332	G258	A197
U1033	U1033	U1033	G966	A889	G824	A759	A694	C623	A553	U480	C410	G332	G259	G198
G1034	G1034	G1034	C967	G890	A825	G760	A695	C624	A554	G481	G411	G337	G260	U199
A1035	A1035	A1035	U968	U891	C826	G761	A696	U625	C556	G482	A412	G338	U261	G200
U1036	U1036	U1036	A969	C892	U827	C762	G700	G628	A559	G484	A413	A339	A262	G201
C1037	C1037	C1037	A970	U893	G828	G763	U701	A629	A559	U485	A414	C339	A263	G202
U1038	U1038	U1038	G971	C894	G829	G764	A702	A630	A560	U486	A415	C345	G264	G203
G1039	G1039	G1039	C972	G895	A766	A767	G703	A631	U561	C490	U421	G346	G265	G204
U1040	U1040	U1040	G973	C899	A768	A768	A704	U632	U562	A495	C422	G347	C267	A205
A1041	A1041	A1041	A974	A800	G832	G769	A705	U633	A563	A496	G423	C351	U268	C206
G1042	G1042	G1042	A975	C901	G833	G769	G706	C634	A564	A497	G424	C352	G269	C207
U1043	U1043	U1043	G976	U896	U835	C770	A707	C634	A565	A498	G425	C352	A270	U208
G1044	G1044	G1044	A977	C906	G836	G771	U707	A635	U565	G497	G424	C352	A270	U208

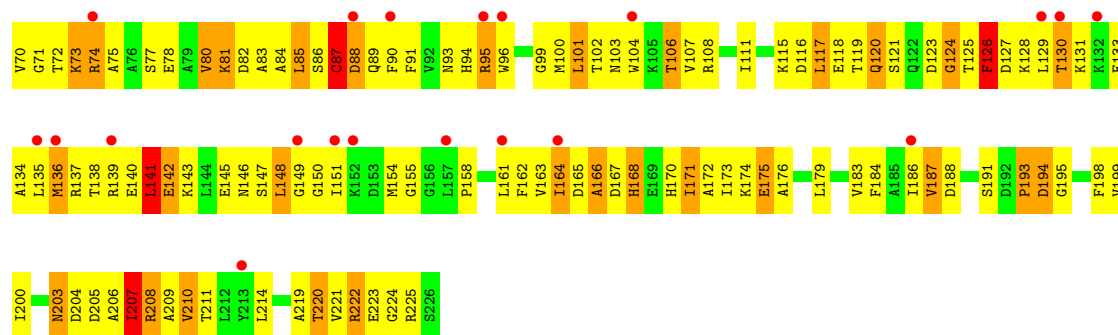


• Molecule 2: 30S ribosomal protein S2

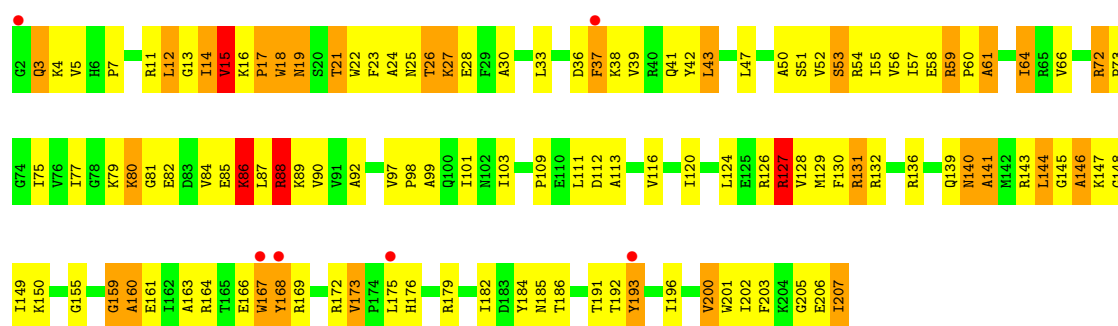
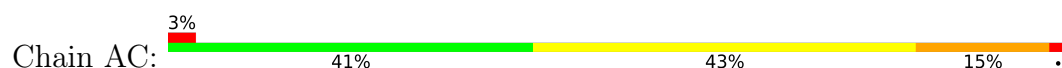


• Molecule 2: 30S ribosomal protein S2

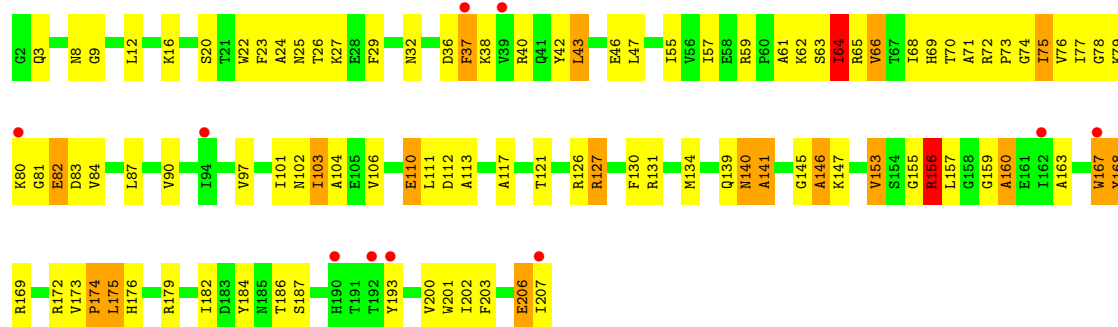




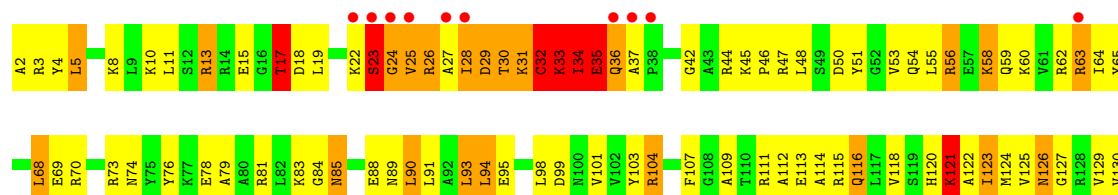
• Molecule 3: 30S ribosomal protein S3

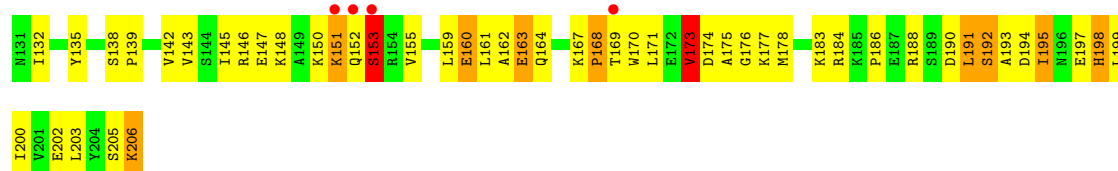


• Molecule 3: 30S ribosomal protein S3

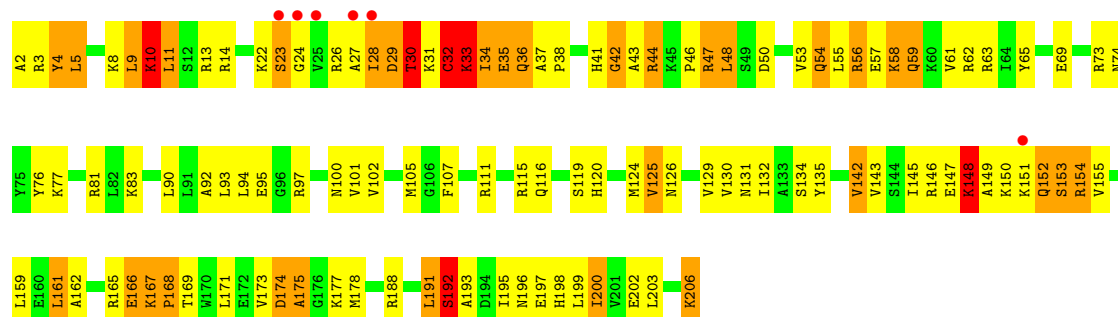
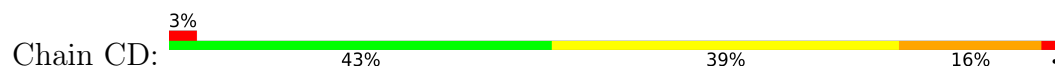


• Molecule 4: 30S ribosomal protein S4

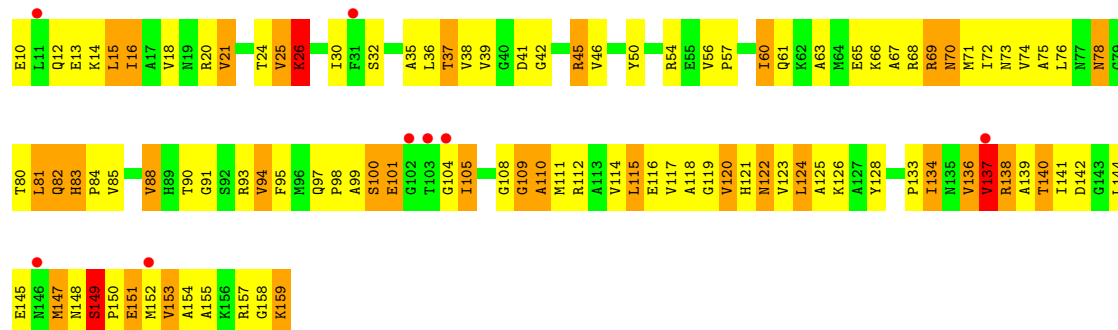




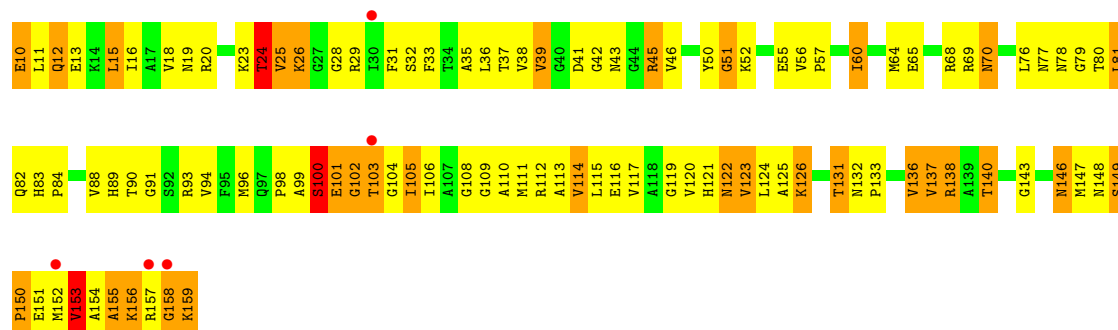
• Molecule 4: 30S ribosomal protein S4



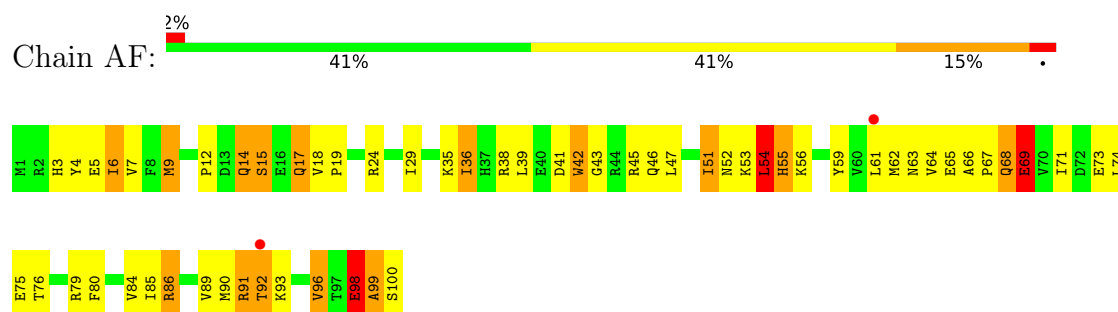
• Molecule 5: 30S ribosomal protein S5



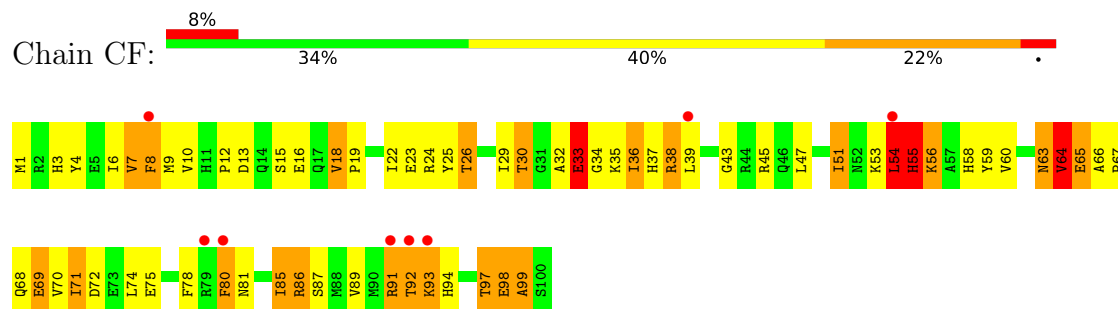
• Molecule 5: 30S ribosomal protein S5



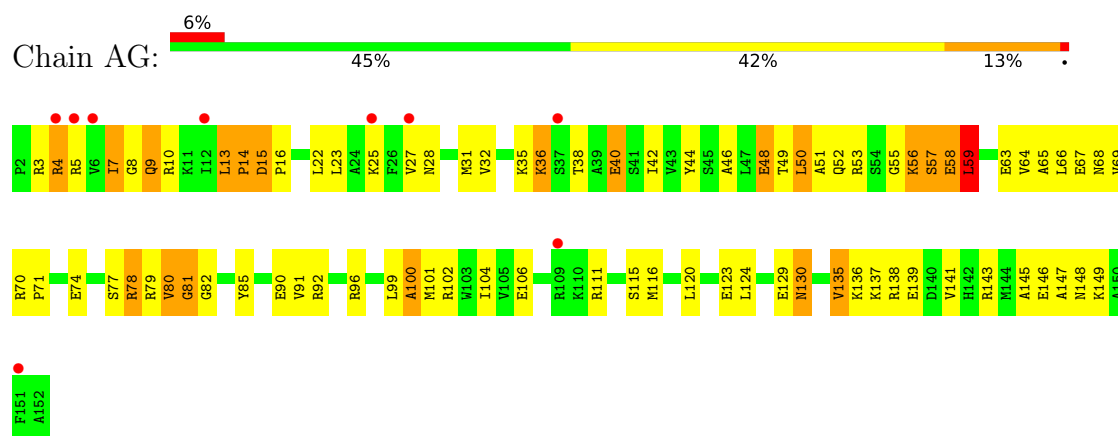
• Molecule 6: 30S ribosomal protein S6



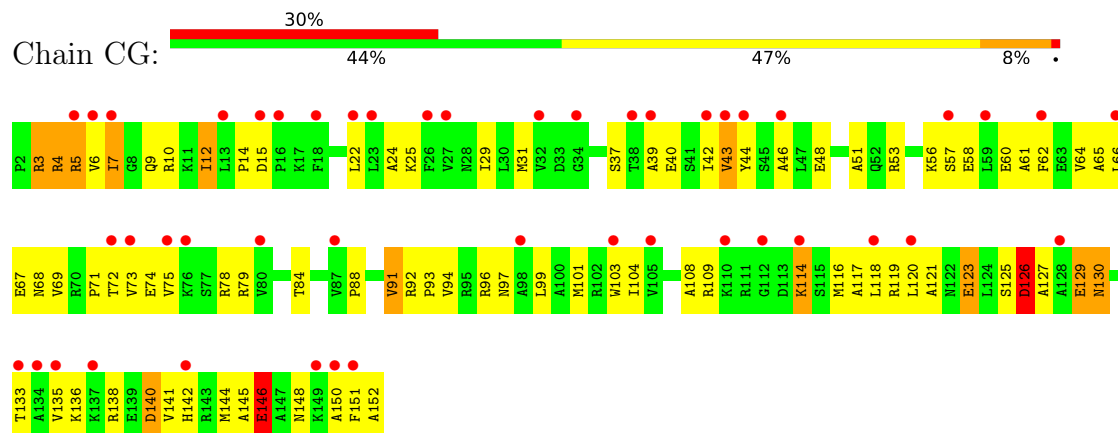
- Molecule 6: 30S ribosomal protein S6



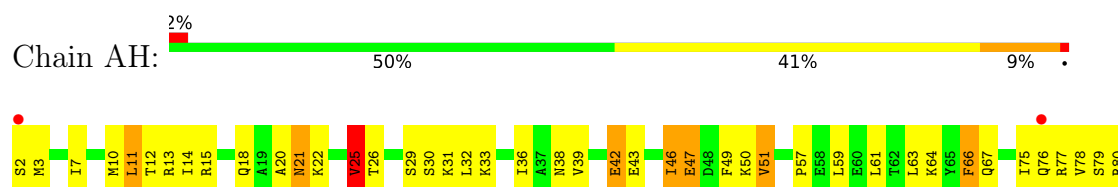
- Molecule 7: 30S ribosomal protein S7



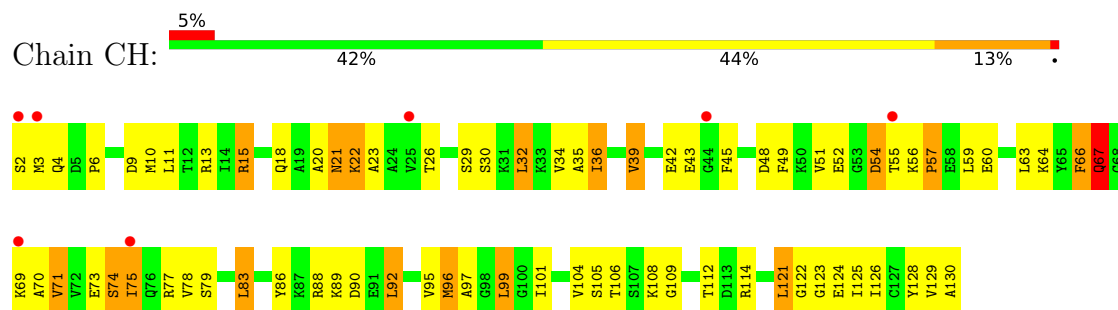
- Molecule 7: 30S ribosomal protein S7



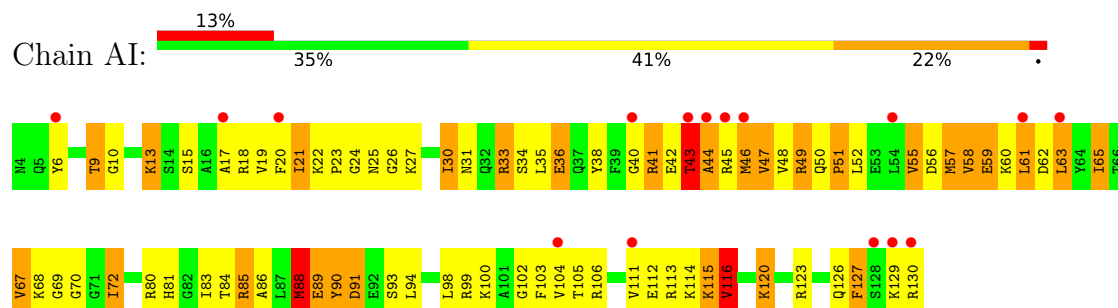
- Molecule 8: 30S ribosomal protein S8



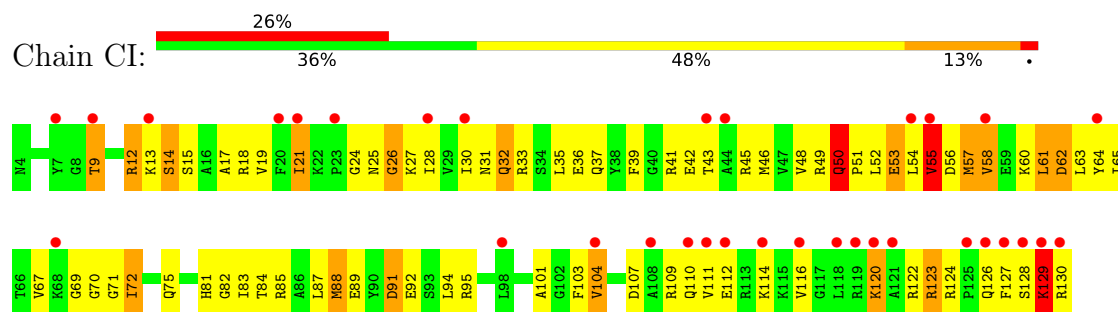
• Molecule 8: 30S ribosomal protein S8



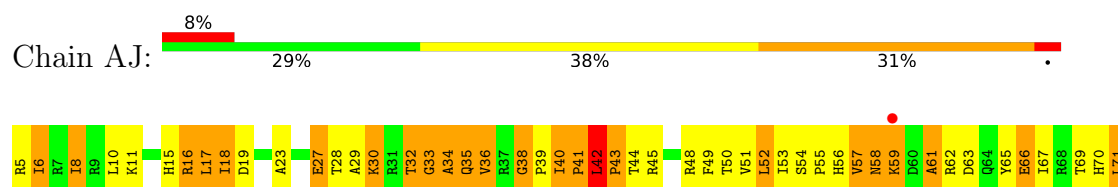
• Molecule 9: 30S ribosomal protein S9

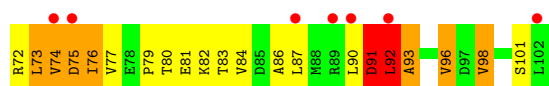


• Molecule 9: 30S ribosomal protein S9

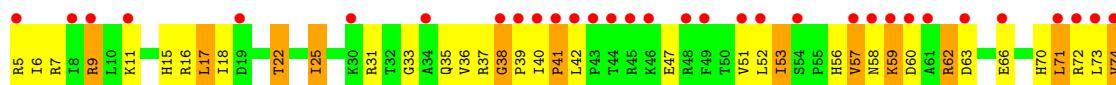


• Molecule 10: 30S ribosomal protein S10

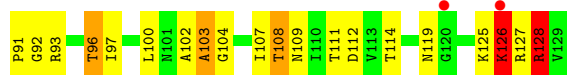




- Molecule 10: 30S ribosomal protein S10



- Molecule 11: 30S ribosomal protein S11



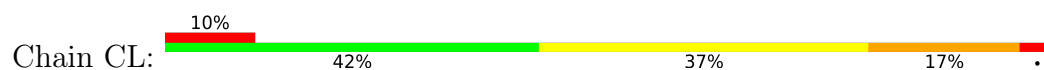
- Molecule 11: 30S ribosomal protein S11

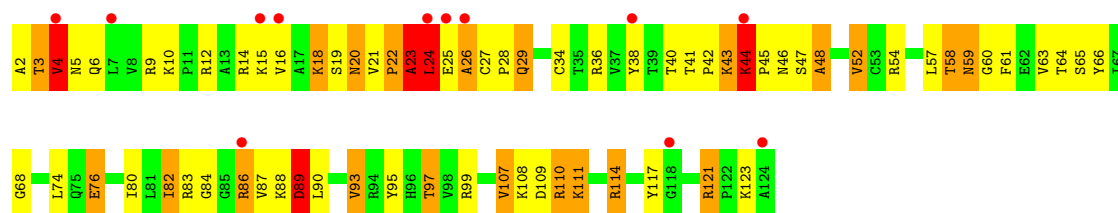


- Molecule 12: 30S ribosomal protein S12

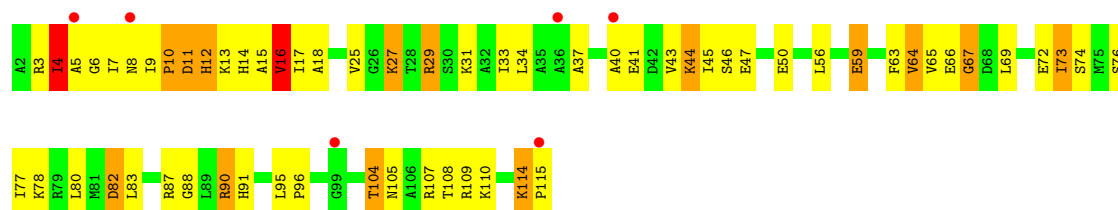


- Molecule 12: 30S ribosomal protein S12

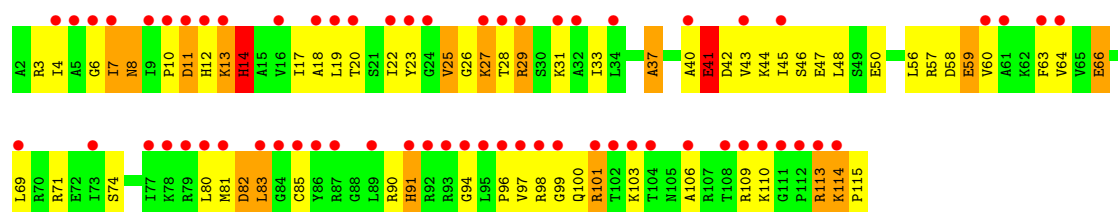




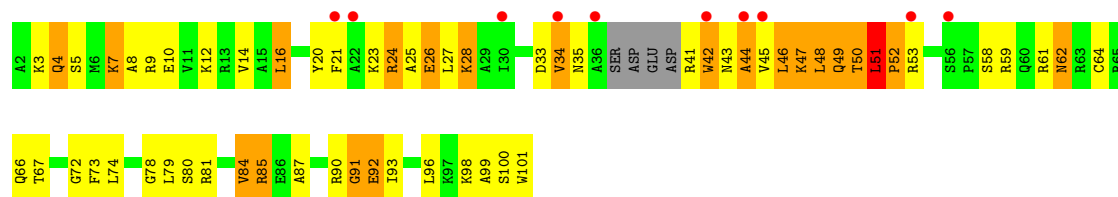
• Molecule 13: 30S ribosomal protein S13



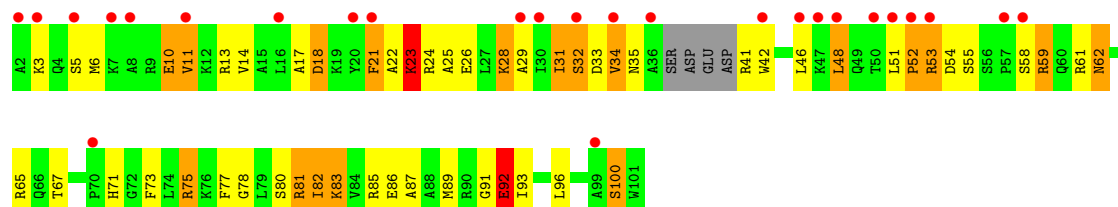
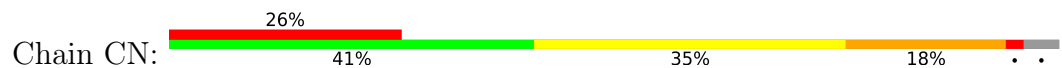
• Molecule 13: 30S ribosomal protein S13



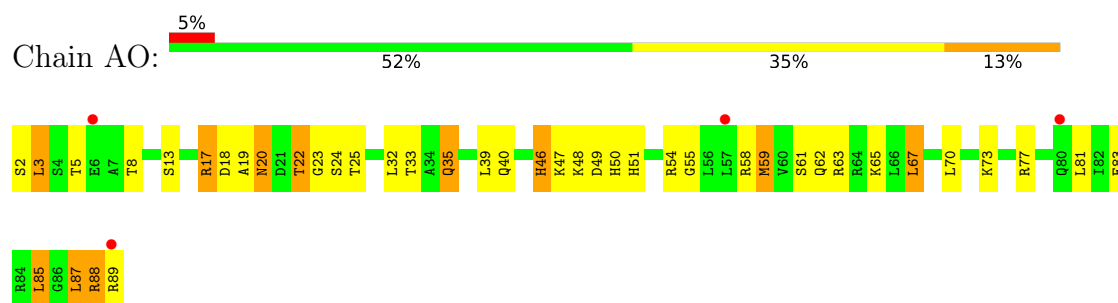
• Molecule 14: 30S ribosomal protein S14



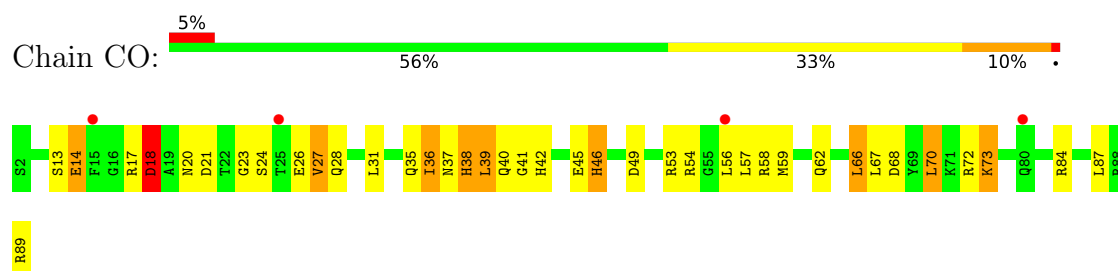
• Molecule 14: 30S ribosomal protein S14



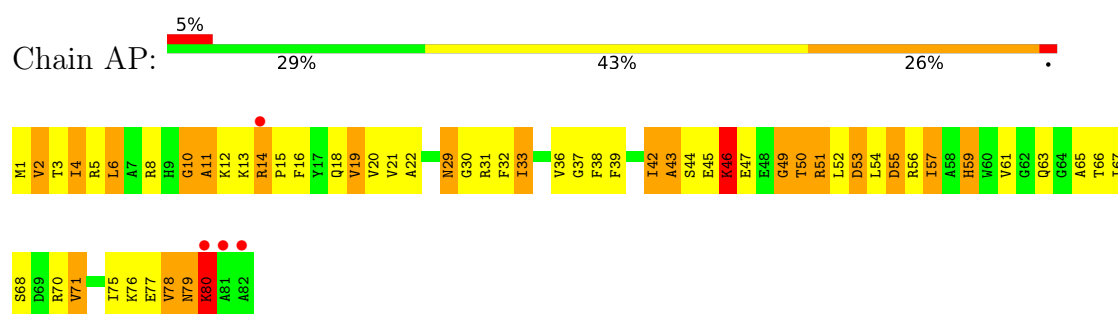
- Molecule 15: 30S ribosomal protein S15



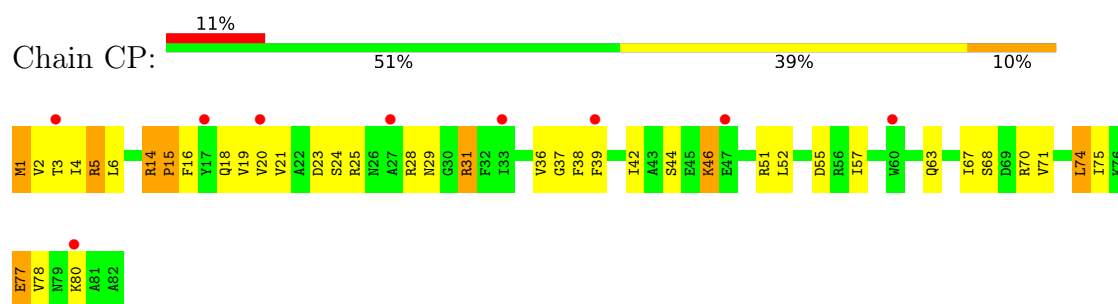
- Molecule 15: 30S ribosomal protein S15



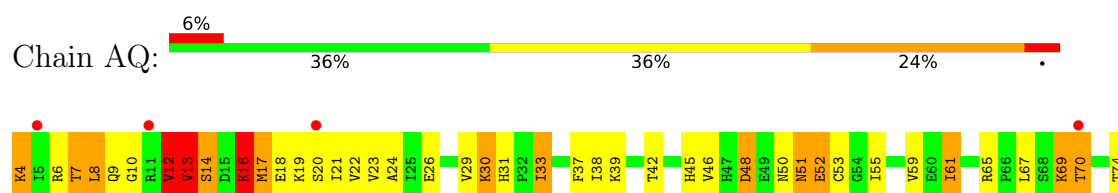
- Molecule 16: 30S ribosomal protein S16



- Molecule 16: 30S ribosomal protein S16

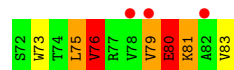
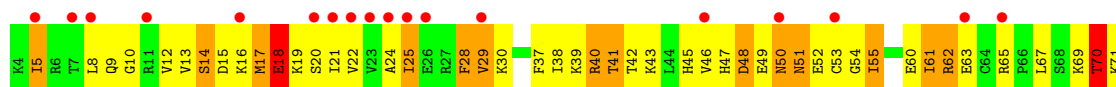


- Molecule 17: 30S ribosomal protein S17

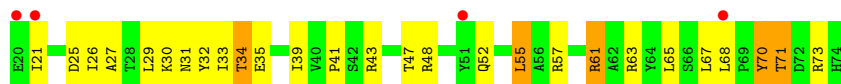




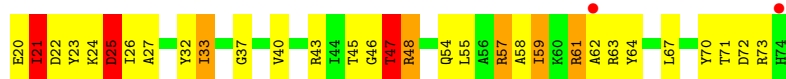
- Molecule 17: 30S ribosomal protein S17



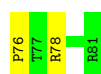
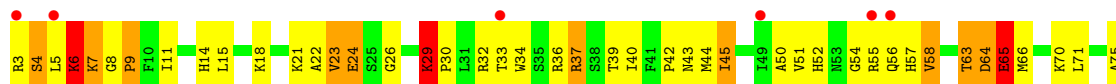
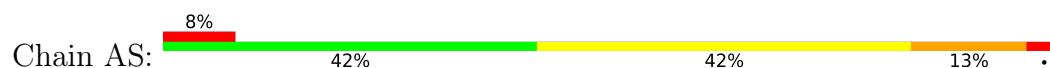
- Molecule 18: 30S ribosomal protein S18



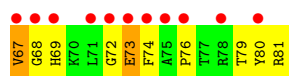
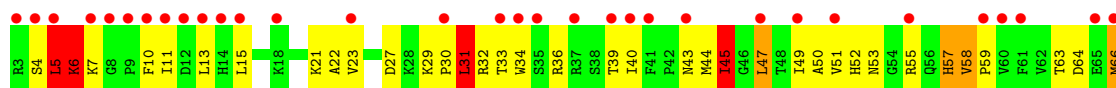
- Molecule 18: 30S ribosomal protein S18



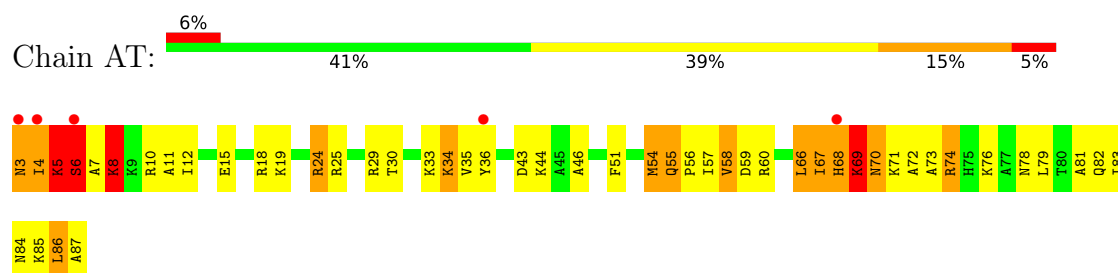
- Molecule 19: 30S ribosomal protein S19



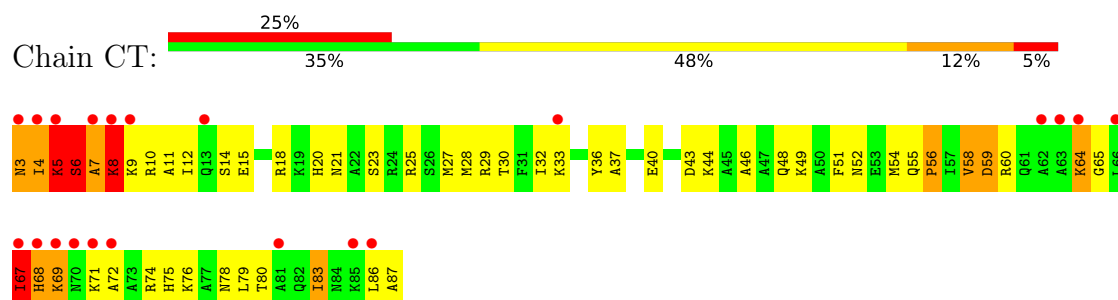
- Molecule 19: 30S ribosomal protein S19



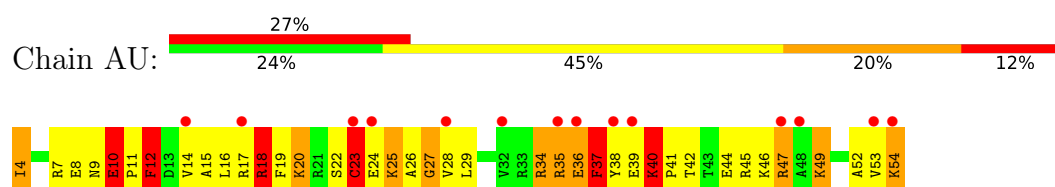
- Molecule 20: 30S ribosomal protein S20



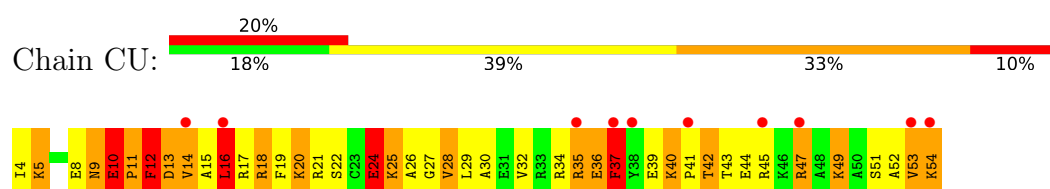
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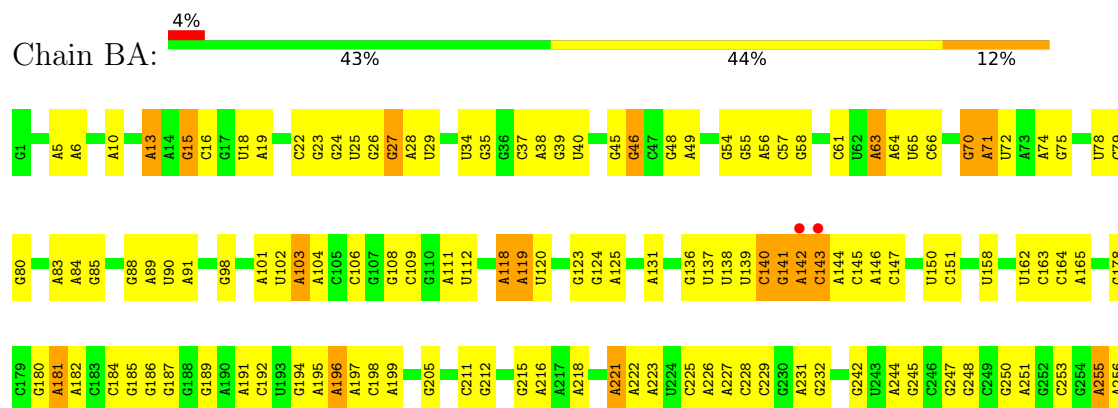
- Molecule 21: 30S ribosomal protein S21



- Molecule 21: 30S ribosomal protein S21

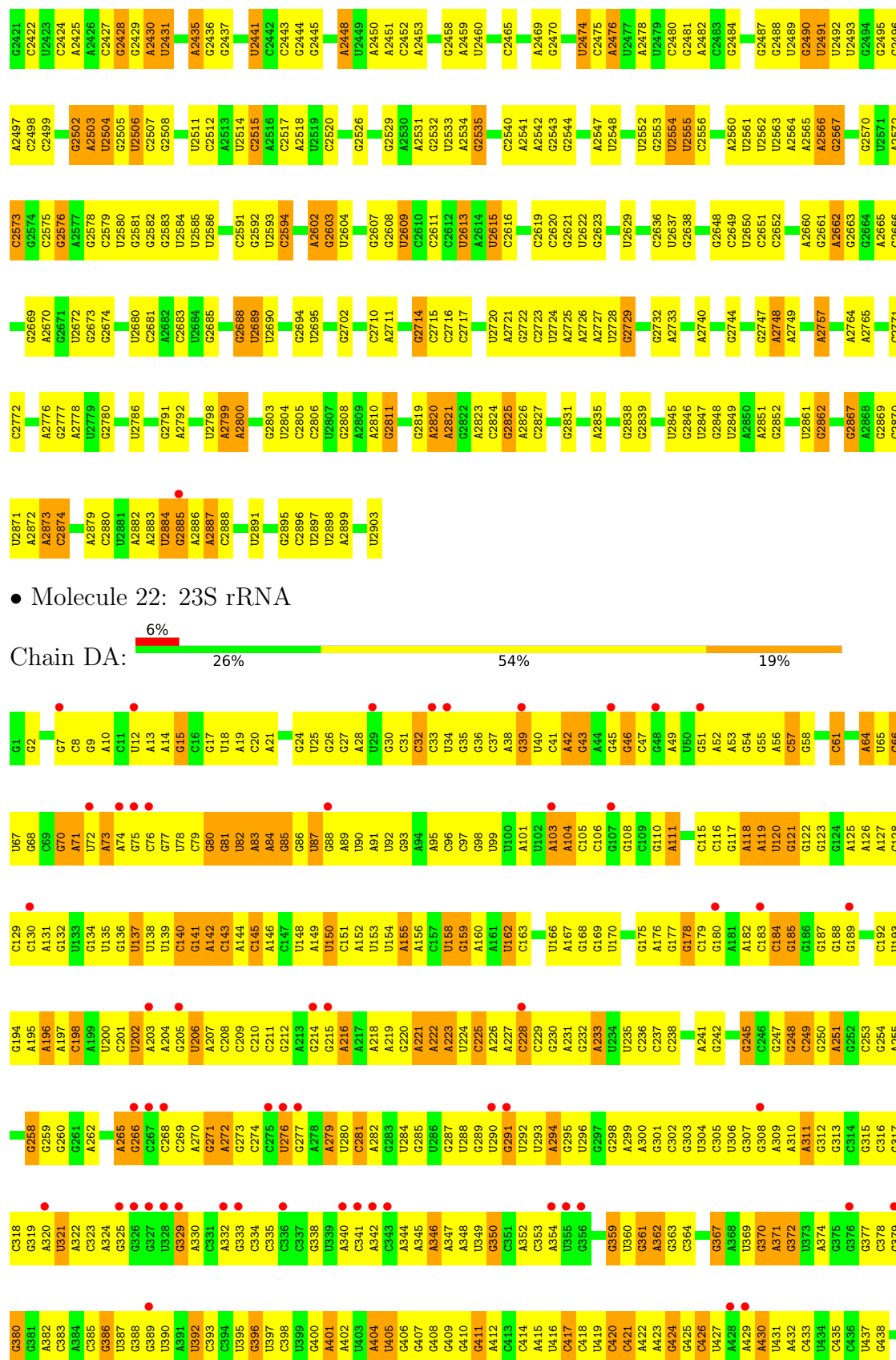


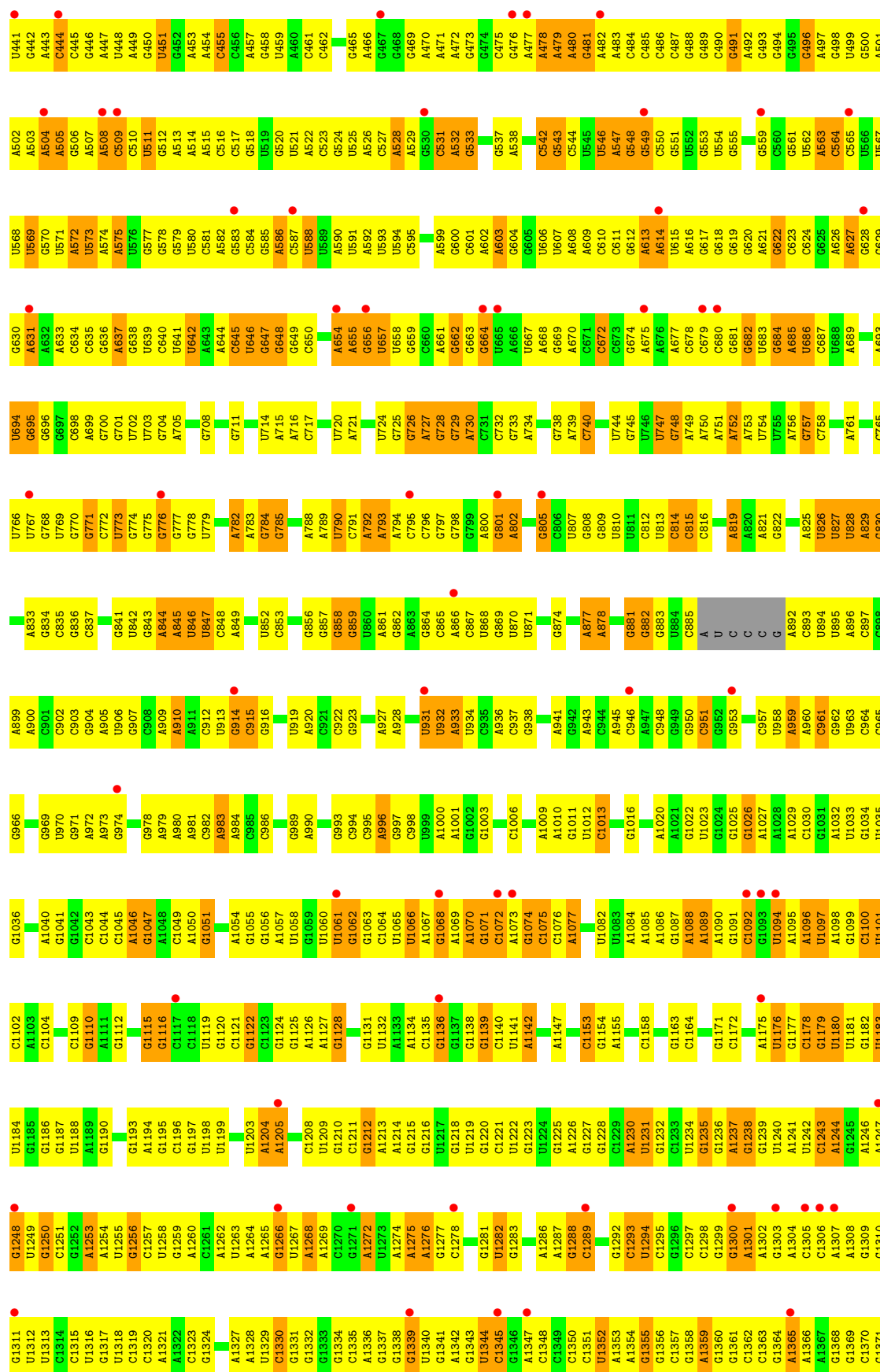
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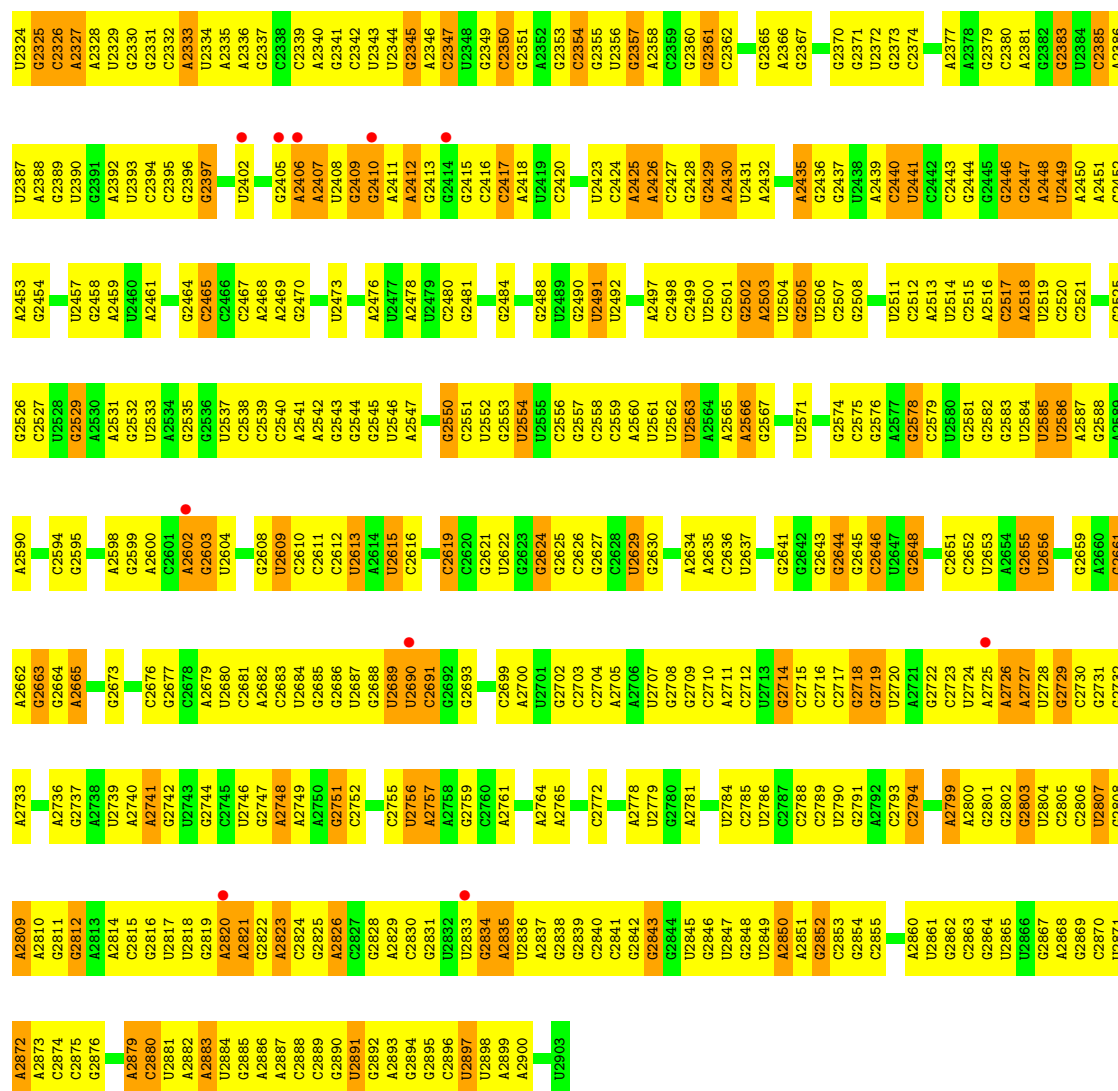
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A1287	C1196	G1112	G1047	A971	C	C814	U740	U653	A582	A502	C420	A342	G259
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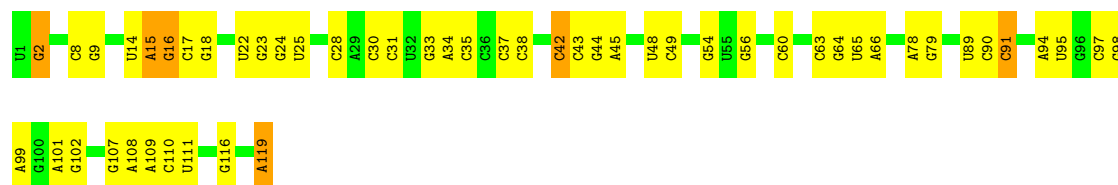


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A2266	A2199	A2134	G2061	C1997	G1930	G1858	A1791	G1724	G1646	U1513	U1438	G1377
A2267	G2200	A2135	A2062	A1998	U1931	A1858	C1793	U1725	U1647	G1514	A1439	A1378
A2268	G2201	G2136	C2063	A1999	U1931	G1863	A1794	C1726	U1648	G1515	U1440	U1379
G2271	U2202	U2137	G2064	C2000	G1935	U1864	A1795	C1727	G1649	A1516	G1441	G1380
U2203	U2203	G2141	C2065	C2001	A1936	U1865	A1796	C1728	A1650	G1519	U1442	G1381
G2204	G2204	A2142	C2066	A1937	A1937	U1866	U1797	G1729	U1651	U1520	U1443	G1382
A2205	A2205	G2143	G2067	U1938	A1938	G1867	U1798	G1730	A1652	G1521	G1444	A1383
A2274	G2206	C2143	U2068	A2005	U1939	G1868	G1799	G1731	G1653	A1522	G1445	A1384
G2275	G2207	G2144	G2069	C2006	U1940	G1869	G1800	C1732	A1654	U1523	G1446	A1385
G2208	G2208	C2145	A2070	U2007	G1945	C1870	A1801	G1733	A1655	G1524	C1447	A1386
G2209	G2209	C2146	A2071	C2008	G1946	A1871	A1802	G1734	A1656	A1525	G1448	A1387
G2280	G2210	A2147	C2072	A2009	U1946	A1872	A1803	A1735	U1657	G1526	G1449	G1388
A2281	A2211	G2148	C2073	G2010	C1947	G1873	G1804	U1736	G1658	G1527	G1389	G1389
G2282	A2212	U2149	U2074	U2011	G1948	C1874	A1805	G1737	G1659	A1528	U1390	U1390
G2283	U2213	C2150	U2075	G2012	G1949	G1875	A1806	G1738	G1660	G1529	G1452	U1391
G2214	G2214	U2151	A2076	A2013	G1950	A1876	G1807	A1739	G1661	G1530	A1453	A1392
G2156	G2215	G2156	U2079	A2014	U1951	A1877	A1808	G1740	U1662	A1531	G1454	A1393
G2216	G2216	G2157	A2080	A2015	A1952	G1878	A1809	G1741	G1663	A1532	G1455	A1394
A2287	G2217	A2158	U2082	U2016	A1953	C1879	A1810	U1742	A1664	C1533	U1457	A1395
A2288	G2218	G2159	G2083	U2017	G1954	U1880	G1811	G1743	A1665	U1534	U1458	A1396
G2221	G2221	C2160	C2084	G2018	U1955	C1881	U1812	A1744	G1666	A1535	G1459	U1397
U2290	G2222	G2161	G2087	A2019	U1956	U1882	G1813	A1745	G1667	G1536	U1460	C1398
U2291	G2223	C2162	G2087	A2020	C1957	U1883	G1814	A1749	A1669	G1537	C1461	C1399
G2223	G2224	A2163	U2092	G2021	A1958	G1884	A1815	G1750	A1670	C1604	G1462	U1400
G2294	G2225	C2164	C2091	U2022	G1959	G1889	C1816	U1751	C1670	C1605	G1463	G1401
G2295	G2226	C2165	U2092	G2024	A1960	A1890	G1817	G1752	C1606	G1606	G1464	U1402
U2296	A2227	U2166	G2093	C2025	G1964	G1891	U1818	G1753	C1607	U1542	G1465	A1403
A2297	G2230	G2167	A2094	U2026	C1965	C1892	U1820	A1754	A1609	A1544	U1466	A1404
A2298	U2231	G2168	C2103	A2030	G1967	C1893	G1826	A1755	A1610	A1545	U1467	U1405
G2300	G2232	A2170	U2105	G2032	G1968	G1895	U1827	G1756	A1676	G1546	U1468	U1406
G2301	G2233	A2171	U2106	A2033	A1969	C1896	G1828	A1757	A1677	C1547	A1470	G1407
G2302	G2234	U2172	G2107	G2034	U1970	U1897	U1829	U1758	A1678	G1548	G1471	G1408
G2303	G2235	C2173	A2108	G2035	G1968	G1898	A1830	A1759	G1682	A1551	G1475	U1410
U2304	U2236	C2175	U2109	G2036	G1968	C1899	G1831	C1761	U1683	A1552	U1476	U1411
G2305	G2237	A2176	G2110	A2037	A1974	G1903	G1834	G1763	U1688	A1553	A1477	A1413
G2306	G2238	C2177	G2111	G2038	G1975	G1903	U1834	G1764	G1618	G1554	C1480	U1414
G2307	G2239	C2178	G2112	U2039	U1976	G1906	G1835	U1765	U1692	G1555	G1480	U1415
G2308	U2240	C2179	U2113	G2040	A1977	G1907	C1836	G1766	U1693	C1556	U1481	G1416
A2309	A2241	U2180	A2114	A2041	C1978	G1907	C1837	G1767	C1694	C1557	G1482	C1417
G2310	G2242	U2181	G2115	A2042	U1979	G1911	C1838	C1768	G1695	C1558	G1483	G1418
A2311	U2243	U2182	G2116	G2043	U1981	U1912	G1839	U1769	U1624	G1559	U1484	A1419
G2312	U2244	A2183	A2117	C2044	A1981	A1912	A1698	A1698	C1625	G1560	C1493	A1420
G2313	U2245	A2184	U2118	C2045	U1982	A1913	A1698	A1698	A1626	C1563	G1493	G1421
G2314	G2246	U2185	A2119	G2048	G1983	C1914	C1843	A1773	A1626	U1562	G1497	G1422
G2315	G2247	G2186	G2120	U2049	G1984	U1915	C1844	C1774	G1627	U1563	U1497	G1423
A2317	G2251	U2187	G2121	G2049	C1985	A1916	G1845	U1775	G1628	C1564	G1500	G1426
G2318	G2252	U2188	U2122	C2050	G1986	U1917	G1846	G1776	G1707	C1565	G1501	A1427
G2319	G2253	U2189	G2123	A2051	C1987	U1918	A1847	U1779	U1709	A1566	A1502	C1428
U2320	G2254	G2190	G2124	A2052	G1988	A1919	G1849	A1780	G1710	G1567	A1503	G1429
U2321	A2321	A2191	G2125	G2053	G1989	C1920	G1850	A1781	A1637	A1569	A1504	G1430
A2322	A2322	A2192	A2126	C2054	C1990	U1920	U1851	U1782	C1639	A1570	A1505	A1431
G2323	G2258	G2193	G2127	C2055	U1991	C1924	U1852	A1783	U1716	A1571	G1432	G1432



• Molecule 23: 5S rRNA

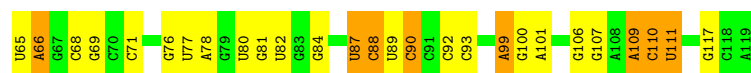
Chain BB: 56% 39% 5%



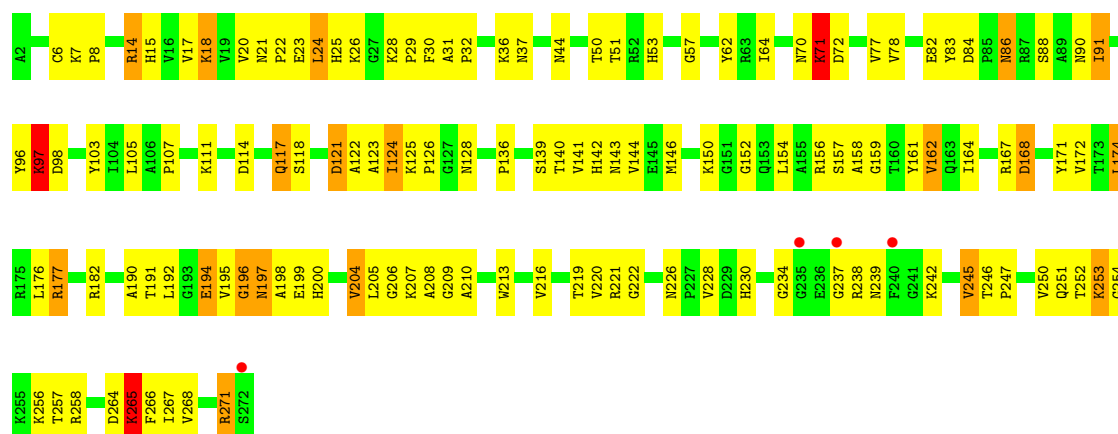
• Molecule 23: 5S rRNA

Chain DB: 38% 52% 9%

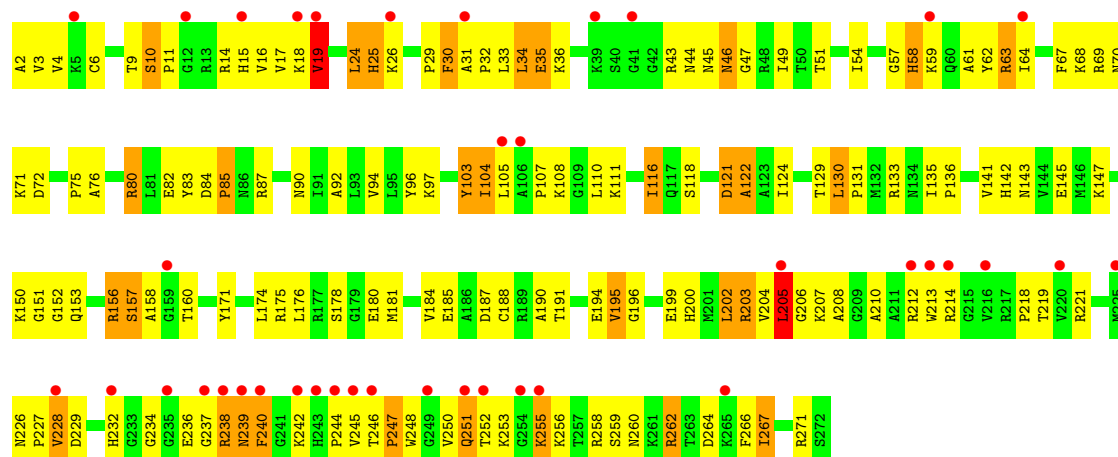




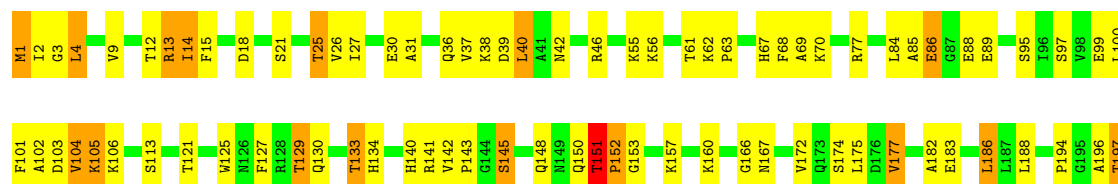
• Molecule 24: 50S ribosomal protein L2



• Molecule 24: 50S ribosomal protein L2

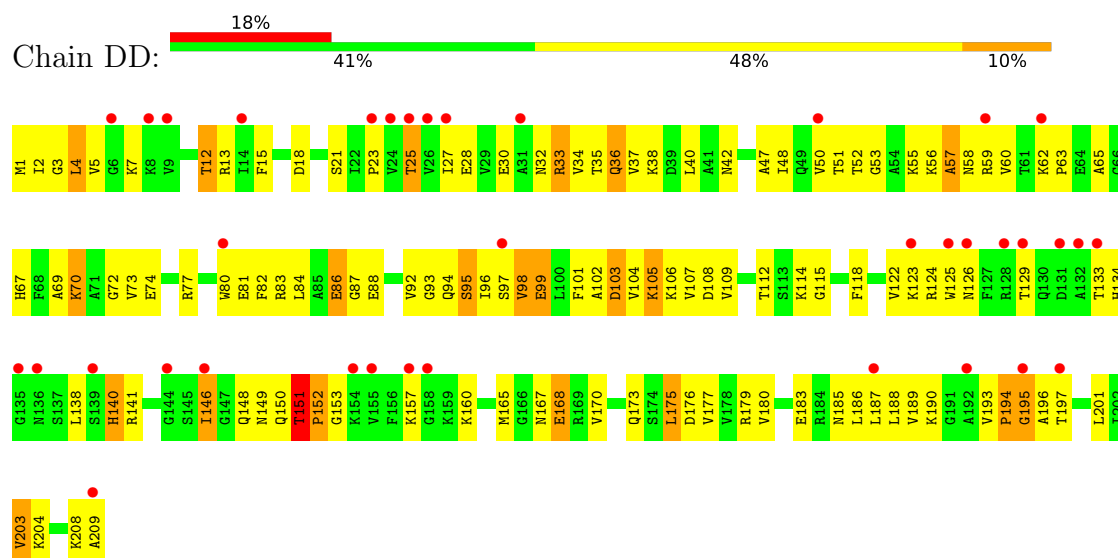


• Molecule 25: 50S ribosomal protein L3

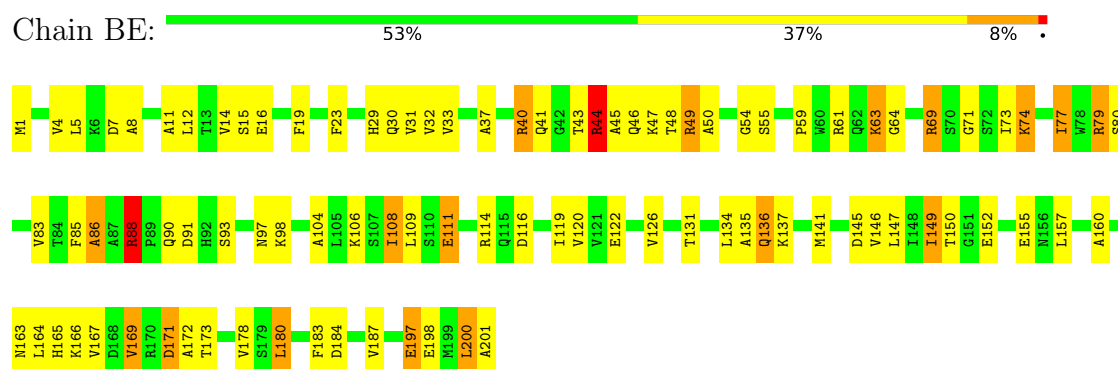




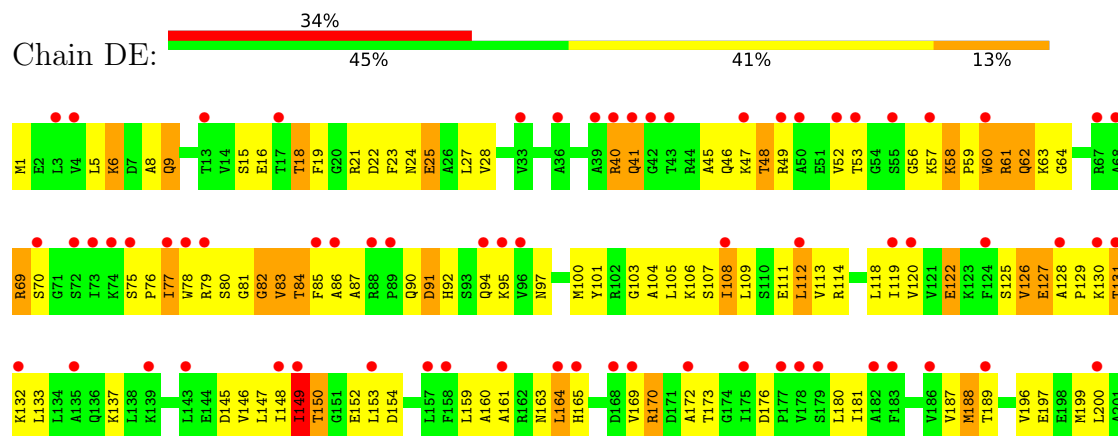
• Molecule 25: 50S ribosomal protein L3



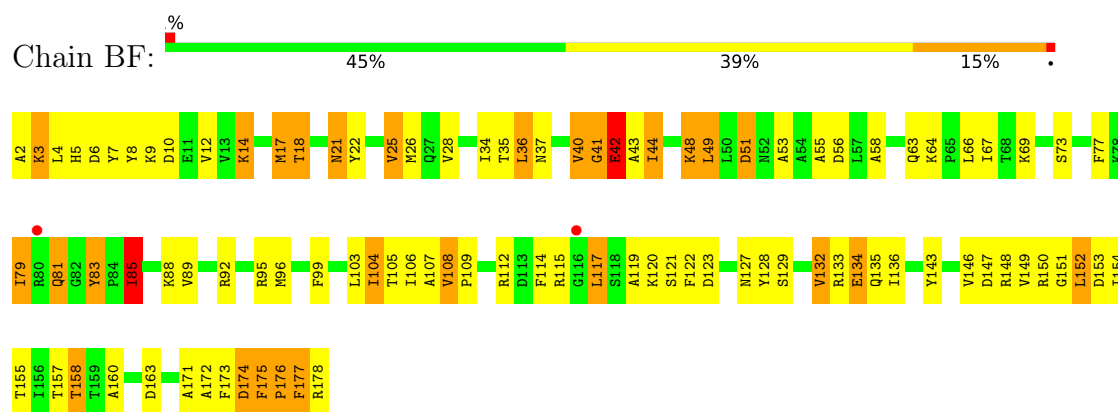
• Molecule 26: 50S ribosomal protein L4



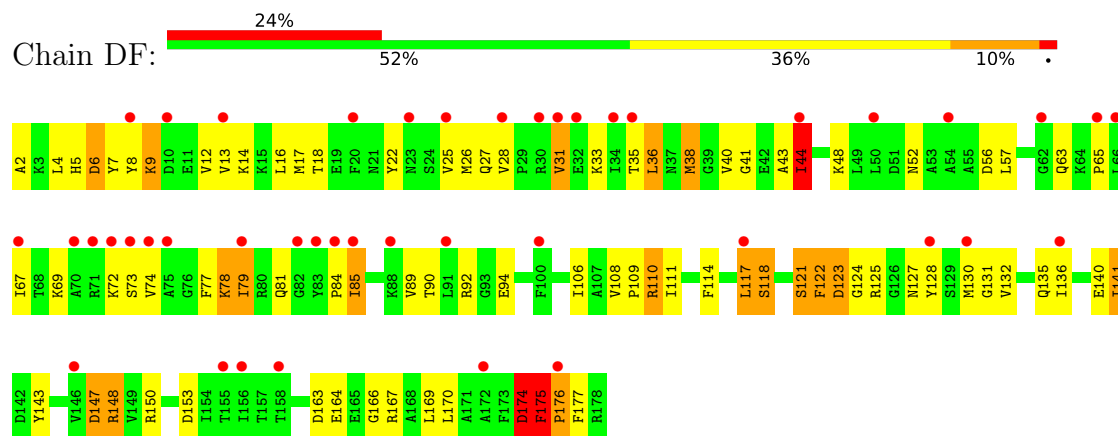
• Molecule 26: 50S ribosomal protein L4



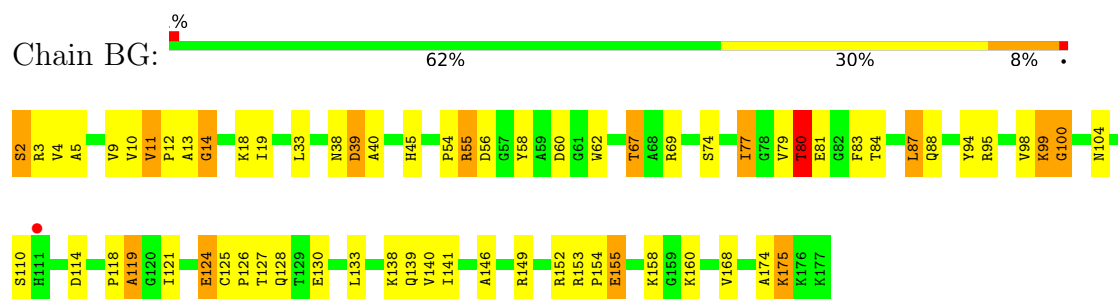
• Molecule 27: 50S ribosomal protein L5



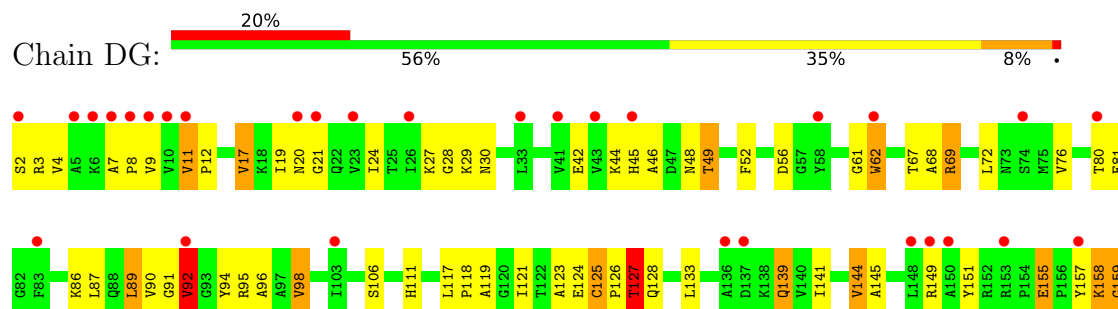
• Molecule 27: 50S ribosomal protein L5



• Molecule 28: 50S ribosomal protein L6

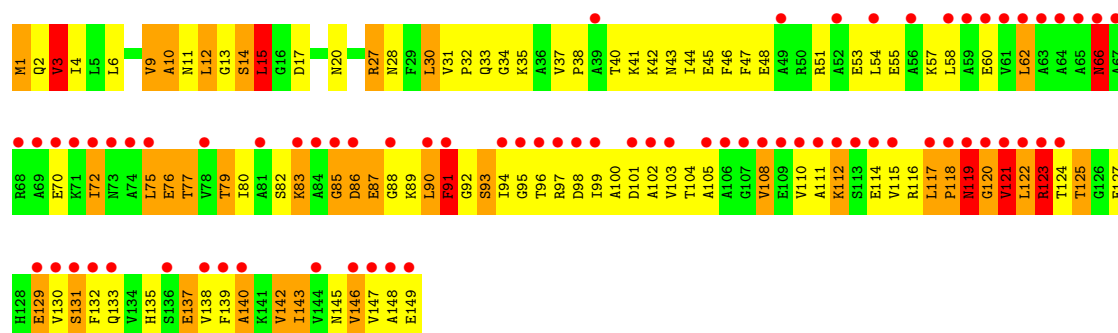


• Molecule 28: 50S ribosomal protein L6

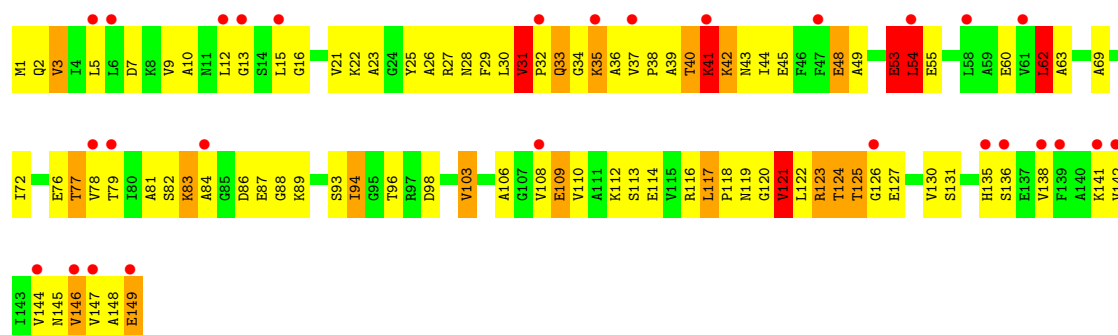




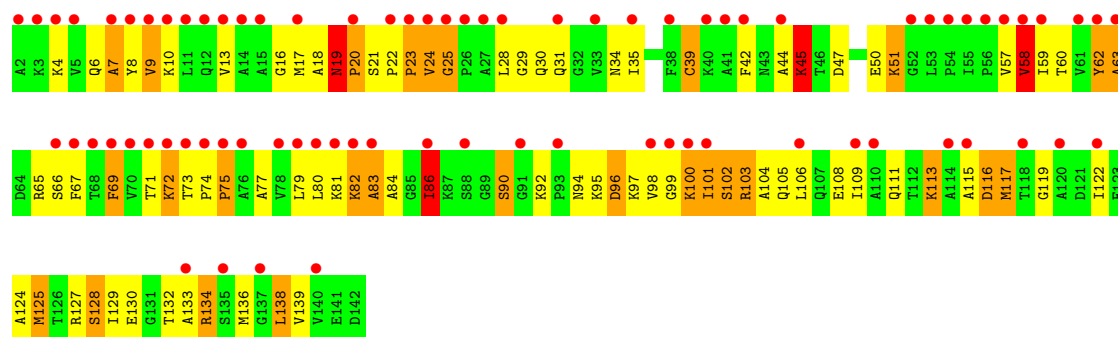
- Molecule 29: 50S ribosomal protein L9



- Molecule 29: 50S ribosomal protein L9

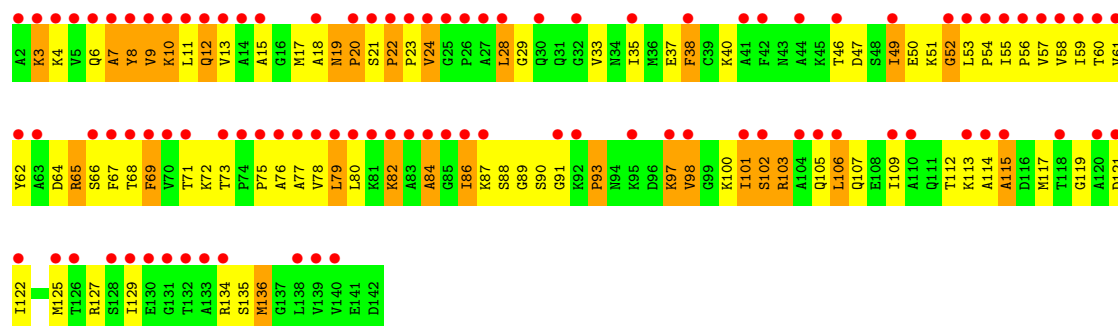


- Molecule 30: 50S ribosomal protein L11

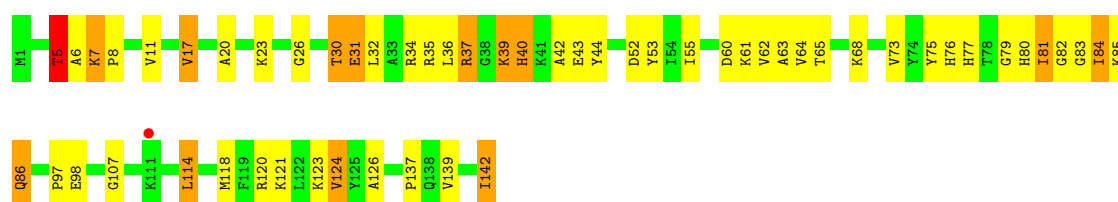


- Molecule 30: 50S ribosomal protein L11

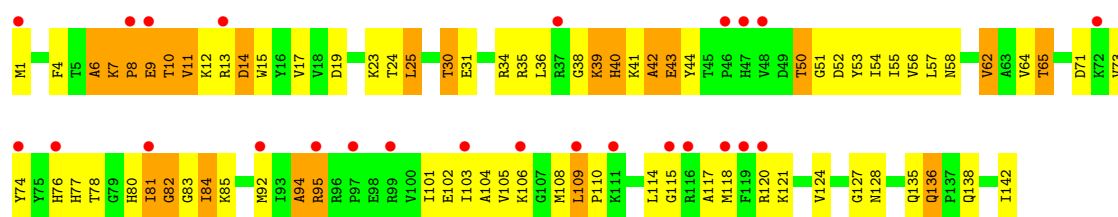




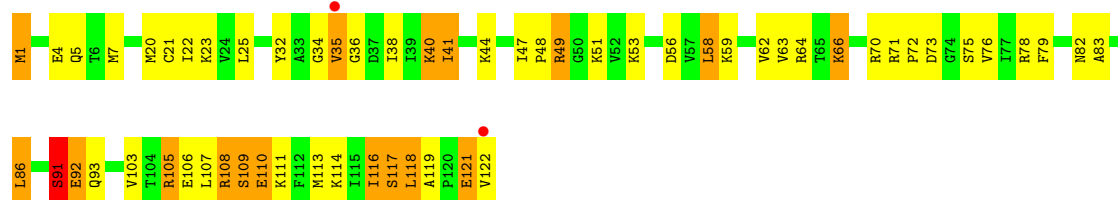
• Molecule 31: 50S ribosomal protein L13



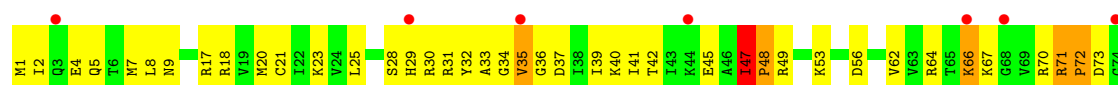
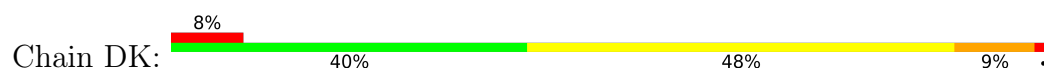
• Molecule 31: 50S ribosomal protein L13



• Molecule 32: 50S ribosomal protein L14



• Molecule 32: 50S ribosomal protein L14

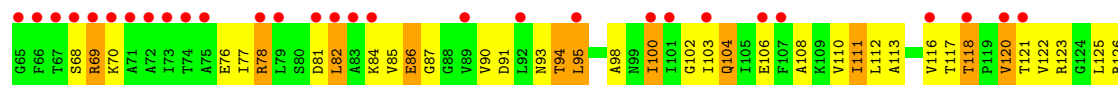
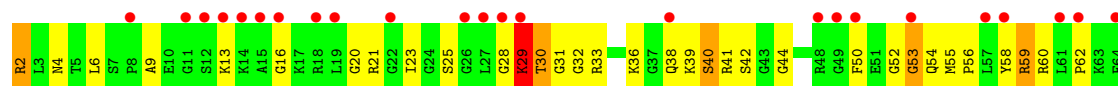
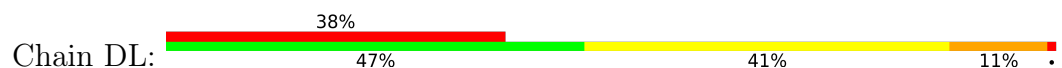




• Molecule 33: 50S ribosomal protein L15



• Molecule 33: 50S ribosomal protein L15



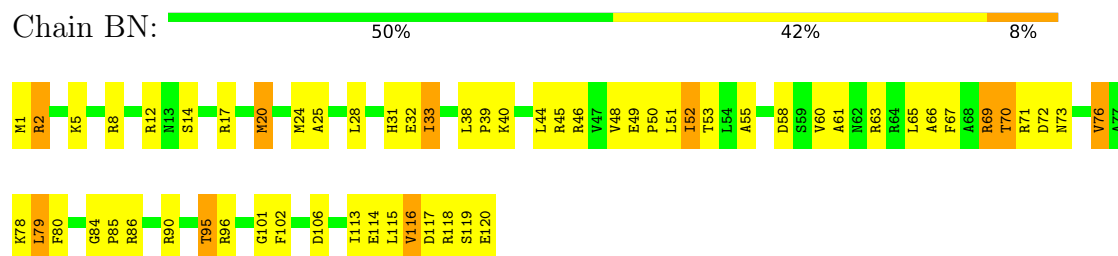
• Molecule 34: 50S ribosomal protein L16



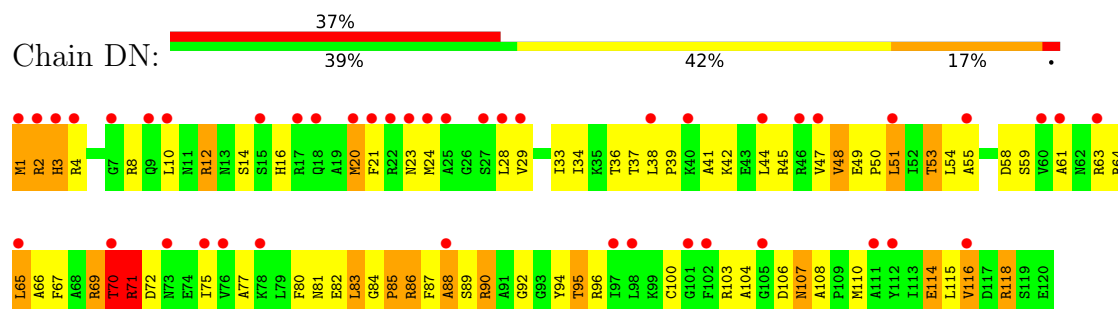
• Molecule 34: 50S ribosomal protein L16



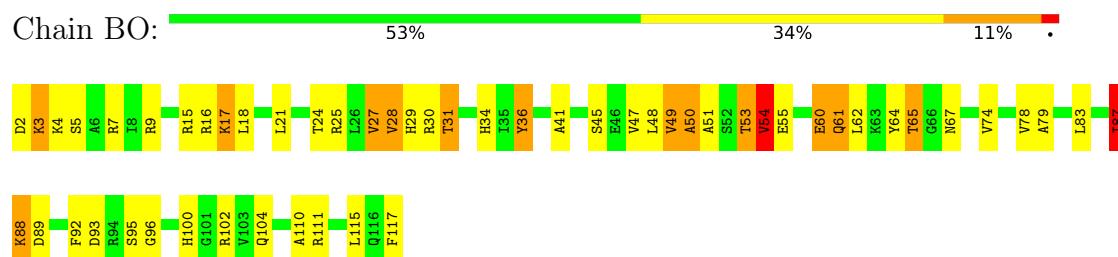
- Molecule 35: 50S ribosomal protein L17



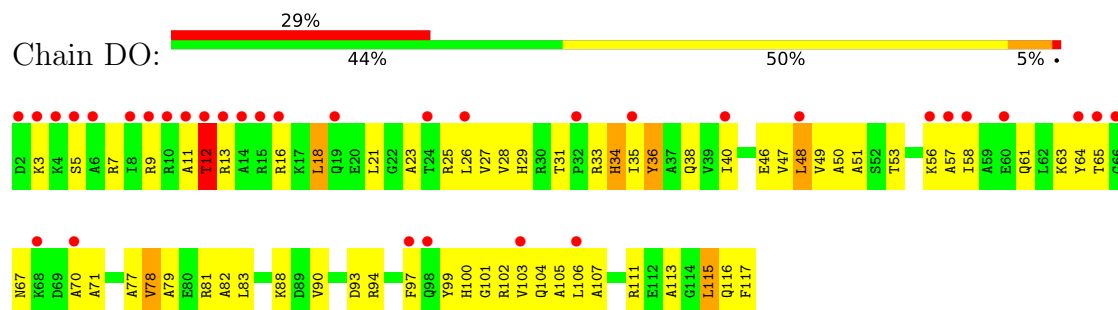
- Molecule 35: 50S ribosomal protein L17



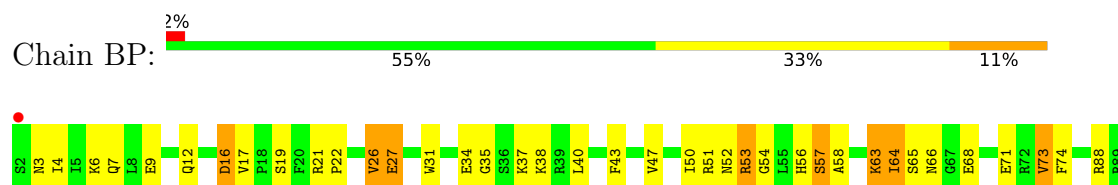
- Molecule 36: 50S ribosomal protein L18



- Molecule 36: 50S ribosomal protein L18



- Molecule 37: 50S ribosomal protein L19





- Molecule 37: 50S ribosomal protein L19



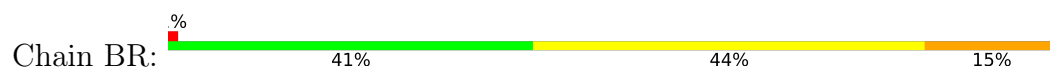
- Molecule 38: 50S ribosomal protein L20



- Molecule 38: 50S ribosomal protein L20

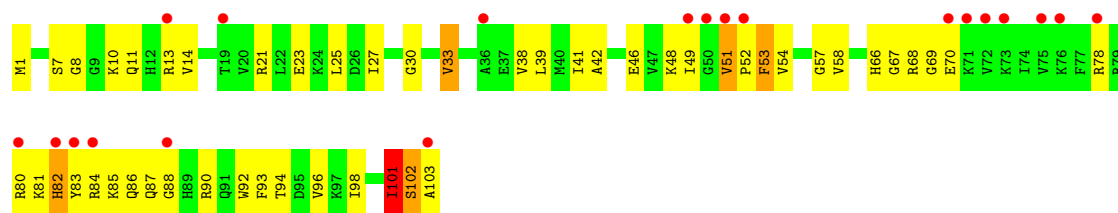


- Molecule 39: 50S ribosomal protein L21

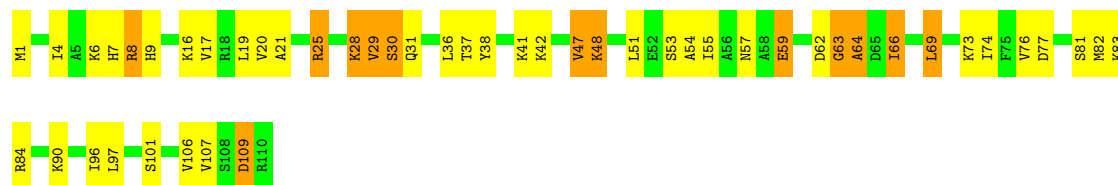


- Molecule 39: 50S ribosomal protein L21

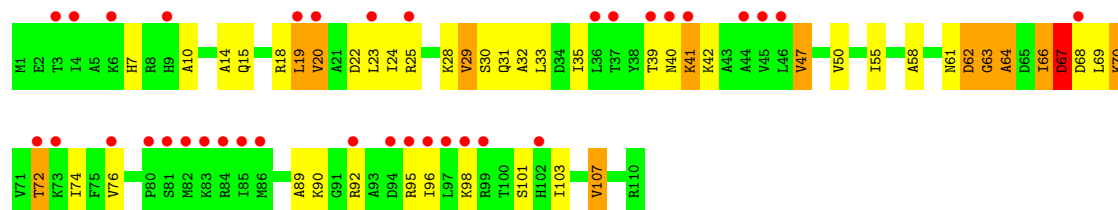




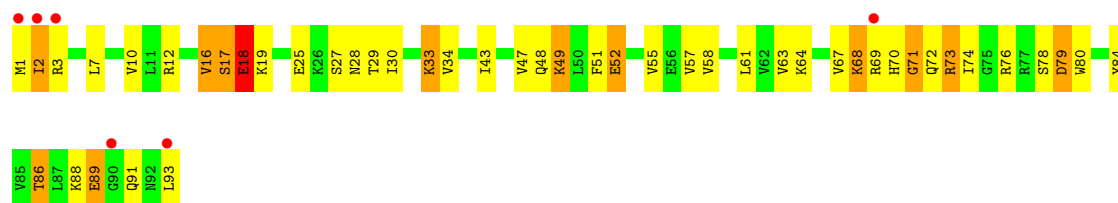
• Molecule 40: 50S ribosomal protein L22



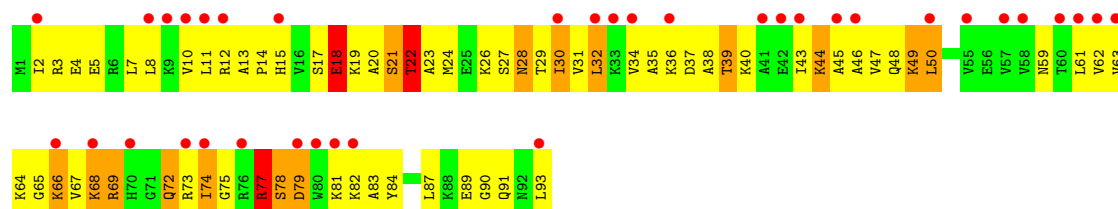
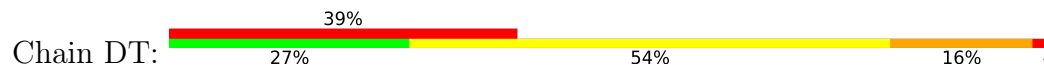
• Molecule 40: 50S ribosomal protein L22



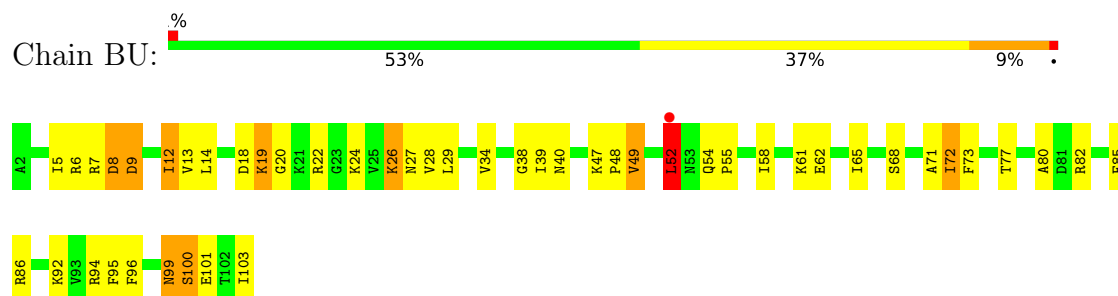
• Molecule 41: 50S ribosomal protein L23



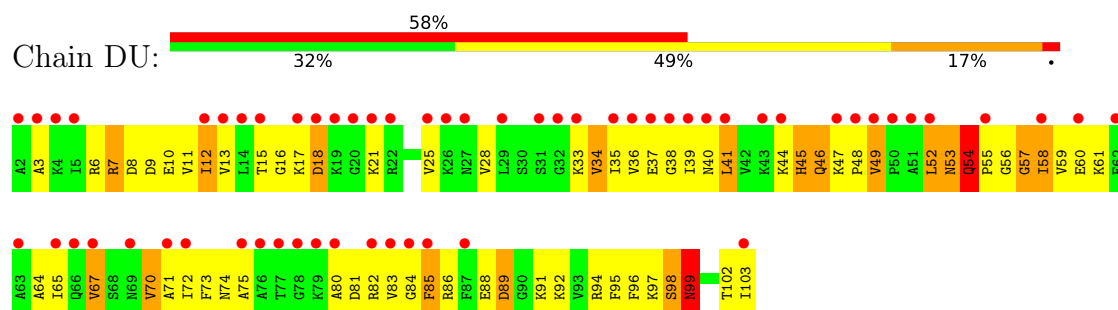
• Molecule 41: 50S ribosomal protein L23



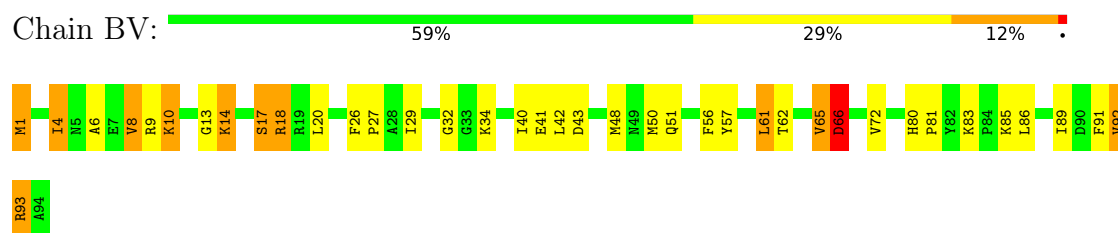
- Molecule 42: 50S ribosomal protein L24



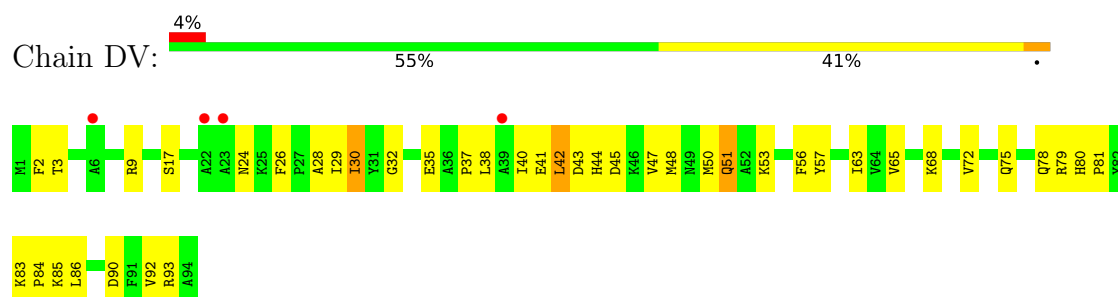
- Molecule 42: 50S ribosomal protein L24



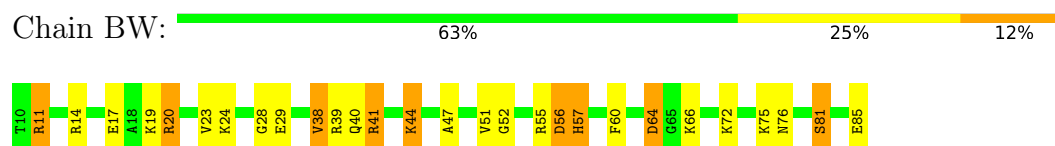
- Molecule 43: 50S ribosomal protein L25



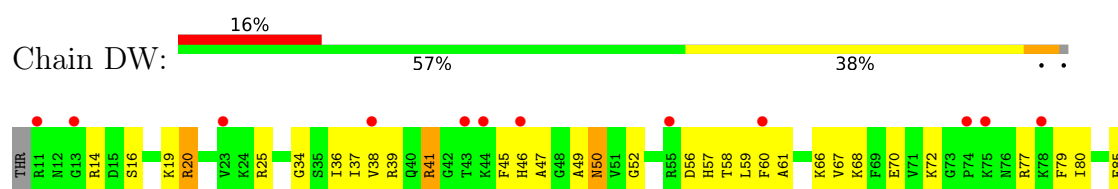
- Molecule 43: 50S ribosomal protein L25



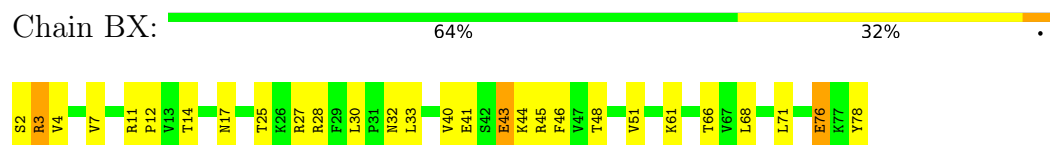
- Molecule 44: 50S ribosomal protein L27



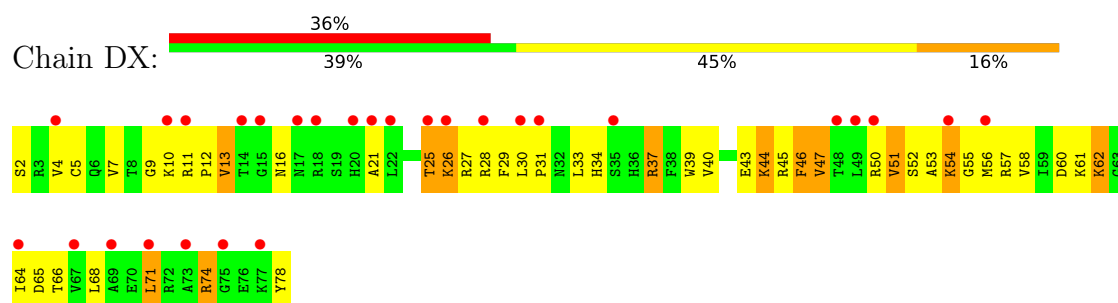
- Molecule 44: 50S ribosomal protein L27



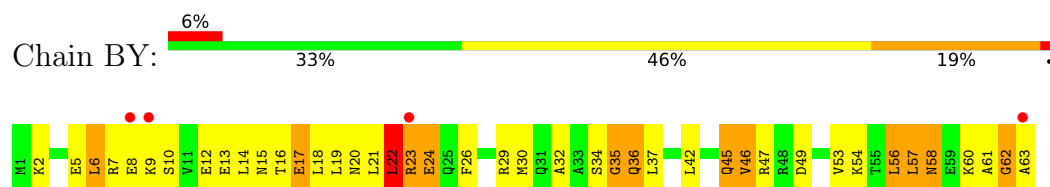
- Molecule 45: 50S ribosomal protein L28



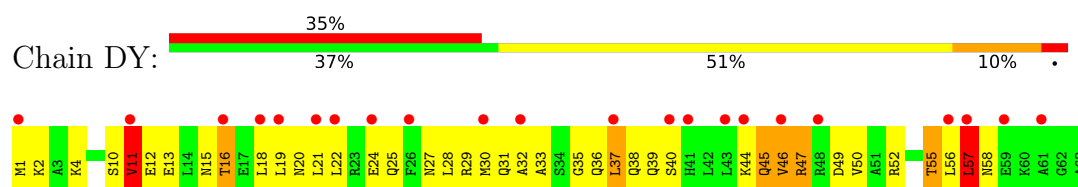
- Molecule 45: 50S ribosomal protein L28



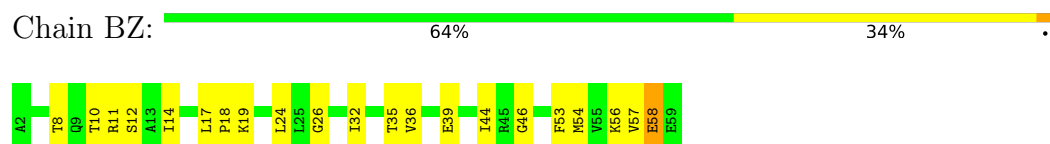
- Molecule 46: 50S ribosomal protein L29



- Molecule 46: 50S ribosomal protein L29

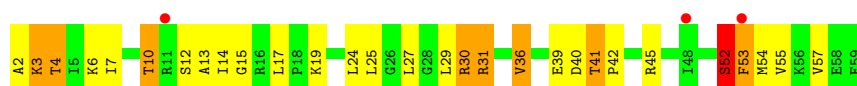


- Molecule 47: 50S ribosomal protein L30

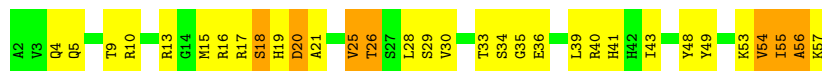


- Molecule 47: 50S ribosomal protein L30

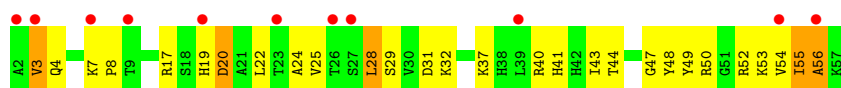




- Molecule 48: 50S ribosomal protein L32



- Molecule 48: 50S ribosomal protein L32



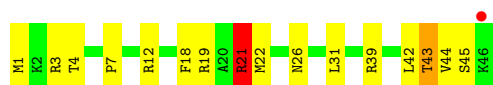
- Molecule 49: 50S ribosomal protein L33



- Molecule 49: 50S ribosomal protein L33



- Molecule 50: 50S ribosomal protein L34

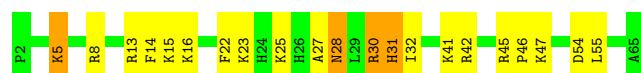


- Molecule 50: 50S ribosomal protein L34



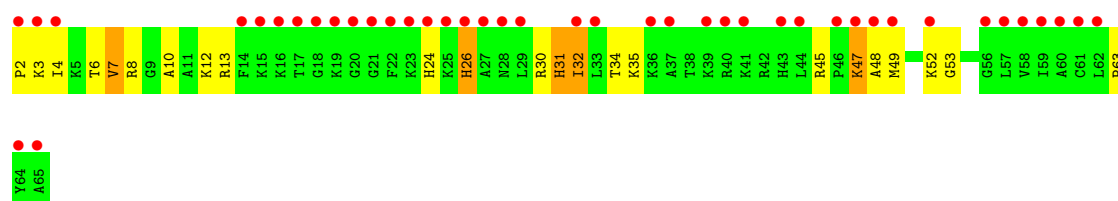
- Molecule 51: 50S ribosomal protein L35

Chain B3: 



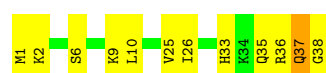
- Molecule 51: 50S ribosomal protein L35

Chain D3: 



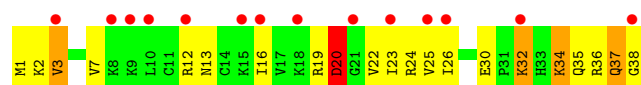
- Molecule 52: 50S ribosomal protein L36

Chain B4: 

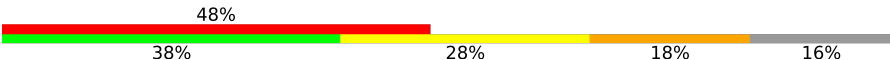


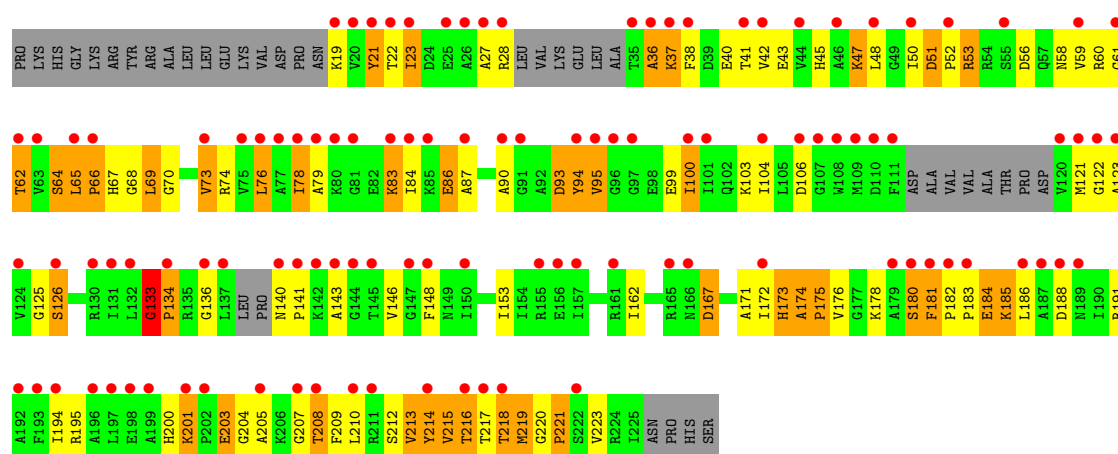
- Molecule 52: 50S ribosomal protein L36

Chain D4: 

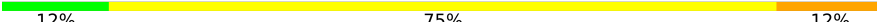


- Molecule 53: 50S ribosomal protein L1

Chain B5: 



- Molecule 54: Quinupristin

Chain B6:  12% 75% 12%



● Molecule 54: Quinupristin

Chain D6:  12% 38% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.26Å 432.34Å 621.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.08 – 2.80 69.08 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.1 (69.08-2.80) 94.1 (69.08-2.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1160)	Depositor
R, R_{free}	0.225 , 0.271 0.228 , 0.273	Depositor DCC
R_{free} test set	5217 reflections (0.40%)	wwPDB-VP
Wilson B-factor (Å ²)	48.8	Xtriage
Anisotropy	0.379	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 47.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	288423	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 1.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: DOL, MG, MHU, MHW, ZN, MHT, 004, DBB, MHV

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	0.19	0/36944	0.37	0/57632
1	CA	0.16	0/36966	0.34	0/57666
2	AB	0.38	0/1736	0.87	4/2338 (0.2%)
2	CB	0.36	0/1736	0.81	1/2338 (0.0%)
3	AC	0.36	0/1652	0.80	2/2225 (0.1%)
3	CC	0.34	0/1652	0.73	0/2225
4	AD	0.35	0/1665	0.80	1/2227 (0.0%)
4	CD	0.39	0/1665	0.79	1/2227 (0.0%)
5	AE	0.42	0/1119	0.86	1/1504 (0.1%)
5	CE	0.40	0/1119	0.85	1/1504 (0.1%)
6	AF	0.40	0/836	0.79	0/1128
6	CF	0.35	0/836	0.76	0/1128
7	AG	0.35	0/1196	0.80	2/1602 (0.1%)
7	CG	0.35	0/1196	0.80	1/1602 (0.1%)
8	AH	0.38	0/989	0.81	0/1326
8	CH	0.31	0/989	0.73	0/1326
9	AI	0.33	0/1034	0.77	0/1375
9	CI	0.32	0/1034	0.78	0/1375
10	AJ	0.40	0/797	0.75	0/1077
10	CJ	0.37	0/797	0.80	0/1077
11	AK	0.38	0/893	0.78	0/1205
11	CK	0.35	0/893	0.83	1/1205 (0.1%)
12	AL	0.39	0/969	0.82	1/1300 (0.1%)
12	CL	0.38	0/969	0.83	0/1300
13	AM	0.39	0/893	0.82	0/1193
13	CM	0.36	0/893	0.77	0/1193
14	AN	0.37	0/785	0.85	2/1043 (0.2%)
14	CN	0.32	0/785	0.74	0/1043
15	AO	0.36	0/718	0.75	0/959
15	CO	0.32	0/718	0.70	0/959
16	AP	0.39	0/659	0.84	2/884 (0.2%)
16	CP	0.34	0/659	0.76	0/884

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.39	0/658	0.77	0/881
17	CQ	0.37	0/658	0.73	0/881
18	AR	0.37	0/463	0.78	1/621 (0.2%)
18	CR	0.36	0/463	0.72	0/621
19	AS	0.36	0/653	0.86	2/877 (0.2%)
19	CS	0.40	0/653	0.84	0/877
20	AT	0.39	0/671	0.81	1/888 (0.1%)
20	CT	0.35	0/671	0.80	1/888 (0.1%)
21	AU	0.46	0/431	0.90	1/570 (0.2%)
21	CU	0.39	0/431	0.78	0/570
22	BA	0.32	0/69659	0.49	0/108672
22	DA	0.15	0/69659	0.33	0/108672
23	BB	0.28	0/2850	0.45	0/4444
23	DB	0.12	0/2828	0.27	0/4410
24	BC	0.49	0/2122	0.90	2/2852 (0.1%)
24	DC	0.34	0/2122	0.77	2/2852 (0.1%)
25	BD	0.55	0/1586	0.95	3/2134 (0.1%)
25	DD	0.33	0/1586	0.77	2/2134 (0.1%)
26	BE	0.51	0/1571	0.86	3/2113 (0.1%)
26	DE	0.36	0/1571	0.80	2/2113 (0.1%)
27	BF	0.38	0/1435	0.78	0/1926
27	DF	0.32	0/1435	0.78	3/1926 (0.2%)
28	BG	0.38	0/1343	0.84	1/1816 (0.1%)
28	DG	0.34	0/1343	0.77	2/1816 (0.1%)
29	BH	0.48	0/1121	0.99	5/1515 (0.3%)
29	DH	0.47	0/1121	0.92	5/1515 (0.3%)
30	BI	0.44	0/1046	0.88	2/1410 (0.1%)
30	DI	0.44	0/1046	0.87	0/1410
31	BJ	0.55	0/1152	0.86	3/1551 (0.2%)
31	DJ	0.34	0/1152	0.78	0/1551
32	BK	0.51	0/948	0.90	0/1268
32	DK	0.34	0/948	0.81	4/1268 (0.3%)
33	BL	0.50	0/1054	0.90	1/1403 (0.1%)
33	DL	0.36	0/1054	0.77	1/1403 (0.1%)
34	BM	0.54	0/1093	0.87	0/1460
34	DM	0.32	0/1093	0.72	0/1460
35	BN	0.62	0/974	0.97	2/1301 (0.2%)
35	DN	0.34	0/974	0.75	1/1301 (0.1%)
36	BO	0.45	0/902	0.86	2/1209 (0.2%)
36	DO	0.34	0/902	0.73	0/1209
37	BP	0.52	0/929	0.85	1/1242 (0.1%)
37	DP	0.33	0/929	0.70	0/1242
38	BQ	0.60	0/960	0.94	0/1278

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DQ	0.33	0/960	0.73	0/1278
39	BR	0.59	0/829	1.02	3/1107 (0.3%)
39	DR	0.29	0/829	0.74	2/1107 (0.2%)
40	BS	0.63	0/864	0.83	0/1156
40	DS	0.37	0/864	0.80	0/1156
41	BT	0.44	0/745	0.81	0/994
41	DT	0.34	0/745	0.71	0/994
42	BU	0.44	0/788	0.80	0/1051
42	DU	0.38	0/788	0.82	0/1051
43	BV	0.47	0/766	0.86	0/1025
43	DV	0.32	0/766	0.70	0/1025
44	BW	0.54	0/587	0.89	1/776 (0.1%)
44	DW	0.27	0/576	0.73	0/762
45	BX	0.44	0/635	0.80	0/848
45	DX	0.36	0/635	0.85	2/848 (0.2%)
46	BY	0.41	0/510	0.89	2/677 (0.3%)
46	DY	0.30	0/510	0.75	0/677
47	BZ	0.58	0/453	0.88	0/605
47	DZ	0.36	0/453	0.77	0/605
48	B0	0.58	0/450	0.94	3/599 (0.5%)
48	D0	0.34	0/450	0.73	0/599
49	B1	0.42	0/417	0.84	2/554 (0.4%)
49	D1	0.35	0/417	0.67	0/554
50	B2	0.55	0/380	1.00	1/498 (0.2%)
50	D2	0.35	0/380	0.85	0/498
51	B3	0.51	0/513	0.86	0/676
51	D3	0.32	0/513	0.69	0/676
52	B4	0.54	0/303	0.93	0/397
52	D4	0.32	0/303	0.73	0/397
53	B5	0.41	0/1145	1.13	13/1556 (0.8%)
54	B6	1.96	0/13	2.89	2/15 (13.3%)
54	D6	1.58	0/13	2.27	1/15 (6.7%)
All	All	0.29	0/310652	0.54	105/464396 (0.0%)

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
6	CF	0	1
11	AK	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
12	CL	0	2
25	BD	0	1
25	DD	0	1
All	All	0	6

There are no bond length outliers.

The worst 5 of 105 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BD	151	THR	CA-C-N	12.47	135.43	119.84
25	BD	151	THR	C-N-CA	12.47	135.43	119.84
53	B5	133	GLY	CA-C-N	10.66	133.16	119.84
53	B5	133	GLY	C-N-CA	10.66	133.16	119.84
53	B5	220	GLY	CA-C-N	10.66	133.16	119.84

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	AK	126	LYS	Peptide
25	BD	151	THR	Peptide
6	CF	54	LEU	Peptide
12	CL	23	ALA	Peptide
12	CL	24	LEU	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32995	0	16607	964	0
1	CA	33015	0	16617	1120	1
2	AB	1705	0	1732	183	0
2	CB	1705	0	1732	147	0
3	AC	1625	0	1696	83	0
3	CC	1625	0	1696	77	0
4	AD	1643	0	1707	131	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	CD	1643	0	1707	126	0
5	AE	1106	0	1148	96	0
5	CE	1106	0	1148	113	0
6	AF	818	0	808	50	0
6	CF	818	0	808	64	0
7	AG	1182	0	1238	64	0
7	CG	1182	0	1238	69	0
8	AH	979	0	1031	56	0
8	CH	979	0	1031	62	0
9	AI	1022	0	1070	94	0
9	CI	1022	0	1070	72	0
10	AJ	787	0	828	84	0
10	CJ	787	0	828	60	0
11	AK	877	0	887	73	0
11	CK	877	0	887	58	0
12	AL	955	0	1016	49	0
12	CL	955	0	1016	81	0
13	AM	884	0	941	47	0
13	CM	884	0	941	51	0
14	AN	774	0	824	62	0
14	CN	774	0	824	54	0
15	AO	710	0	728	34	0
15	CO	710	0	728	34	0
16	AP	649	0	666	58	0
16	CP	649	0	666	37	0
17	AQ	649	0	691	64	0
17	CQ	649	0	691	57	0
18	AR	456	0	478	18	0
18	CR	456	0	478	27	0
19	AS	638	0	665	39	0
19	CS	638	0	665	43	0
20	AT	665	0	714	66	0
20	CT	665	0	714	48	0
21	AU	426	0	449	56	0
21	CU	426	0	449	58	0
22	BA	62195	0	31280	1494	0
22	DA	62195	0	31280	2454	1
23	BB	2549	0	1291	38	0
23	DB	2529	0	1281	67	0
24	BC	2083	0	2154	111	0
24	DC	2083	0	2154	131	0
25	BD	1565	0	1616	71	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	DD	1565	0	1616	101	0
26	BE	1552	0	1619	72	0
26	DE	1552	0	1619	98	0
27	BF	1411	0	1444	88	0
27	DF	1411	0	1444	59	0
28	BG	1323	0	1371	43	0
28	DG	1323	0	1371	47	0
29	BH	1110	0	1147	146	0
29	DH	1110	0	1148	93	0
30	BI	1032	0	1085	78	0
30	DI	1032	0	1085	86	0
31	BJ	1129	0	1162	49	0
31	DJ	1129	0	1162	64	0
32	BK	939	0	1012	50	0
32	DK	939	0	1012	57	0
33	BL	1045	0	1117	60	0
33	DL	1045	0	1117	80	0
34	BM	1074	0	1157	47	0
34	DM	1074	0	1157	44	0
35	BN	961	0	1000	52	0
35	DN	961	0	1000	73	0
36	BO	892	0	923	42	0
36	DO	892	0	923	46	0
37	BP	917	0	962	46	0
37	DP	917	0	962	42	0
38	BQ	947	0	1019	43	0
38	DQ	947	0	1019	47	0
39	BR	816	0	839	73	0
39	DR	816	0	839	45	0
40	BS	857	0	922	35	0
40	DS	857	0	922	39	0
41	BT	739	0	807	42	0
41	DT	739	0	807	61	0
42	BU	780	0	831	38	0
42	DU	780	0	831	71	0
43	BV	753	0	780	30	0
43	DV	753	0	780	26	0
44	BW	580	0	594	20	0
44	DW	569	0	581	24	0
45	BX	625	0	652	16	0
45	DX	625	0	652	50	0
46	BY	509	0	543	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	DY	509	0	543	30	0
47	BZ	449	0	488	10	0
47	DZ	449	0	488	27	0
48	B0	444	0	458	28	0
48	D0	444	0	458	22	0
49	B1	410	0	440	22	0
49	D1	410	0	440	23	0
50	B2	377	0	418	12	0
50	D2	377	0	418	32	0
51	B3	504	0	572	27	0
51	D3	504	0	572	24	0
52	B4	302	0	340	7	0
52	D4	302	0	340	14	0
53	B5	1142	0	865	71	0
54	B6	73	0	64	3	0
54	D6	73	0	65	12	0
55	AA	71	0	0	0	0
55	AM	1	0	0	0	0
55	BA	194	0	0	0	0
55	BB	4	0	0	0	0
55	BQ	1	0	0	0	0
55	CA	56	0	0	0	0
55	D2	1	0	0	0	0
55	DA	166	0	0	0	0
55	DB	3	0	0	0	0
55	DQ	1	0	0	0	0
56	BA	48	0	50	15	0
56	DA	48	0	50	25	0
57	B4	1	0	0	0	0
57	D4	1	0	0	0	0
58	AA	194	0	0	18	0
58	AE	2	0	0	0	0
58	AL	1	0	0	0	0
58	AN	3	0	0	0	0
58	AT	2	0	0	0	0
58	AU	1	0	0	0	0
58	B3	3	0	0	0	0
58	B4	1	0	0	0	0
58	BA	617	0	0	66	0
58	BB	14	0	0	1	0
58	BC	6	0	0	1	0
58	BD	4	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	BE	1	0	0	0	0
58	BF	1	0	0	1	0
58	BG	1	0	0	1	0
58	BJ	1	0	0	0	0
58	BL	7	0	0	0	0
58	BN	5	0	0	0	0
58	BQ	1	0	0	0	0
58	BS	1	0	0	0	0
58	BT	2	0	0	0	0
58	CA	192	0	0	12	0
58	CL	1	0	0	0	0
58	CN	2	0	0	0	0
58	CT	2	0	0	0	0
58	CU	1	0	0	1	0
58	D2	1	0	0	1	0
58	D3	1	0	0	0	0
58	D4	1	0	0	0	0
58	DA	610	0	0	84	0
58	DB	13	0	0	1	0
58	DC	8	0	0	1	0
58	DD	4	0	0	2	0
58	DE	4	0	0	0	0
58	DJ	1	0	0	0	0
58	DL	4	0	0	1	0
58	DN	2	0	0	0	0
58	DS	2	0	0	0	0
58	DT	3	0	0	1	0
58	DU	1	0	0	0	0
58	DV	1	0	0	0	0
All	All	288423	0	193016	10982	1

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 23.

The worst 5 of 10982 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:117:LEU:O	29:BH:121:VAL:HG23	1.34	1.22
22:BA:730:A:OP2	58:BA:3693:HOH:O	1.58	1.21
1:AA:533:A:OP1	58:AA:1848:HOH:O	1.65	1.15
29:BH:117:LEU:O	29:BH:121:VAL:CG2	1.95	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:2498:C:OP2	58:BA:3684:HOH:O	1.64	1.13

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:204:G:OP1	22:DA:289:G:O2'[3_545]	2.12	0.08

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	216/218 (99%)	126 (58%)	45 (21%)	45 (21%)	0	0
2	CB	216/218 (99%)	140 (65%)	51 (24%)	25 (12%)	0	1
3	AC	204/206 (99%)	148 (72%)	35 (17%)	21 (10%)	0	1
3	CC	204/206 (99%)	154 (76%)	39 (19%)	11 (5%)	1	4
4	AD	203/205 (99%)	137 (68%)	39 (19%)	27 (13%)	0	0
4	CD	203/205 (99%)	152 (75%)	32 (16%)	19 (9%)	0	1
5	AE	148/150 (99%)	102 (69%)	27 (18%)	19 (13%)	0	0
5	CE	148/150 (99%)	100 (68%)	33 (22%)	15 (10%)	0	1
6	AF	98/100 (98%)	73 (74%)	15 (15%)	10 (10%)	0	1
6	CF	98/100 (98%)	68 (69%)	15 (15%)	15 (15%)	0	0
7	AG	149/151 (99%)	107 (72%)	29 (20%)	13 (9%)	0	1
7	CG	149/151 (99%)	119 (80%)	22 (15%)	8 (5%)	1	4
8	AH	127/129 (98%)	90 (71%)	28 (22%)	9 (7%)	1	2
8	CH	127/129 (98%)	98 (77%)	19 (15%)	10 (8%)	1	1
9	AI	125/127 (98%)	87 (70%)	24 (19%)	14 (11%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	CI	125/127 (98%)	89 (71%)	18 (14%)	18 (14%)	0	0
10	AJ	96/98 (98%)	64 (67%)	11 (12%)	21 (22%)	0	0
10	CJ	96/98 (98%)	73 (76%)	11 (12%)	12 (12%)	0	0
11	AK	115/117 (98%)	81 (70%)	17 (15%)	17 (15%)	0	0
11	CK	115/117 (98%)	82 (71%)	24 (21%)	9 (8%)	1	2
12	AL	121/123 (98%)	91 (75%)	21 (17%)	9 (7%)	1	2
12	CL	121/123 (98%)	92 (76%)	18 (15%)	11 (9%)	0	1
13	AM	112/114 (98%)	81 (72%)	21 (19%)	10 (9%)	0	1
13	CM	112/114 (98%)	80 (71%)	18 (16%)	14 (12%)	0	0
14	AN	92/100 (92%)	61 (66%)	21 (23%)	10 (11%)	0	1
14	CN	92/100 (92%)	58 (63%)	20 (22%)	14 (15%)	0	0
15	AO	86/88 (98%)	65 (76%)	14 (16%)	7 (8%)	1	1
15	CO	86/88 (98%)	64 (74%)	17 (20%)	5 (6%)	1	4
16	AP	80/82 (98%)	55 (69%)	15 (19%)	10 (12%)	0	0
16	CP	80/82 (98%)	59 (74%)	13 (16%)	8 (10%)	0	1
17	AQ	78/80 (98%)	53 (68%)	18 (23%)	7 (9%)	0	1
17	CQ	78/80 (98%)	56 (72%)	15 (19%)	7 (9%)	0	1
18	AR	53/55 (96%)	42 (79%)	11 (21%)	0	100	100
18	CR	53/55 (96%)	37 (70%)	12 (23%)	4 (8%)	1	2
19	AS	77/79 (98%)	57 (74%)	11 (14%)	9 (12%)	0	1
19	CS	77/79 (98%)	55 (71%)	11 (14%)	11 (14%)	0	0
20	AT	83/85 (98%)	59 (71%)	19 (23%)	5 (6%)	1	3
20	CT	83/85 (98%)	62 (75%)	12 (14%)	9 (11%)	0	1
21	AU	49/51 (96%)	26 (53%)	8 (16%)	15 (31%)	0	0
21	CU	49/51 (96%)	21 (43%)	16 (33%)	12 (24%)	0	0
24	BC	269/271 (99%)	218 (81%)	39 (14%)	12 (4%)	2	7
24	DC	269/271 (99%)	196 (73%)	48 (18%)	25 (9%)	0	1
25	BD	207/209 (99%)	180 (87%)	21 (10%)	6 (3%)	3	13
25	DD	207/209 (99%)	153 (74%)	43 (21%)	11 (5%)	1	5
26	BE	199/201 (99%)	165 (83%)	30 (15%)	4 (2%)	6	21
26	DE	199/201 (99%)	154 (77%)	27 (14%)	18 (9%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	BF	175/177 (99%)	142 (81%)	24 (14%)	9 (5%)	1	5
27	DF	175/177 (99%)	135 (77%)	27 (15%)	13 (7%)	1	2
28	BG	174/176 (99%)	148 (85%)	16 (9%)	10 (6%)	1	4
28	DG	174/176 (99%)	127 (73%)	36 (21%)	11 (6%)	1	3
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%)	78 (56%)	37 (27%)	24 (17%)	0	0
30	DI	139/141 (99%)	82 (59%)	38 (27%)	19 (14%)	0	0
31	BJ	140/142 (99%)	125 (89%)	14 (10%)	1 (1%)	18	47
31	DJ	140/142 (99%)	104 (74%)	23 (16%)	13 (9%)	0	1
32	BK	120/122 (98%)	97 (81%)	14 (12%)	9 (8%)	1	2
32	DK	120/122 (98%)	95 (79%)	15 (12%)	10 (8%)	0	1
33	BL	141/143 (99%)	112 (79%)	21 (15%)	8 (6%)	1	4
33	DL	141/143 (99%)	98 (70%)	31 (22%)	12 (8%)	0	1
34	BM	134/136 (98%)	120 (90%)	11 (8%)	3 (2%)	5	19
34	DM	134/136 (98%)	112 (84%)	17 (13%)	5 (4%)	2	9
35	BN	118/120 (98%)	95 (80%)	21 (18%)	2 (2%)	7	25
35	DN	118/120 (98%)	90 (76%)	18 (15%)	10 (8%)	0	1
36	BO	114/116 (98%)	96 (84%)	14 (12%)	4 (4%)	3	10
36	DO	114/116 (98%)	82 (72%)	24 (21%)	8 (7%)	1	2
37	BP	112/114 (98%)	99 (88%)	8 (7%)	5 (4%)	2	7
37	DP	112/114 (98%)	88 (79%)	18 (16%)	6 (5%)	1	4
38	BQ	115/117 (98%)	102 (89%)	12 (10%)	1 (1%)	14	41
38	DQ	115/117 (98%)	92 (80%)	22 (19%)	1 (1%)	14	41
39	BR	101/103 (98%)	81 (80%)	10 (10%)	10 (10%)	0	1
39	DR	101/103 (98%)	72 (71%)	23 (23%)	6 (6%)	1	3
40	BS	108/110 (98%)	94 (87%)	10 (9%)	4 (4%)	2	9
40	DS	108/110 (98%)	83 (77%)	17 (16%)	8 (7%)	1	2
41	BT	91/93 (98%)	74 (81%)	9 (10%)	8 (9%)	0	1
41	DT	91/93 (98%)	53 (58%)	28 (31%)	10 (11%)	0	1
42	BU	100/102 (98%)	77 (77%)	19 (19%)	4 (4%)	2	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	DU	100/102 (98%)	69 (69%)	19 (19%)	12 (12%)	0	1
43	BV	92/94 (98%)	84 (91%)	7 (8%)	1 (1%)	11	36
43	DV	92/94 (98%)	76 (83%)	14 (15%)	2 (2%)	5	19
44	BW	74/76 (97%)	68 (92%)	4 (5%)	2 (3%)	4	15
44	DW	73/76 (96%)	61 (84%)	12 (16%)	0	100	100
45	BX	75/77 (97%)	68 (91%)	6 (8%)	1 (1%)	9	31
45	DX	75/77 (97%)	58 (77%)	12 (16%)	5 (7%)	1	3
46	BY	61/63 (97%)	43 (70%)	10 (16%)	8 (13%)	0	0
46	DY	61/63 (97%)	44 (72%)	12 (20%)	5 (8%)	0	1
47	BZ	56/58 (97%)	54 (96%)	2 (4%)	0	100	100
47	DZ	56/58 (97%)	41 (73%)	10 (18%)	5 (9%)	0	1
48	B0	54/56 (96%)	46 (85%)	4 (7%)	4 (7%)	1	2
48	D0	54/56 (96%)	37 (68%)	12 (22%)	5 (9%)	0	1
49	B1	48/50 (96%)	40 (83%)	4 (8%)	4 (8%)	0	1
49	D1	48/50 (96%)	36 (75%)	8 (17%)	4 (8%)	0	1
50	B2	44/46 (96%)	37 (84%)	5 (11%)	2 (4%)	2	7
50	D2	44/46 (96%)	34 (77%)	6 (14%)	4 (9%)	0	1
51	B3	62/64 (97%)	56 (90%)	5 (8%)	1 (2%)	7	27
51	D3	62/64 (97%)	52 (84%)	6 (10%)	4 (6%)	1	3
52	B4	36/38 (95%)	31 (86%)	4 (11%)	1 (3%)	4	14
52	D4	36/38 (95%)	32 (89%)	2 (6%)	2 (6%)	1	4
53	B5	183/228 (80%)	87 (48%)	53 (29%)	43 (24%)	0	0
54	B6	2/8 (25%)	2 (100%)	0	0	100	100
54	D6	2/8 (25%)	0	2 (100%)	0	100	100
All	All	11422/11688 (98%)	8528 (75%)	1918 (17%)	976 (8%)	0	1

5 of 976 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	16	PHE
2	AB	20	THR
2	AB	22	TYR
2	AB	25	PRO
2	AB	34	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	180/180 (100%)	127 (71%)	53 (29%)	0	1
2	CB	180/180 (100%)	128 (71%)	52 (29%)	0	1
3	AC	170/170 (100%)	132 (78%)	38 (22%)	1	3
3	CC	170/170 (100%)	144 (85%)	26 (15%)	3	10
4	AD	172/172 (100%)	135 (78%)	37 (22%)	1	4
4	CD	172/172 (100%)	139 (81%)	33 (19%)	1	5
5	AE	113/113 (100%)	79 (70%)	34 (30%)	0	1
5	CE	113/113 (100%)	79 (70%)	34 (30%)	0	1
6	AF	87/87 (100%)	64 (74%)	23 (26%)	0	2
6	CF	87/87 (100%)	58 (67%)	29 (33%)	0	1
7	AG	124/124 (100%)	100 (81%)	24 (19%)	1	5
7	CG	124/124 (100%)	100 (81%)	24 (19%)	1	5
8	AH	104/104 (100%)	79 (76%)	25 (24%)	1	2
8	CH	104/104 (100%)	78 (75%)	26 (25%)	0	2
9	AI	105/105 (100%)	73 (70%)	32 (30%)	0	1
9	CI	105/105 (100%)	91 (87%)	14 (13%)	4	14
10	AJ	86/86 (100%)	64 (74%)	22 (26%)	0	2
10	CJ	86/86 (100%)	65 (76%)	21 (24%)	1	2
11	AK	90/90 (100%)	75 (83%)	15 (17%)	2	8
11	CK	90/90 (100%)	72 (80%)	18 (20%)	1	4
12	AL	103/103 (100%)	86 (84%)	17 (16%)	2	8
12	CL	103/103 (100%)	81 (79%)	22 (21%)	1	4
13	AM	92/92 (100%)	70 (76%)	22 (24%)	1	3
13	CM	92/92 (100%)	73 (79%)	19 (21%)	1	4
14	AN	79/83 (95%)	61 (77%)	18 (23%)	1	3
14	CN	79/83 (95%)	67 (85%)	12 (15%)	3	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	AO	75/76 (99%)	64 (85%)	11 (15%)	3	10
15	CO	75/76 (99%)	65 (87%)	10 (13%)	4	14
16	AP	65/65 (100%)	45 (69%)	20 (31%)	0	1
16	CP	65/65 (100%)	53 (82%)	12 (18%)	1	6
17	AQ	74/74 (100%)	46 (62%)	28 (38%)	0	0
17	CQ	74/74 (100%)	51 (69%)	23 (31%)	0	1
18	AR	48/48 (100%)	38 (79%)	10 (21%)	1	4
18	CR	48/48 (100%)	37 (77%)	11 (23%)	1	3
19	AS	70/70 (100%)	56 (80%)	14 (20%)	1	4
19	CS	70/70 (100%)	55 (79%)	15 (21%)	1	4
20	AT	65/65 (100%)	48 (74%)	17 (26%)	0	2
20	CT	65/65 (100%)	52 (80%)	13 (20%)	1	4
21	AU	44/44 (100%)	27 (61%)	17 (39%)	0	0
21	CU	44/44 (100%)	28 (64%)	16 (36%)	0	0
24	BC	216/216 (100%)	182 (84%)	34 (16%)	2	9
24	DC	216/216 (100%)	189 (88%)	27 (12%)	4	15
25	BD	164/164 (100%)	143 (87%)	21 (13%)	4	15
25	DD	164/164 (100%)	137 (84%)	27 (16%)	2	8
26	BE	165/165 (100%)	129 (78%)	36 (22%)	1	3
26	DE	165/165 (100%)	133 (81%)	32 (19%)	1	5
27	BF	148/148 (100%)	112 (76%)	36 (24%)	1	2
27	DF	148/148 (100%)	118 (80%)	30 (20%)	1	4
28	BG	137/137 (100%)	115 (84%)	22 (16%)	2	8
28	DG	137/137 (100%)	107 (78%)	30 (22%)	1	3
29	BH	114/114 (100%)	81 (71%)	33 (29%)	0	1
29	DH	114/114 (100%)	89 (78%)	25 (22%)	1	3
30	BI	109/109 (100%)	82 (75%)	27 (25%)	1	2
30	DI	109/109 (100%)	77 (71%)	32 (29%)	0	1
31	BJ	116/116 (100%)	100 (86%)	16 (14%)	3	12
31	DJ	116/116 (100%)	99 (85%)	17 (15%)	3	10
32	BK	103/103 (100%)	87 (84%)	16 (16%)	2	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	DK	103/103 (100%)	90 (87%)	13 (13%)	4	15
33	BL	102/102 (100%)	92 (90%)	10 (10%)	7	25
33	DL	102/102 (100%)	84 (82%)	18 (18%)	2	7
34	BM	109/109 (100%)	96 (88%)	13 (12%)	5	17
34	DM	109/109 (100%)	97 (89%)	12 (11%)	6	20
35	BN	100/100 (100%)	90 (90%)	10 (10%)	7	24
35	DN	100/100 (100%)	77 (77%)	23 (23%)	1	3
36	BO	86/86 (100%)	65 (76%)	21 (24%)	1	2
36	DO	86/86 (100%)	69 (80%)	17 (20%)	1	5
37	BP	99/99 (100%)	81 (82%)	18 (18%)	2	6
37	DP	99/99 (100%)	89 (90%)	10 (10%)	7	23
38	BQ	89/89 (100%)	79 (89%)	10 (11%)	6	19
38	DQ	89/89 (100%)	75 (84%)	14 (16%)	2	9
39	BR	84/84 (100%)	70 (83%)	14 (17%)	2	8
39	DR	84/84 (100%)	77 (92%)	7 (8%)	10	32
40	BS	93/93 (100%)	74 (80%)	19 (20%)	1	4
40	DS	93/93 (100%)	81 (87%)	12 (13%)	4	14
41	BT	80/80 (100%)	66 (82%)	14 (18%)	2	7
41	DT	80/80 (100%)	64 (80%)	16 (20%)	1	4
42	BU	83/83 (100%)	67 (81%)	16 (19%)	1	5
42	DU	83/83 (100%)	67 (81%)	16 (19%)	1	5
43	BV	78/78 (100%)	59 (76%)	19 (24%)	1	2
43	DV	78/78 (100%)	67 (86%)	11 (14%)	3	12
44	BW	57/58 (98%)	46 (81%)	11 (19%)	1	5
44	DW	56/58 (97%)	49 (88%)	7 (12%)	4	15
45	BX	67/67 (100%)	60 (90%)	7 (10%)	7	22
45	DX	67/67 (100%)	55 (82%)	12 (18%)	2	6
46	BY	55/55 (100%)	48 (87%)	7 (13%)	4	15
46	DY	55/55 (100%)	44 (80%)	11 (20%)	1	4
47	BZ	48/48 (100%)	41 (85%)	7 (15%)	3	11
47	DZ	48/48 (100%)	36 (75%)	12 (25%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	B0	47/47 (100%)	41 (87%)	6 (13%)	4	15
48	D0	47/47 (100%)	41 (87%)	6 (13%)	4	15
49	B1	45/45 (100%)	41 (91%)	4 (9%)	9	29
49	D1	45/45 (100%)	37 (82%)	8 (18%)	2	6
50	B2	38/38 (100%)	34 (90%)	4 (10%)	6	22
50	D2	38/38 (100%)	30 (79%)	8 (21%)	1	4
51	B3	51/51 (100%)	45 (88%)	6 (12%)	5	17
51	D3	51/51 (100%)	46 (90%)	5 (10%)	7	25
52	B4	34/34 (100%)	30 (88%)	4 (12%)	5	17
52	D4	34/34 (100%)	25 (74%)	9 (26%)	0	2
53	B5	61/180 (34%)	46 (75%)	15 (25%)	1	2
54	B6	2/2 (100%)	2 (100%)	0	100	100
54	D6	2/2 (100%)	2 (100%)	0	100	100
All	All	9390/9522 (99%)	7540 (80%)	1850 (20%)	1	5

5 of 1850 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
50	B2	43	THR
44	DW	39	ARG
7	CG	126	ASP
42	DU	67	VAL
31	DJ	101	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 99 such sidechains are listed below:

Mol	Chain	Res	Type
17	CQ	51	ASN
29	DH	20	ASN
18	CR	74	HIS
24	DC	251	GLN
31	DJ	130	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1537/1539 (99%)	324 (21%)	11 (0%)
1	CA	1538/1539 (99%)	342 (22%)	10 (0%)
22	BA	2895/2903 (99%)	580 (20%)	24 (0%)
22	DA	2895/2903 (99%)	704 (24%)	32 (1%)
23	BB	118/119 (99%)	16 (13%)	0
23	DB	117/119 (98%)	20 (17%)	0
All	All	9100/9122 (99%)	1986 (21%)	77 (0%)

5 of 1986 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	3	A
1	AA	4	U
1	AA	5	U
1	AA	6	G
1	AA	9	G

5 of 77 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	DA	1514	G
22	DA	2326	C
22	DA	1847	A
22	DA	2157	G
22	DA	2756	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
54	MHV	D6	6	54	7,9,10	1.20	0	8,11,13	2.99	3 (37%)
54	MHW	B6	1	54	9,9,10	1.63	1 (11%)	10,11,13	2.89	5 (50%)
54	DBB	B6	3	54	4,5,6	1.37	0	1,5,7	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	DBB	D6	3	54	4,5,6	1.23	0	1,5,7	0.34	0
54	004	D6	7	54	9,10,11	0.82	0	9,12,14	0.69	0
54	004	B6	7	54	9,10,11	1.62	1 (11%)	9,12,14	1.68	2 (22%)
54	MHU	B6	5	54	14,15,16	1.86	3 (21%)	18,19,21	1.31	3 (16%)
54	MHU	D6	5	54	14,15,16	1.68	3 (21%)	18,19,21	1.17	2 (11%)
54	MHW	D6	1	54	9,9,10	1.92	1 (11%)	10,11,13	2.93	3 (30%)
54	MHV	B6	6	54	7,9,10	1.63	1 (14%)	8,11,13	3.21	5 (62%)

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
54	MHV	D6	6	54	-	0/1/12/14	0/1/1/1
54	MHW	B6	1	54	-	0/2/2/4	0/1/1/1
54	DBB	B6	3	54	-	1/3/4/6	-
54	DBB	D6	3	54	-	0/3/4/6	-
54	004	D6	7	54	-	0/4/6/8	0/1/1/1
54	004	B6	7	54	-	0/4/6/8	0/1/1/1
54	MHU	B6	5	54	-	0/9/12/14	0/1/1/1
54	MHU	D6	5	54	-	0/9/12/14	0/1/1/1
54	MHW	D6	1	54	-	0/2/2/4	0/1/1/1
54	MHV	B6	6	54	-	0/1/12/14	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	B6	5	MHU	CZ-NZ	5.24	1.49	1.37
54	D6	1	MHW	CA-C	5.01	1.54	1.48
54	D6	5	MHU	CZ-NZ	4.71	1.48	1.37
54	B6	7	004	CB-CA	-4.57	1.48	1.52
54	B6	1	MHW	CA-C	3.81	1.52	1.48

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	D6	1	MHW	CD-CE-N	6.77	134.13	123.42
54	B6	1	MHW	CD-CE-N	6.08	133.04	123.42
54	B6	6	MHV	CD2-CG-CB	5.42	124.11	115.89
54	D6	6	MHV	CD2-CE-N	-5.25	98.62	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	D6	6	MHV	CD2-CG-CB	5.04	123.53	115.89

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	B6	3	DBB	N-CA-CB-CG

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	D6	6	MHV	1	0
54	D6	3	DBB	1	0
54	D6	7	004	4	0
54	B6	7	004	1	0
54	D6	5	MHU	3	0
54	D6	1	MHW	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	$\# Z > 2$
56	DOL	BA	3001	-	47,50,50	3.24	17 (36%)	57,70,70	2.83	18 (31%)
56	DOL	DA	3001	-	47,50,50	3.30	17 (36%)	57,70,70	2.90	17 (29%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	DOL	BA	3001	-	-	17/64/77/77	0/2/3/3
56	DOL	DA	3001	-	-	13/64/77/77	0/2/3/3

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	DA	3001	DOL	C10-N9	9.53	1.39	1.29
56	BA	3001	DOL	C10-N9	9.35	1.39	1.29
56	DA	3001	DOL	O15-C14	9.00	1.37	1.21
56	BA	3001	DOL	O15-C14	8.64	1.36	1.21
56	DA	3001	DOL	C6-N5	8.00	1.46	1.34

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	DA	3001	DOL	O40-S39-O41	-15.48	100.57	118.13
56	BA	3001	DOL	O40-S39-O41	-14.69	101.47	118.13
56	DA	3001	DOL	O11-C10-C13	6.54	123.74	117.70
56	BA	3001	DOL	C29-C28-C26	-6.27	107.93	122.67
56	BA	3001	DOL	O11-C10-C13	5.78	123.05	117.70

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

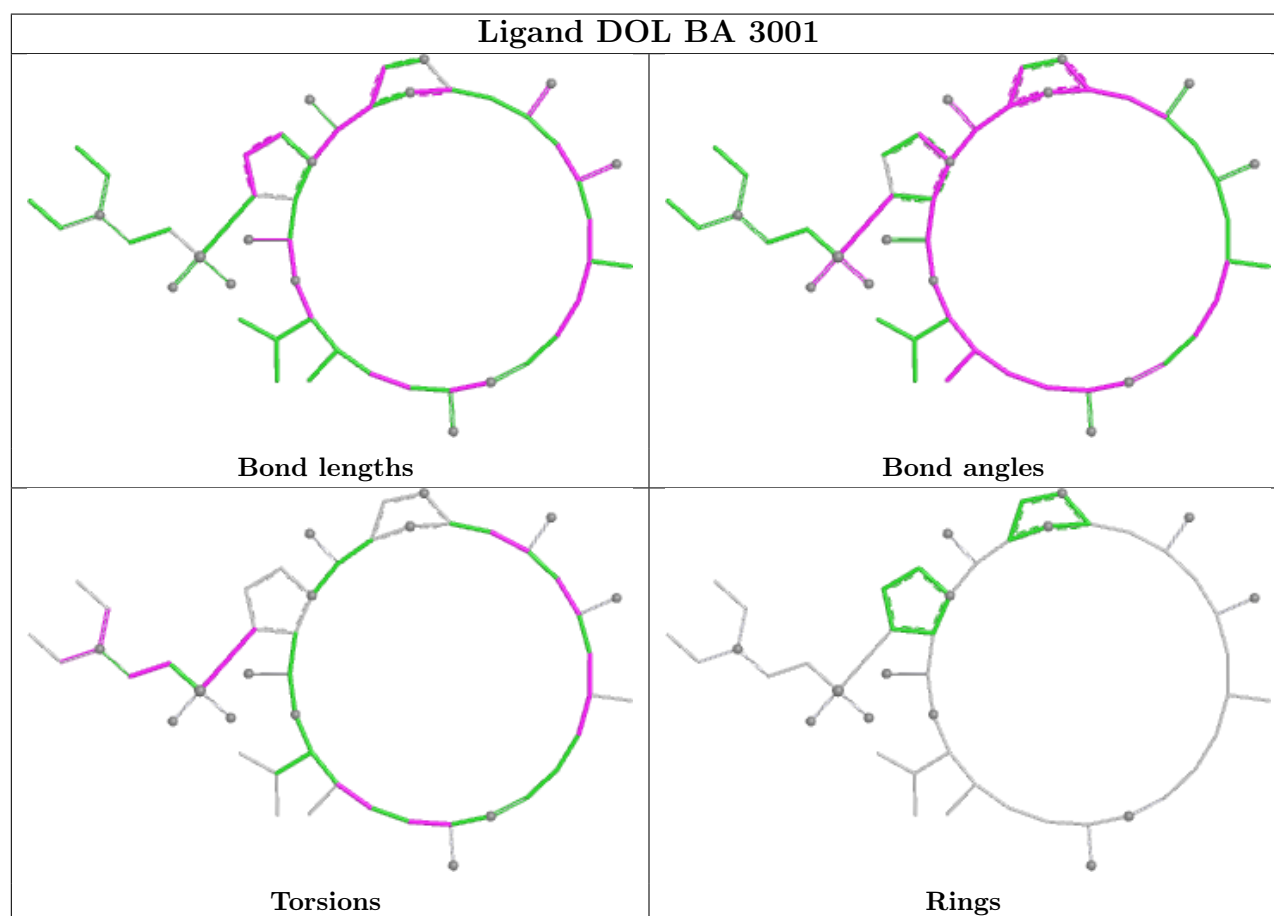
Mol	Chain	Res	Type	Atoms
56	BA	3001	DOL	C1-C2-S39-O40
56	BA	3001	DOL	C1-C2-S39-C42
56	BA	3001	DOL	S39-C42-C43-N44
56	BA	3001	DOL	C14-C16-C17-O18
56	BA	3001	DOL	C21-C20-C22-C23

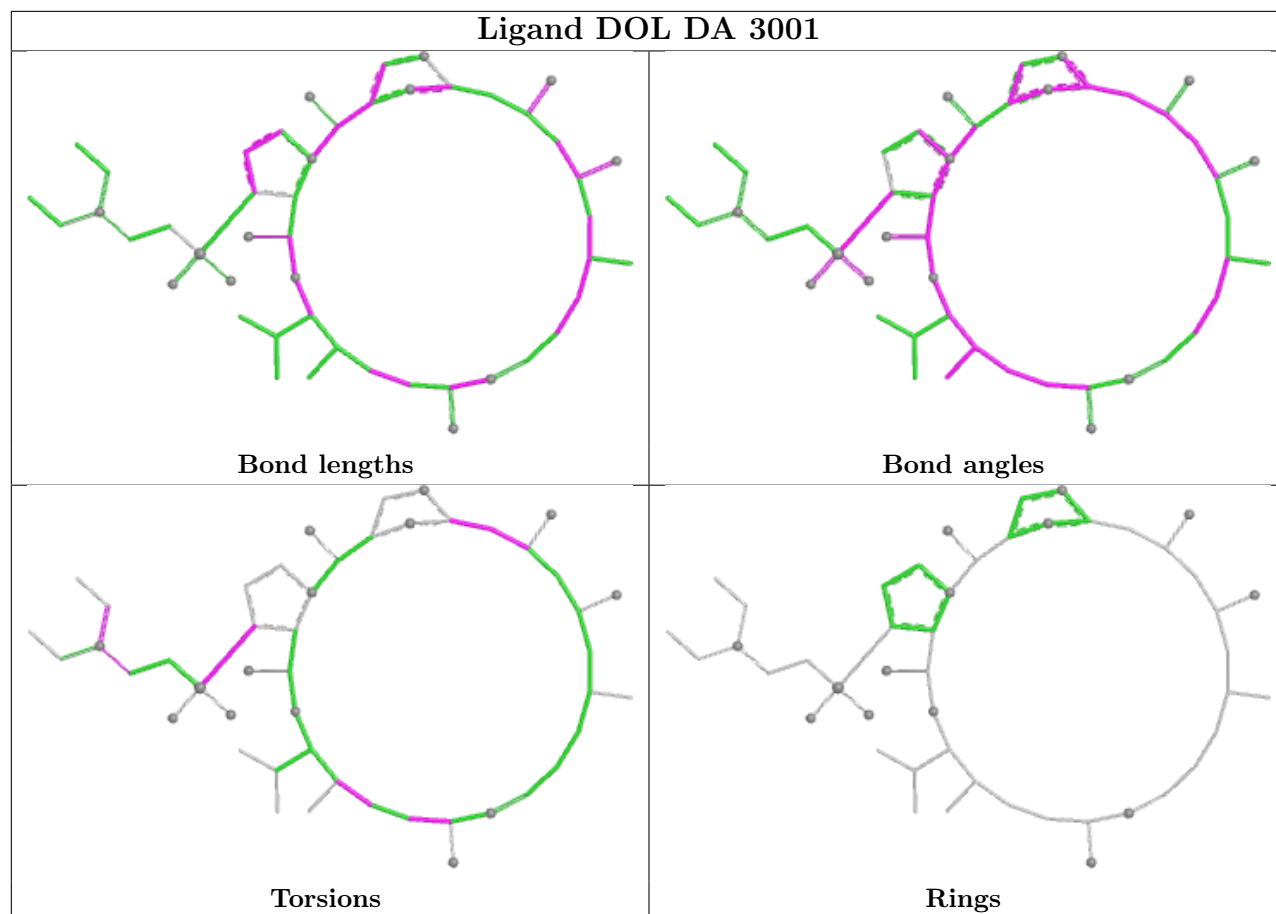
There are no ring outliers.

2 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	BA	3001	DOL	15	0
56	DA	3001	DOL	25	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 than 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.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1538/1539 (99%)	-0.18	18 (1%) 76 68	10, 49, 132, 182	0
1	CA	1539/1539 (100%)	0.34	52 (3%) 48 39	22, 70, 146, 178	0
2	AB	218/218 (100%)	0.74	14 (6%) 25 18	36, 73, 100, 117	0
2	CB	218/218 (100%)	1.00	30 (13%) 6 5	57, 86, 108, 121	0
3	AC	206/206 (100%)	0.26	6 (2%) 53 43	33, 57, 78, 95	0
3	CC	206/206 (100%)	0.70	10 (4%) 35 27	55, 80, 96, 107	0
4	AD	205/205 (100%)	0.49	14 (6%) 23 17	31, 56, 79, 99	0
4	CD	205/205 (100%)	0.06	6 (2%) 53 43	13, 35, 60, 82	0
5	AE	150/150 (100%)	0.38	8 (5%) 32 24	26, 47, 78, 93	0
5	CE	150/150 (100%)	0.38	5 (3%) 49 39	25, 52, 84, 104	0
6	AF	100/100 (100%)	0.32	2 (2%) 65 56	32, 54, 73, 77	0
6	CF	100/100 (100%)	0.59	8 (8%) 18 13	41, 74, 92, 103	0
7	AG	151/151 (100%)	0.66	9 (5%) 27 21	51, 75, 92, 100	0
7	CG	151/151 (100%)	1.67	46 (30%) 1 1	82, 106, 114, 118	0
8	AH	129/129 (100%)	0.11	2 (1%) 70 61	29, 46, 67, 79	0
8	CH	129/129 (100%)	0.59	7 (5%) 31 24	46, 64, 80, 94	0
9	AI	127/127 (100%)	1.01	16 (12%) 8 6	40, 74, 98, 107	0
9	CI	127/127 (100%)	1.53	33 (25%) 1 1	79, 96, 112, 121	0
10	AJ	98/98 (100%)	0.82	8 (8%) 17 13	38, 66, 86, 116	0
10	CJ	98/98 (100%)	1.91	44 (44%) 0 0	72, 97, 115, 123	0
11	AK	117/117 (100%)	0.44	4 (3%) 48 39	25, 60, 89, 119	0
11	CK	117/117 (100%)	0.24	1 (0%) 81 74	35, 68, 79, 90	0
12	AL	123/123 (100%)	0.14	6 (4%) 35 27	20, 34, 65, 97	0
12	CL	123/123 (100%)	0.58	12 (9%) 13 9	30, 50, 74, 95	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	114/114 (100%)	0.60	6 (5%) 32 24	47, 69, 91, 103	0
13	CM	114/114 (100%)	2.31	63 (55%) 0 0	93, 113, 122, 125	0
14	AN	96/100 (96%)	0.94	10 (10%) 11 8	36, 60, 96, 105	0
14	CN	96/100 (96%)	1.59	26 (27%) 1 1	70, 96, 115, 122	0
15	AO	88/88 (100%)	0.25	4 (4%) 38 30	29, 47, 64, 91	0
15	CO	88/88 (100%)	0.56	4 (4%) 38 30	36, 64, 80, 102	0
16	AP	82/82 (100%)	0.47	4 (4%) 35 27	34, 47, 83, 109	0
16	CP	82/82 (100%)	1.15	9 (10%) 10 8	45, 62, 91, 112	0
17	AQ	80/80 (100%)	0.29	5 (6%) 26 19	27, 48, 75, 111	0
17	CQ	80/80 (100%)	1.28	21 (26%) 1 1	42, 77, 97, 99	0
18	AR	55/55 (100%)	0.44	4 (7%) 21 15	40, 52, 77, 102	0
18	CR	55/55 (100%)	0.29	2 (3%) 46 37	36, 54, 78, 108	0
19	AS	79/79 (100%)	0.78	6 (7%) 20 14	54, 70, 88, 97	0
19	CS	79/79 (100%)	2.30	43 (54%) 0 0	95, 114, 122, 128	0
20	AT	85/85 (100%)	0.58	5 (5%) 28 21	35, 48, 68, 96	0
20	CT	85/85 (100%)	1.34	21 (24%) 2 1	53, 78, 96, 101	0
21	AU	51/51 (100%)	1.55	14 (27%) 1 1	41, 74, 95, 105	0
21	CU	51/51 (100%)	1.57	10 (19%) 3 2	42, 69, 98, 102	0
22	BA	2897/2903 (99%)	-0.60	106 (3%) 45 36	0, 14, 129, 195	0
22	DA	2897/2903 (99%)	0.83	165 (5%) 29 22	41, 85, 148, 181	0
23	BB	119/119 (100%)	-0.82	0 100 100	2, 23, 46, 81	0
23	DB	118/119 (99%)	0.66	1 (0%) 82 75	69, 115, 134, 142	0
24	BC	271/271 (100%)	-0.32	4 (1%) 72 63	2, 18, 35, 55	0
24	DC	271/271 (100%)	1.05	39 (14%) 6 5	46, 64, 77, 95	0
25	BD	209/209 (100%)	-0.55	0 100 100	0, 9, 34, 65	0
25	DD	209/209 (100%)	1.27	37 (17%) 4 3	53, 72, 87, 97	0
26	BE	201/201 (100%)	-0.47	0 100 100	1, 23, 54, 88	0
26	DE	201/201 (100%)	1.63	68 (33%) 1 1	52, 89, 105, 113	0
27	BF	177/177 (100%)	0.05	2 (1%) 78 70	21, 40, 74, 88	0
27	DF	177/177 (100%)	1.49	43 (24%) 2 1	94, 113, 124, 131	0
28	BG	176/176 (100%)	-0.20	1 (0%) 85 80	15, 35, 58, 72	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DG	176/176 (100%)	1.47	36 (20%) 2 2	78, 96, 110, 121	0
29	BH	149/149 (100%)	2.06	74 (49%) 0 0	25, 102, 121, 129	0
29	DH	149/149 (100%)	1.30	28 (18%) 3 2	25, 92, 107, 115	0
30	BI	141/141 (100%)	2.39	78 (55%) 0 0	89, 116, 126, 134	0
30	DI	141/141 (100%)	2.84	97 (68%) 0 0	105, 124, 135, 142	0
31	BJ	142/142 (100%)	-0.53	1 (0%) 84 77	1, 6, 26, 35	0
31	DJ	142/142 (100%)	1.00	25 (17%) 4 3	49, 69, 83, 91	0
32	BK	122/122 (100%)	-0.61	2 (1%) 70 61	3, 11, 28, 60	0
32	DK	122/122 (100%)	0.85	10 (8%) 17 13	48, 66, 84, 95	0
33	BL	143/143 (100%)	-0.26	1 (0%) 84 77	1, 18, 42, 65	0
33	DL	143/143 (100%)	1.90	54 (37%) 1 0	43, 87, 98, 115	0
34	BM	136/136 (100%)	-0.61	1 (0%) 84 77	1, 10, 24, 85	0
34	DM	136/136 (100%)	0.80	15 (11%) 10 8	44, 70, 85, 99	0
35	BN	120/120 (100%)	-0.51	0 100 100	2, 7, 17, 65	0
35	DN	120/120 (100%)	1.77	44 (36%) 1 0	58, 78, 92, 112	0
36	BO	116/116 (100%)	-0.39	0 100 100	14, 24, 42, 54	0
36	DO	116/116 (100%)	1.52	34 (29%) 1 1	85, 99, 110, 117	0
37	BP	114/114 (100%)	-0.39	2 (1%) 67 58	6, 16, 41, 71	0
37	DP	114/114 (100%)	1.33	23 (20%) 3 2	61, 74, 86, 94	0
38	BQ	117/117 (100%)	-0.62	0 100 100	0, 3, 12, 30	0
38	DQ	117/117 (100%)	1.28	29 (24%) 2 1	55, 70, 81, 89	0
39	BR	103/103 (100%)	-0.43	1 (0%) 79 72	0, 11, 31, 56	0
39	DR	103/103 (100%)	1.37	20 (19%) 3 2	57, 80, 92, 103	0
40	BS	110/110 (100%)	-0.58	0 100 100	1, 4, 21, 68	0
40	DS	110/110 (100%)	1.70	35 (31%) 1 1	60, 79, 94, 105	0
41	BT	93/93 (100%)	-0.04	6 (6%) 25 18	10, 24, 68, 98	0
41	DT	93/93 (100%)	1.92	36 (38%) 1 0	73, 91, 106, 115	0
42	BU	102/102 (100%)	-0.33	1 (0%) 79 72	10, 25, 58, 77	0
42	DU	102/102 (100%)	2.39	59 (57%) 0 0	77, 95, 109, 120	0
43	BV	94/94 (100%)	-0.45	0 100 100	4, 18, 39, 52	0
43	DV	94/94 (100%)	0.71	4 (4%) 40 31	72, 86, 98, 105	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BW	76/76 (100%)	-0.39	0 100 100	4, 11, 27, 57	0
44	DW	75/76 (98%)	1.42	12 (16%) 5 4	58, 83, 93, 104	0
45	BX	77/77 (100%)	-0.20	0 100 100	8, 22, 48, 68	0
45	DX	77/77 (100%)	1.66	28 (36%) 1 0	47, 72, 87, 91	0
46	BY	63/63 (100%)	0.32	4 (6%) 26 19	18, 38, 71, 94	0
46	DY	63/63 (100%)	1.84	22 (34%) 1 0	81, 99, 106, 109	0
47	BZ	58/58 (100%)	-0.51	0 100 100	2, 6, 25, 34	0
47	DZ	58/58 (100%)	0.99	3 (5%) 33 25	60, 73, 85, 103	0
48	B0	56/56 (100%)	-0.53	0 100 100	0, 7, 33, 60	0
48	D0	56/56 (100%)	1.42	11 (19%) 3 2	51, 82, 95, 103	0
49	B1	50/50 (100%)	-0.27	1 (2%) 65 56	13, 25, 49, 57	0
49	D1	50/50 (100%)	1.55	17 (34%) 1 1	73, 89, 94, 106	0
50	B2	46/46 (100%)	-0.33	1 (2%) 62 52	4, 8, 15, 79	0
50	D2	46/46 (100%)	2.09	21 (45%) 0 0	58, 72, 86, 101	0
51	B3	64/64 (100%)	-0.50	0 100 100	4, 9, 17, 29	0
51	D3	64/64 (100%)	2.53	42 (65%) 0 0	60, 75, 84, 94	0
52	B4	38/38 (100%)	-0.29	0 100 100	5, 15, 29, 52	0
52	D4	38/38 (100%)	1.91	14 (36%) 1 0	62, 77, 88, 98	0
53	B5	191/228 (83%)	2.25	110 (57%) 0 0	100, 121, 133, 141	0
54	B6	2/8 (25%)	-0.26	0 100 100	1, 1, 1, 1	0
54	D6	2/8 (25%)	0.56	0 100 100	46, 46, 46, 51	0
All	All	20738/20810 (99%)	0.45	2086 (10%) 12 9	0, 63, 124, 195	0

The worst 5 of 2086 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	CT	4	ILE	10.7
30	BI	53	LEU	9.0
4	CD	25	VAL	8.5
7	AG	5	ARG	7.1
50	D2	46	LYS	7.0

6.2 Non-standard residues in protein, DNA, RNA chains [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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MHW	D6	1	9/10	0.85	0.12	40,52,59,59	0
54	MHU	D6	5	15/16	0.87	0.17	44,54,60,61	0
54	004	D6	7	10/11	0.87	0.14	42,47,58,59	0
54	MHV	D6	6	9/10	0.91	0.10	45,51,58,60	0
54	DBB	D6	3	6/7	0.92	0.12	36,38,47,51	0
54	MHU	B6	5	15/16	0.95	0.09	0,0,1,2	0
54	MHW	B6	1	9/10	0.95	0.08	0,0,2,9	0
54	DBB	B6	3	6/7	0.96	0.10	0,1,1,2	0
54	004	B6	7	10/11	0.96	0.09	0,0,2,3	0
54	MHV	B6	6	9/10	0.96	0.07	0,0,1,1	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	3048	1/1	0.03	0.18	127,127,127,127	0
55	MG	DA	3131	1/1	0.27	0.35	99,99,99,99	0
55	MG	DA	3075	1/1	0.50	0.13	91,91,91,91	0
55	MG	AA	1657	1/1	0.51	0.23	64,64,64,64	0
55	MG	DA	3041	1/1	0.52	0.30	68,68,68,68	0
55	MG	DA	3026	1/1	0.54	0.36	101,101,101,101	0
55	MG	DA	3135	1/1	0.54	0.23	101,101,101,101	0
55	MG	DA	3071	1/1	0.56	0.19	92,92,92,92	0
55	MG	DA	3144	1/1	0.56	0.18	68,68,68,68	0
55	MG	DA	3133	1/1	0.57	0.31	100,100,100,100	0
55	MG	DA	3077	1/1	0.63	0.21	113,113,113,113	0
55	MG	BA	3125	1/1	0.64	0.30	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	3112	1/1	0.64	0.48	104,104,104,104	0
55	MG	DA	3040	1/1	0.65	0.13	83,83,83,83	0
55	MG	CA	1646	1/1	0.66	0.22	92,92,92,92	0
55	MG	BA	3137	1/1	0.66	0.32	49,49,49,49	0
55	MG	DA	3044	1/1	0.66	0.18	112,112,112,112	0
55	MG	AA	1658	1/1	0.68	0.12	62,62,62,62	0
55	MG	DA	3126	1/1	0.69	0.17	80,80,80,80	0
55	MG	DA	3061	1/1	0.70	0.69	96,96,96,96	0
55	MG	AM	201	1/1	0.70	0.14	62,62,62,62	0
55	MG	DA	3111	1/1	0.70	0.17	107,107,107,107	0
55	MG	DA	3100	1/1	0.71	0.17	77,77,77,77	0
55	MG	BA	3078	1/1	0.72	0.29	79,79,79,79	0
55	MG	DA	3042	1/1	0.72	0.14	87,87,87,87	0
55	MG	DA	3153	1/1	0.72	0.25	53,53,53,53	0
55	MG	CA	1636	1/1	0.73	0.10	126,126,126,126	0
55	MG	DA	3029	1/1	0.73	0.15	73,73,73,73	0
55	MG	DA	3145	1/1	0.74	0.11	71,71,71,71	0
55	MG	BA	3038	1/1	0.75	0.23	42,42,42,42	0
55	MG	DA	3072	1/1	0.76	0.29	90,90,90,90	0
55	MG	DA	3115	1/1	0.76	0.13	111,111,111,111	0
55	MG	DA	3099	1/1	0.76	0.20	86,86,86,86	0
55	MG	DA	3009	1/1	0.77	0.15	90,90,90,90	0
55	MG	CA	1641	1/1	0.77	0.27	73,73,73,73	0
55	MG	DA	3058	1/1	0.77	0.53	109,109,109,109	0
55	MG	DA	3007	1/1	0.77	0.17	121,121,121,121	0
55	MG	DA	3163	1/1	0.77	0.10	54,54,54,54	0
55	MG	DA	3164	1/1	0.77	0.13	57,57,57,57	0
55	MG	AA	1662	1/1	0.78	0.15	57,57,57,57	0
55	MG	DA	3074	1/1	0.78	0.26	77,77,77,77	0
55	MG	DA	3017	1/1	0.78	0.12	98,98,98,98	0
55	MG	DA	3151	1/1	0.78	0.39	59,59,59,59	0
55	MG	CA	1630	1/1	0.78	0.14	120,120,120,120	0
55	MG	DA	3062	1/1	0.78	0.31	82,82,82,82	0
55	MG	BA	3063	1/1	0.78	0.30	31,31,31,31	0
55	MG	DA	3028	1/1	0.79	0.28	103,103,103,103	0
55	MG	BA	3016	1/1	0.79	0.27	58,58,58,58	0
55	MG	DA	3005	1/1	0.79	0.15	102,102,102,102	0
55	MG	DA	3092	1/1	0.79	0.24	113,113,113,113	0
55	MG	DA	3097	1/1	0.79	0.16	91,91,91,91	0
55	MG	AA	1619	1/1	0.80	0.24	73,73,73,73	0
55	MG	DA	3152	1/1	0.81	0.21	52,52,52,52	0
55	MG	BA	3075	1/1	0.81	0.13	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	3158	1/1	0.81	0.14	70,70,70,70	0
55	MG	DA	3119	1/1	0.81	0.18	106,106,106,106	0
55	MG	CA	1652	1/1	0.81	0.12	83,83,83,83	0
55	MG	DA	3113	1/1	0.82	0.12	66,66,66,66	0
55	MG	DA	3003	1/1	0.82	0.21	99,99,99,99	0
55	MG	DA	3057	1/1	0.82	0.12	95,95,95,95	0
55	MG	BA	3153	1/1	0.82	0.12	31,31,31,31	0
55	MG	DA	3027	1/1	0.82	0.10	91,91,91,91	0
55	MG	CA	1654	1/1	0.83	0.14	56,56,56,56	0
55	MG	CA	1635	1/1	0.83	0.09	124,124,124,124	0
55	MG	BA	3167	1/1	0.83	0.08	25,25,25,25	0
55	MG	CA	1615	1/1	0.83	0.19	58,58,58,58	0
55	MG	DA	3078	1/1	0.83	0.11	106,106,106,106	0
55	MG	CA	1628	1/1	0.83	0.11	98,98,98,98	0
55	MG	DA	3093	1/1	0.83	0.10	86,86,86,86	0
55	MG	BA	3134	1/1	0.83	0.29	54,54,54,54	0
55	MG	DA	3019	1/1	0.83	0.09	107,107,107,107	0
55	MG	DA	3166	1/1	0.83	0.09	41,41,41,41	0
55	MG	DQ	201	1/1	0.83	0.17	45,45,45,45	0
55	MG	DA	3080	1/1	0.84	0.09	95,95,95,95	0
55	MG	DA	3103	1/1	0.84	0.12	73,73,73,73	0
55	MG	BA	3136	1/1	0.84	0.12	21,21,21,21	0
55	MG	DA	3056	1/1	0.84	0.26	93,93,93,93	0
55	MG	DA	3157	1/1	0.84	0.17	58,58,58,58	0
55	MG	DA	3011	1/1	0.84	0.13	75,75,75,75	0
55	MG	DA	3137	1/1	0.84	0.26	47,47,47,47	0
55	MG	DA	3140	1/1	0.84	0.20	43,43,43,43	0
55	MG	DA	3142	1/1	0.84	0.18	33,33,33,33	0
55	MG	AA	1664	1/1	0.84	0.08	49,49,49,49	0
55	MG	CA	1653	1/1	0.85	0.23	52,52,52,52	0
55	MG	BA	3059	1/1	0.85	0.24	38,38,38,38	0
55	MG	DA	3146	1/1	0.85	0.11	43,43,43,43	0
55	MG	DA	3124	1/1	0.85	0.10	89,89,89,89	0
55	MG	DA	3098	1/1	0.85	0.10	66,66,66,66	0
55	MG	DA	3127	1/1	0.85	0.11	71,71,71,71	0
55	MG	CA	1656	1/1	0.85	0.10	54,54,54,54	0
55	MG	BA	3104	1/1	0.85	0.19	17,17,17,17	0
55	MG	BA	3061	1/1	0.85	0.22	30,30,30,30	0
55	MG	BA	3187	1/1	0.85	0.12	33,33,33,33	0
55	MG	BA	3049	1/1	0.85	0.11	44,44,44,44	0
55	MG	DA	3167	1/1	0.85	0.13	100,100,100,100	0
55	MG	BA	3050	1/1	0.85	0.09	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	3178	1/1	0.86	0.30	30,30,30,30	0
55	MG	DA	3160	1/1	0.86	0.19	43,43,43,43	0
55	MG	DA	3045	1/1	0.86	0.09	94,94,94,94	0
55	MG	DA	3060	1/1	0.86	0.16	77,77,77,77	0
55	MG	DA	3165	1/1	0.86	0.26	42,42,42,42	0
55	MG	BA	3100	1/1	0.86	0.26	52,52,52,52	0
55	MG	DA	3155	1/1	0.86	0.14	62,62,62,62	0
55	MG	BA	3113	1/1	0.86	0.07	22,22,22,22	0
55	MG	DA	3148	1/1	0.87	0.25	65,65,65,65	0
55	MG	DA	3149	1/1	0.87	0.28	35,35,35,35	0
55	MG	CA	1627	1/1	0.87	0.15	89,89,89,89	0
55	MG	DA	3031	1/1	0.87	0.07	69,69,69,69	0
55	MG	BA	3027	1/1	0.87	0.22	46,46,46,46	0
55	MG	BA	3057	1/1	0.87	0.25	73,73,73,73	0
55	MG	DA	3079	1/1	0.87	0.08	96,96,96,96	0
55	MG	BA	3058	1/1	0.87	0.23	15,15,15,15	0
55	MG	DA	3090	1/1	0.87	0.12	90,90,90,90	0
55	MG	AA	1667	1/1	0.87	0.07	49,49,49,49	0
55	MG	DA	3143	1/1	0.87	0.13	60,60,60,60	0
55	MG	AA	1671	1/1	0.87	0.24	59,59,59,59	0
55	MG	DA	3120	1/1	0.87	0.10	79,79,79,79	0
55	MG	CA	1626	1/1	0.87	0.07	48,48,48,48	0
55	MG	DA	3147	1/1	0.87	0.26	54,54,54,54	0
56	DOL	DA	3001	48/48	0.87	0.14	26,45,58,63	0
55	MG	BA	3191	1/1	0.88	0.13	12,12,12,12	0
55	MG	AA	1629	1/1	0.88	0.10	61,61,61,61	0
55	MG	AA	1669	1/1	0.88	0.25	51,51,51,51	0
55	MG	DA	3089	1/1	0.88	0.13	83,83,83,83	0
55	MG	DA	3039	1/1	0.88	0.09	57,57,57,57	0
55	MG	BA	3181	1/1	0.88	0.12	24,24,24,24	0
55	MG	AA	1644	1/1	0.88	0.06	44,44,44,44	0
55	MG	CA	1629	1/1	0.88	0.09	91,91,91,91	0
55	MG	DA	3107	1/1	0.89	0.11	75,75,75,75	0
55	MG	AA	1654	1/1	0.89	0.14	43,43,43,43	0
55	MG	DA	3012	1/1	0.89	0.14	73,73,73,73	0
55	MG	CA	1606	1/1	0.89	0.09	89,89,89,89	0
55	MG	BA	3176	1/1	0.89	0.09	20,20,20,20	0
55	MG	DA	3116	1/1	0.89	0.16	76,76,76,76	0
55	MG	BA	3146	1/1	0.89	0.23	30,30,30,30	0
55	MG	AA	1661	1/1	0.89	0.10	29,29,29,29	0
55	MG	DA	3123	1/1	0.89	0.09	57,57,57,57	0
55	MG	CA	1645	1/1	0.89	0.13	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	3159	1/1	0.89	0.13	14,14,14,14	0
55	MG	CA	1651	1/1	0.89	0.10	44,44,44,44	0
55	MG	D2	101	1/1	0.89	0.10	83,83,83,83	0
55	MG	DA	3033	1/1	0.89	0.09	71,71,71,71	0
55	MG	DA	3084	1/1	0.90	0.08	105,105,105,105	0
55	MG	AA	1646	1/1	0.90	0.08	49,49,49,49	0
55	MG	DA	3150	1/1	0.90	0.14	56,56,56,56	0
55	MG	CA	1643	1/1	0.90	0.16	50,50,50,50	0
55	MG	AA	1635	1/1	0.90	0.10	66,66,66,66	0
55	MG	AA	1659	1/1	0.90	0.30	50,50,50,50	0
55	MG	DA	3032	1/1	0.90	0.11	68,68,68,68	0
55	MG	CA	1649	1/1	0.90	0.22	52,52,52,52	0
55	MG	DA	3064	1/1	0.90	0.10	48,48,48,48	0
55	MG	DA	3035	1/1	0.90	0.09	79,79,79,79	0
55	MG	CA	1631	1/1	0.90	0.10	95,95,95,95	0
55	MG	CA	1632	1/1	0.90	0.08	73,73,73,73	0
55	MG	DA	3108	1/1	0.90	0.11	59,59,59,59	0
55	MG	AA	1665	1/1	0.90	0.11	37,37,37,37	0
55	MG	BA	3090	1/1	0.90	0.14	19,19,19,19	0
55	MG	DA	3024	1/1	0.90	0.12	46,46,46,46	0
55	MG	DA	3025	1/1	0.90	0.17	69,69,69,69	0
55	MG	CA	1655	1/1	0.90	0.12	44,44,44,44	0
55	MG	CA	1608	1/1	0.91	0.12	84,84,84,84	0
55	MG	DA	3136	1/1	0.91	0.12	91,91,91,91	0
55	MG	DA	3154	1/1	0.91	0.20	40,40,40,40	0
55	MG	DA	3049	1/1	0.91	0.10	84,84,84,84	0
55	MG	AA	1649	1/1	0.91	0.07	32,32,32,32	0
55	MG	BA	3186	1/1	0.91	0.10	29,29,29,29	0
55	MG	AA	1651	1/1	0.91	0.36	61,61,61,61	0
55	MG	DA	3008	1/1	0.91	0.09	100,100,100,100	0
55	MG	BA	3189	1/1	0.91	0.12	45,45,45,45	0
55	MG	DA	3105	1/1	0.91	0.12	80,80,80,80	0
55	MG	DA	3125	1/1	0.91	0.10	62,62,62,62	0
55	MG	DA	3106	1/1	0.91	0.08	52,52,52,52	0
55	MG	AA	1668	1/1	0.91	0.07	29,29,29,29	0
55	MG	AA	1648	1/1	0.91	0.13	47,47,47,47	0
55	MG	DA	3014	1/1	0.91	0.12	73,73,73,73	0
55	MG	BA	3089	1/1	0.92	0.10	33,33,33,33	0
55	MG	BA	3165	1/1	0.92	0.25	43,43,43,43	0
55	MG	DA	3094	1/1	0.92	0.07	84,84,84,84	0
55	MG	DA	3141	1/1	0.92	0.18	40,40,40,40	0
55	MG	AA	1650	1/1	0.92	0.17	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	3046	1/1	0.92	0.09	62,62,62,62	0
55	MG	DA	3047	1/1	0.92	0.10	73,73,73,73	0
55	MG	BA	3169	1/1	0.92	0.09	35,35,35,35	0
55	MG	DA	3010	1/1	0.92	0.06	80,80,80,80	0
55	MG	AA	1660	1/1	0.92	0.17	51,51,51,51	0
55	MG	CA	1633	1/1	0.92	0.22	64,64,64,64	0
55	MG	AA	1670	1/1	0.92	0.14	33,33,33,33	0
55	MG	BA	3111	1/1	0.92	0.10	6,6,6,6	0
55	MG	AA	1630	1/1	0.92	0.11	73,73,73,73	0
55	MG	CA	1642	1/1	0.92	0.17	25,25,25,25	0
55	MG	BA	3119	1/1	0.92	0.09	20,20,20,20	0
55	MG	DA	3068	1/1	0.92	0.08	65,65,65,65	0
55	MG	AA	1652	1/1	0.92	0.24	49,49,49,49	0
55	MG	AA	1638	1/1	0.92	0.08	87,87,87,87	0
55	MG	CA	1647	1/1	0.92	0.12	41,41,41,41	0
55	MG	DA	3159	1/1	0.92	0.14	43,43,43,43	0
55	MG	CA	1601	1/1	0.92	0.09	39,39,39,39	0
55	MG	AA	1639	1/1	0.92	0.07	65,65,65,65	0
55	MG	AA	1643	1/1	0.92	0.11	28,28,28,28	0
55	MG	CA	1609	1/1	0.92	0.08	89,89,89,89	0
55	MG	CA	1614	1/1	0.92	0.06	50,50,50,50	0
55	MG	BA	3042	1/1	0.92	0.21	0,0,0,0	0
55	MG	BA	3149	1/1	0.92	0.09	38,38,38,38	0
55	MG	DA	3134	1/1	0.92	0.11	58,58,58,58	0
55	MG	BA	3081	1/1	0.92	0.09	24,24,24,24	0
55	MG	BB	202	1/1	0.93	0.07	16,16,16,16	0
55	MG	DA	3102	1/1	0.93	0.08	62,62,62,62	0
55	MG	DA	3030	1/1	0.93	0.10	60,60,60,60	0
55	MG	AA	1655	1/1	0.93	0.09	35,35,35,35	0
55	MG	DA	3006	1/1	0.93	0.06	93,93,93,93	0
55	MG	CA	1604	1/1	0.93	0.06	95,95,95,95	0
55	MG	DA	3070	1/1	0.93	0.05	108,108,108,108	0
55	MG	DA	3109	1/1	0.93	0.16	42,42,42,42	0
55	MG	DA	3034	1/1	0.93	0.11	69,69,69,69	0
55	MG	CA	1605	1/1	0.93	0.10	86,86,86,86	0
55	MG	DA	3037	1/1	0.93	0.07	93,93,93,93	0
55	MG	DA	3038	1/1	0.93	0.08	63,63,63,63	0
55	MG	BA	3069	1/1	0.93	0.08	4,4,4,4	0
55	MG	BA	3033	1/1	0.93	0.08	11,11,11,11	0
55	MG	BA	3170	1/1	0.93	0.10	38,38,38,38	0
55	MG	AA	1656	1/1	0.93	0.11	43,43,43,43	0
55	MG	AA	1663	1/1	0.93	0.12	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	3086	1/1	0.93	0.08	76,76,76,76	0
55	MG	AA	1614	1/1	0.93	0.20	69,69,69,69	0
55	MG	BA	3185	1/1	0.93	0.21	16,16,16,16	0
55	MG	DA	3161	1/1	0.93	0.07	57,57,57,57	0
55	MG	DA	3128	1/1	0.93	0.08	80,80,80,80	0
55	MG	DA	3020	1/1	0.93	0.08	54,54,54,54	0
55	MG	BA	3151	1/1	0.93	0.10	12,12,12,12	0
55	MG	BA	3120	1/1	0.93	0.13	37,37,37,37	0
55	MG	BA	3155	1/1	0.93	0.10	20,20,20,20	0
55	MG	DB	201	1/1	0.93	0.06	116,116,116,116	0
55	MG	BA	3124	1/1	0.93	0.07	11,11,11,11	0
55	MG	BA	3195	1/1	0.93	0.33	23,23,23,23	0
55	MG	DA	3138	1/1	0.93	0.15	40,40,40,40	0
55	MG	DA	3002	1/1	0.94	0.06	78,78,78,78	0
55	MG	BA	3086	1/1	0.94	0.14	14,14,14,14	0
55	MG	DA	3091	1/1	0.94	0.07	77,77,77,77	0
55	MG	BA	3156	1/1	0.94	0.13	19,19,19,19	0
55	MG	AA	1653	1/1	0.94	0.08	28,28,28,28	0
55	MG	BA	3162	1/1	0.94	0.10	36,36,36,36	0
55	MG	DA	3095	1/1	0.94	0.12	91,91,91,91	0
55	MG	AA	1632	1/1	0.94	0.09	55,55,55,55	0
55	MG	DA	3063	1/1	0.94	0.08	54,54,54,54	0
55	MG	CA	1603	1/1	0.94	0.06	44,44,44,44	0
55	MG	AA	1626	1/1	0.94	0.07	23,23,23,23	0
55	MG	AA	1666	1/1	0.94	0.10	46,46,46,46	0
55	MG	BA	3139	1/1	0.94	0.23	0,0,0,0	0
55	MG	BA	3173	1/1	0.94	0.09	27,27,27,27	0
55	MG	BA	3175	1/1	0.94	0.06	27,27,27,27	0
55	MG	BA	3142	1/1	0.94	0.26	2,2,2,2	0
55	MG	BA	3005	1/1	0.94	0.08	34,34,34,34	0
55	MG	BA	3180	1/1	0.94	0.07	32,32,32,32	0
55	MG	DA	3110	1/1	0.94	0.11	33,33,33,33	0
55	MG	BA	3147	1/1	0.94	0.07	9,9,9,9	0
55	MG	AA	1605	1/1	0.94	0.09	23,23,23,23	0
55	MG	AA	1608	1/1	0.94	0.06	17,17,17,17	0
55	MG	BA	3082	1/1	0.94	0.10	6,6,6,6	0
55	MG	AA	1628	1/1	0.95	0.07	48,48,48,48	0
55	MG	BA	3004	1/1	0.95	0.04	26,26,26,26	0
55	MG	BA	3115	1/1	0.95	0.05	20,20,20,20	0
55	MG	BA	3116	1/1	0.95	0.18	34,34,34,34	0
55	MG	BA	3085	1/1	0.95	0.18	27,27,27,27	0
55	MG	BA	3062	1/1	0.95	0.26	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	3104	1/1	0.95	0.06	79,79,79,79	0
55	MG	DA	3132	1/1	0.95	0.13	54,54,54,54	0
55	MG	DA	3156	1/1	0.95	0.16	41,41,41,41	0
55	MG	AA	1612	1/1	0.95	0.10	47,47,47,47	0
55	MG	AA	1620	1/1	0.95	0.07	69,69,69,69	0
55	MG	CA	1638	1/1	0.95	0.05	76,76,76,76	0
55	MG	DA	3081	1/1	0.95	0.07	60,60,60,60	0
55	MG	BA	3127	1/1	0.95	0.06	9,9,9,9	0
55	MG	DA	3162	1/1	0.95	0.14	38,38,38,38	0
55	MG	BA	3132	1/1	0.95	0.13	23,23,23,23	0
55	MG	BA	3157	1/1	0.95	0.07	24,24,24,24	0
55	MG	CA	1644	1/1	0.95	0.09	42,42,42,42	0
55	MG	AA	1631	1/1	0.95	0.10	46,46,46,46	0
55	MG	DA	3114	1/1	0.95	0.07	65,65,65,65	0
55	MG	CA	1618	1/1	0.95	0.05	37,37,37,37	0
55	MG	AA	1609	1/1	0.95	0.08	36,36,36,36	0
55	MG	BA	3163	1/1	0.95	0.25	15,15,15,15	0
55	MG	DA	3016	1/1	0.95	0.12	62,62,62,62	0
55	MG	CA	1624	1/1	0.96	0.05	45,45,45,45	0
55	MG	CA	1625	1/1	0.96	0.07	22,22,22,22	0
55	MG	DA	3088	1/1	0.96	0.06	74,74,74,74	0
55	MG	BA	3121	1/1	0.96	0.07	3,3,3,3	0
55	MG	BA	3152	1/1	0.96	0.06	6,6,6,6	0
55	MG	BA	3183	1/1	0.96	0.09	12,12,12,12	0
55	MG	DA	3043	1/1	0.96	0.07	66,66,66,66	0
55	MG	BA	3093	1/1	0.96	0.05	58,58,58,58	0
55	MG	BA	3094	1/1	0.96	0.07	31,31,31,31	0
55	MG	BA	3095	1/1	0.96	0.04	21,21,21,21	0
55	MG	AA	1617	1/1	0.96	0.07	52,52,52,52	0
55	MG	BA	3190	1/1	0.96	0.06	31,31,31,31	0
55	MG	BA	3036	1/1	0.96	0.15	11,11,11,11	0
55	MG	DA	3050	1/1	0.96	0.05	56,56,56,56	0
55	MG	DA	3053	1/1	0.96	0.06	40,40,40,40	0
55	MG	DA	3054	1/1	0.96	0.06	55,55,55,55	0
55	MG	DA	3055	1/1	0.96	0.09	72,72,72,72	0
55	MG	BA	3076	1/1	0.96	0.11	14,14,14,14	0
55	MG	BA	3112	1/1	0.96	0.07	20,20,20,20	0
55	MG	CA	1639	1/1	0.96	0.05	43,43,43,43	0
55	MG	BB	204	1/1	0.96	0.28	16,16,16,16	0
55	MG	BA	3077	1/1	0.96	0.07	8,8,8,8	0
55	MG	BA	3166	1/1	0.96	0.08	19,19,19,19	0
55	MG	BA	3141	1/1	0.96	0.06	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	3168	1/1	0.96	0.11	35,35,35,35	0
55	MG	DA	3067	1/1	0.96	0.06	58,58,58,58	0
55	MG	BA	3087	1/1	0.96	0.07	4,4,4,4	0
55	MG	CA	1607	1/1	0.96	0.08	54,54,54,54	0
55	MG	CA	1648	1/1	0.96	0.13	22,22,22,22	0
55	MG	BA	3031	1/1	0.96	0.12	14,14,14,14	0
55	MG	CA	1650	1/1	0.96	0.14	35,35,35,35	0
55	MG	DA	3121	1/1	0.96	0.05	52,52,52,52	0
55	MG	BA	3079	1/1	0.96	0.05	22,22,22,22	0
55	MG	BA	3148	1/1	0.96	0.15	29,29,29,29	0
55	MG	BA	3092	1/1	0.96	0.04	19,19,19,19	0
55	MG	CA	1617	1/1	0.96	0.07	39,39,39,39	0
55	MG	DB	203	1/1	0.96	0.05	85,85,85,85	0
55	MG	DA	3036	1/1	0.96	0.06	62,62,62,62	0
55	MG	BA	3150	1/1	0.96	0.06	37,37,37,37	0
56	DOL	BA	3001	48/48	0.96	0.09	0,3,25,36	0
55	MG	DA	3083	1/1	0.96	0.08	69,69,69,69	0
55	MG	CA	1623	1/1	0.97	0.11	50,50,50,50	0
55	MG	DA	3122	1/1	0.97	0.06	41,41,41,41	0
55	MG	DA	3069	1/1	0.97	0.10	79,79,79,79	0
55	MG	BA	3171	1/1	0.97	0.06	24,24,24,24	0
55	MG	BA	3021	1/1	0.97	0.06	1,1,1,1	0
55	MG	BA	3174	1/1	0.97	0.04	12,12,12,12	0
55	MG	DA	3073	1/1	0.97	0.09	60,60,60,60	0
55	MG	AA	1637	1/1	0.97	0.04	15,15,15,15	0
55	MG	DA	3129	1/1	0.97	0.06	45,45,45,45	0
55	MG	BA	3030	1/1	0.97	0.05	9,9,9,9	0
55	MG	DA	3076	1/1	0.97	0.10	69,69,69,69	0
55	MG	BA	3144	1/1	0.97	0.07	15,15,15,15	0
55	MG	BA	3145	1/1	0.97	0.18	28,28,28,28	0
55	MG	BA	3064	1/1	0.97	0.06	5,5,5,5	0
55	MG	BA	3182	1/1	0.97	0.14	33,33,33,33	0
55	MG	BA	3103	1/1	0.97	0.06	0,0,0,0	0
55	MG	DA	3082	1/1	0.97	0.07	60,60,60,60	0
55	MG	DA	3139	1/1	0.97	0.17	30,30,30,30	0
55	MG	AA	1625	1/1	0.97	0.06	47,47,47,47	0
55	MG	BA	3071	1/1	0.97	0.05	60,60,60,60	0
55	MG	AA	1602	1/1	0.97	0.14	46,46,46,46	0
55	MG	AA	1640	1/1	0.97	0.10	36,36,36,36	0
55	MG	BA	3002	1/1	0.97	0.04	18,18,18,18	0
55	MG	AA	1613	1/1	0.97	0.06	24,24,24,24	0
55	MG	BA	3192	1/1	0.97	0.06	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	3193	1/1	0.97	0.05	38,38,38,38	0
55	MG	BA	3154	1/1	0.97	0.09	25,25,25,25	0
55	MG	BA	3117	1/1	0.97	0.09	1,1,1,1	0
55	MG	BA	3043	1/1	0.97	0.04	16,16,16,16	0
55	MG	BA	3047	1/1	0.97	0.07	4,4,4,4	0
55	MG	CA	1602	1/1	0.97	0.09	88,88,88,88	0
55	MG	BA	3048	1/1	0.97	0.05	8,8,8,8	0
55	MG	BA	3160	1/1	0.97	0.04	10,10,10,10	0
55	MG	DA	3101	1/1	0.97	0.06	57,57,57,57	0
55	MG	BA	3084	1/1	0.97	0.12	6,6,6,6	0
55	MG	AA	1634	1/1	0.97	0.05	35,35,35,35	0
55	MG	BA	3164	1/1	0.97	0.04	4,4,4,4	0
55	MG	BA	3006	1/1	0.97	0.08	50,50,50,50	0
55	MG	BA	3129	1/1	0.97	0.08	4,4,4,4	0
55	MG	CA	1610	1/1	0.97	0.04	63,63,63,63	0
55	MG	CA	1611	1/1	0.97	0.12	90,90,90,90	0
55	MG	CA	1613	1/1	0.97	0.04	19,19,19,19	0
55	MG	BA	3051	1/1	0.97	0.04	6,6,6,6	0
55	MG	BA	3008	1/1	0.97	0.09	37,37,37,37	0
55	MG	CA	1616	1/1	0.97	0.05	37,37,37,37	0
55	MG	BA	3009	1/1	0.97	0.04	4,4,4,4	0
55	MG	AA	1606	1/1	0.97	0.04	44,44,44,44	0
55	MG	DB	202	1/1	0.97	0.07	66,66,66,66	0
55	MG	CA	1619	1/1	0.97	0.06	33,33,33,33	0
55	MG	CA	1621	1/1	0.97	0.04	64,64,64,64	0
55	MG	DA	3118	1/1	0.97	0.09	60,60,60,60	0
55	MG	DA	3013	1/1	0.97	0.05	44,44,44,44	0
55	MG	CA	1622	1/1	0.97	0.07	51,51,51,51	0
55	MG	DA	3066	1/1	0.98	0.03	47,47,47,47	0
55	MG	DA	3015	1/1	0.98	0.05	55,55,55,55	0
55	MG	AA	1610	1/1	0.98	0.09	65,65,65,65	0
55	MG	BA	3105	1/1	0.98	0.03	4,4,4,4	0
55	MG	BA	3072	1/1	0.98	0.05	3,3,3,3	0
55	MG	AA	1621	1/1	0.98	0.05	39,39,39,39	0
55	MG	DA	3021	1/1	0.98	0.10	63,63,63,63	0
55	MG	DA	3022	1/1	0.98	0.05	52,52,52,52	0
55	MG	BA	3046	1/1	0.98	0.05	17,17,17,17	0
55	MG	BA	3114	1/1	0.98	0.07	0,0,0,0	0
55	MG	DA	3130	1/1	0.98	0.04	81,81,81,81	0
55	MG	BA	3012	1/1	0.98	0.08	14,14,14,14	0
55	MG	CA	1634	1/1	0.98	0.04	49,49,49,49	0
55	MG	BA	3013	1/1	0.98	0.07	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	1624	1/1	0.98	0.06	41,41,41,41	0
55	MG	CA	1637	1/1	0.98	0.06	64,64,64,64	0
55	MG	BA	3194	1/1	0.98	0.04	8,8,8,8	0
55	MG	BA	3080	1/1	0.98	0.03	39,39,39,39	0
55	MG	BA	3020	1/1	0.98	0.04	22,22,22,22	0
55	MG	BA	3158	1/1	0.98	0.11	19,19,19,19	0
55	MG	DA	3085	1/1	0.98	0.04	67,67,67,67	0
55	MG	BQ	201	1/1	0.98	0.05	3,3,3,3	0
55	MG	DA	3087	1/1	0.98	0.04	54,54,54,54	0
55	MG	AA	1616	1/1	0.98	0.04	50,50,50,50	0
55	MG	BA	3083	1/1	0.98	0.04	0,0,0,0	0
55	MG	BA	3161	1/1	0.98	0.15	31,31,31,31	0
55	MG	BA	3053	1/1	0.98	0.03	2,2,2,2	0
55	MG	BA	3126	1/1	0.98	0.04	6,6,6,6	0
55	MG	BA	3054	1/1	0.98	0.08	9,9,9,9	0
55	MG	BA	3056	1/1	0.98	0.04	5,5,5,5	0
55	MG	BA	3022	1/1	0.98	0.07	2,2,2,2	0
55	MG	DA	3096	1/1	0.98	0.04	57,57,57,57	0
55	MG	BA	3133	1/1	0.98	0.10	32,32,32,32	0
55	MG	AA	1601	1/1	0.98	0.05	58,58,58,58	0
55	MG	AA	1645	1/1	0.98	0.08	42,42,42,42	0
55	MG	CA	1612	1/1	0.98	0.04	40,40,40,40	0
55	MG	BA	3003	1/1	0.98	0.10	17,17,17,17	0
55	MG	BA	3138	1/1	0.98	0.25	1,1,1,1	0
55	MG	BA	3172	1/1	0.98	0.07	31,31,31,31	0
55	MG	DA	3051	1/1	0.98	0.05	28,28,28,28	0
55	MG	DA	3052	1/1	0.98	0.06	56,56,56,56	0
55	MG	DA	3004	1/1	0.98	0.07	76,76,76,76	0
55	MG	AA	1627	1/1	0.98	0.09	37,37,37,37	0
55	MG	BA	3140	1/1	0.98	0.16	0,0,0,0	0
55	MG	AA	1636	1/1	0.98	0.10	27,27,27,27	0
55	MG	AA	1603	1/1	0.98	0.10	44,44,44,44	0
55	MG	BA	3177	1/1	0.98	0.12	17,17,17,17	0
55	MG	DA	3059	1/1	0.98	0.04	51,51,51,51	0
55	MG	BA	3143	1/1	0.98	0.20	12,12,12,12	0
55	MG	BA	3179	1/1	0.98	0.10	26,26,26,26	0
55	MG	BA	3099	1/1	0.98	0.05	4,4,4,4	0
55	MG	BA	3065	1/1	0.98	0.04	0,0,0,0	0
55	MG	DA	3117	1/1	0.98	0.04	67,67,67,67	0
55	MG	BA	3041	1/1	0.98	0.05	6,6,6,6	0
55	MG	DA	3065	1/1	0.98	0.03	36,36,36,36	0
55	MG	BA	3096	1/1	0.99	0.02	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	3184	1/1	0.99	0.09	6,6,6,6	0
55	MG	BA	3097	1/1	0.99	0.05	4,4,4,4	0
55	MG	BA	3098	1/1	0.99	0.03	2,2,2,2	0
55	MG	BA	3034	1/1	0.99	0.04	6,6,6,6	0
55	MG	BA	3188	1/1	0.99	0.02	10,10,10,10	0
55	MG	AA	1615	1/1	0.99	0.03	47,47,47,47	0
55	MG	BA	3101	1/1	0.99	0.04	1,1,1,1	0
55	MG	BA	3102	1/1	0.99	0.03	7,7,7,7	0
55	MG	BA	3066	1/1	0.99	0.05	0,0,0,0	0
55	MG	CA	1640	1/1	0.99	0.07	26,26,26,26	0
55	MG	BA	3068	1/1	0.99	0.07	0,0,0,0	0
55	MG	AA	1607	1/1	0.99	0.04	44,44,44,44	0
55	MG	BA	3106	1/1	0.99	0.05	16,16,16,16	0
55	MG	BB	201	1/1	0.99	0.04	20,20,20,20	0
55	MG	BA	3108	1/1	0.99	0.07	0,0,0,0	0
55	MG	BB	203	1/1	0.99	0.04	7,7,7,7	0
55	MG	BA	3109	1/1	0.99	0.05	12,12,12,12	0
55	MG	BA	3110	1/1	0.99	0.07	3,3,3,3	0
55	MG	BA	3040	1/1	0.99	0.04	0,0,0,0	0
55	MG	BA	3010	1/1	0.99	0.03	0,0,0,0	0
55	MG	BA	3074	1/1	0.99	0.06	1,1,1,1	0
55	MG	BA	3011	1/1	0.99	0.05	1,1,1,1	0
55	MG	AA	1647	1/1	0.99	0.03	48,48,48,48	0
55	MG	BA	3045	1/1	0.99	0.03	9,9,9,9	0
55	MG	AA	1622	1/1	0.99	0.10	16,16,16,16	0
55	MG	BA	3118	1/1	0.99	0.03	1,1,1,1	0
55	MG	AA	1623	1/1	0.99	0.03	46,46,46,46	0
55	MG	BA	3017	1/1	0.99	0.05	2,2,2,2	0
55	MG	AA	1604	1/1	0.99	0.03	48,48,48,48	0
55	MG	BA	3122	1/1	0.99	0.07	18,18,18,18	0
55	MG	BA	3123	1/1	0.99	0.03	0,0,0,0	0
55	MG	AA	1618	1/1	0.99	0.03	37,37,37,37	0
55	MG	AA	1641	1/1	0.99	0.03	19,19,19,19	0
55	MG	BA	3052	1/1	0.99	0.02	11,11,11,11	0
55	MG	BA	3024	1/1	0.99	0.06	0,0,0,0	0
55	MG	BA	3025	1/1	0.99	0.04	2,2,2,2	0
55	MG	BA	3130	1/1	0.99	0.04	0,0,0,0	0
55	MG	CA	1620	1/1	0.99	0.05	61,61,61,61	0
55	MG	BA	3131	1/1	0.99	0.04	1,1,1,1	0
55	MG	AA	1642	1/1	0.99	0.04	23,23,23,23	0
55	MG	BA	3028	1/1	0.99	0.04	5,5,5,5	0
55	MG	BA	3029	1/1	0.99	0.14	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	3018	1/1	0.99	0.04	60,60,60,60	0
55	MG	BA	3091	1/1	0.99	0.04	3,3,3,3	0
55	MG	AA	1633	1/1	0.99	0.03	30,30,30,30	0
55	MG	AA	1611	1/1	0.99	0.03	21,21,21,21	0
55	MG	BA	3032	1/1	0.99	0.04	4,4,4,4	0
55	MG	DA	3023	1/1	0.99	0.04	69,69,69,69	0
55	MG	BA	3007	1/1	0.99	0.03	22,22,22,22	0
57	ZN	B4	101	1/1	0.99	0.04	33,33,33,33	0
57	ZN	D4	101	1/1	0.99	0.03	87,87,87,87	0
55	MG	BA	3128	1/1	1.00	0.01	0,0,0,0	0
55	MG	BA	3026	1/1	1.00	0.02	3,3,3,3	0
55	MG	BA	3015	1/1	1.00	0.05	2,2,2,2	0
55	MG	BA	3018	1/1	1.00	0.06	0,0,0,0	0
55	MG	BA	3044	1/1	1.00	0.02	3,3,3,3	0
55	MG	BA	3067	1/1	1.00	0.06	0,0,0,0	0
55	MG	BA	3055	1/1	1.00	0.04	0,0,0,0	0
55	MG	BA	3135	1/1	1.00	0.02	2,2,2,2	0
55	MG	BA	3035	1/1	1.00	0.08	0,0,0,0	0
55	MG	BA	3070	1/1	1.00	0.06	0,0,0,0	0
55	MG	BA	3023	1/1	1.00	0.02	1,1,1,1	0
55	MG	BA	3037	1/1	1.00	0.04	0,0,0,0	0
55	MG	BA	3088	1/1	1.00	0.10	2,2,2,2	0
55	MG	BA	3073	1/1	1.00	0.11	7,7,7,7	0
55	MG	BA	3019	1/1	1.00	0.04	11,11,11,11	0
55	MG	BA	3107	1/1	1.00	0.09	0,0,0,0	0
55	MG	BA	3060	1/1	1.00	0.04	15,15,15,15	0
55	MG	BA	3039	1/1	1.00	0.10	0,0,0,0	0
55	MG	BA	3014	1/1	1.00	0.05	0,0,0,0	0

6.5 Other polymers ⓘ

There are no such residues in this entry.